



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:23 AM GMT

PDB ID : 2A74
Title : Human Complement Component C3c
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Nilsson-Ekdahl, K.; Nilsson, B.; Gros, P.
Deposited on : 2005-07-04
Resolution : 2.40 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

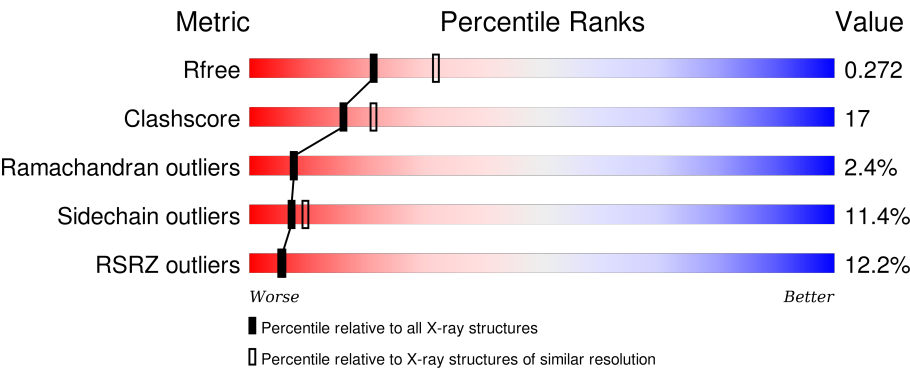
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	643	<div><div>9%</div><div>65%26%6% ..</div></div>
1	D	643	<div><div>11%</div><div>66%24%7% ..</div></div>
2	B	188	<div><div>10%</div><div>78%14%5% .</div></div>
2	E	188	<div><div>25%</div><div>69%21%6% ..</div></div>
3	C	343	<div><div>11%</div><div>51%26%7% .14%</div></div>

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Mol	Chain	Length	Quality of chain
3	F	343	

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
4	NDG	A	645	X	-	-	-
4	NDG	D	644	-	-	-	X
4	NDG	D	645	X	-	-	-
5	GOL	A	712	-	-	X	X
5	GOL	A	713	-	-	-	X
5	GOL	B	702	-	-	-	X
5	GOL	C	709	-	-	-	X
5	GOL	D	711	-	-	X	X
5	GOL	E	705	-	-	-	X
5	GOL	E	706	-	-	-	X
5	GOL	F	707	-	-	-	X
6	NO3	C	801	-	X	-	X
6	NO3	F	802	-	X	-	X
6	NO3	F	803	-	X	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 18389 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 Complement Component C3c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total	C	N	O	S	0	0	0
			4907	3127	828	937	15			
1	D	633	Total	C	N	O	S	0	0	0
			4933	3144	833	941	15			

- Molecule 2 is a protein called Complement Component C3c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1480	950	249	276	5			
2	E	184	Total	C	N	O	S	0	0	0
			1484	954	250	275	5			

- Molecule 3 is a protein called Complement Component C3c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	296	Total	C	N	O	S	0	0	0
			2407	1517	395	475	20			
3	F	298	Total	C	N	O	S	0	0	0
			2421	1524	397	480	20			

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

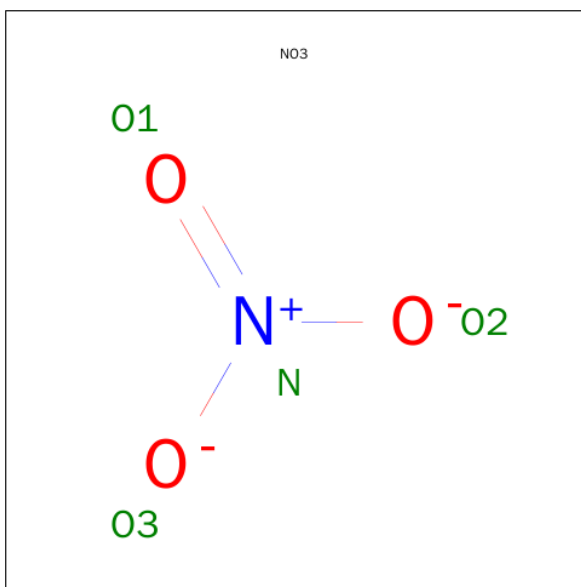
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	N	O	0	0
			4	1	3		
6	F	1	Total	N	O	0	0
			4	1	3		
6	F	1	Total	N	O	0	0
			4	1	3		

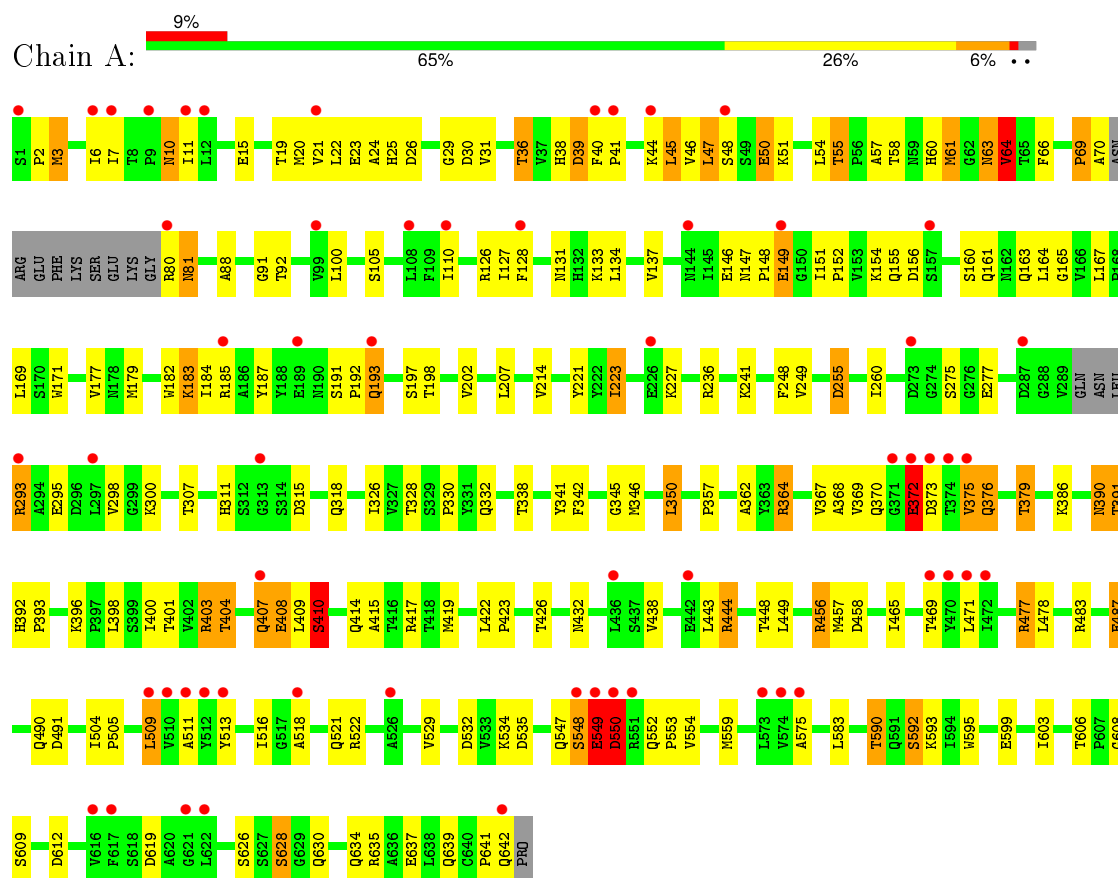
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	188	Total	O	0	0
			188	188		
7	B	58	Total	O	0	0
			58	58		
7	C	71	Total	O	0	0
			71	71		
7	D	148	Total	O	0	0
			148	148		
7	E	53	Total	O	0	0
			53	53		
7	F	93	Total	O	0	0
			93	93		

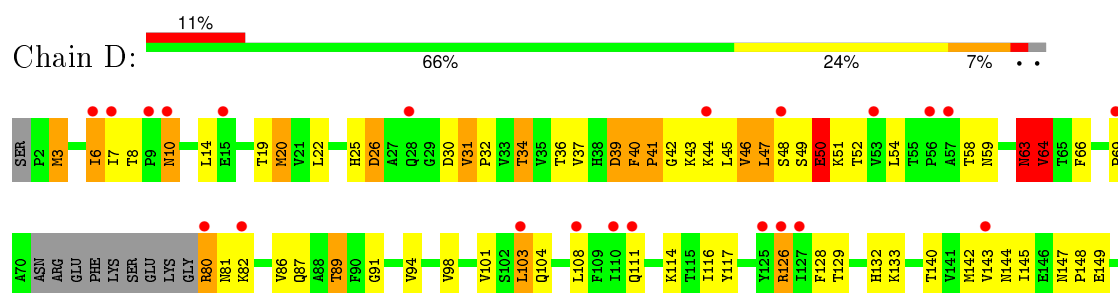
3 Residue-property plots [i](#)

