



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 PM GMT

PDB ID : 3WGV
Title : Crystal structure of a Na⁺-bound Na⁺,K⁺-ATPase preceding the E1P state with oligomycin
Authors : Kanai, R.; Ogawa, H.; Vilsen, B.; Cornelius, F.; Toyoshima, C.
Deposited on : 2013-08-09
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

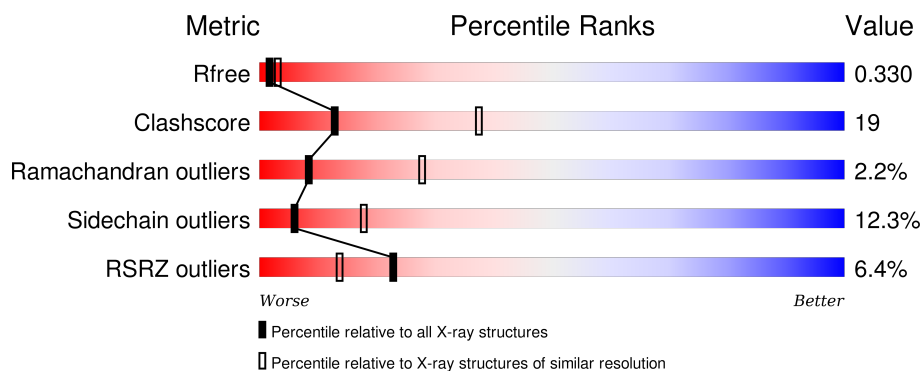
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1016	<div> <div>2%</div> <div>55%</div> <div>36%</div> <div>7%</div> <div>.</div> </div>
1	C	1016	<div> <div>4%</div> <div>59%</div> <div>34%</div> <div>5%</div> <div>.</div> </div>
2	B	303	<div> <div>17%</div> <div>52%</div> <div>42%</div> <div>6%</div> </div>
2	D	303	<div> <div>17%</div> <div>53%</div> <div>39%</div> <div>7%</div> </div>
3	E	65	<div> <div>8%</div> <div>20%</div> <div>29%</div> <div>.</div> <div>.</div> <div>46%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	65	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	EFO	A	2015	-	-	-	X
10	EFO	C	2013	-	-	-	X
5	ALF	C	2002	-	-	X	-
7	NA	A	2007	-	-	-	X
7	NA	C	2005	-	-	-	X
7	NA	C	2006	-	-	-	X
8	CLR	A	2010	-	-	-	X
8	CLR	D	3002	-	-	-	X
9	PC1	A	2012	-	-	-	X
9	PC1	C	2011	-	-	-	X
9	PC1	C	2012	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21909 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7714	4918	1300	1449	47			
1	C	994	Total	C	N	O	S	0	0	0
			7714	4918	1300	1449	47			

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2479	1603	408	454	14			
2	D	303	Total	C	N	O	S	0	0	0
			2479	1603	408	454	14			

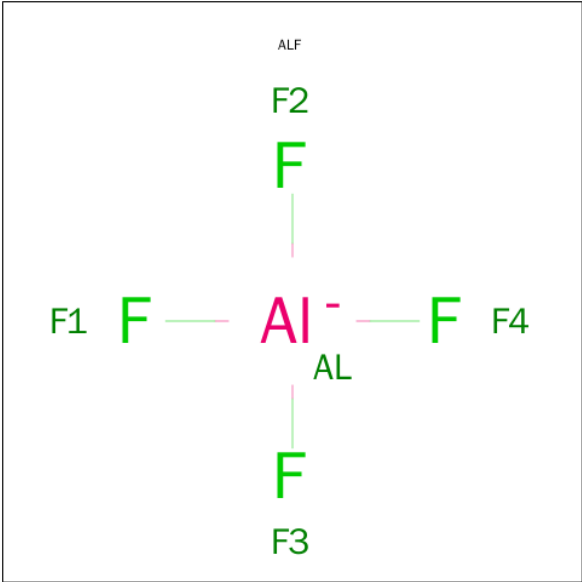
- Molecule 3 is a protein called Na⁺/K⁺ ATPase gamma subunit transcript variant a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	34	Total	C	N	O	0	0	0
			270	183	39	48			
3	E	35	Total	C	N	O	0	0	0
			281	189	43	49			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

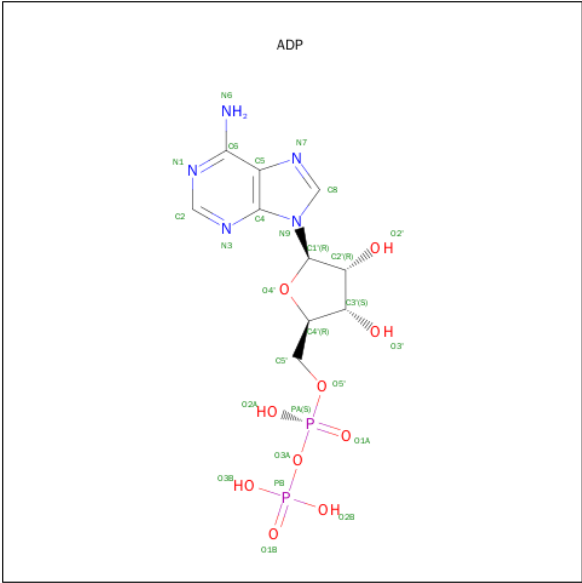
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			5	1	4		
5	C	1	Total	Al	F	0	0
			5	1	4		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			27	10	5	10		

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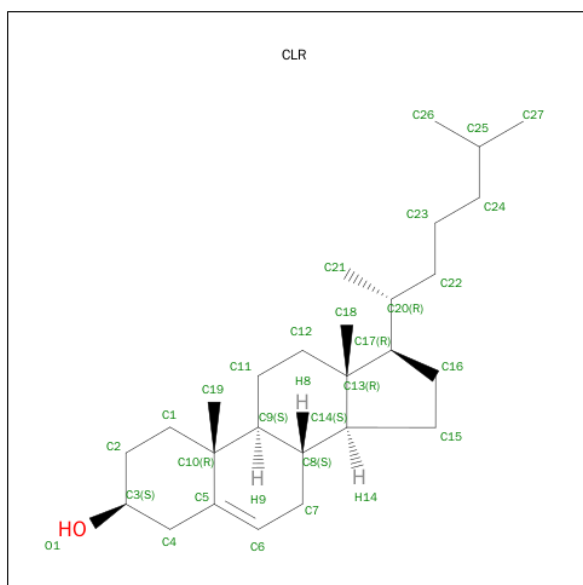
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

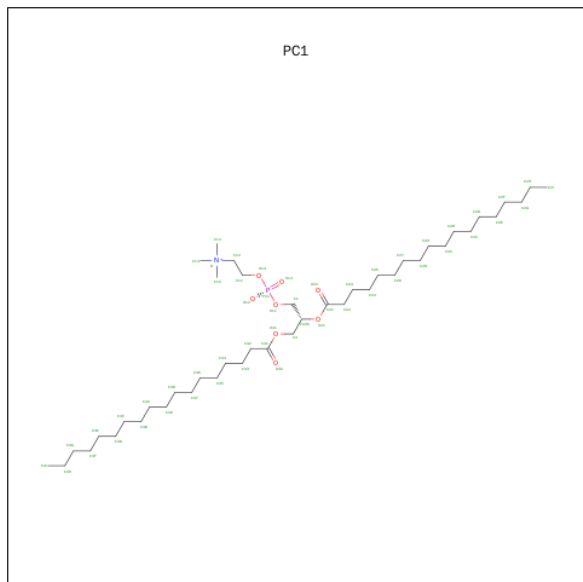
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Na	0	0
			4	4		
7	C	4	Total	Na	0	0
			4	4		

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



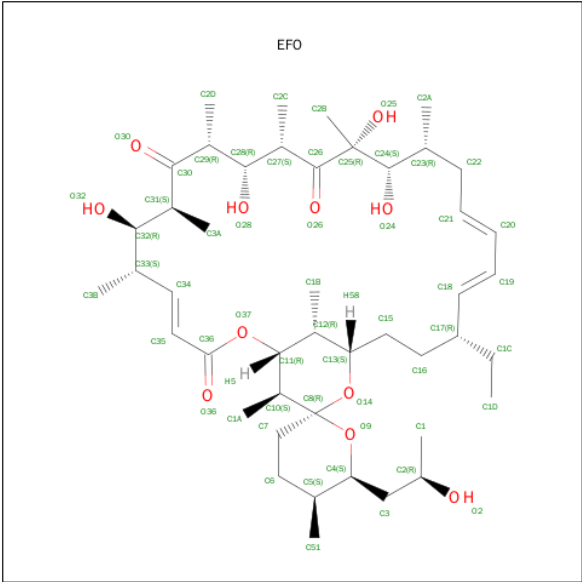
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			28	27	1		
8	A	1	Total	C	O	0	0
			28	27	1		
8	G	1	Total	C	O	0	0
			28	27	1		
8	D	1	Total	C	O	0	0
			28	27	1		
8	D	1	Total	C	O	0	0
			28	27	1		
8	E	1	Total	C	O	0	0
			28	27	1		

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



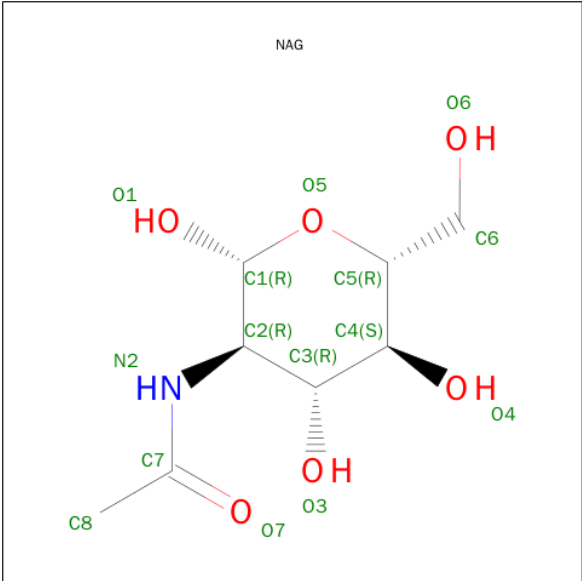
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	D	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 10 is OLIGOMYCIN A (three-letter code: EFO) (formula: $C_{45}H_{74}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			56	45	11		
10	C	1	Total	C	O	0	0
			56	45	11		

- Molecule 11 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			14	8	1	5		

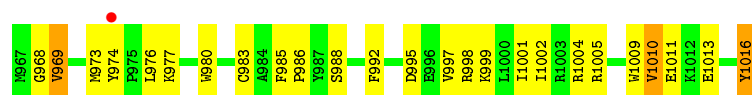
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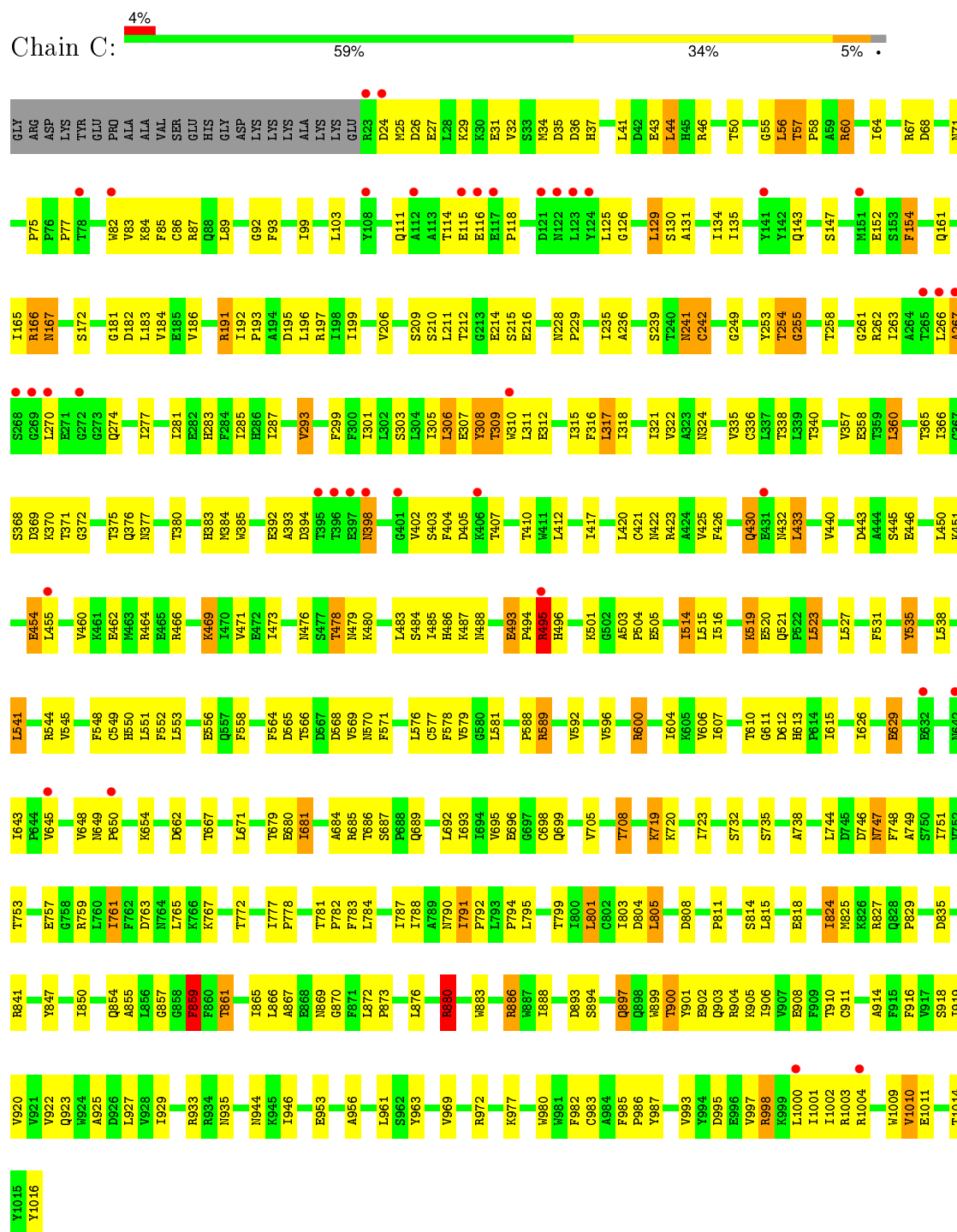
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	24	Total	O	0	0
			24	24		
12	B	2	Total	O	0	0
			2	2		
12	C	20	Total	O	0	0
			20	20		
12	D	2	Total	O	0	0
			2	2		