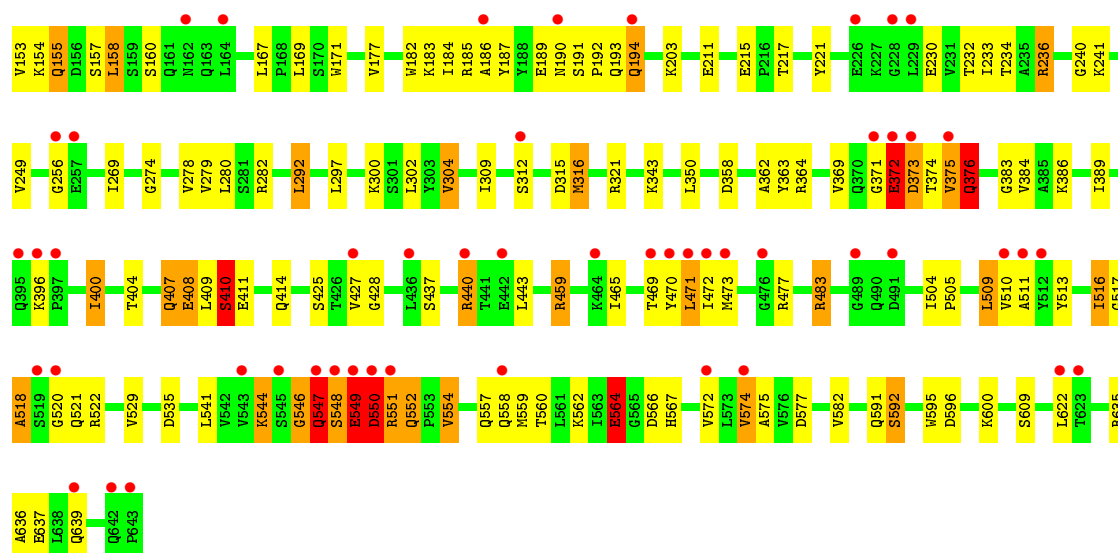
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Complement Component C3c

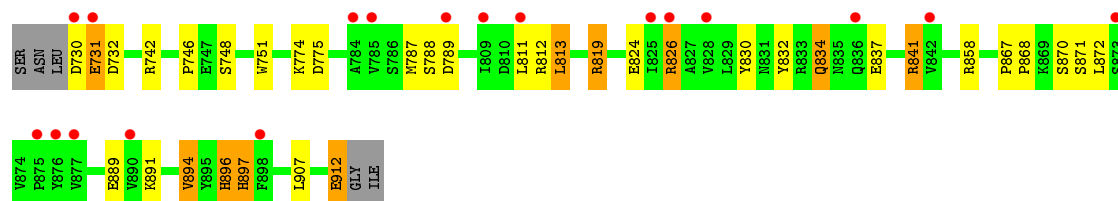
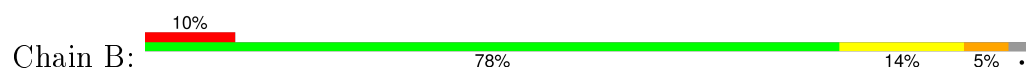


• Molecule 1: Complement Component C3c

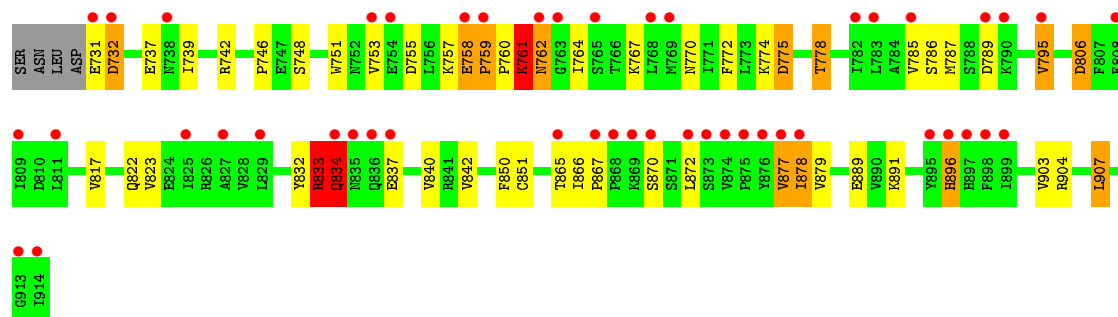




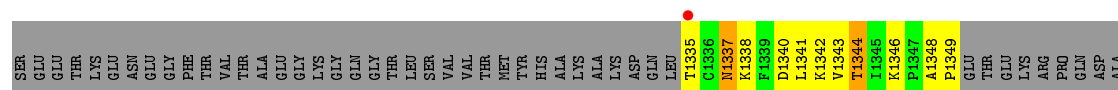
• Molecule 2: Complement Component C3c

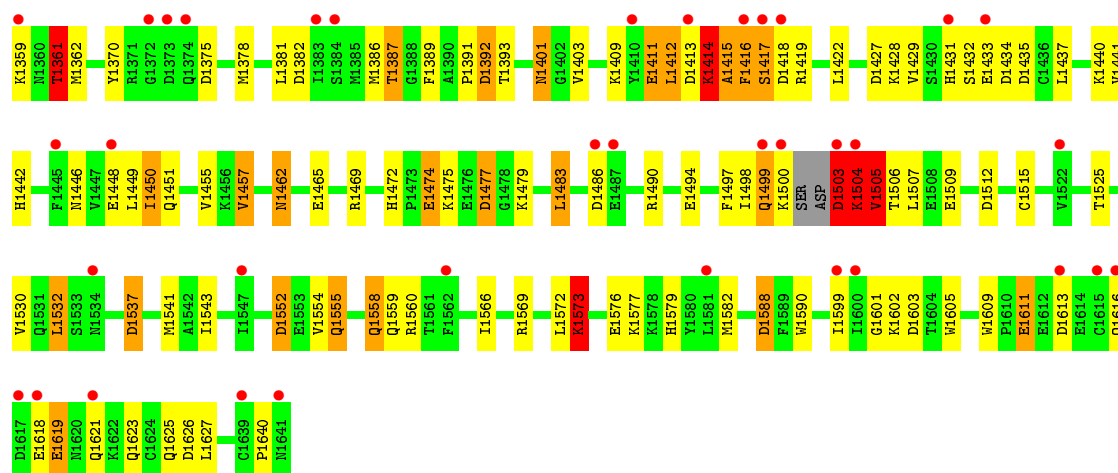


• Molecule 2: Complement Component C3c

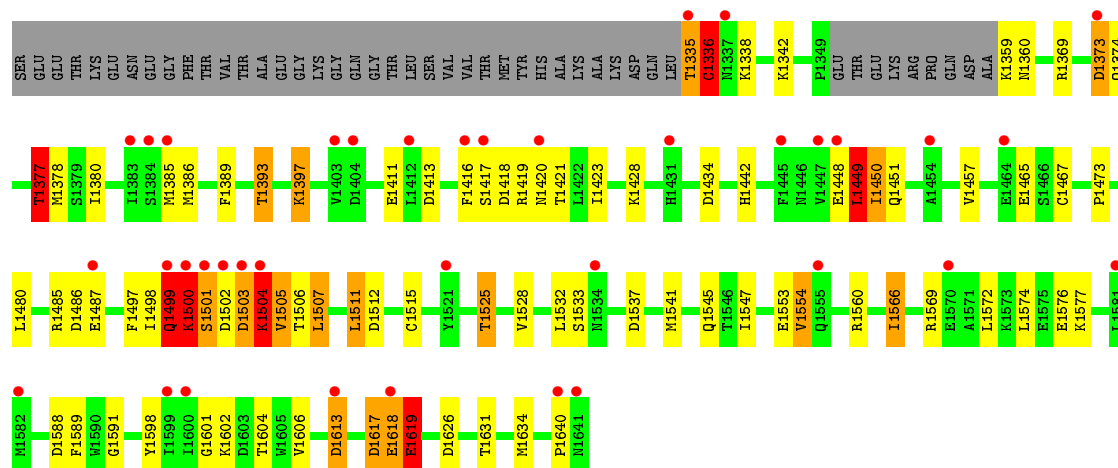


• Molecule 3: Complement Component C3c





• Molecule 3: Complement Component C3c



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	126.87Å 246.86Å 87.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 28.35 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-2.40) 95.0 (28.35-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.215 , 0.275 0.213 , 0.272	Depositor DCC
R_{free} test set	3124 reflections (3.06%)	DCC
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 116257 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18389	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.48 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7203e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NDG, NO3

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	0.45	2/5004 (0.0%)	0.72	11/6799 (0.2%)
1	D	0.65	10/5032 (0.2%)	0.71	10/6839 (0.1%)
2	B	0.49	1/1512 (0.1%)	0.70	1/2055 (0.0%)
2	E	1.21	16/1516 (1.1%)	0.76	6/2060 (0.3%)
3	C	0.40	1/2453 (0.0%)	0.76	16/3305 (0.5%)
3	F	0.59	7/2468 (0.3%)	0.78	11/3327 (0.3%)
All	All	0.62	37/17985 (0.2%)	0.73	55/24385 (0.2%)

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
1	A	0	5
1	D	0	8
3	C	0	1
3	F	0	3
4	A	1	0
4	D	1	0
All	All	2	17

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	564	GLU	CG-CD	19.98	1.81	1.51
2	E	837	GLU	CD-OE1	16.09	1.43	1.25
2	E	761	LYS	CE-NZ	13.09	1.81	1.49
2	E	758	GLU	CD-OE2	12.47	1.39	1.25
3	F	1397	LYS	CE-NZ	12.42	1.80	1.49
1	D	544	LYS	CE-NZ	12.09	1.79	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	837	GLU	CD-OE2	11.71	1.38	1.25
2	E	896	HIS	CG-CD2	11.11	1.54	1.35
2	E	896	HIS	CE1-NE2	10.37	1.56	1.32
2	E	761	LYS	C-O	10.18	1.42	1.23
1	A	149	GLU	CD-OE2	9.62	1.36	1.25
3	F	1618	GLU	CG-CD	9.11	1.65	1.51
1	D	549	GLU	CD-OE1	8.61	1.35	1.25
2	E	758	GLU	CG-CD	8.04	1.64	1.51
1	A	149	GLU	CD-OE1	7.78	1.34	1.25
2	E	761	LYS	CD-CE	7.71	1.70	1.51
1	D	149	GLU	CD-OE1	7.50	1.33	1.25
1	D	544	LYS	CD-CE	7.49	1.70	1.51
1	D	559	MET	C-O	7.41	1.37	1.23
1	D	562	LYS	CD-CE	7.33	1.69	1.51
1	D	564	GLU	CD-OE1	6.45	1.32	1.25
3	F	1617	ASP	CG-OD1	6.26	1.39	1.25
2	E	896	HIS	CG-ND1	6.19	1.52	1.38
1	D	547	GLN	CG-CD	6.09	1.65	1.51
1	D	546	GLY	C-O	6.06	1.33	1.23
2	E	767	LYS	C-O	6.04	1.34	1.23
2	E	834	GLN	C-O	6.02	1.34	1.23
3	F	1397	LYS	CD-CE	5.80	1.65	1.51
3	C	1409	LYS	CE-NZ	5.76	1.63	1.49
3	F	1617	ASP	CG-OD2	5.55	1.38	1.25
2	E	759	PRO	CA-C	5.52	1.63	1.52
3	F	1618	GLU	CD-OE2	5.51	1.31	1.25
2	B	896	HIS	CE1-NE2	5.29	1.44	1.32
2	E	764	ILE	CB-CG1	5.22	1.68	1.54
2	E	762	ASN	CG-OD1	5.21	1.35	1.24
3	F	1618	GLU	CD-OE1	5.13	1.31	1.25
2	E	762	ASN	C-N	5.07	1.42	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	564	GLU	OE1-CD-OE2	7.91	132.80	123.30
2	E	761	LYS	CD-CE-NZ	-7.19	95.16	111.70
3	C	1413	ASP	CB-CG-OD2	6.27	123.94	118.30
3	F	1397	LYS	CD-CE-NZ	-6.14	97.58	111.70
1	A	30	ASP	CB-CG-OD2	5.94	123.65	118.30
2	E	755	ASP	CB-CG-OD2	5.90	123.61	118.30
3	F	1512	ASP	CB-CG-OD2	5.90	123.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	315	ASP	CB-CG-OD2	5.84	123.56	118.30
3	C	1435	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	373	ASP	CB-CG-OD2	5.77	123.49	118.30
3	F	1373	ASP	CB-CG-OD2	5.75	123.47	118.30
3	C	1603	ASP	CB-CG-OD2	5.70	123.43	118.30
3	F	1486	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	156	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	149	GLU	OE1-CD-OE2	5.64	130.07	123.30
3	C	1552	ASP	CB-CG-OD2	5.60	123.34	118.30
3	C	1486	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	612	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	491	ASP	CB-CG-OD2	5.49	123.24	118.30
2	E	732	ASP	CB-CG-OD2	5.47	123.23	118.30
1	D	39	ASP	CB-CG-OD2	5.46	123.21	118.30
3	C	1340	ASP	CB-CG-OD2	5.44	123.19	118.30
3	F	1503	ASP	CB-CG-OD2	5.43	123.19	118.30
3	F	1626	ASP	CB-CG-OD2	5.42	123.18	118.30
3	C	1427	ASP	CB-CG-OD2	5.42	123.18	118.30
3	C	1434	ASP	CB-CG-OD2	5.42	123.18	118.30
3	C	1588	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	39	ASP	CB-CG-OD2	5.36	123.12	118.30
3	F	1613	ASP	CB-CG-OD2	5.35	123.12	118.30
2	E	806	ASP	CB-CG-OD2	5.34	123.10	118.30
1	D	26	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	509	LEU	CA-CB-CG	5.25	127.37	115.30
2	B	789	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	564	GLU	CG-CD-OE1	-5.25	107.81	118.30
1	D	30	ASP	CB-CG-OD2	5.22	123.00	118.30
3	C	1392	ASP	CB-CG-OD2	5.22	123.00	118.30
3	C	1626	ASP	CB-CG-OD2	5.21	122.99	118.30
3	C	1512	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	544	LYS	CD-CE-NZ	-5.18	99.78	111.70
3	C	1537	ASP	CB-CG-OD2	5.17	122.96	118.30
3	F	1434	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	619	ASP	CB-CG-OD2	5.16	122.94	118.30
3	F	1502	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	566	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	26	ASP	CB-CG-OD2	5.08	122.88	118.30
3	F	1588	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	458	ASP	CB-CG-OD2	5.07	122.87	118.30
3	C	1477	ASP	CB-CG-OD2	5.05	122.84	118.30
2	E	775	ASP	CB-CG-OD2	5.04	122.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	789	ASP	CB-CG-OD2	5.02	122.82	118.30
3	F	1413	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	550	ASP	CB-CG-OD2	5.02	122.82	118.30
3	C	1503	ASP	CB-CG-OD2	5.02	122.81	118.30
1	D	358	ASP	CB-CG-OD2	5.01	122.81	118.30
3	C	1382	ASP	CB-CG-OD2	5.00	122.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	645	NDG	C1
4	D	645	NDG	C1

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ASP	Peptide
1	A	403	ARG	Peptide
1	A	549	GLU	Peptide
1	A	63	ASN	Peptide
1	A	69	PRO	Peptide
3	C	1415	ALA	Peptide
1	D	374	THR	Peptide
1	D	40	PHE	Peptide
1	D	428	GLY	Peptide
1	D	44	LYS	Peptide
1	D	548	SER	Peptide
1	D	549	GLU	Peptide
1	D	63	ASN	Peptide
1	D	80	ARG	Peptide
3	F	1417	SER	Peptide
3	F	1500	LYS	Peptide
3	F	1640	PRO	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	4907	0	4970	204	0
1	D	4933	0	4996	195	0
2	B	1480	0	1501	30	0
2	E	1484	0	1511	46	0
3	C	2407	0	2316	97	0
3	F	2421	0	2326	62	0
4	A	28	0	25	2	0
4	D	28	0	21	1	0
5	A	18	0	24	6	0
5	B	12	0	16	2	0
5	C	12	0	16	0	0
5	D	6	0	8	5	0
5	E	18	0	24	2	0
5	F	12	0	16	4	0
6	C	4	0	0	0	0
6	F	8	0	0	0	0
7	A	188	0	0	11	0
7	B	58	0	0	0	0
7	C	71	0	0	6	0
7	D	148	0	0	3	0
7	E	53	0	0	2	0
7	F	93	0	0	2	0
All	All	18389	0	17770	601	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 17.