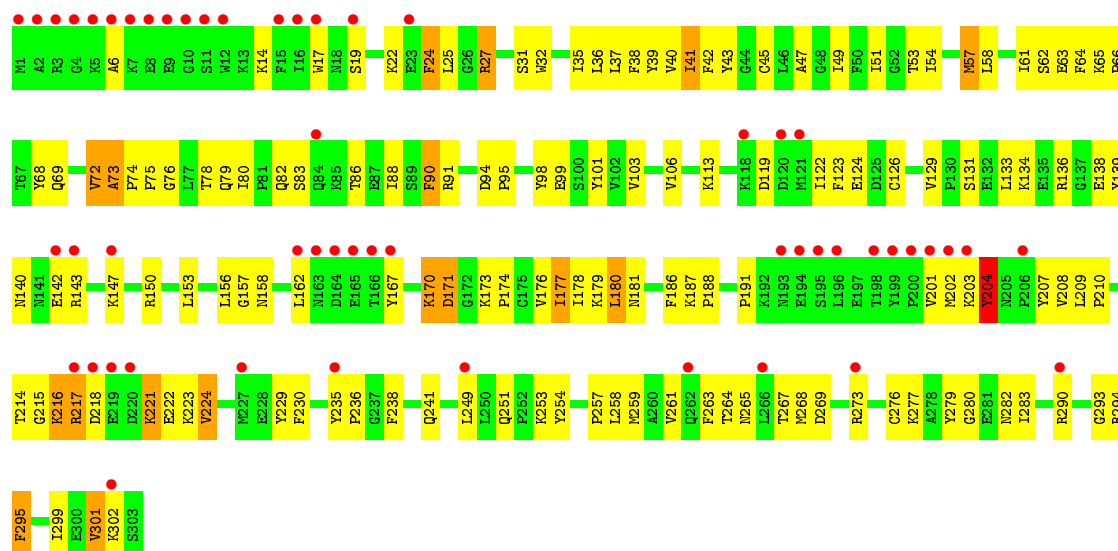


• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

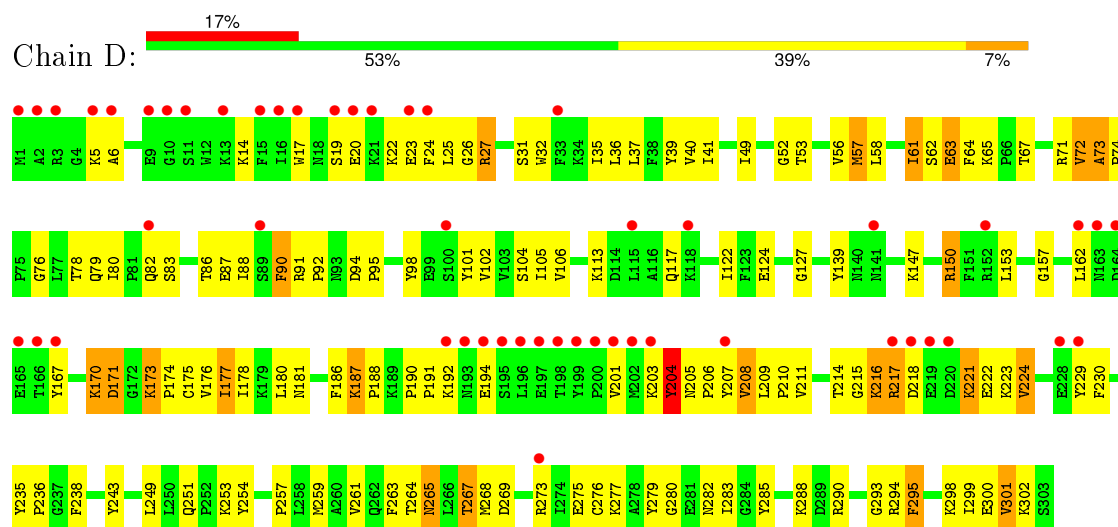


• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

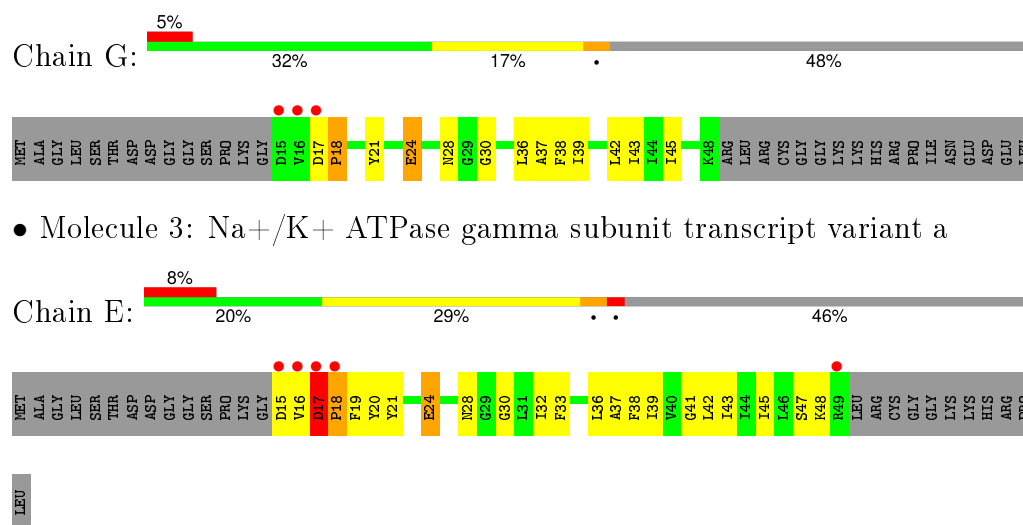




• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



• Molecule 3: Na⁺/K⁺ ATPase gamma subunit transcript variant a



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.28Å 210.18Å 256.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.99 – 2.80 15.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (15.99-2.80) 94.4 (15.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.270 , 0.298 0.316 , 0.330	Depositor DCC
R_{free} test set	3965 reflections (3.08%)	DCC
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 132832 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	21909	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAG, ADP, ALF, NA, PC1, EFO, CLR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	1/7864 (0.0%)	0.66	7/10671 (0.1%)
1	C	0.39	0/7864	0.58	2/10671 (0.0%)
2	B	0.34	0/2544	0.53	1/3426 (0.0%)
2	D	0.34	0/2544	0.53	0/3426
3	E	0.35	0/287	0.56	0/389
3	G	0.38	0/276	0.54	0/375
All	All	0.41	1/21379 (0.0%)	0.60	10/28958 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	656	CYS	CB-SG	-5.07	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	ARG	CB-CA-C	-9.36	91.69	110.40
1	A	600	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	A	600	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	239	SER	CB-CA-C	-6.59	97.57	110.10
1	C	239	SER	CB-CA-C	-6.45	97.85	110.10
1	C	495	ARG	CB-CA-C	-6.36	97.67	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	34	MET	N-CA-CB	-5.44	100.81	110.60
2	B	73	ALA	C-N-CD	5.16	139.24	128.40
1	A	508	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	17	ASP	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7714	0	7770	303	0
1	C	7714	0	7769	264	0
2	B	2479	0	2458	103	0
2	D	2479	0	2458	98	0
3	E	281	0	285	14	0
3	G	270	0	272	12	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	A	5	0	0	1	0
5	C	5	0	0	2	0
6	A	27	0	12	3	0
6	C	27	0	12	6	0
7	A	4	0	0	0	0
7	C	4	0	0	0	0
8	A	56	0	92	27	0
8	D	56	0	92	29	0
8	E	28	0	45	13	0
8	G	28	0	45	9	0
9	A	216	0	352	14	0
9	B	54	0	88	2	0
9	C	216	0	352	15	0
9	D	54	0	88	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	56	0	74	0	0
10	C	56	0	74	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	A	24	0	0	0	0
12	B	2	0	0	0	0
12	C	20	0	0	2	0
12	D	2	0	0	0	0
All	All	21909	0	22364	851	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (851) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2009:CLR:C11	8:A:2009:CLR:C9	1.77	1.62
8:D:3002:CLR:C11	8:D:3002:CLR:C12	1.74	1.60
8:A:2010:CLR:C9	8:A:2010:CLR:C11	1.76	1.59
8:D:3001:CLR:C9	8:D:3001:CLR:C11	1.78	1.57
8:E:101:CLR:C11	8:E:101:CLR:C9	1.78	1.56
8:D:3002:CLR:C11	8:D:3002:CLR:C9	1.78	1.55
8:G:101:CLR:C11	8:G:101:CLR:C9	1.79	1.54
1:C:495:ARG:HG3	1:C:495:ARG:O	1.42	1.11
1:C:493:GLU:HG2	1:C:495:ARG:H	1.24	1.03
1:A:600:ARG:HH11	1:A:600:ARG:HG2	1.33	0.94
2:D:221:LYS:HE3	2:D:223:LYS:HB2	1.49	0.93
1:A:417:ILE:HD11	1:A:548:PHE:HB3	1.48	0.93
1:A:493:GLU:HG2	1:A:495:ARG:H	1.35	0.91
8:A:2010:CLR:C10	8:A:2010:CLR:C11	2.50	0.90
1:C:44:LEU:HD11	1:C:197:ARG:HG2	1.54	0.90
2:B:76:GLY:HA2	2:B:293:GLY:H	1.37	0.90
2:B:221:LYS:HE3	2:B:223:LYS:HB2	1.52	0.90
1:A:790:ASN:HD22	1:A:880:ARG:HD2	1.38	0.88
1:C:166:ARG:NH1	1:C:182:ASP:OD1	2.06	0.88
1:A:57:THR:HG23	1:A:60:ARG:HB2	1.56	0.87
2:D:124:GLU:HB2	2:D:147:LYS:HD3	1.56	0.87
2:B:188:PRO:HB3	2:B:209:LEU:HD22	1.56	0.86
8:A:2009:CLR:C11	8:A:2009:CLR:C10	2.52	0.86
8:D:3002:CLR:C11	8:D:3002:CLR:C10	2.54	0.86
2:D:216:LYS:HG2	2:D:221:LYS:HB2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:ASP:HA	2:D:302:LYS:HA	1.56	0.85
1:A:480:LYS:HE3	6:A:2004:ADP:H5'2	1.57	0.85
8:D:3001:CLR:C11	8:D:3001:CLR:C10	2.55	0.84
1:A:443:ASP:HB2	1:A:446:GLU:HB2	1.60	0.84
1:A:494:PRO:HG2	1:A:552:PHE:HB3	1.59	0.83
8:E:101:CLR:C11	8:E:101:CLR:C10	2.56	0.82
1:A:679:THR:HG23	1:A:680:GLU:HG3	1.61	0.82
1:C:454:GLU:HG2	1:C:460:VAL:HG23	1.59	0.82
2:B:216:LYS:HG2	2:B:221:LYS:HB2	1.62	0.81
1:C:763:ASP:OD2	12:C:2114:HOH:O	1.97	0.81
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.62	0.81
1:C:195:ASP:HB2	1:C:253:TYR:HB2	1.61	0.81
1:A:495:ARG:HG3	1:A:495:ARG:O	1.77	0.81
1:C:495:ARG:O	1:C:495:ARG:CG	2.27	0.80
1:C:384:MET:HE1	1:C:393:ALA:HB2	1.62	0.80
1:C:165:ILE:HB	1:C:183:LEU:HD21	1.62	0.80
1:C:872:LEU:HD12	1:C:873:PRO:HD2	1.64	0.79
8:D:3001:CLR:H212	8:D:3001:CLR:H121	1.64	0.78
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.19	0.78
2:D:79:GLN:HB3	2:D:295:PHE:HZ	1.46	0.78
2:B:79:GLN:HB3	2:B:295:PHE:HZ	1.49	0.78
1:C:514:ILE:HG13	1:C:523:LEU:HG	1.66	0.77
1:C:565:ASP:H	1:C:570:ASN:HB2	1.51	0.76
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.21	0.75
1:C:57:THR:HG23	1:C:60:ARG:HB2	1.68	0.75
1:C:600:ARG:HB3	1:C:600:ARG:HH11	1.52	0.75
1:A:472:GLU:HB2	1:A:484:SER:HB3	1.68	0.75
2:B:124:GLU:HB2	2:B:147:LYS:HD3	1.69	0.75
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.70	0.74
1:A:165:ILE:HB	1:A:183:LEU:HD21	1.67	0.74
1:C:986:PRO:HG3	8:D:3002:CLR:H152	1.70	0.74
2:D:122:ILE:HG21	2:D:253:LYS:HE2	1.70	0.74
2:D:173:LYS:HG2	2:D:264:THR:HA	1.69	0.74
8:E:101:CLR:H121	8:E:101:CLR:H212	1.70	0.74
1:A:495:ARG:O	1:A:495:ARG:CG	2.35	0.73
1:C:309:THR:HG23	1:C:312:GLU:HB2	1.70	0.73
8:G:101:CLR:C11	8:G:101:CLR:C8	2.66	0.73
1:C:946:ILE:HG13	3:E:45:ILE:HD11	1.70	0.73
2:D:188:PRO:HB3	2:D:209:LEU:HD22	1.71	0.72
2:B:269:ASP:HA	2:B:302:LYS:HA	1.71	0.72
1:C:759:ARG:HH12	1:C:829:PRO:HA	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ILE:HG21	2:B:253:LYS:HE2	1.70	0.72
1:A:963:TYR:CE2	8:G:101:CLR:H21	2.24	0.71
1:C:56:LEU:HD11	1:C:182:ASP:HB3	1.72	0.71
2:D:187:LYS:O	2:D:282:ASN:ND2	2.22	0.71
8:G:101:CLR:C11	8:G:101:CLR:C10	2.63	0.71
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.72	0.71
1:A:44:LEU:HD11	1:A:197:ARG:HG2	1.72	0.71
1:C:685:ARG:NH2	6:C:2004:ADP:O3'	2.22	0.70
1:A:473:ILE:HD11	1:A:483:LEU:HD23	1.72	0.70
1:C:1003:ARG:HD2	9:C:2011:PC1:H122	1.72	0.70
8:D:3002:CLR:C11	8:D:3002:CLR:C8	2.68	0.70
8:A:2010:CLR:C11	8:A:2010:CLR:C8	2.64	0.70
1:C:643:ILE:HD11	1:C:648:VAL:HG22	1.73	0.70
1:A:255:GLY:O	1:A:258:THR:HG22	1.92	0.70
1:C:277:ILE:HD12	1:C:358:GLU:HG3	1.74	0.69
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.28	0.69
8:A:2009:CLR:H212	8:A:2009:CLR:H121	1.73	0.69
1:A:166:ARG:NH1	1:A:182:ASP:OD1	2.25	0.69
9:C:2012:PC1:H351	9:C:2012:PC1:H251	1.75	0.69
8:D:3001:CLR:C8	8:D:3001:CLR:C11	2.67	0.69
1:A:50:THR:HG22	1:A:56:LEU:HB3	1.75	0.69
1:A:551:LEU:HD22	1:A:553:LEU:HD23	1.75	0.69
1:C:50:THR:HG22	1:C:56:LEU:HD23	1.75	0.68
1:C:600:ARG:NH1	12:C:2120:HOH:O	2.25	0.68
1:C:696:GLU:HG3	1:C:720:LYS:HE2	1.75	0.68
2:B:14:LYS:HA	2:B:17:TRP:HB3	1.75	0.68
8:A:2010:CLR:H212	8:A:2010:CLR:H121	1.73	0.68
1:C:241:ASN:OD1	1:C:241:ASN:N	2.24	0.68
9:A:2013:PC1:H3B2	9:A:2013:PC1:H292	1.74	0.68
1:A:1002:ILE:HG23	1:A:1011:GLU:HB2	1.76	0.68
3:G:17:ASP:HB3	3:G:18:PRO:HD2	1.76	0.68
1:A:239:SER:OG	1:A:239:SER:O	2.11	0.68
1:A:493:GLU:HG2	1:A:495:ARG:N	2.09	0.67
3:G:24:GLU:O	3:G:28:ASN:ND2	2.26	0.67
1:C:867:ALA:HB2	1:C:873:PRO:HD3	1.76	0.67
2:D:209:LEU:HD21	2:D:283:ILE:HD11	1.77	0.67
2:D:191:PRO:HG3	2:D:280:GLY:HA2	1.77	0.67
2:B:88:ILE:HB	2:B:299:ILE:HG22	1.76	0.67
1:C:488:ASN:HB3	1:C:493:GLU:HG3	1.75	0.66
1:C:417:ILE:HD11	1:C:548:PHE:HB3	1.75	0.66
2:D:216:LYS:HB3	2:D:273:ARG:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:PHE:CD2	2:B:98:TYR:HB3	2.31	0.66
2:D:14:LYS:HA	2:D:17:TRP:HB3	1.77	0.66
1:A:108:TYR:HA	1:A:111:GLN:HE21	1.60	0.66
1:A:394:ASP:N	1:A:394:ASP:OD1	2.28	0.66
1:C:445:SER:OG	1:C:544:ARG:NH1	2.29	0.66
1:A:154:PHE:HB3	1:A:350:LEU:HD13	1.78	0.66
1:C:719:LYS:NZ	1:C:738:ALA:O	2.28	0.65
1:A:505:GLU:HG3	1:A:506:ARG:H	1.61	0.65
9:C:2009:PC1:H2D2	9:C:2012:PC1:H3F2	1.78	0.65
8:D:3002:CLR:C11	8:D:3002:CLR:C13	2.68	0.65
1:A:759:ARG:HH12	1:A:829:PRO:HA	1.60	0.65
2:D:229:TYR:HD1	2:D:261:VAL:HG12	1.60	0.65
9:C:2009:PC1:H3I1	9:C:2009:PC1:H2I3	1.78	0.65
1:A:514:ILE:HG12	1:A:578:PHE:HB3	1.77	0.65
1:A:842:LEU:HD12	1:A:1016:TYR:HD2	1.61	0.65
1:A:258:THR:HG23	1:A:261:GLY:H	1.60	0.65
1:C:777:ILE:HD11	1:C:847:TYR:HA	1.79	0.64
1:C:372:GLY:HA2	1:C:377:ASN:HB2	1.79	0.64
1:C:679:THR:HG23	1:C:680:GLU:HG3	1.79	0.64
8:A:2010:CLR:H193	8:A:2010:CLR:H111	1.79	0.64
1:A:790:ASN:ND2	1:A:880:ARG:HD2	2.11	0.64
2:D:217:ARG:HD2	2:D:218:ASP:H	1.62	0.64
1:A:274:GLN:HE22	1:A:279:ALA:HB2	1.62	0.64
2:B:27:ARG:HD3	2:B:32:TRP:HE3	1.62	0.64
1:C:211:LEU:HD23	1:C:212:THR:HG23	1.80	0.64
1:A:1009:TRP:HZ2	2:B:35:ILE:HG22	1.63	0.64
1:A:613:HIS:CD2	1:A:615:ILE:HG12	2.33	0.63
1:A:613:HIS:NE2	1:A:615:ILE:HG12	2.14	0.63
8:A:2009:CLR:C8	8:A:2009:CLR:C11	2.65	0.63
1:C:299:PHE:HB3	1:C:316:PHE:HE2	1.64	0.63
3:E:33:PHE:CE1	8:E:101:CLR:H183	2.34	0.63
1:C:426:PHE:HE2	1:C:454:GLU:HG3	1.63	0.63
2:B:173:LYS:HG2	2:B:264:THR:HA	1.81	0.63
2:B:224:VAL:HB	2:B:267:THR:HG21	1.81	0.62
1:C:963:TYR:CE2	8:E:101:CLR:H21	2.33	0.62
1:A:36:ASP:OD1	1:A:47:LYS:NZ	2.32	0.62
9:C:2011:PC1:H2H2	8:D:3002:CLR:H272	1.80	0.62
2:B:216:LYS:H	2:B:216:LYS:HD2	1.63	0.62
1:A:152:GLU:HA	1:A:155:LYS:HG2	1.82	0.62
1:A:209:SER:HB3	1:A:215:SER:HA	1.82	0.62
1:C:998:ARG:HE	1:C:1014:THR:HB	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:TYR:HD1	2:B:261:VAL:HG12	1.64	0.62
1:C:854:GLN:HG2	1:C:922:VAL:HB	1.81	0.62
1:C:266:LEU:HD22	1:C:270:LEU:HA	1.82	0.62
1:A:324:ASN:HA	1:A:776:ASN:OD1	2.00	0.61
1:A:708:THR:HG22	1:A:725:VAL:HB	1.81	0.61
2:D:83:SER:HB3	2:D:86:THR:HA	1.80	0.61
1:C:258:THR:HG23	1:C:261:GLY:H	1.64	0.61
1:A:483:LEU:HD21	1:A:571:PHE:HE2	1.65	0.61
1:A:946:ILE:HG13	3:G:45:ILE:HD11	1.81	0.61
1:C:777:ILE:HD12	1:C:777:ILE:H	1.65	0.61
1:C:480:LYS:HG2	6:C:2004:ADP:H5'1	1.83	0.61
1:C:186:VAL:HG11	1:C:192:ILE:HD13	1.81	0.61
1:A:1016:TYR:H	1:A:1016:TYR:HD1	1.48	0.61
1:C:956:ALA:HB2	3:E:37:ALA:HB3	1.83	0.61
1:C:982:PHE:HA	1:C:985:PHE:CD1	2.36	0.60
2:B:209:LEU:HD21	2:B:283:ILE:HD11	1.82	0.60
1:C:471:VAL:HG21	1:C:564:PHE:HB2	1.83	0.60
8:A:2009:CLR:H111	8:A:2009:CLR:H193	1.82	0.60
2:D:91:ARG:HG3	2:D:302:LYS:O	2.01	0.60