All (601) 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)
1:D:564:GLU:CG	1:D:564:GLU:CD	1.81	1.49
3:F:1397:LYS:CE	3:F:1397:LYS:NZ	1.80	1.44
1:D:544:LYS:NZ	1:D:544:LYS:CE	1.79	1.43
2:E:761:LYS:CE	2:E:761:LYS:NZ	1.81	1.42
1:A:6:ILE:HD11	1:A:20:MET:CG	1.53	1.39
1:A:6:ILE:CD1	1:A:20:MET:HG3	1.50	1.38
1:D:292:LEU:CD2	1:D:292:LEU:H	1.42	1.27
1:D:375:VAL:HG23	1:D:376:GLN:H	1.12	1.14
1:A:403:ARG:HB3	1:A:404:THR:HG22	1.16	1.14
1:D:6:ILE:HD11	1:D:20:MET:SD	1.88	1.14
1:A:404:THR:HG23	1:A:414:GLN:HB3	1.26	1.14
1:A:372:GLU:HA	1:A:373:ASP:HB3	1.13	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:LEU:N	1:D:292:LEU:HD23	1.63	1.11
1:D:20:MET:CE	1:D:86:VAL:CG1	2.29	1.10
1:A:375:VAL:HG12	1:A:376:GLN:H	0.99	1.09
1:D:20:MET:HE3	1:D:86:VAL:CG1	1.84	1.08
1:D:80:ARG:HD3	1:D:637:GLU:HA	1.13	1.07
1:A:36:THR:HG21	1:A:38:HIS:CE1	1.91	1.06
3:C:1525:THR:OG1	3:C:1541:MET:HE2	1.57	1.05
3:F:1533:SER:O	3:F:1566:ILE:HD11	1.56	1.04
1:A:606:THR:HG21	7:A:652:HOH:O	1.58	1.03
3:C:1411:GLU:HG2	3:C:1422:LEU:HD12	1.42	1.01
3:F:1504:LYS:HG2	3:F:1505:VAL:H	1.25	1.01
1:A:409:LEU:O	1:A:410:SER:HB3	1.61	1.00
1:D:20:MET:CE	1:D:86:VAL:HG11	1.90	1.00
3:C:1391:PRO:HG2	3:C:1419:ARG:HD2	1.40	1.00
3:F:1504:LYS:HG2	3:F:1505:VAL:N	1.77	1.00
1:D:160:SER:HB3	1:D:167:LEU:HD11	1.44	0.99
1:A:36:THR:HG21	1:A:38:HIS:HE1	1.27	0.98
1:A:315:ASP:HA	5:A:703:GOL:H31	1.41	0.98
1:D:292:LEU:H	1:D:292:LEU:HD23	0.81	0.97
1:A:293:ARG:HH21	1:A:295:GLU:HB2	1.30	0.97
1:A:372:GLU:HA	1:A:373:ASP:CB	1.90	0.97
1:D:63:ASN:HA	7:D:781:HOH:O	1.65	0.97
1:A:36:THR:CG2	1:A:38:HIS:CE1	2.48	0.96
3:C:1525:THR:CB	3:C:1541:MET:HE2	1.96	0.96
1:D:535:ASP:HB3	5:D:711:GOL:H32	1.48	0.96
1:D:473:MET:CE	1:D:622:LEU:HD21	1.96	0.96
1:A:426:THR:CG2	7:A:829:HOH:O	2.15	0.95
3:F:1386:MET:HB3	3:F:1450:ILE:HD12	1.48	0.95
1:D:20:MET:HE3	1:D:86:VAL:HG11	1.44	0.95
1:A:375:VAL:HG12	1:A:376:GLN:N	1.82	0.95
1:A:404:THR:CG2	1:A:414:GLN:HB3	1.96	0.94
3:F:1448:GLU:O	3:F:1449:LEU:HB2	1.68	0.93
1:A:403:ARG:CB	1:A:404:THR:HG22	1.98	0.93
3:F:1386:MET:HB3	3:F:1450:ILE:CD1	1.98	0.93
1:A:372:GLU:CA	1:A:373:ASP:HB3	1.99	0.93
1:D:160:SER:HB3	1:D:167:LEU:CD1	1.98	0.92
1:A:6:ILE:HD13	1:A:20:MET:HE3	1.53	0.91
1:A:404:THR:HG21	1:A:415:ALA:O	1.71	0.89
1:D:404:THR:HG22	1:D:414:GLN:OE1	1.73	0.89
3:F:1591:GLY:H	5:F:707:GOL:H31	1.35	0.88
1:A:248:PHE:HD1	3:C:1378:MET:HE3	1.39	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PHE:HD1	3:C:1378:MET:CE	1.87	0.87
1:A:548:SER:O	1:A:549:GLU:HB2	1.73	0.86
1:A:375:VAL:CG1	1:A:376:GLN:H	1.84	0.86
1:A:369:VAL:O	1:A:372:GLU:HG2	1.75	0.85
1:A:362:ALA:O	1:A:379:THR:HG21	1.73	0.85
1:D:375:VAL:HG23	1:D:376:GLN:N	1.90	0.85
3:C:1415:ALA:HB3	3:C:1417:SER:HB3	1.56	0.85
1:D:375:VAL:CG2	1:D:376:GLN:H	1.88	0.85
1:D:549:GLU:HB3	1:D:550:ASP:CA	2.07	0.85
1:D:577:ASP:OD1	2:E:778:THR:HG21	1.77	0.85
1:A:31:VAL:HG13	1:A:54:LEU:HB2	1.59	0.85
1:A:248:PHE:CD1	3:C:1378:MET:HE3	2.13	0.84
1:D:6:ILE:CD1	1:D:20:MET:SD	2.65	0.84
1:A:477:ARG:HH11	1:A:477:ARG:CG	1.90	0.83
3:C:1387:THR:CG2	3:C:1451:GLN:H	1.91	0.83
1:D:80:ARG:HD3	1:D:637:GLU:CA	2.04	0.83
1:A:128:PHE:HB3	2:B:787:MET:HE1	1.59	0.82
1:D:47:LEU:HD13	1:D:66:PHE:HB2	1.59	0.82
1:D:549:GLU:CB	1:D:550:ASP:HB2	2.08	0.82
3:C:1348:ALA:HB1	3:C:1349:PRO:HD2	1.62	0.82
2:B:824:GLU:OE1	2:B:826:ARG:NH1	2.12	0.81
1:D:3:MET:HE2	1:D:522:ARG:HG2	1.61	0.81
1:A:404:THR:CG2	1:A:415:ALA:O	2.28	0.80
1:A:403:ARG:HB3	1:A:404:THR:CG2	2.08	0.80
1:D:473:MET:HE1	1:D:622:LEU:HD21	1.62	0.80
3:C:1525:THR:OG1	3:C:1541:MET:CE	2.30	0.80
1:D:47:LEU:CD1	1:D:66:PHE:HB2	2.10	0.80
1:A:393:PRO:HD3	7:A:722:HOH:O	1.80	0.80
1:A:20:MET:CE	1:A:88:ALA:HB2	2.10	0.80
1:D:372:GLU:HG3	1:D:375:VAL:HG22	1.63	0.80
1:D:292:LEU:CD2	1:D:292:LEU:N	2.24	0.78
1:A:362:ALA:O	1:A:379:THR:CG2	2.32	0.78
1:A:20:MET:HE1	1:A:88:ALA:HB2	1.64	0.78
1:A:606:THR:HG22	1:A:608:GLY:H	1.48	0.78
1:A:6:ILE:CD1	1:A:20:MET:CG	2.30	0.77
1:A:6:ILE:CD1	1:A:20:MET:HE3	2.15	0.77
3:C:1498:ILE:HG22	3:C:1499:GLN:HG2	1.67	0.77
2:E:889:GLU:HG3	2:E:904:ARG:HB3	1.65	0.77
1:D:386:LYS:HB3	1:D:440:ARG:HD2	1.65	0.77
1:A:426:THR:HG22	7:A:829:HOH:O	1.78	0.76
1:D:386:LYS:CB	1:D:440:ARG:HD2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ASN:ND2	1:D:155:GLN:HG3	2.01	0.76
1:D:473:MET:HE3	1:D:622:LEU:HD21	1.65	0.76
1:A:426:THR:HG23	7:A:829:HOH:O	1.78	0.76