2:D:106:VAL:HG22	2:D:167:TYR:HB2	1.83	0.60
1:C:732:SER:HG	1:C:735:SER:HG	1.49	0.60
3:E:17:ASP:HB3	3:E:18:PRO:HD2	1.81	0.60
2:D:87:GLU:HA	2:D:298:LYS:O	2.02	0.60
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.83	0.60
1:A:343:ARG:HD2	1:A:757:GLU:OE2	2.02	0.60
1:A:360:LEU:HA	1:A:723:ILE:HD13	1.83	0.60
1:C:125:LEU:O	1:C:129:LEU:HB2	2.01	0.60
1:A:818:GLU:HG2	1:A:944:ASN:HD22	1.66	0.60
1:C:494:PRO:HG2	1:C:552:PHE:HB3	1.82	0.60
1:C:469:LYS:HA	1:C:486:HIS:HA	1.83	0.60
1:A:35:ASP:HB2	1:A:37:HIS:ND1	2.16	0.60
1:C:385:TRP:HB3	1:C:581:LEU:HB2	1.83	0.60
2:D:88:ILE:HB	2:D:299:ILE:HG22	1.82	0.60
1:A:514:ILE:HG13	1:A:523:LEU:HG	1.84	0.59
1:A:80:PRO:HG2	1:A:83:VAL:HB	1.83	0.59
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.84	0.59
1:C:398:ASN:HB2	1:C:455:LEU:HD13	1.84	0.59
8:D:3002:CLR:H111	8:D:3002:CLR:H193	1.84	0.59
1:C:31:GLU:HG3	1:C:32:VAL:H	1.68	0.59
1:C:827:ARG:HH12	1:C:933:ARG:HH21	1.50	0.59
2:D:76:GLY:HA2	2:D:293:GLY:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LEU:HD12	1:A:437:LYS:HB3	1.85	0.59
1:A:372:GLY:HA2	1:A:377:ASN:HB2	1.85	0.59
1:C:365:THR:HB	1:C:705:VAL:HG12	1.84	0.59
1:C:191:ARG:HA	1:C:241:ASN:HB3	1.85	0.58
1:C:549:CYS:HA	1:C:579:VAL:HG23	1.84	0.58
1:A:986:PRO:CG	8:A:2010:CLR:H181	2.33	0.58
5:A:2002:ALF:F1	6:A:2004:ADP:O3B	2.11	0.58
1:A:874:ILE:HD12	1:A:874:ILE:H	1.68	0.58
2:B:214:THR:OG1	2:B:215:GLY:N	2.35	0.58
1:A:496:HIS:HB2	1:A:553:LEU:HB2	1.84	0.58
8:D:3002:CLR:H212	8:D:3002:CLR:H121	1.85	0.58
2:B:216:LYS:HB3	2:B:273:ARG:HB2	1.85	0.58
1:C:281:ILE:HD11	1:C:765:LEU:HD13	1.85	0.58
1:A:831:ASN:HD21	2:B:6:ALA:HB2	1.69	0.58
1:C:496:HIS:HB2	1:C:553:LEU:HB2	1.84	0.58
1:A:824:ILE:HD12	1:A:825:MET:H	1.68	0.58
1:A:889:ASN:HD22	1:A:900:THR:HB	1.69	0.58
1:C:902:GLU:O	1:C:906:ILE:HG12	2.03	0.58
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.86	0.58
8:A:2010:CLR:C11	8:A:2010:CLR:C19	2.82	0.57
1:A:927:LEU:HG	1:A:947:LEU:HD21	1.87	0.57
1:C:553:LEU:HD22	1:C:558:PHE:CE2	2.39	0.57
8:A:2010:CLR:C9	8:A:2010:CLR:C12	2.79	0.57
1:C:551:LEU:HD12	1:C:576:LEU:HA	1.87	0.57
2:D:186:PHE:CZ	2:D:282:ASN:HB3	2.40	0.57
1:C:303:SER:O	1:C:308:TYR:HB2	2.04	0.57
1:A:340:THR:HG22	1:A:757:GLU:OE1	2.04	0.57
1:A:857:GLY:O	1:A:861:THR:HG23	2.04	0.57
1:A:628:SER:OG	1:A:680:GLU:OE2	2.21	0.57
1:A:300:PHE:HB2	1:A:317:LEU:HB2	1.86	0.57
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.39	0.56
1:A:263:ILE:HG13	1:A:263:ILE:O	2.05	0.56
2:D:14:LYS:HZ3	2:D:17:TRP:HE3	1.53	0.56
1:C:60:ARG:O	1:C:64:ILE:HG13	2.05	0.56
1:C:126:GLY:O	1:C:130:SER:OG	2.17	0.56
1:A:370:LYS:NZ	1:A:612:ASP:OD2	2.37	0.56
1:A:671:LEU:O	1:A:675:LEU:HD22	2.06	0.56
1:A:420:LEU:HD13	1:A:486:HIS:ND1	2.20	0.56
1:A:902:GLU:O	1:A:906:ILE:HG12	2.05	0.56
1:A:638:ALA:HB2	1:A:648:VAL:HG21	1.87	0.56
1:C:206:VAL:HA	1:C:242:CYS:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:987:TYR:OH	2:D:53:THR:HG21	2.06	0.56
1:C:538:LEU:HA	1:C:541:LEU:HD22	1.88	0.56
9:C:2012:PC1:H361	9:C:2012:PC1:H3B2	1.88	0.56
2:D:268:MET:HA	2:D:301:VAL:HG23	1.87	0.56
1:C:99:ILE:O	1:C:103:LEU:HG	2.06	0.56
1:A:963:TYR:HE1	1:A:976:LEU:H	1.54	0.56
1:C:985:PHE:HZ	8:E:101:CLR:H221	1.72	0.55
1:C:369:ASP:OD1	5:C:2002:ALF:F1	2.14	0.55
1:A:892:GLU:HA	1:A:897:GLN:O	2.06	0.55
1:A:777:ILE:HD11	1:A:847:TYR:CG	2.41	0.55
1:C:565:ASP:H	1:C:570:ASN:CB	2.19	0.55
2:B:217:ARG:HD2	2:B:218:ASP:H	1.71	0.55
1:A:469:LYS:HB2	1:A:486:HIS:CD2	2.42	0.55
2:B:27:ARG:HD3	2:B:32:TRP:CE3	2.41	0.55
1:C:67:ARG:NH1	1:C:68:ASP:OD2	2.39	0.55
2:D:61:ILE:HG23	2:D:67:THR:HG23	1.87	0.55
1:A:963:TYR:CD2	3:G:30:GLY:HA3	2.41	0.55
1:A:768:SER:HA	1:A:815:LEU:HD23	1.89	0.55
1:A:350:LEU:HD23	1:A:742:ILE:HD12	1.88	0.55
2:B:178:ILE:HD11	2:B:276:CYS:SG	2.47	0.55
8:E:101:CLR:H111	8:E:101:CLR:H193	1.88	0.55
1:C:469:LYS:HB3	1:C:486:HIS:CE1	2.40	0.55
2:D:27:ARG:HD3	2:D:32:TRP:HE3	1.71	0.55
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.72	0.55
1:A:607:ILE:HG12	1:A:681:ILE:HG13	1.88	0.55
1:C:460:VAL:HG11	1:C:464:ARG:HH21	1.71	0.55
1:A:55:GLY:HA3	1:A:165:ILE:O	2.07	0.55
1:C:152:GLU:C	1:C:154:PHE:H	2.09	0.55
9:C:2012:PC1:H3B1	9:C:2012:PC1:H282	1.87	0.55
1:A:706:ALA:HA	1:A:723:ILE:HG13	1.88	0.55
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.88	0.55
2:B:80:ILE:HB	2:B:177:ILE:HG23	1.89	0.55
1:A:183:LEU:HD23	1:A:183:LEU:H	1.73	0.54
1:A:777:ILE:HD11	1:A:847:TYR:HA	1.90	0.54
1:A:475:PHE:H	1:A:482:GLN:HG3	1.72	0.54
1:C:255:GLY:O	1:C:258:THR:HG22	2.07	0.54
2:B:138:GLU:O	2:B:140:ASN:N	2.39	0.54
1:A:60:ARG:O	1:A:64:ILE:HG13	2.07	0.54
1:C:861:THR:HG21	1:C:918:SER:OG	2.07	0.54
1:A:666:MET:HG3	1:A:670:GLN:HB3	1.90	0.54
1:C:747:ASN:HD21	1:C:749:ALA:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:3001:CLR:C9	8:D:3001:CLR:C12	2.84	0.54
9:A:2014:PC1:H122	2:B:25:LEU:HD11	1.89	0.54
1:C:306:LEU:HD12	1:C:880:ARG:HE	1.73	0.54
3:G:17:ASP:CB	3:G:18:PRO:HD2	2.38	0.54
1:A:977:LYS:HD3	2:B:68:TYR:CE1	2.43	0.54
2:B:90:PHE:HD2	2:B:98:TYR:HB3	1.72	0.54
1:C:801:LEU:O	1:C:805:LEU:HG	2.07	0.54
1:A:336:CYS:O	1:A:340:THR:HG23	2.08	0.54
1:A:888:ILE:O	1:A:904:ARG:NH2	2.41	0.54
1:C:143:GLN:HE21	1:C:335:VAL:HG22	1.73	0.54
1:A:854:GLN:HE22	1:A:923:GLN:HE21	1.55	0.54
1:C:613:HIS:HD2	1:C:615:ILE:HB	1.72	0.54
1:A:472:GLU:CB	1:A:484:SER:HB3	2.36	0.53
1:C:814:SER:HB3	1:C:946:ILE:HG22	1.89	0.53
1:A:603:GLY:HA3	1:A:829:PRO:HD3	1.90	0.53
1:A:440:VAL:HG12	1:A:441:ALA:H	1.74	0.53
1:A:131:ALA:O	1:A:135:ILE:HG12	2.09	0.53
1:C:854:GLN:HE22	1:C:923:GLN:HE21	1.57	0.53
1:A:899:TRP:CE3	2:B:72:VAL:HG13	2.43	0.53
1:C:906:ILE:O	1:C:910:THR:OG1	2.22	0.53
1:A:476:ASN:OD1	1:A:478:THR:HG23	2.08	0.53
8:A:2009:CLR:C19	8:A:2009:CLR:C11	2.87	0.53
9:A:2013:PC1:H292	9:A:2013:PC1:C3B	2.39	0.53
2:B:83:SER:HB3	2:B:86:THR:HA	1.89	0.53
1:C:317:LEU:O	1:C:321:ILE:HG12	2.09	0.53
1:A:861:THR:HG21	1:A:918:SER:OG	2.08	0.53
2:B:106:VAL:HG22	2:B:167:TYR:HB2	1.91	0.53
1:A:505:GLU:OE2	1:A:613:HIS:ND1	2.34	0.53
2:B:176:VAL:HB	2:B:261:VAL:HG23	1.90	0.53
1:A:951:LEU:O	1:A:955:THR:HG23	2.08	0.53
1:C:440:VAL:HG21	1:C:451:LYS:HE3	1.90	0.53
1:A:609:VAL:HG12	1:A:691:LYS:HE2	1.89	0.53
1:A:335:VAL:HG11	1:A:817:TYR:CE2	2.43	0.53
1:A:1001:ILE:CG2	1:A:1010:VAL:HG21	2.39	0.53
8:E:101:CLR:C11	8:E:101:CLR:C8	2.69	0.53
8:E:101:CLR:C9	8:E:101:CLR:C12	2.83	0.52
2:D:176:VAL:HB	2:D:261:VAL:HG23	1.90	0.52
1:A:421:CYS:O	1:A:482:GLN:NE2	2.42	0.52
1:C:58:PRO:HD3	1:C:167:ASN:HB2	1.91	0.52
1:C:184:VAL:HG11	1:C:193:PRO:HG3	1.91	0.52
1:C:916:PHE:O	1:C:920:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2010:CLR:C21	8:A:2010:CLR:H121	2.39	0.52
2:D:224:VAL:HB	2:D:267:THR:HG21	1.91	0.52
1:A:997:VAL:O	1:A:1001:ILE:HG13	2.09	0.52
9:C:2009:PC1:H291	9:C:2009:PC1:H3A1	1.92	0.52
1:A:771:TYR:CE1	1:A:927:LEU:HB2	2.44	0.52
1:A:1009:TRP:CZ2	2:B:35:ILE:HG22	2.43	0.52
1:A:184:VAL:HG11	1:A:193:PRO:HG2	1.91	0.52
1:A:393:ALA:HA	1:A:402:VAL:HA	1.91	0.52
2:D:90:PHE:CD2	2:D:98:TYR:HB3	2.44	0.52
1:A:921:VAL:HG22	1:A:924:TRP:CH2	2.45	0.52
1:A:89:LEU:HD21	1:A:134:ILE:HA	1.91	0.52
1:A:422:ASN:OD1	1:A:423:ARG:N	2.42	0.52
1:C:986:PRO:CG	8:D:3002:CLR:H152	2.39	0.52
1:C:421:CYS:O	1:C:501:LYS:NZ	2.23	0.52
8:A:2010:CLR:H193	8:A:2010:CLR:C11	2.40	0.52
1:C:801:LEU:HD12	1:C:805:LEU:HD11	1.92	0.52
1:C:493:GLU:HG2	1:C:495:ARG:N	2.08	0.52
1:C:514:ILE:HD12	1:C:527:LEU:HD13	1.90	0.52
1:A:56:LEU:HG	1:A:182:ASP:HB3	1.91	0.52
1:A:777:ILE:H	1:A:777:ILE:HD12	1.74	0.52
2:B:76:GLY:H	2:B:181:ASN:HD22	1.56	0.52
1:A:501:LYS:HE3	6:A:2004:ADP:N1	2.24	0.52
9:D:3003:PC1:H242	8:E:101:CLR:H6	1.92	0.51
1:A:258:THR:HG23	1:A:261:GLY:N	2.24	0.51
1:C:893:ASP:OD2	1:C:897:GLN:HG3	2.10	0.51
1:C:531:PHE:HE2	1:C:581:LEU:HD21	1.75	0.51
1:C:115:GLU:HG2	1:C:116:GLU:H	1.74	0.51
1:C:283:HIS:NE2	1:C:287:ILE:HD11	2.25	0.51
2:B:251:GLN:HB3	2:B:254:TYR:HB2	1.92	0.51
1:A:986:PRO:HG3	8:A:2010:CLR:H181	1.92	0.51
1:A:818:GLU:OE2	1:A:931:LYS:NZ	2.39	0.51
1:C:551:LEU:HD13	1:C:576:LEU:HD23	1.92	0.51
2:B:202:MET:SD	2:B:236:PRO:HG2	2.50	0.51
1:C:43:GLU:O	1:C:46:ARG:HG2	2.10	0.51
1:A:347:LYS:HG3	1:A:753:THR:HG21	1.92	0.51
1:C:600:ARG:HH21	1:C:680:GLU:HG2	1.76	0.51
1:C:196:LEU:HB2	1:C:236:ALA:HB3	1.93	0.51
1:C:340:THR:HG21	1:C:357:VAL:HG11	1.91	0.51
1:C:997:VAL:O	1:C:1001:ILE:HG13	2.11	0.51
1:A:889:ASN:ND2	1:A:901:TYR:H	2.08	0.51
1:A:263:ILE:HD12	1:A:265:THR:OG1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:PRO:HG3	8:A:2010:CLR:H152	1.91	0.51
1:A:44:LEU:HD11	1:A:197:ARG:CG	2.38	0.51
1:C:827:ARG:NH1	1:C:933:ARG:HH21	2.08	0.51
3:E:24:GLU:O	3:E:28:ASN:ND2	2.43	0.51
1:C:698:CYS:HB2	1:C:705:VAL:HG11	1.93	0.51
1:C:375:THR:HA	1:C:588:PRO:HA	1.92	0.51
1:A:443:ASP:O	1:A:447:SER:OG	2.29	0.51
1:A:31:GLU:HG3	1:A:32:VAL:H	1.76	0.51
2:D:192:LYS:HZ1	2:D:205:ASN:HB3	1.75	0.51
2:B:136:ARG:HD2	2:B:143:ARG:HH12	1.76	0.50
1:C:689:GLN:O	1:C:693:ILE:HG12	2.10	0.50
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.93	0.50
1:C:972:ARG:HH12	2:D:288:LYS:HZ1	1.59	0.50
1:C:782:PRO:HG3	1:C:795:LEU:HD23	1.94	0.50
1:C:376:GLN:HG3	1:C:589:ARG:HA	1.93	0.50
1:A:420:LEU:HB3	1:A:486:HIS:HE1	1.73	0.50
2:B:90:PHE:CZ	2:B:174:PRO:HG3	2.46	0.50
1:C:824:ILE:HD12	1:C:825:MET:H	1.77	0.50
1:A:298:SER:HB2	9:A:2014:PC1:H3F1	1.93	0.50
1:A:185:GLU:HG3	1:A:248:ARG:HG2	1.93	0.50
2:D:117:GLN:HB3	2:D:150:ARG:HD3	1.93	0.50
1:A:211:LEU:HD12	1:A:260:MET:SD	2.52	0.50
2:B:280:GLY:HA3	2:B:283:ILE:HD13	1.94	0.50
1:C:757:GLU:O	1:C:761:ILE:HG22	2.11	0.50
1:A:769:ILE:HA	1:A:772:THR:HG22	1.94	0.50
8:D:3002:CLR:C11	8:D:3002:CLR:C14	2.89	0.49
1:A:620:ILE:O	1:A:624:VAL:HG13	2.12	0.49
1:A:781:THR:HG22	8:A:2009:CLR:C27	2.41	0.49
2:D:56:VAL:HG11	8:D:3002:CLR:H122	1.92	0.49
1:A:759:ARG:HH22	1:A:829:PRO:HG3	1.76	0.49
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.93	0.49
1:C:131:ALA:O	1:C:135:ILE:HG12	2.12	0.49
8:A:2009:CLR:H191	2:B:39:TYR:CZ	2.46	0.49
9:C:2009:PC1:H391	9:C:2009:PC1:H291	1.94	0.49
2:B:191:PRO:HG3	2:B:280:GLY:HA2	1.93	0.49
1:A:928:VAL:O	1:A:931:LYS:HB3	2.12	0.49
1:C:503:ALA:HB1	1:C:685:ARG:NH1	2.26	0.49
2:B:35:ILE:HG13	2:B:36:LEU:N	2.26	0.49
1:A:998:ARG:HA	1:A:1001:ILE:HD12	1.94	0.49
2:D:251:GLN:HB3	2:D:254:TYR:HB2	1.93	0.49
2:D:178:ILE:HD11	2:D:276:CYS:SG	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:GLU:HG3	2:B:140:ASN:ND2	2.27	0.49
1:C:861:THR:O	1:C:865:ILE:HD12	2.12	0.49
2:B:42:PHE:HD2	2:B:43:TYR:CD1	2.30	0.49
1:A:545:VAL:HG22	1:A:583:SER:HB3	1.94	0.49
1:C:93:PHE:CZ	1:C:285:ILE:HG23	2.48	0.49
1:C:430:GLN:HA	1:C:430:GLN:HE21	1.76	0.49
2:D:57:MET:HA	8:D:3002:CLR:H11	1.93	0.49
8:E:101:CLR:C11	8:E:101:CLR:C19	2.90	0.49
8:G:101:CLR:H183	8:G:101:CLR:H212	1.94	0.49
1:A:413:ALA:O	1:A:417:ILE:HG23	2.12	0.49
1:C:777:ILE:CD1	1:C:847:TYR:HA	2.43	0.49
1:A:192:ILE:HD12	1:A:236:ALA:HB1	1.95	0.49
1:A:454:GLU:HG2	1:A:460:VAL:HG23	1.94	0.49
2:B:37:LEU:O	2:B:41:ILE:HG23	2.13	0.49
8:D:3002:CLR:C11	8:D:3002:CLR:C19	2.91	0.49
1:A:688:PRO:HG3	1:A:713:ASN:HB2	1.94	0.49
2:D:36:LEU:O	2:D:40:VAL:HG23	2.13	0.49
1:A:861:THR:HG22	1:A:983:CYS:HB3	1.95	0.49
1:A:317:LEU:O	1:A:321:ILE:HG12	2.13	0.49
1:A:710:ASP:OD1	1:A:711:GLY:N	2.44	0.49
1:A:283:HIS:O	1:A:287:ILE:HG12	2.12	0.49
1:A:191:ARG:HA	1:A:241:ASN:HB3	1.95	0.49
1:A:777:ILE:CD1	1:A:847:TYR:HA	2.42	0.49
1:A:882:ASN:HB3	1:A:888:ILE:HD12	1.95	0.49
2:D:90:PHE:CZ	2:D:174:PRO:HG3	2.48	0.49
2:B:157:GLY:H	2:B:230:PHE:HB3	1.78	0.49
1:C:607:ILE:HG23	1:C:681:ILE:HG13	1.93	0.49
1:C:426:PHE:CE2	1:C:454:GLU:HG3	2.47	0.48
1:C:763:ASP:O	1:C:767:LYS:HG3	2.13	0.48
1:C:1009:TRP:HZ2	2:D:35:ILE:HG22	1.78	0.48
2:D:214:THR:OG1	2:D:215:GLY:N	2.45	0.48
8:D:3001:CLR:C21	8:D:3001:CLR:H121	2.40	0.48
1:C:50:THR:HG21	1:C:181:GLY:C	2.33	0.48
2:B:91:ARG:NH2	2:D:94:ASP:OD1	2.45	0.48
1:C:611:GLY:O	6:C:2004:ADP:H5'2	2.12	0.48
1:A:944:ASN:ND2	1:A:947:LEU:HB2	2.29	0.48
2:B:14:LYS:HZ3	2:B:17:TRP:HE3	1.61	0.48
1:A:182:ASP:O	1:A:251:VAL:HG23	2.13	0.48
2:B:268:MET:HA	2:B:301:VAL:HG23	1.95	0.48
1:C:1001:ILE:CG2	1:C:1010:VAL:HG21	2.43	0.48
1:A:752:VAL:O	1:A:755:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2010:CLR:H111	8:A:2010:CLR:C19	2.44	0.48
2:B:209:LEU:HD12	2:B:210:PRO:HD2	1.96	0.48
1:A:340:THR:HG21	1:A:761:ILE:CD1	2.43	0.48
1:A:937:VAL:HG21	1:A:992:PHE:CE1	2.49	0.48
1:C:565:ASP:CB	1:C:570:ASN:HD22	2.26	0.48
1:A:838:VAL:HG13	1:A:842:LEU:HD22	1.95	0.48
2:B:36:LEU:O	2:B:40:VAL:HG23	2.14	0.48
1:A:185:GLU:HG3	1:A:248:ARG:CG	2.43	0.48
3:G:38:PHE:O	3:G:42:LEU:HG	2.12	0.48
2:D:216:LYS:HD2	2:D:216:LYS:H	1.77	0.48
2:B:238:PHE:CD1	2:B:257:PRO:HB2	2.49	0.48
2:D:192:LYS:NZ	2:D:205:ASN:HB3	2.29	0.48
1:C:899:TRP:CE3	2:D:72:VAL:HG13	2.49	0.48
1:A:565:ASP:HB3	1:A:570:ASN:HB2	1.95	0.48
8:E:101:CLR:C21	8:E:101:CLR:H121	2.43	0.48
1:A:793:LEU:O	1:A:912:HIS:NE2	2.43	0.48
1:C:692:LEU:O	1:C:696:GLU:HB2	2.14	0.48
1:A:777:ILE:N	1:A:777:ILE:HD12	2.29	0.48
1:C:613:HIS:CD2	1:C:615:ILE:HB	2.48	0.48
1:C:147:SER:HB2	1:C:338:THR:HG23	1.96	0.48
1:A:387:ASP:O	1:A:389:GLN:N	2.46	0.48
1:C:556:GLU:N	1:C:556:GLU:OE1	2.43	0.48
8:A:2009:CLR:H111	8:A:2009:CLR:C19	2.44	0.47
2:D:52:GLY:O	2:D:56:VAL:HG23	2.13	0.47
9:A:2013:PC1:H261	9:A:2013:PC1:H291	1.68	0.47
1:A:37:HIS:CE1	1:A:229:PRO:HG3	2.49	0.47
2:D:204:TYR:CE2	2:D:207:TYR:HB2	2.48	0.47
1:A:303:SER:O	1:A:308:TYR:HB2	2.14	0.47
2:B:38:PHE:HD2	2:B:39:TYR:CD1	2.32	0.47
1:A:1009:TRP:CE2	1:A:1013:GLU:HG3	2.48	0.47
1:A:956:ALA:HB2	3:G:37:ALA:HB3	1.95	0.47
2:B:277:LYS:HD2	2:B:279:TYR:CE2	2.49	0.47
8:D:3001:CLR:H111	8:D:3001:CLR:H193	1.96	0.47
1:A:815:LEU:HA	1:A:815:LEU:HD12	1.71	0.47
2:D:17:TRP:CZ2	2:D:19:SER:HB3	2.49	0.47
1:A:402:VAL:HG21	1:A:404:PHE:CZ	2.49	0.47
2:B:99:GLU:O	2:B:103:VAL:HG23	2.14	0.47
9:D:3003:PC1:H282	9:D:3003:PC1:H2B2	1.60	0.47
1:C:103:LEU:HD12	1:C:318:ILE:HD11	1.95	0.47
1:A:790:ASN:C	1:A:880:ARG:HB2	2.35	0.47
2:D:98:TYR:CZ	2:D:171:ASP:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:TYR:HB3	2:B:208:VAL:HB	1.97	0.47
2:B:131:SER:HB2	2:B:241:GLN:HB3	1.97	0.47
1:A:512:SER:OG	1:A:575:ASN:HA	2.13	0.47
1:A:349:CYS:SG	1:A:741:MET:HG2	2.55	0.47
1:A:803:ILE:HG23	1:A:919:ILE:HG21	1.96	0.47
1:C:804:ASP:O	1:C:808:ASP:HB2	2.15	0.47
1:C:25:MET:O	1:C:29:LYS:HG3	2.15	0.47
2:B:186:PHE:CZ	2:B:282:ASN:HB3	2.50	0.47
2:B:173:LYS:HA	2:B:174:PRO:HD3	1.79	0.47
2:D:49:ILE:O	2:D:53:THR:HG22	2.14	0.47
1:A:192:ILE:HA	1:A:193:PRO:HD3	1.71	0.47
2:D:102:VAL:HA	2:D:105:ILE:HG22	1.95	0.47
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.78	0.47
2:B:170:LYS:N	2:B:170:LYS:HD2	2.30	0.47
1:A:814:SER:HB2	1:A:946:ILE:HG22	1.97	0.47
1:A:861:THR:HG22	1:A:983:CYS:CB	2.45	0.47
1:C:613:HIS:CD2	1:C:615:ILE:H	2.32	0.47
1:A:864:VAL:HG22	2:B:57:MET:SD	2.54	0.47
1:C:972:ARG:HH12	2:D:288:LYS:NZ	2.12	0.46
1:A:188:GLY:HA2	1:A:244:GLU:HA	1.97	0.46
1:A:920:VAL:HG13	1:A:954:GLU:HG2	1.97	0.46
1:C:544:ARG:NH2	6:C:2004:ADP:O1B	2.48	0.46
1:A:504:PRO:HB3	1:A:581:LEU:CD2	2.45	0.46
3:E:39:ILE:O	3:E:43:ILE:HG12	2.15	0.46
2:D:277:LYS:HD2	2:D:279:TYR:CE2	2.51	0.46
1:C:778:PRO:HB3	1:C:855:ALA:HA	1.97	0.46
1:C:901:TYR:OH	1:C:905:LYS:HE3	2.15	0.46
3:E:47:SER:OG	3:E:47:SER:O	2.29	0.46
1:A:670:GLN:O	1:A:674:ILE:HG13	2.15	0.46
1:C:83:VAL:O	1:C:87:ARG:HG2	2.15	0.46
1:A:280:GLU:OE1	1:A:830:ARG:NH2	2.48	0.46
1:C:370:LYS:HB2	1:C:610:THR:HB	1.97	0.46
1:A:985:PHE:HZ	8:G:101:CLR:H221	1.80	0.46
2:D:101:TYR:O	2:D:104:SER:OG	2.33	0.46
1:C:914:ALA:O	1:C:918:SER:N	2.44	0.46
1:C:430:GLN:O	1:C:432:ASN:N	2.41	0.46
1:A:301:ILE:HD11	9:A:2014:PC1:H3I1	1.98	0.46
1:C:324:ASN:N	1:C:324:ASN:HD22	2.13	0.46
1:A:488:ASN:OD1	1:A:490:ASN:ND2	2.49	0.46
1:A:977:LYS:HD3	2:B:68:TYR:CZ	2.50	0.46
2:D:23:GLU:HG2	2:D:24:PHE:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:ARG:NH2	1:A:934:ARG:HD3	2.30	0.46
2:B:49:ILE:O	2:B:53:THR:HG22	2.16	0.46
1:A:85:PHE:CZ	1:A:138:CYS:HB3	2.51	0.46
1:A:551:LEU:HD12	1:A:576:LEU:HD23	1.97	0.46
1:A:36:ASP:HB3	1:A:39:LEU:HD12	1.97	0.46
1:A:847:TYR:CD2	9:A:2011:PC1:H381	2.51	0.46
1:C:781:THR:N	1:C:782:PRO:HD2	2.31	0.46
1:A:410:THR:HG23	1:A:515:LEU:HD22	1.98	0.46
1:C:1002:ILE:HG23	1:C:1011:GLU:HB2	1.98	0.46
1:C:935:ASN:HA	1:C:1003:ARG:HD3	1.98	0.46
1:A:898:GLN:OE1	2:B:181:ASN:HA	2.16	0.46
1:A:473:ILE:H	1:A:473:ILE:HG12	1.64	0.46
1:C:883:TRP:HZ2	1:C:908:GLU:HB2	1.81	0.46
1:C:901:TYR:HA	1:C:904:ARG:CZ	2.46	0.46
1:C:383:HIS:CD2	1:C:392:GLU:HG2	2.51	0.46
1:A:968:GLY:HA2	1:A:973:MET:N	2.30	0.46
1:A:781:THR:HG22	8:A:2009:CLR:H273	1.98	0.45
2:D:76:GLY:H	2:D:181:ASN:HD22	1.62	0.45
1:A:977:LYS:HG2	3:G:21:TYR:CE2	2.52	0.45
1:C:75:PRO:O	1:C:77:PRO:HD3	2.16	0.45
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.97	0.45
2:D:275:GLU:HA	2:D:295:PHE:O	2.15	0.45
1:A:1016:TYR:N	1:A:1016:TYR:CD1	2.84	0.45
1:C:589:ARG:NH1	1:C:746:ASP:HB3	2.32	0.45
2:D:180:LEU:HD13	2:D:181:ASN:N	2.30	0.45
1:C:360:LEU:HA	1:C:723:ILE:HD13	1.98	0.45
1:A:226:ASN:HB3	1:A:231:GLU:HB2	1.99	0.45
1:A:860:PHE:CE1	2:B:53:THR:HG23	2.51	0.45
1:A:747:ASN:HD21	1:A:749:ALA:HB3	1.80	0.45
8:D:3002:CLR:H111	8:D:3002:CLR:C19	2.47	0.45
8:D:3001:CLR:C19	8:D:3001:CLR:C11	2.94	0.45
1:C:183:LEU:HB2	1:C:249:GLY:O	2.16	0.45
2:D:27:ARG:HD3	2:D:32:TRP:CE3	2.51	0.45
9:A:2014:PC1:H361	9:A:2014:PC1:H2B2	1.98	0.45
1:C:753:THR:O	1:C:757:GLU:HG2	2.17	0.45
1:C:71:ASN:OD1	1:C:254:THR:HG22	2.17	0.45
1:A:436:LEU:HG	1:A:455:LEU:HD11	1.97	0.45
1:A:318:ILE:HD13	1:A:318:ILE:HA	1.81	0.45
1:C:483:LEU:HD21	1:C:571:PHE:HE2	1.81	0.45
1:C:993:VAL:O	1:C:997:VAL:HG13	2.15	0.45
2:B:203:LYS:HB2	2:B:235:TYR:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ALA:HA	1:A:238:PHE:HB2	1.99	0.45
1:A:475:PHE:N	1:A:482:GLN:HG3	2.32	0.45
1:A:968:GLY:HA3	1:A:974:TYR:CE2	2.52	0.45
2:D:80:ILE:HB	2:D:177:ILE:HG23	1.97	0.45
1:A:50:THR:CG2	1:A:56:LEU:HD23	2.47	0.45
2:B:157:GLY:N	2:B:230:PHE:HB3	2.32	0.45
1:C:886:ARG:HA	1:C:901:TYR:CD1	2.51	0.45
2:D:24:PHE:C	2:D:26:GLY:H	2.20	0.45
1:A:445:SER:OG	1:A:544:ARG:NH1	2.50	0.45
1:C:425:VAL:HG12	1:C:426:PHE:O	2.16	0.45
2:B:91:ARG:HH21	2:B:94:ASP:HB2	1.82	0.45
2:B:95:PRO:HA	2:B:98:TYR:CE1	2.51	0.45
2:D:229:TYR:CD1	2:D:261:VAL:HG12	2.47	0.45
1:A:977:LYS:N	1:A:980:TRP:CD1	2.80	0.45
1:A:1001:ILE:HG21	1:A:1010:VAL:HG21	1.99	0.45
2:D:95:PRO:HA	2:D:98:TYR:CE1	2.52	0.45
2:B:134:LYS:HB2	2:B:136:ARG:HH12	1.82	0.45
1:C:55:GLY:HA2	1:C:183:LEU:HD22	1.98	0.45
1:C:565:ASP:OD2	1:C:568:ASP:HB2	2.16	0.45
2:B:98:TYR:HA	2:B:101:TYR:HD1	1.81	0.45
1:A:214:GLU:HB2	1:A:216:GLU:HG3	1.99	0.45
1:C:977:LYS:HG2	3:E:21:TYR:HE2	1.82	0.45
1:C:565:ASP:HB2	1:C:570:ASN:HD22	1.82	0.45
1:C:611:GLY:HA2	1:C:686:THR:H	1.82	0.45
1:A:654:LYS:HD3	1:A:654:LYS:HA	1.75	0.44
1:A:927:LEU:HD11	1:A:947:LEU:HG	1.99	0.44
1:C:695:VAL:O	1:C:699:GLN:HG3	2.18	0.44
8:A:2009:CLR:H193	8:A:2009:CLR:C11	2.47	0.44
9:C:2009:PC1:H3H2	9:C:2012:PC1:H2H1	1.99	0.44
1:A:238:PHE:CD2	1:A:258:THR:HG21	2.52	0.44
2:B:42:PHE:HD2	2:B:43:TYR:HD1	1.63	0.44
2:B:203:LYS:HB3	2:B:203:LYS:HE2	1.82	0.44
2:D:37:LEU:O	2:D:41:ILE:HG23	2.16	0.44
3:G:45:ILE:HA	3:G:45:ILE:HD12	1.71	0.44
1:A:900:THR:HG23	1:A:903:GLN:NE2	2.33	0.44
1:A:450:LEU:HD23	1:A:460:VAL:HG21	1.99	0.44
2:D:204:TYR:HD2	2:D:207:TYR:H	1.65	0.44
9:A:2012:PC1:H2A2	9:A:2012:PC1:H2E2	1.99	0.44
1:A:81:GLU:HG3	1:A:82:TRP:H	1.83	0.44
8:D:3001:CLR:H212	8:D:3001:CLR:C12	2.42	0.44
2:D:88:ILE:HG23	2:D:101:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:GLU:HB2	1:A:825:MET:SD	2.57	0.44
1:C:870:GLY:O	1:C:893:ASP:HB2	2.18	0.44
1:C:199:ILE:HA	1:C:199:ILE:HD13	1.57	0.44
1:C:929:ILE:HB	1:C:995:ASP:OD2	2.16	0.44
1:C:460:VAL:HG12	1:C:464:ARG:HE	1.82	0.44
1:A:350:LEU:HB2	1:A:744:LEU:HD21	1.98	0.44
3:E:28:ASN:O	3:E:32:ILE:HG12	2.17	0.44
1:C:592:VAL:O	1:C:596:VAL:HG13	2.18	0.44
1:C:487:LYS:HB3	1:C:487:LYS:HE2	1.85	0.44
1:A:695:VAL:O	1:A:699:GLN:HG3	2.17	0.44
2:D:31:SER:O	2:D:35:ILE:HG23	2.17	0.44
2:B:204:TYR:CE2	2:B:207:TYR:HB2	2.52	0.44
1:C:305:ILE:C	1:C:307:GLU:H	2.21	0.44
1:A:821:GLU:HA	1:A:940:GLN:OE1	2.17	0.44
1:A:763:ASP:O	1:A:767:LYS:HG3	2.18	0.44
1:A:315:ILE:HA	1:A:315:ILE:HD13	1.88	0.44
1:C:613:HIS:NE2	1:C:615:ILE:HD13	2.32	0.44
1:A:1001:ILE:O	1:A:1005:ARG:HB2	2.17	0.44
2:D:98:TYR:OH	2:D:171:ASP:HB3	2.18	0.44
1:C:37:HIS:HB3	1:C:235:ILE:HD11	1.98	0.44
1:C:759:ARG:HE	1:C:825:MET:CE	2.30	0.44
2:B:17:TRP:CZ2	2:B:19:SER:HB3	2.52	0.44
9:A:2013:PC1:H2C2	9:B:401:PC1:H3I1	1.99	0.44
1:A:618:LYS:O	1:A:621:ALA:HB3	2.17	0.44
1:C:228:ASN:HA	1:C:229:PRO:HD3	1.86	0.44
1:A:488:ASN:O	1:A:493:GLU:HG3	2.17	0.44
9:A:2013:PC1:H3F1	9:B:401:PC1:H3H2	2.00	0.44
1:C:1001:ILE:HG21	1:C:1010:VAL:HG21	1.99	0.44