2:B:819:ARG:HH11	2:B:819:ARG:HB3	1.51	0.76
1:D:6:ILE:HD11	1:D:20:MET:CG	2.16	0.75
1:D:549:GLU:OE1	1:D:549:GLU:HA	1.85	0.75
1:D:58:THR:HG23	1:D:58:THR:O	1.86	0.75
1:A:372:GLU:CA	1:A:373:ASP:CB	2.63	0.75
1:A:372:GLU:HB3	1:A:375:VAL:HB	1.67	0.75
1:A:404:THR:O	1:A:404:THR:HG23	1.86	0.74
1:D:6:ILE:HD13	1:D:7:ILE:N	2.02	0.74
1:D:80:ARG:CD	1:D:637:GLU:HA	2.07	0.74
3:C:1341:LEU:HD22	3:C:1457:VAL:HG22	1.68	0.74
3:C:1525:THR:CB	3:C:1541:MET:CE	2.65	0.74
3:C:1361:THR:HA	3:C:1441:VAL:O	1.86	0.73
3:C:1490:ARG:NE	7:C:526:HOH:O	2.16	0.73
1:D:371:GLY:O	1:D:372:GLU:HB2	1.88	0.73
1:A:29:GLY:O	1:A:60:HIS:HE1	1.70	0.73
3:F:1448:GLU:O	3:F:1449:LEU:CB	2.35	0.73
1:D:3:MET:HE3	1:D:522:ARG:HD2	1.69	0.73
3:F:1576:GLU:O	3:F:1577:LYS:HB2	1.87	0.73
1:D:549:GLU:HB3	1:D:550:ASP:HB2	1.71	0.73
1:D:20:MET:HE3	1:D:86:VAL:HG13	1.70	0.73
2:B:896:HIS:C	2:B:897:HIS:HD1	1.91	0.73
1:A:6:ILE:HG12	1:A:20:MET:CE	2.18	0.72
1:A:191:SER:HA	1:A:193:GLN:HE21	1.54	0.72
2:B:837:GLU:HB3	2:B:868:PRO:HD3	1.70	0.71
1:A:367:VAL:HG12	1:A:404:THR:H	1.53	0.71
1:D:312:SER:O	7:D:786:HOH:O	2.07	0.71
1:D:111:GLN:OE1	1:D:126:ARG:HD3	1.90	0.71
1:D:473:MET:CE	1:D:622:LEU:CD2	2.69	0.71
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.73	0.71
1:D:549:GLU:HB3	1:D:550:ASP:HA	1.73	0.70
2:B:858:ARG:NH2	3:C:1494:GLU:HA	2.07	0.70
1:A:370:GLN:CG	1:A:401:THR:HB	2.22	0.70
1:D:549:GLU:HB3	1:D:550:ASP:CB	2.21	0.70
3:F:1449:LEU:N	3:F:1449:LEU:HD23	2.07	0.70
1:D:3:MET:CE	1:D:522:ARG:HG2	2.21	0.70
1:A:592:SER:HA	5:A:712:GOL:H32	1.74	0.70
2:B:819:ARG:CB	2:B:819:ARG:HH11	2.05	0.70
2:E:822:GLN:HE22	3:F:1480:LEU:H	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ARG:HG2	1:A:477:ARG:HH11	1.57	0.69
1:A:69:PRO:HA	1:A:70:ALA:HB3	1.73	0.69
3:C:1337:ASN:HD22	3:C:1337:ASN:H	1.41	0.69
1:D:473:MET:HE1	1:D:622:LEU:CD2	2.22	0.69
1:A:154:LYS:HD2	1:A:171:TRP:CD1	2.26	0.69
1:A:47:LEU:CD1	1:A:66:PHE:HB2	2.23	0.68
1:A:370:GLN:HG2	1:A:401:THR:HB	1.76	0.68
3:F:1428:LYS:HE3	7:F:68:HOH:O	1.93	0.68
3:C:1572:LEU:O	3:C:1573:LYS:HD2	1.94	0.68
3:C:1525:THR:HB	3:C:1541:MET:CE	2.23	0.68
3:C:1465:GLU:HG3	3:C:1465:GLU:O	1.91	0.68
3:C:1411:GLU:HG2	3:C:1422:LEU:CD1	2.19	0.68
1:D:6:ILE:CG1	1:D:20:MET:SD	2.82	0.67
1:D:592:SER:HB3	5:D:711:GOL:H11	1.74	0.67
1:D:369:VAL:HG22	1:D:400:ILE:HD11	1.77	0.66
2:B:819:ARG:HH11	2:B:819:ARG:CG	2.07	0.66
3:C:1381:LEU:CD2	3:C:1457:VAL:HG13	2.25	0.66
1:A:23:GLU:HG2	1:A:61:MET:HG2	1.77	0.66
1:D:541:LEU:HD22	2:E:786:SER:HB3	1.78	0.66
3:C:1499:GLN:HG3	3:C:1500:LYS:N	2.10	0.66
1:D:409:LEU:O	1:D:410:SER:HB3	1.96	0.66
3:F:1525:THR:CG2	3:F:1541:MET:SD	2.84	0.65
1:D:6:ILE:HD13	1:D:7:ILE:H	1.61	0.65
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.27	0.65
1:A:345:GLY:H	1:A:391:THR:HG22	1.62	0.65
2:E:761:LYS:NZ	2:E:761:LYS:CD	2.60	0.65
1:A:6:ILE:HD12	1:A:21:VAL:O	1.95	0.64
1:A:80:ARG:O	1:A:81:ASN:HB2	1.96	0.64
1:D:103:LEU:H	1:D:103:LEU:HD22	1.62	0.64
1:D:160:SER:CB	1:D:167:LEU:HD11	2.24	0.64
2:B:819:ARG:NH1	2:B:912:GLU:OE2	2.31	0.64
2:B:894:VAL:CG2	2:B:897:HIS:HB2	2.27	0.64
1:A:350:LEU:HD23	1:A:419:MET:CE	2.27	0.64
1:D:549:GLU:CB	1:D:550:ASP:CB	2.76	0.64
3:F:1397:LYS:CD	3:F:1397:LYS:NZ	2.60	0.64
3:C:1448:GLU:O	3:C:1449:LEU:HB2	1.97	0.64
1:D:40:PHE:CD2	1:D:41:PRO:HD3	2.33	0.64
1:D:20:MET:CE	1:D:86:VAL:HG12	2.27	0.63
2:E:785:VAL:HG22	2:E:795:VAL:HB	1.79	0.63
1:D:3:MET:CE	1:D:522:ARG:CG	2.77	0.63
1:D:6:ILE:HD11	1:D:20:MET:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:HG12	1:A:20:MET:SD	2.38	0.63
2:B:858:ARG:HH22	3:C:1494:GLU:HA	1.64	0.63
1:D:3:MET:HE3	1:D:522:ARG:CD	2.29	0.62
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.81	0.62
1:A:7:ILE:HG21	1:A:471:LEU:HD22	1.81	0.62
3:C:1537:ASP:OD2	3:C:1569:ARG:HD3	2.00	0.62
3:F:1386:MET:HB3	3:F:1450:ILE:HD11	1.82	0.62
1:A:293:ARG:HH21	1:A:295:GLU:CB	2.10	0.61
1:D:472:ILE:HD13	1:D:509:LEU:HD22	1.82	0.61
1:D:309:ILE:HG12	1:D:316:MET:HG3	1.82	0.61
1:D:20:MET:HE2	1:D:86:VAL:HG11	1.80	0.61
3:C:1515:CYS:SG	3:C:1640:PRO:HD3	2.40	0.61
1:A:404:THR:CG2	1:A:404:THR:O	2.48	0.61
1:D:547:GLN:H	1:D:547:GLN:HE21	1.47	0.61
1:D:472:ILE:CD1	1:D:509:LEU:HD22	2.31	0.61
1:D:233:ILE:HD13	1:D:269:ILE:HD11	1.83	0.61
1:A:6:ILE:HD11	1:A:20:MET:SD	2.40	0.60
1:A:535:ASP:HB3	5:A:712:GOL:H11	1.83	0.60
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.82	0.60
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.84	0.60
3:C:1381:LEU:HD23	3:C:1457:VAL:HG13	1.83	0.60
3:C:1525:THR:HB	3:C:1541:MET:HE2	1.76	0.60
3:C:1359:LYS:NZ	3:C:1446:ASN:HB2	2.17	0.60
1:A:47:LEU:HD21	1:A:50:GLU:HG2	1.81	0.60
1:D:558:GLN:NE2	2:E:770:ASN:OD1	2.33	0.60
1:A:6:ILE:CD1	1:A:20:MET:SD	2.89	0.60
1:D:6:ILE:HG12	1:D:22:LEU:HD23	1.83	0.60
3:C:1483:LEU:HD23	3:C:1599:ILE:HD12	1.82	0.60
1:D:19:THR:HG21	4:D:644:NDG:H8C1	1.83	0.60
3:F:1507:LEU:HD22	3:F:1511:LEU:HD22	1.84	0.59
1:A:477:ARG:HH11	1:A:477:ARG:HG3	1.66	0.59
1:D:45:LEU:HD21	1:D:48:SER:OG	2.02	0.59
3:F:1386:MET:SD	3:F:1473:PRO:HD3	2.42	0.59
1:D:549:GLU:HB2	1:D:550:ASP:HB2	1.83	0.59
1:A:6:ILE:HD12	1:A:7:ILE:H	1.68	0.59
3:F:1537:ASP:OD2	3:F:1569:ARG:HG2	2.02	0.59
1:D:473:MET:HE3	1:D:622:LEU:CD2	2.33	0.59
1:D:409:LEU:O	1:D:410:SER:CB	2.50	0.59
1:D:80:ARG:HB3	1:D:636:ALA:O	2.02	0.59
1:A:350:LEU:HD23	1:A:419:MET:HE2	1.84	0.59
1:D:108:LEU:CD2	1:D:129:THR:HG22	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ARG:NH1	1:A:477:ARG:HG2	2.18	0.59
1:D:20:MET:HE1	1:D:86:VAL:CG1	2.28	0.58
1:A:367:VAL:O	1:A:376:GLN:HA	2.03	0.58
1:D:143:VAL:HG11	1:D:169:LEU:CD1	2.33	0.58
3:C:1613:ASP:HA	3:C:1616:GLN:HE21	1.68	0.58
1:A:6:ILE:HD11	1:A:20:MET:HG3	0.68	0.57
1:A:3:MET:HE3	1:A:522:ARG:CG	2.33	0.57
3:C:1387:THR:HG23	3:C:1451:GLN:H	1.66	0.57
1:D:8:THR:HG22	1:D:20:MET:HG2	1.86	0.57
1:A:15:GLU:HG2	1:A:70:ALA:HB2	1.85	0.57
2:E:867:PRO:HG2	2:E:870:SER:OG	2.05	0.57
3:C:1555:GLN:HG2	7:C:579:HOH:O	2.05	0.57
2:E:877:VAL:HG13	3:F:1451:GLN:CG	2.35	0.57
2:E:877:VAL:HG13	3:F:1451:GLN:HG2	1.87	0.57
3:C:1588:ASP:OD2	7:C:561:HOH:O	2.17	0.57
1:D:50:GLU:HB3	1:D:64:VAL:HB	1.86	0.57
1:D:386:LYS:H	1:D:440:ARG:CZ	2.17	0.57
1:D:577:ASP:CG	2:E:778:THR:HG21	2.25	0.56
1:D:386:LYS:HB2	1:D:440:ARG:HD2	1.87	0.56
3:C:1391:PRO:CG	3:C:1419:ARG:HD2	2.26	0.56
3:F:1634:MET:HE2	3:F:1634:MET:HA	1.87	0.56
1:D:544:LYS:NZ	1:D:544:LYS:CD	2.66	0.56
3:C:1543:ILE:HD12	3:C:1554:VAL:HG21	1.88	0.56
1:A:6:ILE:CD1	1:A:20:MET:CE	2.83	0.56
1:A:255:ASP:HB2	1:A:300:LYS:HG2	1.88	0.56
2:E:907:LEU:H	2:E:907:LEU:HD12	1.70	0.56
1:A:404:THR:HG21	1:A:415:ALA:N	2.20	0.56
1:A:69:PRO:CA	1:A:70:ALA:HB3	2.35	0.56
1:A:487:GLU:H	1:A:490:GLN:NE2	2.04	0.56
1:A:6:ILE:CG1	1:A:20:MET:CE	2.83	0.56
2:B:837:GLU:HB2	2:B:867:PRO:HA	1.88	0.56
3:F:1338:LYS:HG3	3:F:1465:GLU:HB3	1.87	0.56
1:A:61:MET:HG3	1:A:483:ARG:CZ	2.36	0.55
1:D:504:ILE:CG2	1:D:505:PRO:HA	2.35	0.55
1:D:147:ASN:HB2	1:D:148:PRO:CD	2.36	0.55
3:F:1335:THR:O	3:F:1335:THR:OG1	2.21	0.55
1:A:590:THR:HG23	7:A:724:HOH:O	2.06	0.55
3:C:1346:LYS:O	3:C:1362:MET:HB3	2.06	0.55
1:A:6:ILE:CG1	1:A:20:MET:HE3	2.37	0.55
1:D:6:ILE:HG13	1:D:20:MET:CE	2.37	0.55
2:B:834:GLN:HE21	2:B:834:GLN:HA	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:THR:HG21	1:A:419:MET:CE	2.37	0.55
2:B:858:ARG:CZ	3:C:1449:LEU:HD11	2.37	0.55
1:A:409:LEU:O	1:A:410:SER:CB	2.44	0.55
3:F:1515:CYS:SG	3:F:1634:MET:HE3	2.47	0.55
1:A:504:ILE:HG23	1:A:505:PRO:HA	1.89	0.55
2:E:903:VAL:HG21	5:E:705:GOL:H11	1.88	0.55
1:A:444:ARG:NH2	1:A:534:LYS:HE2	2.21	0.55
3:C:1419:ARG:HD3	3:C:1422:LEU:HD13	1.89	0.55
3:C:1621:GLN:O	3:C:1625:GLN:HG3	2.07	0.54
3:F:1499:GLN:CG	3:F:1500:LYS:H	2.21	0.54
1:A:20:MET:HE2	1:A:88:ALA:HB2	1.89	0.54
1:D:160:SER:HB3	1:D:167:LEU:HD13	1.89	0.54
3:C:1499:GLN:CG	3:C:1500:LYS:H	2.20	0.54
1:D:128:PHE:HD1	2:E:787:MET:CE	2.19	0.54
3:F:1525:THR:HG23	3:F:1541:MET:SD	2.48	0.54
1:A:346:MET:O	1:A:391:THR:HB	2.07	0.54
1:A:315:ASP:HA	5:A:703:GOL:C3	2.28	0.54
1:D:25:HIS:O	1:D:26:ASP:HB2	2.07	0.54
1:D:596:ASP:O	1:D:600:LYS:HG2	2.08	0.54
3:C:1370:TYR:HB2	3:C:1429:VAL:HG22	1.89	0.54
3:C:1506:THR:OG1	3:C:1509:GLU:HG2	2.06	0.54
1:D:504:ILE:HG23	1:D:505:PRO:HA	1.90	0.54
3:C:1391:PRO:HG2	3:C:1419:ARG:CD	2.27	0.53
1:D:548:SER:O	1:D:549:GLU:HB2	2.06	0.53
1:A:504:ILE:CG2	1:A:505:PRO:HA	2.38	0.53
3:C:1504:LYS:O	3:C:1505:VAL:HG23	2.07	0.53
1:A:595:TRP:HD1	5:A:712:GOL:H12	1.72	0.53
3:C:1375:ASP:OD1	3:C:1431:HIS:HD2	1.91	0.53
1:A:487:GLU:H	1:A:490:GLN:HE21	1.56	0.53
1:A:634:GLN:HG3	7:A:795:HOH:O	2.09	0.53
3:C:1401:ASN:N	3:C:1401:ASN:HD22	2.05	0.53
2:E:834:GLN:HG3	7:E:577:HOH:O	2.08	0.53
1:D:230:GLU:HG2	1:D:279:VAL:HG22	1.91	0.53
3:C:1337:ASN:H	3:C:1337:ASN:ND2	2.04	0.53
1:A:177:VAL:HG22	1:A:182:TRP:HZ2	1.73	0.53
1:D:37:VAL:N	1:D:47:LEU:O	2.32	0.53