1:A:303:SER:HB2	1:A:308:TYR:CD2	2.52	0.44
1:C:925:ALA:O	1:C:929:ILE:HG12	2.18	0.44
1:A:724:GLY:N	1:A:740:ASP:OD2	2.41	0.44
1:C:841:ARG:HB2	1:C:1016:TYR:HA	2.00	0.44
8:A:2010:CLR:C11	8:A:2010:CLR:C1	2.95	0.43
1:C:50:THR:CG2	1:C:56:LEU:HD23	2.44	0.43
9:A:2013:PC1:H122	9:A:2013:PC1:H11	1.99	0.43
1:A:300:PHE:HE1	1:A:314:VAL:HG12	1.83	0.43
1:A:609:VAL:O	1:A:691:LYS:HE2	2.18	0.43
1:C:794:PRO:HG2	1:C:859:PHE:HE2	1.83	0.43
2:D:157:GLY:H	2:D:230:PHE:HB3	1.83	0.43
1:A:781:THR:HA	1:A:784:LEU:HD12	2.00	0.43
2:B:88:ILE:HG23	2:B:101:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:GLU:OE2	1:C:613:HIS:ND1	2.49	0.43
2:D:62:SER:C	2:D:64:PHE:H	2.22	0.43
1:C:366:ILE:HG13	1:C:604:ILE:HG21	2.00	0.43
8:A:2009:CLR:H121	8:A:2009:CLR:C21	2.46	0.43
2:D:209:LEU:HD12	2:D:210:PRO:HD2	2.00	0.43
1:C:503:ALA:HA	1:C:504:PRO:HD3	1.88	0.43
1:C:258:THR:HG23	1:C:261:GLY:N	2.31	0.43
1:C:430:GLN:HE21	1:C:433:LEU:HD21	1.83	0.43
1:A:304:LEU:HA	1:A:304:LEU:HD23	1.84	0.43
1:A:35:ASP:HB2	1:A:37:HIS:CE1	2.53	0.43
1:A:418:ALA:O	1:A:422:ASN:HB2	2.18	0.43
1:A:624:VAL:CG2	1:A:626:ILE:HG12	2.49	0.43
1:A:206:VAL:HA	1:A:242:CYS:HA	2.00	0.43
1:A:471:VAL:HG21	1:A:564:PHE:HB2	2.00	0.43
1:A:115:GLU:HG2	1:A:116:GLU:N	2.34	0.43
1:C:873:PRO:HA	1:C:876:LEU:HD12	1.99	0.43
1:C:514:ILE:HG22	1:C:516:ILE:HG12	2.01	0.43
2:D:178:ILE:HD13	2:D:211:VAL:HG11	2.01	0.43
1:C:483:LEU:HD12	1:C:484:SER:N	2.33	0.43
3:G:39:ILE:O	3:G:43:ILE:HG12	2.19	0.43
2:D:203:LYS:HE2	2:D:203:LYS:HB3	1.79	0.43
1:A:697:GLY:HA2	1:A:700:ARG:NH2	2.34	0.43
1:C:963:TYR:CZ	8:E:101:CLR:H21	2.53	0.43
1:C:654:LYS:HB3	1:C:679:THR:HG22	2.00	0.43
2:B:98:TYR:CZ	2:B:171:ASP:HB3	2.54	0.43
1:A:815:LEU:O	1:A:818:GLU:HB2	2.18	0.43
1:C:372:GLY:O	1:C:589:ARG:NH2	2.52	0.43
1:A:292:ALA:O	1:A:321:ILE:HD13	2.18	0.43
1:A:977:LYS:HG2	3:G:21:TYR:HE2	1.83	0.43
1:A:621:ALA:O	1:A:626:ILE:N	2.49	0.43
2:B:186:PHE:HZ	2:B:282:ASN:HB3	1.84	0.43
1:A:864:VAL:HA	2:B:57:MET:SD	2.58	0.43
1:C:612:ASP:O	1:C:684:ALA:HB1	2.19	0.43
2:D:113:LYS:HA	2:D:153:LEU:HD11	2.01	0.43
1:A:781:THR:N	1:A:782:PRO:HD2	2.34	0.43
1:A:1009:TRP:CZ2	1:A:1013:GLU:HG3	2.54	0.43
1:C:549:CYS:HB2	1:C:577:CYS:O	2.19	0.43
1:A:752:VAL:HA	1:A:755:VAL:HG12	2.01	0.43
2:D:277:LYS:HG2	2:D:285:TYR:CE2	2.54	0.43
1:C:263:ILE:HG13	1:C:267:ALA:HA	1.99	0.43
1:C:900:THR:H	1:C:903:GLN:HE21	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:SER:OG	2:B:65:LYS:HG2	2.19	0.43
2:B:123:PHE:HB3	2:B:150:ARG:HG3	2.00	0.43
2:B:88:ILE:HG23	2:B:101:TYR:CD2	2.54	0.43
1:C:462:GLU:O	1:C:466:ARG:HG3	2.18	0.43
2:D:39:TYR:CE2	8:D:3001:CLR:H182	2.54	0.43
1:A:654:LYS:O	1:A:679:THR:HG22	2.19	0.43
1:A:901:TYR:HA	1:A:904:ARG:CZ	2.49	0.43
2:D:90:PHE:O	2:D:92:PRO:HD3	2.19	0.43
2:D:204:TYR:HB3	2:D:208:VAL:HB	2.00	0.43
1:C:89:LEU:HD22	1:C:134:ILE:HD13	2.01	0.43
1:A:692:LEU:HD12	1:A:716:PRO:HB2	2.01	0.43
1:A:358:GLU:O	1:A:361:GLY:N	2.45	0.43
1:A:957:LEU:HD22	1:A:957:LEU:HA	1.87	0.43
1:C:963:TYR:CD2	3:E:30:GLY:HA3	2.53	0.42
1:A:571:PHE:HB2	1:A:572:PRO:HD2	2.00	0.42
1:C:483:LEU:HD12	1:C:484:SER:H	1.84	0.42
2:D:62:SER:OG	2:D:65:LYS:HG2	2.19	0.42
1:C:410:THR:HG23	1:C:515:LEU:HD22	2.00	0.42
1:C:982:PHE:O	1:C:985:PHE:HB2	2.19	0.42
1:C:55:GLY:HA3	1:C:165:ILE:O	2.19	0.42
1:C:514:ILE:HG12	1:C:578:PHE:HB3	2.00	0.42
1:C:340:THR:CG2	1:C:357:VAL:HG11	2.48	0.42
1:C:360:LEU:HG	1:C:723:ILE:HD13	2.00	0.42
1:A:366:ILE:HG13	1:A:604:ILE:HG21	2.01	0.42
1:A:841:ARG:HH11	1:A:841:ARG:HG3	1.82	0.42
1:A:483:LEU:HD12	1:A:499:VAL:O	2.18	0.42
1:A:765:LEU:O	1:A:769:ILE:HG13	2.19	0.42
1:A:565:ASP:OD2	1:A:568:ASP:HB2	2.17	0.42
2:D:238:PHE:CD1	2:D:257:PRO:HB2	2.54	0.42
2:B:47:ALA:O	2:B:51:ILE:HG13	2.19	0.42
1:A:503:ALA:HB3	1:A:506:ARG:HB2	2.02	0.42
1:A:430:GLN:HB3	1:A:438:ARG:HB3	2.01	0.42
1:A:600:ARG:NH1	1:A:600:ARG:HG2	2.11	0.42
1:C:31:GLU:HG3	1:C:32:VAL:N	2.31	0.42
1:A:450:LEU:HB3	1:A:451:LYS:H	1.73	0.42
1:A:293:VAL:HA	1:A:321:ILE:CD1	2.50	0.42
1:A:470:ILE:H	1:A:470:ILE:HG13	1.70	0.42
9:C:2011:PC1:H272	9:C:2011:PC1:H2A1	1.70	0.42
2:B:180:LEU:HD13	2:B:181:ASN:N	2.34	0.42
1:C:479:ASN:O	1:C:480:LYS:HB2	2.20	0.42
1:A:503:ALA:HA	1:A:504:PRO:HD3	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:ARG:HG3	2:B:31:SER:HB3	2.02	0.42
3:E:18:PRO:HB2	3:E:19:PHE:H	1.52	0.42
2:B:177:ILE:HD11	2:B:258:LEU:HD13	2.00	0.42
1:C:899:TRP:CH2	2:D:72:VAL:HG22	2.55	0.42
1:C:209:SER:HB3	1:C:215:SER:HA	2.02	0.42
1:A:538:LEU:HA	1:A:538:LEU:HD23	1.76	0.42
9:C:2012:PC1:H221	9:C:2012:PC1:H2	1.78	0.42
1:A:867:ALA:HB2	1:A:873:PRO:HD3	2.02	0.42
1:A:952:PHE:HD2	3:G:37:ALA:HA	1.84	0.42
1:C:311:LEU:O	1:C:315:ILE:HG12	2.20	0.42
1:A:778:PRO:HB3	1:A:855:ALA:HA	2.00	0.42
1:C:165:ILE:HB	1:C:183:LEU:CD2	2.44	0.42
1:C:565:ASP:HB3	1:C:570:ASN:HB2	2.00	0.42
5:C:2002:ALF:F1	6:C:2004:ADP:O3B	2.28	0.42
1:A:360:LEU:HD23	1:A:723:ILE:CD1	2.50	0.42
1:A:331:ALA:O	1:A:335:VAL:HG23	2.20	0.42
1:C:27:GLU:C	1:C:29:LYS:H	2.23	0.42
1:A:968:GLY:HA2	1:A:973:MET:H	1.85	0.42
3:E:38:PHE:CZ	3:E:42:LEU:HD11	2.55	0.42
1:A:187:LYS:HG2	1:A:190:ASP:OD2	2.20	0.42
1:C:649:ASN:HA	1:C:650:PRO:HD3	1.91	0.42
9:C:2009:PC1:H132	9:C:2009:PC1:H112	1.80	0.42
8:G:101:CLR:C12	8:G:101:CLR:C9	2.89	0.42
2:D:190:PRO:HA	2:D:191:PRO:HD3	1.85	0.42
1:A:192:ILE:CD1	1:A:236:ALA:HB1	2.50	0.42
2:D:277:LYS:HB3	2:D:279:TYR:CE1	2.55	0.42
1:C:422:ASN:OD1	1:C:446:GLU:HB3	2.20	0.42
1:C:24:ASP:OD2	1:C:26:ASP:HB2	2.20	0.42
1:C:535:TYR:CE2	1:C:545:VAL:HB	2.55	0.42
1:A:587:PRO:HA	1:A:588:PRO:HD3	1.92	0.42
1:A:638:ALA:HB2	1:A:648:VAL:CG2	2.49	0.41
1:A:854:GLN:NE2	1:A:923:GLN:HE21	2.16	0.41
1:A:609:VAL:CG1	1:A:691:LYS:HG2	2.49	0.41
1:C:606:VAL:HG11	1:C:626:ILE:HD12	2.00	0.41
8:D:3002:CLR:H212	8:D:3002:CLR:C12	2.49	0.41
2:B:57:MET:HE3	2:B:58:LEU:HA	2.02	0.41
1:A:864:VAL:HG13	2:B:57:MET:HG3	2.01	0.41
1:C:791:ILE:HG12	1:C:792:PRO:O	2.20	0.41
1:A:48:TYR:OH	1:A:252:VAL:HB	2.20	0.41
1:C:908:GLU:O	1:C:911:CYS:HB2	2.19	0.41
1:A:827:ARG:HH21	1:A:934:ARG:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:VAL:HG11	1:A:566:THR:HB	2.02	0.41
2:D:300:GLU:HG2	2:D:302:LYS:HB2	2.01	0.41
1:A:301:ILE:HG13	1:A:302:LEU:N	2.36	0.41
1:A:387:ASP:C	1:A:389:GLN:H	2.23	0.41
1:C:883:TRP:O	1:C:904:ARG:HD2	2.21	0.41
1:C:368:SER:HB2	1:C:708:THR:OG1	2.20	0.41
2:D:71:ARG:HA	2:D:71:ARG:HE	1.85	0.41
1:C:519:LYS:HG2	1:C:519:LYS:H	1.69	0.41
2:D:57:MET:HE2	2:D:58:LEU:HA	2.03	0.41
2:D:216:LYS:HE2	2:D:273:ARG:O	2.21	0.41
1:C:460:VAL:CG1	1:C:464:ARG:HH21	2.32	0.41
1:C:293:VAL:HA	1:C:321:ILE:HD12	2.02	0.41
1:C:1009:TRP:CZ2	2:D:35:ILE:HG22	2.55	0.41
2:D:277:LYS:HB3	2:D:279:TYR:CZ	2.54	0.41
1:C:803:ILE:HD12	1:C:919:ILE:HG21	2.03	0.41
6:C:2004:ADP:H3'	6:C:2004:ADP:O2B	2.19	0.41
1:C:32:VAL:O	1:C:262:ARG:NH1	2.54	0.41
1:A:89:LEU:HA	1:A:89:LEU:HD23	1.89	0.41
2:D:35:ILE:HG13	2:D:36:LEU:N	2.36	0.41
2:B:62:SER:C	2:B:64:PHE:H	2.23	0.41
2:B:179:LYS:HE2	2:B:179:LYS:HB3	1.80	0.41
2:B:24:PHE:HA	2:B:24:PHE:HD2	1.73	0.41
1:A:966:GLY:O	1:A:969:VAL:HG22	2.21	0.41
8:D:3001:CLR:C1	8:D:3001:CLR:C11	2.99	0.41
2:B:216:LYS:HE2	2:B:273:ARG:HB2	2.02	0.41
1:C:763:ASP:HB3	1:C:767:LYS:HE3	2.03	0.41
1:A:866:LEU:HD13	1:A:876:LEU:HD21	2.02	0.41
1:A:370:LYS:HB2	1:A:610:THR:HB	2.02	0.41
1:C:861:THR:HG22	1:C:983:CYS:HB3	2.02	0.41
1:A:430:GLN:C	1:A:432:ASN:H	2.24	0.41
8:D:3002:CLR:C11	8:D:3002:CLR:C1	2.98	0.41
9:C:2009:PC1:H272	8:D:3001:CLR:H14	2.03	0.41
8:G:101:CLR:C21	8:G:101:CLR:H121	2.50	0.41
1:C:777:ILE:HD12	1:C:777:ILE:N	2.32	0.41
1:C:589:ARG:HD3	1:C:746:ASP:O	2.20	0.41
1:A:274:GLN:HB3	1:A:274:GLN:HE21	1.59	0.41
1:A:369:ASP:HB3	1:A:373:THR:OG1	2.21	0.41
1:A:337:LEU:HD12	1:A:337:LEU:HA	1.90	0.41
1:A:505:GLU:CD	1:A:685:ARG:HH11	2.24	0.41
1:C:471:VAL:HG11	1:C:566:THR:HB	2.03	0.41
1:C:857:GLY:O	1:C:861:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:HIS:HD2	1:C:615:ILE:H	1.68	0.41
1:A:402:VAL:HG21	1:A:404:PHE:CE1	2.55	0.41
2:B:204:TYR:HD2	2:B:207:TYR:H	1.68	0.41
2:B:66:PRO:HG2	2:B:69:GLN:HG3	2.02	0.41
1:C:866:LEU:HD23	1:C:866:LEU:HA	1.86	0.41
9:C:2009:PC1:H2A1	9:C:2009:PC1:H3C2	2.03	0.41
1:C:953:GLU:OE2	3:E:41:GLY:HA3	2.20	0.41
1:A:537:GLU:O	1:A:541:LEU:HD22	2.20	0.41
8:G:101:CLR:H121	8:G:101:CLR:H212	2.03	0.40
1:C:565:ASP:N	1:C:570:ASN:HB2	2.28	0.40
2:D:188:PRO:HG2	2:D:243:TYR:CD1	2.57	0.40
2:B:91:ARG:HG3	2:B:302:LYS:O	2.21	0.40
2:B:74:PRO:HA	2:B:75:PRO:HD3	1.86	0.40
1:A:648:VAL:HG23	1:A:648:VAL:H	1.68	0.40
1:C:900:THR:H	1:C:903:GLN:NE2	2.19	0.40
1:A:629:GLU:OE1	1:A:629:GLU:N	2.55	0.40
1:A:870:GLY:O	1:A:893:ASP:HB2	2.21	0.40
1:C:318:ILE:O	1:C:322:VAL:HG23	2.20	0.40
1:A:998:ARG:NH1	1:A:999:LYS:HG3	2.37	0.40
1:C:799:THR:O	1:C:803:ILE:HG12	2.21	0.40
2:D:5:LYS:HB3	2:D:6:ALA:H	1.73	0.40
1:C:783:PHE:O	1:C:787:ILE:HG13	2.21	0.40
1:C:784:LEU:O	1:C:788:ILE:HG12	2.20	0.40
1:A:189:GLY:HA2	1:A:734:VAL:HG21	2.04	0.40
2:D:170:LYS:N	2:D:170:LYS:HD2	2.36	0.40
3:E:15:ASP:HB3	3:E:16:VAL:H	1.64	0.40
1:C:476:ASN:O	1:C:478:THR:N	2.53	0.40
1:A:95:MET:HE3	1:A:96:LEU:N	2.36	0.40
1:A:793:LEU:HD12	1:A:794:PRO:HD2	2.02	0.40
1:C:850:ILE:O	1:C:854:GLN:HG3	2.21	0.40
2:B:126:CYS:HB3	2:B:241:GLN:OE1	2.21	0.40
9:A:2012:PC1:H152	9:A:2012:PC1:H112	1.88	0.40
1:C:111:GLN:HB3	1:C:118:PRO:CB	2.51	0.40
2:D:235:TYR:HA	2:D:236:PRO:HD3	1.70	0.40
1:C:84:LYS:HE2	1:C:84:LYS:HB3	1.93	0.40
1:A:309:THR:HG23	1:A:312:GLU:HB2	2.02	0.40
8:A:2010:CLR:H191	8:A:2010:CLR:H8	1.92	0.40
2:B:94:ASP:HA	2:B:95:PRO:HD3	1.84	0.40
9:A:2013:PC1:H381	9:A:2013:PC1:H2C1	2.02	0.40
1:C:854:GLN:NE2	1:C:923:GLN:HE21	2.17	0.40
2:D:265:ASN:HD22	2:D:267:THR:HG23	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ILE:O	1:C:305:ILE:HG12	2.22	0.40
1:C:214:GLU:HB2	1:C:216:GLU:HG3	2.03	0.40
1:C:405:ASP:C	1:C:407:THR:H	2.23	0.40
1:C:748:PHE:O	1:C:751:ILE:HD12	2.21	0.40
1:C:790:ASN:C	1:C:880:ARG:HB2	2.42	0.40
1:A:921:VAL:HG12	1:A:988:SER:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	992/1016 (98%)	859 (87%)	114 (12%)	19 (2%)	10	32
1	C	992/1016 (98%)	884 (89%)	91 (9%)	17 (2%)	11	36
2	B	301/303 (99%)	238 (79%)	55 (18%)	8 (3%)	6	21
2	D	301/303 (99%)	231 (77%)	59 (20%)	11 (4%)	4	14
3	E	33/65 (51%)	31 (94%)	1 (3%)	1 (3%)	5	18
3	G	32/65 (49%)	27 (84%)	4 (12%)	1 (3%)	5	17
All	All	2651/2768 (96%)	2270 (86%)	324 (12%)	57 (2%)	8	28