1:D:103:LEU:N	1:D:103:LEU:HD22	2.23	0.53
1:D:407:GLN:O	1:D:408:GLU:HG2	2.08	0.53
1:A:69:PRO:HA	1:A:70:ALA:CB	2.38	0.53
1:A:20:MET:CE	1:A:22:LEU:HD21	2.38	0.53
3:C:1490:ARG:HD2	3:C:1590:TRP:CZ3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:THR:O	1:D:58:THR:CG2	2.57	0.52
1:A:3:MET:CE	1:A:522:ARG:HG2	2.38	0.52
3:C:1344:THR:CG2	3:C:1346:LYS:HE2	2.38	0.52
1:D:554:VAL:HG12	1:D:557:GLN:HB2	1.91	0.52
1:D:574:VAL:HG13	2:E:751:TRP:HE3	1.75	0.52
1:A:248:PHE:CD1	3:C:1378:MET:CE	2.76	0.52
1:A:444:ARG:HH22	1:A:534:LYS:HE2	1.73	0.52
3:C:1359:LYS:NZ	3:C:1446:ASN:CB	2.72	0.52
1:A:628:SER:HB2	1:A:630:GLN:OE1	2.10	0.52
1:D:104:GLN:HE21	1:D:132:HIS:CE1	2.27	0.52
1:D:564:GLU:CD	1:D:564:GLU:CB	2.71	0.52
3:C:1381:LEU:HD21	3:C:1457:VAL:HG13	1.90	0.52
1:D:128:PHE:HB3	2:E:787:MET:HE1	1.91	0.52
3:C:1462:ASN:HD22	3:C:1465:GLU:H	1.57	0.52
1:D:187:TYR:CD1	1:D:192:PRO:HA	2.44	0.52
1:A:469:THR:O	1:A:511:ALA:HA	2.10	0.52
3:C:1344:THR:HG21	3:C:1346:LYS:HE2	1.91	0.52
1:A:187:TYR:CD1	1:A:192:PRO:HA	2.45	0.52
1:A:223:ILE:HD11	1:A:328:THR:HG22	1.90	0.52
3:C:1530:VAL:HG12	3:C:1532:LEU:HD13	1.92	0.52
3:F:1499:GLN:O	3:F:1500:LYS:HB3	2.08	0.51
1:D:221:TYR:OH	1:D:282:ARG:HG3	2.10	0.51
3:C:1386:MET:HB3	3:C:1450:ILE:CD1	2.40	0.51
3:C:1483:LEU:HD23	3:C:1599:ILE:CD1	2.40	0.51
1:D:372:GLU:HA	1:D:372:GLU:OE1	2.09	0.51
3:F:1498:ILE:HG22	3:F:1499:GLN:HG3	1.93	0.51
1:D:104:GLN:HE21	1:D:132:HIS:HE1	1.57	0.51
1:A:19:THR:HG21	4:A:644:NDG:H8C1	1.91	0.51
2:E:889:GLU:CG	2:E:904:ARG:HB3	2.39	0.51
2:E:746:PRO:CG	2:E:774:LYS:HG2	2.40	0.51
1:A:403:ARG:CA	1:A:404:THR:HG22	2.40	0.51
3:F:1591:GLY:N	5:F:707:GOL:H31	2.15	0.51
3:F:1525:THR:HG21	3:F:1541:MET:SD	2.50	0.51
1:A:149:GLU:OE2	1:D:363:TYR:OH	2.24	0.51
1:D:470:TYR:C	1:D:471:LEU:HG	2.32	0.51
2:E:822:GLN:NE2	3:F:1480:LEU:H	2.08	0.51
1:D:591:GLN:NE2	2:E:795:VAL:H	2.08	0.51
1:A:160:SER:HA	1:A:167:LEU:HD21	1.91	0.51
1:D:104:GLN:HG3	1:D:194:GLN:OE1	2.10	0.51
1:D:550:ASP:O	1:D:552:GLN:N	2.40	0.50
1:A:45:LEU:CG	1:A:48:SER:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:THR:HG21	1:A:419:MET:HE1	1.92	0.50
3:F:1537:ASP:OD2	3:F:1569:ARG:CG	2.60	0.50
3:C:1552:ASP:OD2	3:C:1560:ARG:HD2	2.12	0.50
1:A:20:MET:HE2	1:A:22:LEU:HD21	1.94	0.50
1:D:20:MET:HE1	1:D:86:VAL:HG12	1.92	0.50
1:A:128:PHE:HA	1:A:165:GLY:O	2.11	0.50
1:A:375:VAL:CG1	1:A:376:GLN:N	2.55	0.50
3:F:1606:VAL:O	5:F:710:GOL:H12	2.11	0.50
1:D:40:PHE:CD2	1:D:41:PRO:CD	2.95	0.50
1:A:575:ALA:O	2:B:748:SER:HA	2.11	0.50
3:F:1416:PHE:HZ	3:F:1442:HIS:HB2	1.77	0.50
1:D:126:ARG:HA	1:D:167:LEU:O	2.12	0.50
3:C:1499:GLN:CG	3:C:1500:LYS:N	2.70	0.50
1:D:45:LEU:CD2	1:D:48:SER:OG	2.59	0.50
1:A:547:GLN:OE1	1:A:559:MET:HB2	2.12	0.50
1:A:133:LYS:O	1:A:134:LEU:HB2	2.11	0.50
2:B:819:ARG:HH11	2:B:819:ARG:HG2	1.76	0.49
1:A:177:VAL:HG22	1:A:182:TRP:CZ2	2.47	0.49
1:D:564:GLU:OE1	1:D:564:GLU:CG	2.55	0.49
3:C:1386:MET:HB3	3:C:1450:ILE:HD13	1.93	0.49
1:D:592:SER:CB	5:D:711:GOL:H11	2.43	0.49
2:B:841:ARG:HD2	5:B:701:GOL:O2	2.13	0.49
3:C:1582:MET:HA	3:C:1605:TRP:O	2.12	0.49
1:A:407:GLN:O	1:A:409:LEU:N	2.46	0.49
1:A:3:MET:HE3	1:A:522:ARG:HG2	1.94	0.49
1:D:211:GLU:HB3	1:D:582:VAL:HG22	1.95	0.49
1:D:595:TRP:HD1	5:D:711:GOL:H31	1.78	0.49
3:C:1344:THR:HG22	7:C:505:HOH:O	2.13	0.49
1:A:375:VAL:O	1:A:376:GLN:HB2	2.12	0.49
3:F:1504:LYS:O	3:F:1505:VAL:HB	2.13	0.49
1:A:370:GLN:HG3	1:A:401:THR:HB	1.92	0.49
1:D:558:GLN:HB3	2:E:772:PHE:CE2	2.47	0.48
1:A:332:GLN:HE21	1:A:357:PRO:HA	1.78	0.48
1:D:375:VAL:CG2	1:D:376:GLN:N	2.58	0.48
1:A:595:TRP:CD1	5:A:712:GOL:H12	2.48	0.48
1:A:407:GLN:C	1:A:409:LEU:H	2.17	0.48
1:A:47:LEU:CD2	1:A:66:PHE:HB2	2.43	0.48
3:C:1359:LYS:HZ3	3:C:1446:ASN:HB2	1.78	0.48
1:D:36:THR:HG22	1:D:48:SER:HA	1.95	0.48
3:C:1509:GLU:HB2	7:C:494:HOH:O	2.12	0.48
3:F:1393:THR:CG2	3:F:1419:ARG:HH12	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:GLU:HG3	7:A:690:HOH:O	2.13	0.48
3:C:1609:TRP:CG	3:C:1627:LEU:HD13	2.49	0.48
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.94	0.48
1:A:183:LYS:HD3	1:A:197:SER:HB3	1.94	0.48
1:D:6:ILE:CD1	1:D:7:ILE:N	2.76	0.48
1:D:350:LEU:HD21	1:D:400:ILE:HG12	1.94	0.48
3:C:1504:LYS:O	3:C:1505:VAL:CG2	2.62	0.48
1:D:241:LYS:HG3	2:E:832:TYR:CE1	2.49	0.48
1:A:55:THR:HG22	1:A:58:THR:H	1.79	0.48
3:C:1525:THR:HB	3:C:1541:MET:HE3	1.94	0.48
1:D:47:LEU:HD11	1:D:66:PHE:HB2	1.95	0.48