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	A	402	VAL
2	B	82	GLN
2	B	139	TYR
3	G	18	PRO
1	C	267	ALA

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Mol	Chain	Res	Type
1	C	398	ASN
1	C	880	ARG
3	E	18	PRO
1	A	381	VAL
1	A	710	ASP
2	B	201	VAL
2	B	204	TYR
2	B	265	ASN
1	C	34	MET
1	C	92	GLY
1	C	629	GLU
1	C	961	LEU
2	D	82	GLN
2	D	201	VAL
2	D	204	TYR
2	D	265	ASN
1	A	450	LEU
1	A	721	ALA
1	A	775	SER
1	A	821	GLU
2	B	133	LEU
2	B	156	LEU
1	C	167	ASN
1	C	210	SER
1	C	404	PHE
1	C	569	VAL
1	C	859	PHE
2	D	63	GLU
1	A	359	THR
1	A	451	LYS
1	A	590	ALA
2	B	142	GLU
1	C	944	ASN
2	D	194	GLU
2	D	206	PRO
1	A	92	GLY
1	A	118	PRO
1	A	394	ASP
1	C	306	LEU
1	C	835	ASP
2	D	139	TYR
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	569	VAL
2	D	25	LEU
1	C	255	GLY
2	D	73	ALA
1	A	188	GLY
1	C	402	VAL
2	D	127	GLY
1	A	91	GLY
1	A	489	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	844/861 (98%)	725 (86%)	119 (14%)	4	12
1	C	844/861 (98%)	755 (90%)	89 (10%)	8	24
2	B	269/269 (100%)	235 (87%)	34 (13%)	5	17
2	D	269/269 (100%)	237 (88%)	32 (12%)	6	19
3	E	29/52 (56%)	24 (83%)	5 (17%)	2	7
3	G	28/52 (54%)	26 (93%)	2 (7%)	18	46
All	All	2283/2364 (97%)	2002 (88%)	281 (12%)	6	18

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	41	LEU
1	A	44	LEU
1	A	57	THR
1	A	60	ARG
1	A	82	TRP
1	A	83	VAL
1	A	94	SER
1	A	121	ASP

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Mol	Chain	Res	Type
1	A	125	LEU
1	A	129	LEU
1	A	152	GLU
1	A	158	VAL
1	A	161	GLN
1	A	164	VAL
1	A	166	ARG
1	A	170	LYS
1	A	171	MET
1	A	172	SER
1	A	210	SER
1	A	216	GLU
1	A	239	SER
1	A	241	ASN
1	A	242	CYS
1	A	252	VAL
1	A	266	LEU
1	A	268	SER
1	A	270	LEU
1	A	274	GLN
1	A	287	ILE
1	A	308	TYR
1	A	309	THR
1	A	310	TRP
1	A	317	LEU
1	A	318	ILE
1	A	337	LEU
1	A	360	LEU
1	A	364	SER
1	A	371	THR
1	A	379	MET
1	A	380	THR
1	A	384	MET
1	A	394	ASP
1	A	396	THR
1	A	415	SER
1	A	425	VAL
1	A	430	GLN
1	A	432	ASN
1	A	433	LEU
1	A	437	LYS
1	A	445	SER

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Mol	Chain	Res	Type
1	A	447	SER
1	A	449	LEU
1	A	450	LEU
1	A	453	ILE
1	A	455	LEU
1	A	461	LYS
1	A	469	LYS
1	A	471	VAL
1	A	473	ILE
1	A	478	THR
1	A	485	ILE
1	A	487	LYS
1	A	493	GLU
1	A	495	ARG
1	A	514	ILE
1	A	515	LEU
1	A	519	LYS
1	A	521	GLN
1	A	523	LEU
1	A	535	TYR
1	A	541	LEU
1	A	589	ARG
1	A	600	ARG
1	A	624	VAL
1	A	628	SER
1	A	629	GLU
1	A	635	GLU
1	A	645	VAL
1	A	663	LEU
1	A	666	MET
1	A	667	THR
1	A	671	LEU
1	A	675	LEU
1	A	681	ILE
1	A	687	SER
1	A	705	VAL
1	A	715	SER
1	A	732	SER
1	A	740	ASP
1	A	744	LEU
1	A	747	ASN
1	A	750	SER

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Mol	Chain	Res	Type
1	A	751	ILE
1	A	753	THR
1	A	775	SER
1	A	791	ILE
1	A	805	LEU
1	A	814	SER
1	A	815	LEU
1	A	818	GLU
1	A	819	GLN
1	A	822	SER
1	A	823	ASP
1	A	824	ILE
1	A	830	ARG
1	A	835	ASP
1	A	880	ARG
1	A	881	VAL
1	A	882	ASN
1	A	900	THR
1	A	911	CYS
1	A	922	VAL
1	A	957	LEU
1	A	969	VAL
1	A	995	ASP
1	A	1004	ARG
1	A	1010	VAL
1	A	1016	TYR
2	B	22	LYS
2	B	24	PHE
2	B	27	ARG
2	B	41	ILE
2	B	45	CYS
2	B	54	ILE
2	B	57	MET
2	B	61	ILE
2	B	63	GLU
2	B	72	VAL
2	B	78	THR
2	B	90	PHE
2	B	119	ASP
2	B	129	VAL
2	B	158	ASN
2	B	162	LEU

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Mol	Chain	Res	Type
2	B	170	LYS
2	B	171	ASP
2	B	177	ILE
2	B	180	LEU
2	B	187	LYS
2	B	204	TYR
2	B	216	LYS
2	B	217	ARG
2	B	221	LYS
2	B	222	GLU
2	B	224	VAL
2	B	249	LEU
2	B	259	MET
2	B	263	PHE
2	B	290	ARG
2	B	294	ARG
2	B	295	PHE
2	B	301	VAL
3	G	24	GLU
3	G	36	LEU
1	C	35	ASP
1	C	36	ASP
1	C	41	LEU
1	C	44	LEU
1	C	56	LEU
1	C	57	THR
1	C	60	ARG
1	C	82	TRP
1	C	85	PHE
1	C	86	CYS
1	C	114	THR
1	C	129	LEU
1	C	154	PHE
1	C	161	GLN
1	C	166	ARG
1	C	172	SER
1	C	191	ARG
1	C	241	ASN
1	C	242	CYS
1	C	254	THR
1	C	274	GLN
1	C	293	VAL

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Mol	Chain	Res	Type
1	C	308	TYR
1	C	309	THR
1	C	310	TRP
1	C	317	LEU
1	C	336	CYS
1	C	360	LEU
1	C	371	THR
1	C	380	THR
1	C	394	ASP
1	C	403	SER
1	C	412	LEU
1	C	423	ARG
1	C	430	GLN
1	C	433	LEU
1	C	443	ASP
1	C	450	LEU
1	C	454	GLU
1	C	469	LYS
1	C	473	ILE
1	C	478	THR
1	C	485	ILE
1	C	493	GLU
1	C	495	ARG
1	C	514	ILE
1	C	519	LYS
1	C	520	GLU
1	C	521	GLN
1	C	523	LEU
1	C	535	TYR
1	C	541	LEU
1	C	550	HIS
1	C	589	ARG
1	C	600	ARG
1	C	629	GLU
1	C	645	VAL
1	C	662	ASP
1	C	667	THR
1	C	671	LEU
1	C	681	ILE
1	C	687	SER
1	C	708	THR
1	C	719	LYS

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Mol	Chain	Res	Type
1	C	744	LEU
1	C	747	ASN
1	C	761	ILE
1	C	772	THR
1	C	791	ILE
1	C	801	LEU
1	C	805	LEU
1	C	815	LEU
1	C	818	GLU
1	C	824	ILE
1	C	859	PHE
1	C	861	THR
1	C	869	ASN
1	C	880	ARG
1	C	886	ARG
1	C	888	ILE
1	C	894	SER
1	C	897	GLN
1	C	900	THR
1	C	969	VAL
1	C	980	TRP
1	C	998	ARG
1	C	1000	LEU
1	C	1004	ARG
1	C	1010	VAL
2	D	20	GLU
2	D	22	LYS
2	D	27	ARG
2	D	57	MET
2	D	61	ILE
2	D	63	GLU
2	D	72	VAL
2	D	78	THR
2	D	90	PHE
2	D	150	ARG
2	D	162	LEU
2	D	170	LYS
2	D	171	ASP
2	D	173	LYS
2	D	175	CYS
2	D	177	ILE
2	D	187	LYS

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Mol	Chain	Res	Type
2	D	204	TYR
2	D	208	VAL
2	D	216	LYS
2	D	217	ARG
2	D	221	LYS
2	D	222	GLU
2	D	224	VAL
2	D	249	LEU
2	D	259	MET
2	D	263	PHE
2	D	267	THR
2	D	290	ARG
2	D	294	ARG
2	D	295	PHE
2	D	301	VAL
3	E	17	ASP
3	E	20	TYR
3	E	24	GLU
3	E	36	LEU
3	E	48	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	156	ASN
1	A	161	GLN
1	A	274	GLN
1	A	324	ASN
1	A	388	ASN
1	A	430	GLN
1	A	479	ASN
1	A	550	HIS
1	A	699	GLN
1	A	701	GLN
1	A	747	ASN
1	A	790	ASN
1	A	854	GLN
1	A	882	ASN
1	A	889	ASN
1	A	903	GLN
1	A	923	GLN

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Mol	Chain	Res	Type
1	A	935	ASN
1	A	944	ASN
2	B	181	ASN
2	B	262	GLN
2	B	292	GLN
3	G	28	ASN
1	C	111	GLN
1	C	119	GLN
1	C	120	ASN
1	C	143	GLN
1	C	156	ASN
1	C	161	GLN
1	C	274	GLN
1	C	324	ASN
1	C	388	ASN
1	C	399	GLN
1	C	430	GLN
1	C	550	HIS
1	C	570	ASN
1	C	790	ASN
1	C	819	GLN
1	C	889	ASN
1	C	903	GLN
1	C	923	GLN
2	D	140	ASN
2	D	158	ASN
2	D	181	ASN
2	D	262	GLN
3	E	28	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ALF	A	2002	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	A	2004	4	22,29,29	1.12	2 (9%)	27,45,45	2.00	5 (18%)
8	CLR	A	2009	-	31,31,31	4.18	11 (35%)	48,48,48	2.03	13 (27%)
8	CLR	A	2010	-	31,31,31	4.15	11 (35%)	48,48,48	2.10	12 (25%)
9	PC1	A	2011	-	53,53,53	0.88	4 (7%)	57,61,61	1.30	5 (8%)
9	PC1	A	2012	-	53,53,53	0.89	1 (1%)	57,61,61	1.41	8 (14%)
9	PC1	A	2013	-	53,53,53	0.86	3 (5%)	57,61,61	1.15	4 (7%)
9	PC1	A	2014	-	53,53,53	0.88	3 (5%)	57,61,61	1.34	4 (7%)
10	EFO	A	2015	-	55,58,58	2.09	17 (30%)	63,85,85	3.43	17 (26%)
9	PC1	B	401	-	53,53,53	0.87	4 (7%)	57,61,61	1.27	4 (7%)
11	NAG	B	402	-	14,14,15	0.21	0	15,19,21	0.36	0
5	ALF	C	2002	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	C	2004	-	22,29,29	0.90	1 (4%)	27,45,45	1.92	3 (11%)
9	PC1	C	2009	-	53,53,53	0.89	3 (5%)	57,61,61	1.26	4 (7%)
9	PC1	C	2010	-	53,53,53	0.87	3 (5%)	57,61,61	1.38	5 (8%)
9	PC1	C	2011	-	53,53,53	0.91	4 (7%)	57,61,61	1.29	5 (8%)
9	PC1	C	2012	-	53,53,53	0.88	3 (5%)	57,61,61	1.26	4 (7%)
10	EFO	C	2013	-	55,58,58	2.15	18 (32%)	63,85,85	3.38	18 (28%)
8	CLR	D	3001	-	31,31,31	4.19	12 (38%)	48,48,48	2.03	15 (31%)
8	CLR	D	3002	-	31,31,31	4.24	12 (38%)	48,48,48	1.81	12 (25%)
9	PC1	D	3003	-	53,53,53	0.88	3 (5%)	57,61,61	1.20	4 (7%)
11	NAG	D	3004	-	14,14,15	0.22	0	15,19,21	0.46	0
8	CLR	E	101	-	31,31,31	4.34	12 (38%)	48,48,48	2.32	14 (29%)
8	CLR	G	101	-	31,31,31	4.35	12 (38%)	48,48,48	2.52	12 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ALF	A	2002	-	-	0/0/0/0	0/0/0/0
6	ADP	A	2004	4	-	0/12/32/32	0/3/3/3
8	CLR	A	2009	-	-	0/10/68/68	0/4/4/4
8	CLR	A	2010	-	-	0/10/68/68	0/4/4/4
9	PC1	A	2011	-	-	0/57/57/57	0/0/0/0
9	PC1	A	2012	-	-	0/57/57/57	0/0/0/0
9	PC1	A	2013	-	-	0/57/57/57	0/0/0/0
9	PC1	A	2014	-	-	0/57/57/57	0/0/0/0
10	EFO	A	2015	-	-	0/72/110/110	0/1/3/3
9	PC1	B	401	-	-	0/57/57/57	0/0/0/0
11	NAG	B	402	-	-	0/6/23/26	0/1/1/1
5	ALF	C	2002	-	-	0/0/0/0	0/0/0/0
6	ADP	C	2004	-	-	0/12/32/32	0/3/3/3
9	PC1	C	2009	-	-	0/57/57/57	0/0/0/0
9	PC1	C	2010	-	-	0/57/57/57	0/0/0/0
9	PC1	C	2011	-	-	0/57/57/57	0/0/0/0
9	PC1	C	2012	-	-	2/57/57/57	0/0/0/0
10	EFO	C	2013	-	-	0/72/110/110	0/1/3/3
8	CLR	D	3001	-	-	0/10/68/68	0/4/4/4
8	CLR	D	3002	-	-	0/10/68/68	0/4/4/4
9	PC1	D	3003	-	-	0/57/57/57	0/0/0/0
11	NAG	D	3004	-	-	0/6/23/26	0/1/1/1
8	CLR	E	101	-	-	0/10/68/68	0/4/4/4
8	CLR	G	101	-	-	0/10/68/68	0/4/4/4

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2010	CLR	C10-C9	-11.29	1.35	1.56
8	E	101	CLR	C10-C9	-11.26	1.35	1.56
8	A	2009	CLR	C10-C9	-11.17	1.35	1.56
8	G	101	CLR	C10-C9	-11.16	1.35	1.56
8	D	3002	CLR	C10-C9	-11.08	1.36	1.56
8	D	3001	CLR	C10-C9	-10.85	1.36	1.56
10	C	2013	EFO	C15-C13	-7.20	1.36	1.52
10	A	2015	EFO	C15-C13	-6.92	1.37	1.52
8	E	101	CLR	C8-C14	-6.16	1.41	1.53
8	A	2010	CLR	C13-C14	-5.86	1.43	1.55
8	E	101	CLR	C13-C14	-5.77	1.43	1.55
8	D	3001	CLR	C13-C14	-5.60	1.43	1.55
8	D	3002	CLR	C13-C14	-5.46	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2009	CLR	C13-C14	-5.33	1.44	1.55
8	A	2010	CLR	C8-C14	-5.32	1.43	1.53
8	G	101	CLR	C13-C14	-5.03	1.44	1.55
8	D	3001	CLR	C8-C14	-4.93	1.43	1.53
8	G	101	CLR	C8-C14	-4.92	1.43	1.53
8	A	2009	CLR	C8-C14	-4.85	1.44	1.53
8	G	101	CLR	C12-C13	-4.58	1.45	1.54
10	C	2013	EFO	C6-C5	-4.47	1.43	1.53
8	A	2010	CLR	C12-C13	-4.40	1.45	1.54
10	A	2015	EFO	C6-C5	-4.38	1.43	1.53
8	D	3002	CLR	C8-C14	-4.33	1.45	1.53
8	E	101	CLR	C12-C13	-4.24	1.46	1.54
8	A	2009	CLR	C12-C13	-4.10	1.46	1.54
8	D	3001	CLR	C12-C13	-3.89	1.46	1.54
8	D	3002	CLR	C12-C13	-3.88	1.46	1.54
10	A	2015	EFO	C10-C11	-3.46	1.43	1.53
10	C	2013	EFO	C10-C11	-3.44	1.43	1.53
10	C	2013	EFO	C7-C6	-3.30	1.46	1.53
10	A	2015	EFO	C7-C6	-3.28	1.46	1.53
8	G	101	CLR	C20-C17	-3.08	1.48	1.54
8	E	101	CLR	C20-C17	-3.04	1.48	1.54
8	D	3001	CLR	C20-C17	-2.92	1.48	1.54
10	A	2015	EFO	C12-C11	-2.83	1.47	1.53
10	A	2015	EFO	C2D-C29	-2.80	1.46	1.53
10	C	2013	EFO	C2D-C29	-2.73	1.46	1.53
8	E	101	CLR	O1-C3	-2.69	1.35	1.43
10	C	2013	EFO	C12-C11	-2.67	1.47	1.53
8	A	2010	CLR	C20-C17	-2.62	1.49	1.54
10	C	2013	EFO	C8-C10	-2.55	1.50	1.53
9	A	2013	PC1	O21-C2	-2.42	1.40	1.46
8	G	101	CLR	O1-C3	-2.32	1.36	1.43
9	C	2009	PC1	O21-C2	-2.31	1.40	1.46
9	C	2011	PC1	C2A-C29	-2.25	1.38	1.51
9	D	3003	PC1	O21-C2	-2.21	1.40	1.46
9	B	401	PC1	O21-C2	-2.20	1.41	1.46
9	A	2011	PC1	C3A-C39	-2.19	1.38	1.51
9	C	2011	PC1	C3A-C39	-2.18	1.38	1.51
9	A	2013	PC1	C3A-C39	-2.17	1.39	1.51
10	A	2015	EFO	C8-C10	-2.16	1.50	1.53
8	D	3001	CLR	O1-C3	-2.16	1.37	1.43
9	B	401	PC1	C3A-C39	-2.15	1.39	1.51
9	A	2011	PC1	O21-C2	-2.15	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	2012	PC1	C3A-C39	-2.13	1.39	1.51
8	D	3002	CLR	O1-C3	-2.11	1.37	1.43
9	C	2009	PC1	C3A-C39	-2.11	1.39	1.51
9	D	3003	PC1	C3A-C39	-2.11	1.39	1.51
9	C	2010	PC1	C3A-C39	-2.07	1.39	1.51
9	A	2014	PC1	C3A-C39	-2.05	1.39	1.51
8	A	2009	CLR	C20-C17	-2.05	1.50	1.54
8	D	3002	CLR	C7-C6	2.00	1.54	1.50
8	E	101	CLR	C15-C14	2.04	1.59	1.54
9	B	401	PC1	O21-C21	2.07	1.40	1.34
8	D	3002	CLR	C15-C14	2.09	1.59	1.54
9	C	2011	PC1	O21-C21	2.11	1.40	1.34
9	C	2010	PC1	O21-C21	2.13	1.40	1.34
8	D	3001	CLR	C15-C14	2.14	1.59	1.54
10	A	2015	EFO	O30-C30	2.17	1.25	1.21
9	C	2012	PC1	O21-C21	2.17	1.40	1.34
9	A	2014	PC1	O21-C21	2.21	1.40	1.34
10	C	2013	EFO	O30-C30	2.27	1.25	1.21
9	A	2011	PC1	O21-C21	2.31	1.41	1.34
6	C	2004	ADP	C5-C4	2.34	1.45	1.40
8	E	101	CLR	C10-C5	2.35	1.57	1.52
8	D	3001	CLR	C10-C5	2.36	1.58	1.52
8	D	3002	CLR	C10-C5	2.36	1.58	1.52
10	A	2015	EFO	O37-C36	2.48	1.40	1.34
10	C	2013	EFO	C19-C20	2.49	1.51	1.44
10	A	2015	EFO	C19-C20	2.51	1.51	1.44
10	C	2013	EFO	O37-C36	2.51	1.40	1.34
10	C	2013	EFO	C27-C28	2.52	1.59	1.54
8	A	2009	CLR	C15-C14	2.53	1.60	1.54
8	A	2010	CLR	C15-C14	2.59	1.60	1.54
8	A	2010	CLR	C10-C5	2.67	1.58	1.52
8	G	101	CLR	C15-C14	2.68	1.60	1.54
8	A	2009	CLR	C10-C5	2.69	1.58	1.52
9	A	2013	PC1	O31-C31	2.77	1.41	1.33
6	A	2004	ADP	C5-C4	2.78	1.46	1.40
9	A	2011	PC1	O31-C31	2.80	1.41	1.33
10	A	2015	EFO	C19-C18	2.84	1.45	1.33
6	A	2004	ADP	O4'-C1'	2.85	1.44	1.41
8	G	101	CLR	C10-C5	2.90	1.59	1.52
10	C	2013	EFO	C19-C18	2.92	1.45	1.33
10	A	2015	EFO	C17-C18	2.93	1.56	1.50
10	C	2013	EFO	C17-C18	2.99	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	401	PC1	O31-C31	2.99	1.42	1.33
9	C	2012	PC1	O31-C31	3.05	1.42	1.33
9	C	2011	PC1	O31-C31	3.09	1.42	1.33
9	C	2009	PC1	O31-C31	3.09	1.42	1.33
9	D	3003	PC1	O31-C31	3.10	1.42	1.33
10	C	2013	EFO	C20-C21	3.11	1.42	1.32
10	A	2015	EFO	C35-C34	3.16	1.40	1.32
10	A	2015	EFO	C20-C21	3.18	1.42	1.32
10	A	2015	EFO	C1A-C10	3.21	1.60	1.53
10	C	2013	EFO	C1A-C10	3.27	1.60	1.53
9	A	2014	PC1	O31-C31	3.33	1.43	1.33
9	C	2010	PC1	O31-C31	3.35	1.43	1.33
10	C	2013	EFO	C35-C34	3.35	1.41	1.32
9	A	2012	PC1	O31-C31	3.36	1.43	1.33
10	A	2015	EFO	O14-C13	3.48	1.51	1.44
10	C	2013	EFO	O14-C13	3.50	1.52	1.44
8	A	2010	CLR	C16-C15	3.79	1.64	1.54
8	D	3001	CLR	C16-C15	3.86	1.64	1.54
8	G	101	CLR	C16-C15	3.88	1.65	1.54
8	E	101	CLR	C16-C15	3.91	1.65	1.54
8	D	3002	CLR	C16-C15	4.08	1.65	1.54
8	A	2009	CLR	C16-C15	4.28	1.66	1.54
10	A	2015	EFO	O37-C11	4.32	1.51	1.44
10	C	2013	EFO	O37-C11	4.36	1.51	1.44
8	G	101	CLR	C6-C5	5.80	1.47	1.33
8	A	2010	CLR	C6-C5	5.95	1.47	1.33
8	D	3001	CLR	C6-C5	5.97	1.47	1.33
8	D	3002	CLR	C6-C5	6.00	1.47	1.33
8	A	2009	CLR	C6-C5	6.10	1.48	1.33
8	E	101	CLR	C6-C5	6.18	1.48	1.33
8	A	2010	CLR	C12-C11	8.32	1.71	1.53
8	E	101	CLR	C12-C11	8.74	1.72	1.53
8	A	2009	CLR	C12-C11	8.80	1.72	1.53
8	D	3001	CLR	C12-C11	9.02	1.73	1.53
8	G	101	CLR	C12-C11	9.32	1.74	1.53
8	D	3002	CLR	C12-C11	9.70	1.74	1.53
8	A	2010	CLR	C11-C9	12.94	1.76	1.53
8	A	2009	CLR	C11-C9	13.31	1.77	1.53
8	D	3001	CLR	C11-C9	13.74	1.78	1.53
8	E	101	CLR	C11-C9	13.85	1.78	1.53
8	D	3002	CLR	C11-C9	13.99	1.78	1.53
8	G	101	CLR	C11-C9	14.55	1.79	1.53

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	101	CLR	C7-C8-C14	-8.67	97.33	110.86
8	E	101	CLR	C15-C14-C8	-8.39	105.77	119.03
8	G	101	CLR	C15-C14-C8	-8.13	106.18	119.03
6	C	2004	ADP	N3-C2-N1	-7.24	123.35	128.89
8	E	101	CLR	C7-C8-C14	-6.81	100.23	110.86
10	A	2015	EFO	O14-C13-C12	-6.73	102.23	109.78
6	A	2004	ADP	N3-C2-N1	-6.46	123.95	128.89
8	A	2010	CLR	C11-C9-C10	-5.40	105.96	113.11
8	A	2010	CLR	C7-C8-C14	-5.18	102.78	110.86
8	A	2009	CLR	C11-C9-C10	-4.91	106.61	113.11
8	G	101	CLR	C12-C13-C17	-4.90	107.85	116.56
8	D	3001	CLR	C7-C8-C14	-4.90	103.22	110.86
10	C	2013	EFO	O14-C13-C12	-4.82	104.37	109.78
8	A	2009	CLR	C7-C8-C14	-4.78	103.40	110.86
8	A	2009	CLR	C12-C13-C17	-4.77	108.08	116.56
8	D	3001	CLR	C15-C14-C8	-4.76	111.51	119.03
8	D	3002	CLR	C11-C9-C10	-4.55	107.08	113.11
8	D	3002	CLR	C15-C14-C8	-4.52	111.88	119.03
8	A	2009	CLR	C15-C14-C8	-4.52	111.89	119.03
8	A	2010	CLR	C12-C13-C17	-4.42	108.70	116.56
8	G	101	CLR	C16-C15-C14	-4.40	96.26	105.12
8	A	2010	CLR	C15-C14-C8	-4.36	112.13	119.03
10	C	2013	EFO	C8-O14-C13	-4.27	105.35	114.86
6	C	2004	ADP	C2'-C1'-N9	-4.23	107.83	114.29
6	A	2004	ADP	PA-O3A-PB	-4.16	118.73	132.67
10	A	2015	EFO	C8-O14-C13	-4.15	105.63	114.86
10	C	2013	EFO	C8-O9-C4	-4.09	105.77	114.86
10	A	2015	EFO	C8-O9-C4	-4.02	105.92	114.86
8	G	101	CLR	C11-C12-C13	-3.99	105.71	112.84
10	C	2013	EFO	C22-C21-C20	-3.94	119.86	125.34
8	E	101	CLR	C11-C12-C13	-3.84	105.97	112.84
6	A	2004	ADP	C4-C5-N7	-3.84	105.94	109.48
8	D	3001	CLR	C12-C13-C17	-3.83	109.75	116.56
8	A	2010	CLR	C11-C9-C8	-3.76	106.29	111.74
8	A	2010	CLR	C12-C11-C9	-3.74	106.79	113.10
8	G	101	CLR	C11-C9-C8	-3.74	106.31	111.74
8	E	101	CLR	C8-C7-C6	-3.71	107.15	112.75
8	D	3001	CLR	C11-C9-C10	-3.65	108.27	113.11
8	E	101	CLR	C12-C13-C17	-3.59	110.18	116.56
8	A	2010	CLR	C22-C20-C17	-3.57	102.75	110.24
8	A	2009	CLR	C11-C9-C8	-3.56	106.57	111.74
8	A	2010	CLR	C11-C12-C13	-3.50	106.59	112.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	101	CLR	C22-C20-C17	-3.41	103.07	110.24
8	E	101	CLR	C11-C9-C10	-3.39	108.62	113.11
8	D	3002	CLR	C7-C8-C14	-3.38	105.58	110.86
8	G	101	CLR	C8-C7-C6	-3.22	107.88	112.75
10	C	2013	EFO	O37-C36-O36	-3.18	118.35	123.30
8	D	3002	CLR	C11-C9-C8	-3.14	107.18	111.74
10	A	2015	EFO	C22-C21-C20	-3.13	120.98	125.34
8	E	101	CLR	C12-C11-C9	-3.09	107.89	113.10
8	D	3001	CLR	C11-C9-C8	-2.99	107.40	111.74
8	D	3001	CLR	C12-C11-C9	-2.98	108.08	113.10
8	E	101	CLR	C16-C15-C14	-2.93	99.22	105.12
8	D	3002	CLR	C12-C13-C17	-2.93	111.35	116.56
8	D	3001	CLR	C16-C17-C20	-2.84	106.98	112.05
9	A	2011	PC1	O31-C31-O32	-2.83	116.19	123.49
8	A	2009	CLR	C22-C20-C17	-2.83	104.30	110.24
8	A	2009	CLR	C11-C12-C13	-2.76	107.90	112.84
10	A	2015	EFO	O25-C25-C26	-2.69	105.34	108.66
8	A	2009	CLR	C10-C5-C6	-2.68	117.97	122.92
8	D	3001	CLR	C22-C20-C17	-2.63	104.72	110.24
8	D	3001	CLR	C11-C12-C13	-2.62	108.16	112.84
8	D	3001	CLR	C10-C5-C6	-2.54	118.22	122.92
10	C	2013	EFO	O9-C4-C5	-2.51	106.91	110.46
6	C	2004	ADP	C4-C5-N7	-2.46	107.21	109.48
8	D	3002	CLR	C8-C7-C6	-2.45	109.06	112.75
8	D	3002	CLR	C2-C1-C10	-2.39	107.67	112.75
10	C	2013	EFO	C51-C5-C4	-2.37	109.24	112.72
9	C	2011	PC1	O31-C31-O32	-2.30	117.56	123.49
8	D	3001	CLR	C18-C13-C17	-2.29	107.26	111.75
8	E	101	CLR	C16-C17-C20	-2.28	107.98	112.05
8	A	2010	CLR	C10-C5-C6	-2.28	118.71	122.92
8	A	2009	CLR	C8-C7-C6	-2.26	109.33	112.75
8	D	3002	CLR	C10-C5-C6	-2.26	118.75	122.92
8	E	101	CLR	C10-C5-C6	-2.22	118.82	122.92
8	D	3002	CLR	C2-C3-C4	-2.20	106.39	110.32
10	A	2015	EFO	O37-C36-O36	-2.16	119.93	123.30
8	A	2009	CLR	C12-C11-C9	-2.16	109.46	113.10
8	A	2010	CLR	C2-C3-C4	-2.16	106.48	110.32
8	A	2009	CLR	C7-C8-C9	-2.10	106.85	109.71
10	C	2013	EFO	C2C-C27-C28	-2.10	108.68	112.37
8	G	101	CLR	C19-C10-C5	-2.09	105.13	108.36
8	G	101	CLR	C2-C3-C4	-2.03	106.71	110.32
9	A	2012	PC1	O21-C21-O22	-2.01	118.29	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	2013	EFO	C2B-C25-C26	2.03	111.06	107.50
9	A	2012	PC1	C34-C33-C32	2.07	120.86	113.29
8	E	101	CLR	C15-C14-C13	2.07	106.50	103.82
10	C	2013	EFO	C32-C31-C30	2.10	113.38	109.84
9	A	2013	PC1	O31-C31-C32	2.12	118.36	111.90
10	C	2013	EFO	C12-C11-C10	2.13	116.38	112.19
6	A	2004	ADP	C4'-O4'-C1'	2.18	112.12	109.72
9	A	2012	PC1	C3-O31-C31	2.25	123.13	116.85
9	C	2011	PC1	O31-C3-C2	2.26	114.77	108.69
8	A	2010	CLR	C17-C13-C14	2.26	102.75	100.09
10	C	2013	EFO	O28-C28-C29	2.29	113.99	108.72
10	A	2015	EFO	O28-C28-C29	2.30	114.02	108.72
9	B	401	PC1	O31-C31-C32	2.33	119.00	111.90
9	C	2009	PC1	O31-C31-C32	2.35	119.06	111.90
8	E	101	CLR	C17-C13-C14	2.36	102.86	100.09
8	D	3001	CLR	C12-C13-C14	2.37	111.16	107.31
9	C	2012	PC1	O31-C31-C32	2.38	119.15	111.90
10	A	2015	EFO	C23-C22-C21	2.38	117.40	113.81
9	D	3003	PC1	O21-C21-C22	2.41	116.77	111.53
8	D	3001	CLR	C19-C10-C9	2.43	114.78	111.67
10	A	2015	EFO	C6-C7-C8	2.44	116.60	112.05
8	G	101	CLR	C4-C5-C10	2.49	120.06	116.43
9	A	2012	PC1	C2-O21-C21	2.53	123.97	117.89
8	A	2009	CLR	C4-C5-C10	2.54	120.13	116.43
8	D	3001	CLR	C4-C5-C10	2.55	120.14	116.43
9	A	2012	PC1	O31-C31-C32	2.59	119.79	111.90
9	A	2011	PC1	O31-C31-C32	2.63	119.90	111.90
9	A	2013	PC1	O31-C3-C2	2.63	115.76	108.69
10	A	2015	EFO	C12-C11-C10	2.64	117.39	112.19
8	D	3002	CLR	C12-C13-C14	2.69	111.67	107.31
9	D	3003	PC1	O31-C31-C32	2.70	120.11	111.90
10	A	2015	EFO	C11-O37-C36	2.72	121.33	117.27
9	A	2011	PC1	O31-C3-C2	2.79	116.20	108.69
8	G	101	CLR	C19-C10-C9	2.89	115.36	111.67
9	B	401	PC1	O31-C3-C2	2.91	116.53	108.69
9	A	2014	PC1	O31-C31-C32	2.92	120.78	111.90
9	C	2010	PC1	O31-C31-C32	2.93	120.84	111.90
8	E	101	CLR	C12-C13-C14	2.96	112.12	107.31
9	C	2011	PC1	O31-C31-C32	2.98	120.98	111.90
9	C	2010	PC1	C2-O21-C21	3.00	125.09	117.89
8	D	3002	CLR	C19-C10-C9	3.01	115.51	111.67
10	A	2015	EFO	C32-C31-C30	3.03	114.94	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2004	ADP	O4'-C1'-N9	3.06	114.50	108.10
8	A	2010	CLR	C4-C5-C10	3.16	121.03	116.43
9	C	2010	PC1	O21-C21-C22	3.21	118.51	111.53
10	C	2013	EFO	C23-C22-C21	3.22	118.67	113.81
10	C	2013	EFO	C1A-C10-C8	3.23	117.59	112.15
9	A	2012	PC1	O21-C21-C22	3.32	118.75	111.53
9	C	2009	PC1	O31-C3-C2	3.35	117.72	108.69
8	D	3002	CLR	C13-C14-C8	3.42	119.71	114.37
9	C	2012	PC1	C15-N-C13	3.48	117.92	108.98
10	A	2015	EFO	O37-C36-C35	3.53	120.17	111.42
8	G	101	CLR	C21-C20-C17	3.56	118.89	112.96
9	D	3003	PC1	C15-N-C13	3.56	118.15	108.98
9	A	2013	PC1	C15-N-C13	3.69	118.47	108.98
9	A	2014	PC1	C15-N-C13	3.71	118.52	108.98
9	C	2011	PC1	C15-N-C13	3.72	118.53	108.98
8	A	2009	CLR	C17-C13-C14	3.73	104.47	100.09
8	D	3001	CLR	C17-C13-C14	3.73	104.47	100.09
9	C	2012	PC1	O31-C3-C2	3.85	119.06	108.69
9	A	2012	PC1	O31-C3-C2	3.86	119.07	108.69
9	A	2011	PC1	C15-N-C13	3.88	118.96	108.98
9	A	2012	PC1	C15-N-C13	3.92	119.06	108.98
9	C	2009	PC1	O21-C21-C22	3.93	120.07	111.53
9	A	2013	PC1	O21-C21-C22	3.97	120.15	111.53
9	C	2009	PC1	C15-N-C13	4.00	119.25	108.98
9	A	2014	PC1	O21-C21-C22	4.05	120.32	111.53
10	C	2013	EFO	O37-C36-C35	4.06	121.50	111.42
9	C	2010	PC1	C15-N-C13	4.10	119.53	108.98
9	D	3003	PC1	O31-C3-C2	4.13	119.80	108.69
9	B	401	PC1	C15-N-C13	4.17	119.70	108.98
9	C	2010	PC1	O31-C3-C2	4.20	119.99	108.69
9	C	2012	PC1	O21-C21-C22	4.24	120.75	111.53
10	A	2015	EFO	C1A-C10-C8	4.30	119.40	112.15
9	C	2011	PC1	O21-C21-C22	4.34	120.95	111.53
9	A	2014	PC1	O31-C3-C2	4.40	120.52	108.69
9	B	401	PC1	O21-C21-C22	4.41	121.12	111.53
9	A	2011	PC1	O21-C21-C22	4.56	121.44	111.53
10	C	2013	EFO	O14-C13-C15	6.03	113.04	106.07
10	A	2015	EFO	O14-C13-C15	6.67	113.78	106.07
10	A	2015	EFO	O9-C4-C3	7.74	116.14	105.88
10	C	2013	EFO	O9-C4-C3	9.45	118.41	105.88
10	C	2013	EFO	O9-C8-O14	19.78	160.24	109.60
10	A	2015	EFO	O9-C8-O14	20.35	161.70	109.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	2012	PC1	C2-O21-C21-O22
9	C	2012	PC1	C2-O21-C21-C22

There are no ring outliers.

19 monomers are involved in 116 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2002	ALF	1	0
6	A	2004	ADP	3	0
8	A	2009	CLR	12	0
8	A	2010	CLR	15	0
9	A	2011	PC1	1	0
9	A	2012	PC1	2	0
9	A	2013	PC1	7	0
9	A	2014	PC1	4	0
9	B	401	PC1	2	0
5	C	2002	ALF	2	0
6	C	2004	ADP	6	0
9	C	2009	PC1	8	0
9	C	2011	PC1	3	0
9	C	2012	PC1	6	0
8	D	3001	CLR	12	0
8	D	3002	CLR	17	0
9	D	3003	PC1	2	0
8	E	101	CLR	13	0
8	G	101	CLR	9	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	994/1016 (97%)	-0.29	21 (2%) 67 56	17, 57, 117, 181	0
1	C	994/1016 (97%)	0.02	38 (3%) 44 32	34, 74, 143, 199	0
2	B	303/303 (100%)	0.90	53 (17%) 2 1	59, 130, 199, 229	0
2	D	303/303 (100%)	0.93	51 (16%) 2 1	68, 127, 205, 239	0
3	E	35/65 (53%)	0.81	5 (14%) 4 2	70, 88, 165, 168	0
3	G	34/65 (52%)	0.52	3 (8%) 12 6	75, 91, 164, 175	0
All	All	2663/2768 (96%)	0.13	171 (6%) 23 14	17, 77, 161, 239	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	218	ASP	17.9
2	D	219	GLU	14.8
2	B	1	MET	9.9
2	D	167	TYR	9.9
3	E	16	VAL	9.7
2	D	166	THR	9.1
3	E	15	ASP	9.1
2	D	1	MET	8.8
1	C	396	THR	8.6
3	G	15	ASP	8.2
2	B	165	GLU	7.9
2	B	198	THR	7.5
1	C	268	SER	7.3
2	B	166	THR	7.2
2	D	217	ARG	7.0
2	D	196	LEU	6.9
2	D	195	SER	6.6
1	A	272	GLY	6.6
2	B	220	ASP	6.2

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Mol	Chain	Res	Type	RSRZ
2	D	17	TRP	6.1
2	B	15	PHE	6.0
1	C	265	THR	6.0
2	B	201	VAL	6.0
2	D	162	LEU	5.9
2	B	163	ASN	5.8
2	B	164	ASP	5.8
3	E	17	ASP	5.5
2	B	218	ASP	5.4
3	G	16	VAL	5.4
2	D	228	GLU	5.4
2	D	2	ALA	5.3
2	B	217	ARG	5.3
2	D	16	ILE	5.3
1	C	397	GLU	5.2
2	D	15	PHE	5.2
1	A	268	SER	5.2
1	C	395	THR	5.2
2	D	203	LYS	5.0
2	D	198	THR	5.0
2	D	197	GLU	5.0
2	B	219	GLU	5.0
3	E	18	PRO	5.0
2	B	7	LYS	4.9
2	D	163	ASN	4.8
1	A	400	SER	4.8
2	D	201	VAL	4.6
2	B	17	TRP	4.5
1	A	23	ARG	4.5
2	B	4	GLY	4.5
2	B	196	LEU	4.5
1	A	271	GLU	4.5
2	B	194	GLU	4.5
2	B	195	SER	4.4
2	D	164	ASP	4.4
2	D	9	GLU	4.4
1	C	269	GLY	4.4
2	D	11	SER	4.3
2	B	6	ALA	4.2
2	B	302	LYS	4.1
2	B	227	MET	4.1
2	D	202	MET	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	117	GLU	4.1
3	G	17	ASP	4.1
2	B	167	TYR	4.0
1	C	82	TRP	4.0
2	D	165	GLU	4.0
2	B	200	PRO	4.0
1	A	270	LEU	4.0
2	D	220	ASP	4.0
1	A	273	GLY	3.9
1	C	24	ASP	3.8
2	B	9	GLU	3.8
1	C	642	ASN	3.6
2	D	23	GLU	3.6
1	C	398	ASN	3.6
1	A	395	THR	3.5
1	A	82	TRP	3.5
2	D	82	GLN	3.5
1	C	78	THR	3.5
2	B	3	ARG	3.4
2	D	118	LYS	3.4
1	C	141	TYR	3.4
2	D	200	PRO	3.4
1	C	650	PRO	3.3
1	C	270	LEU	3.3
2	D	89	SER	3.3
1	C	645	VAL	3.3
1	A	399	GLN	3.3
1	A	114	THR	3.2
1	A	265	THR	3.2
1	A	269	GLY	3.1
2	B	23	GLU	3.1
2	D	194	GLU	3.1
1	C	121	ASP	3.1
2	B	5	LYS	3.1
2	D	10	GLY	3.1
2	B	12	TRP	3.0
1	A	264	ALA	3.0
2	D	21	LYS	3.0
1	C	632	GLU	3.0
1	A	401	GLY	3.0
1	C	151	MET	3.0
2	D	193	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	142	GLU	2.9
2	B	273	ARG	2.9
1	C	1004	ARG	2.9
2	B	290	ARG	2.8
1	C	495	ARG	2.8
2	B	235	TYR	2.8
1	C	267	ALA	2.8
2	D	192	LYS	2.8
2	B	262	GLN	2.8
2	B	147	LYS	2.7
2	B	16	ILE	2.7
2	B	2	ALA	2.7
2	B	19	SER	2.7
2	B	11	SER	2.6
1	C	124	TYR	2.6
1	C	116	GLU	2.6
1	C	117	GLU	2.6
2	D	5	LYS	2.5
1	C	1000	LEU	2.5
2	D	19	SER	2.5
2	B	10	GLY	2.5
2	B	202	MET	2.5
2	B	193	ASN	2.5
2	D	207	TYR	2.5
2	B	118	LYS	2.5
2	D	141	ASN	2.5
1	C	266	LEU	2.5
2	B	120	ASP	2.5
2	D	13	LYS	2.5
2	B	206	PRO	2.4
2	D	229	TYR	2.4
2	B	203	LYS	2.4
2	D	273	ARG	2.4
2	B	121	MET	2.4
2	B	162	LEU	2.4
1	C	122	ASN	2.4
2	D	6	ALA	2.4
1	C	23	ARG	2.4
2	D	100	SER	2.4
1	A	24	ASP	2.4
1	A	495	ARG	2.3
1	C	272	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	3	ARG	2.3
1	C	431	GLU	2.3
2	B	8	GLU	2.3
2	D	115	LEU	2.3
2	D	152	ARG	2.3
1	A	120	ASN	2.3
1	C	112	ALA	2.3
1	C	310	TRP	2.2
3	E	49	ARG	2.2
2	D	199	TYR	2.2
1	A	266	LEU	2.2
1	C	123	LEU	2.2
1	A	974	TYR	2.2
2	D	24	PHE	2.2
1	C	115	GLU	2.2
2	B	84	GLN	2.1
2	B	266	LEU	2.1
2	B	199	TYR	2.1
2	D	20	GLU	2.1
2	B	249	LEU	2.1
1	C	406	LYS	2.1
1	C	108	TYR	2.1
1	C	455	LEU	2.1
2	D	33	PHE	2.1
1	C	401	GLY	2.1
2	B	143	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	NA	C	2006	1/1	0.22	0.42	7.31	83,83,83,83	0
9	PC1	A	2012	54/54	0.79	0.36	3.93	61,117,163,176	0
7	NA	A	2007	1/1	0.90	0.28	3.52	98,98,98,98	0
9	PC1	C	2012	54/54	0.76	0.35	3.38	79,133,162,185	0
8	CLR	D	3002	28/28	0.87	0.29	3.02	13,97,131,141	0
7	NA	C	2005	1/1	0.88	0.29	2.96	103,103,103,103	0
10	EFO	C	2013	56/56	0.78	0.41	2.89	49,150,194,195	0
8	CLR	A	2010	28/28	0.89	0.32	2.55	60,98,131,138	0
10	EFO	A	2015	56/56	0.82	0.33	2.28	91,134,150,160	0
9	PC1	C	2011	54/54	0.83	0.42	2.01	77,117,163,173	0
7	NA	C	2007	1/1	0.95	0.26	1.94	77,77,77,77	0
9	PC1	C	2010	54/54	0.82	0.32	1.55	68,101,143,205	0
9	PC1	B	401	54/54	0.82	0.27	1.38	61,90,146,170	0
9	PC1	A	2013	54/54	0.88	0.28	1.37	71,103,124,174	0
7	NA	A	2005	1/1	0.92	0.18	1.21	95,95,95,95	0
9	PC1	D	3003	54/54	0.88	0.23	1.20	44,80,121,142	0
5	ALF	A	2002	5/5	0.98	0.17	1.16	14,14,28,29	0
9	PC1	A	2014	54/54	0.81	0.36	0.59	86,123,160,189	0
9	PC1	C	2009	54/54	0.88	0.26	0.49	59,107,140,145	0
8	CLR	A	2009	28/28	0.89	0.22	0.42	62,93,107,147	0
9	PC1	A	2011	54/54	0.90	0.26	0.29	57,97,128,130	0
8	CLR	G	101	28/28	0.91	0.17	-0.12	54,91,100,131	0
8	CLR	E	101	28/28	0.92	0.16	-0.16	37,77,109,172	0
7	NA	A	2006	1/1	0.93	0.16	-0.29	65,65,65,65	0
5	ALF	C	2002	5/5	0.99	0.15	-0.47	20,24,71,106	0
8	CLR	D	3001	28/28	0.91	0.18	-0.57	35,83,89,92	0
4	MG	A	2003	1/1	1.00	0.11	-0.69	15,15,15,15	0
6	ADP	C	2004	27/27	0.96	0.14	-0.79	31,47,57,60	0
6	ADP	A	2004	27/27	0.97	0.11	-0.82	10,23,38,47	0
4	MG	C	2003	1/1	0.98	0.12	-1.21	51,51,51,51	0
7	NA	A	2008	1/1	0.72	0.17	-	59,59,59,59	0
4	MG	C	2001	1/1	0.84	0.23	-	54,54,54,54	0
11	NAG	D	3004	14/15	0.84	0.31	-	96,123,132,133	0
4	MG	A	2001	1/1	0.94	0.39	-	61,61,61,61	0
7	NA	C	2008	1/1	0.95	0.16	-	46,46,46,46	0
11	NAG	B	402	14/15	0.84	0.34	-	126,137,144,146	0

6.5 Other polymers ⓘ

There are no such residues in this entry.