1:A:63:ASN:O	1:A:64:VAL:HG22	2.14	0.48
3:F:1532:LEU:HD22	3:F:1569:ARG:HD3	1.95	0.48
1:D:177:VAL:CG2	1:D:182:TRP:CZ2	2.97	0.48
3:F:1385:MET:HE3	7:F:183:HOH:O	2.14	0.48
3:F:1497:PHE:HA	3:F:1601:GLY:O	2.14	0.48
1:D:249:VAL:HG11	1:D:278:VAL:HG11	1.96	0.47
1:D:595:TRP:HD1	5:D:711:GOL:C3	2.27	0.47
1:A:3:MET:HE1	1:A:630:GLN:OE1	2.14	0.47
1:A:364:ARG:HG2	1:A:364:ARG:HH11	1.79	0.47
1:A:341:TYR:HA	1:A:422:LEU:O	2.14	0.47
1:D:3:MET:HE3	1:D:522:ARG:CG	2.44	0.47
3:C:1555:GLN:HB2	3:C:1558:GLN:NE2	2.29	0.47
1:A:606:THR:HG22	1:A:608:GLY:N	2.24	0.47
3:F:1572:LEU:HB3	3:F:1574:LEU:HG	1.95	0.47
1:D:157:SER:C	1:D:158:LEU:HG	2.35	0.47
1:A:477:ARG:NH1	1:A:477:ARG:CG	2.60	0.47
1:D:215:GLU:HG2	7:D:712:HOH:O	2.14	0.47
3:C:1497:PHE:HA	3:C:1601:GLY:O	2.15	0.47
1:A:532:ASP:OD1	7:A:812:HOH:O	2.20	0.47
1:D:31:VAL:HG13	1:D:54:LEU:HB2	1.96	0.47
3:F:1547:ILE:HG12	3:F:1631:THR:HG23	1.96	0.47
1:D:183:LYS:HD2	1:D:185:ARG:CZ	2.44	0.47
1:D:547:GLN:N	1:D:547:GLN:HE21	2.13	0.46
1:A:330:PRO:O	1:A:357:PRO:HD3	2.15	0.46
3:C:1465:GLU:O	3:C:1465:GLU:CG	2.60	0.46
1:A:20:MET:HE3	1:A:22:LEU:CD2	2.45	0.46
1:D:126:ARG:HD2	2:E:751:TRP:CZ2	2.50	0.46
1:A:3:MET:HG3	1:A:628:SER:OG	2.15	0.46
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.50	0.46
1:A:6:ILE:CG1	1:A:20:MET:SD	3.02	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:TRP:CD1	1:A:202:VAL:HG23	2.51	0.46
1:A:590:THR:HG22	1:A:593:LYS:H	1.81	0.46
1:A:45:LEU:HG	1:A:48:SER:HB3	1.98	0.46
1:D:59:ASN:O	1:D:483:ARG:NH2	2.49	0.46
1:D:369:VAL:O	1:D:372:GLU:HG2	2.16	0.46
3:F:1499:GLN:O	3:F:1500:LYS:CB	2.63	0.46
1:D:34:THR:O	1:D:34:THR:HG22	2.15	0.46
1:D:465:ILE:HD12	1:D:513:TYR:CD1	2.49	0.46
3:C:1579:HIS:HD2	3:C:1611:GLU:OE1	1.99	0.46
1:D:517:GLY:O	1:D:518:ALA:C	2.54	0.46
1:A:6:ILE:HD13	1:A:20:MET:CG	2.35	0.45
1:A:45:LEU:HD21	1:A:48:SER:HB3	1.98	0.45
1:D:46:VAL:HG12	1:D:69:PRO:HD2	1.97	0.45
2:B:841:ARG:CD	5:B:701:GOL:O2	2.64	0.45
1:D:567:HIS:CE1	2:E:760:PRO:HD3	2.51	0.45
1:D:304:VAL:HG13	1:D:321:ARG:HB3	1.98	0.45
1:A:11:ILE:HG12	1:A:100:LEU:HD23	1.98	0.45
3:F:1554:VAL:HG13	3:F:1560:ARG:HE	1.81	0.45
3:F:1420:ASN:OD1	3:F:1421:THR:HG23	2.17	0.45
3:C:1462:ASN:ND2	3:C:1465:GLU:H	2.13	0.45
1:A:641:PRO:O	1:A:642:GLN:HB2	2.15	0.45
3:F:1589:PHE:HE1	3:F:1598:TYR:CE2	2.34	0.45
1:A:3:MET:CE	1:A:630:GLN:OE1	2.65	0.45
1:D:10:ASN:HD22	1:D:10:ASN:HA	1.59	0.45
1:D:6:ILE:HG13	1:D:20:MET:HE2	1.97	0.45
1:A:338:THR:HG23	1:A:350:LEU:HA	1.98	0.45
1:A:50:GLU:HB3	1:A:64:VAL:HB	1.99	0.45
1:D:145:ILE:HG12	1:D:184:ILE:HG12	1.99	0.45
2:E:823:VAL:HG23	2:E:878:ILE:HG23	1.99	0.45
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.99	0.45
1:D:126:ARG:HD2	2:E:751:TRP:CH2	2.52	0.45
1:D:574:VAL:HG13	2:E:751:TRP:CE3	2.52	0.45
1:A:110:ILE:HB	1:A:198:THR:OG1	2.16	0.45
3:F:1501:SER:HB2	3:F:1503:ASP:O	2.17	0.45
2:E:732:ASP:OD1	2:E:896:HIS:HA	2.15	0.45
1:D:116:ILE:HD11	1:D:203:LYS:HD2	1.99	0.45
1:A:2:PRO:HA	1:A:25:HIS:O	2.17	0.45
3:F:1499:GLN:HG3	3:F:1500:LYS:H	1.81	0.45
1:A:184:ILE:O	1:A:197:SER:HA	2.17	0.45
1:A:40:PHE:HA	1:A:41:PRO:HA	1.72	0.45
1:A:147:ASN:CB	1:A:148:PRO:CD	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:HD12	2:E:762:ASN:CG	2.37	0.44
1:D:516:ILE:HD11	1:D:520:GLY:HA2	1.97	0.44
2:E:737:GLU:CD	2:E:737:GLU:H	2.20	0.44
3:F:1393:THR:HG23	3:F:1419:ARG:HH12	1.81	0.44
1:A:3:MET:SD	1:A:626:SER:HB2	2.57	0.44
3:C:1362:MET:HE2	3:C:1389:PHE:CZ	2.53	0.44
2:B:746:PRO:CG	2:B:774:LYS:HG3	2.47	0.44
2:B:819:ARG:NH1	2:B:819:ARG:HG2	2.33	0.44
3:F:1497:PHE:HB2	3:F:1604:THR:O	2.17	0.44
1:A:368:ALA:N	1:A:403:ARG:O	2.40	0.44
1:D:50:GLU:HA	1:D:50:GLU:OE1	2.17	0.44
1:A:61:MET:HB3	1:A:61:MET:HE3	1.75	0.44
1:A:55:THR:CG2	1:A:57:ALA:H	2.31	0.44
3:C:1472:HIS:CE1	3:C:1474:GLU:HG2	2.53	0.44
1:A:422:LEU:HB3	1:A:423:PRO:HD2	2.00	0.44
2:E:851:CYS:HB3	2:E:879:VAL:HB	2.00	0.44
1:D:49:SER:HB2	1:D:50:GLU:OE2	2.17	0.44
3:C:1503:ASP:O	3:C:1504:LYS:HB3	2.18	0.44
1:D:142:MET:HG3	1:D:187:TYR:CE1	2.53	0.44
2:B:830:TYR:CD1	2:B:871:SER:HB3	2.53	0.44
3:C:1504:LYS:HG2	3:C:1505:VAL:N	2.32	0.43
2:E:806:ASP:HB3	2:E:833:ARG:HG2	2.00	0.43
3:F:1617:ASP:O	3:F:1619:GLU:N	2.50	0.43
3:C:1415:ALA:CB	3:C:1417:SER:H	2.31	0.43
1:D:143:VAL:HG11	1:D:169:LEU:HD11	2.00	0.43
1:D:148:PRO:HD3	1:D:182:TRP:CE2	2.53	0.43
1:D:546:GLY:HA3	1:D:560:THR:HG22	2.01	0.43
1:A:603:ILE:HA	7:A:757:HOH:O	2.17	0.43
1:D:575:ALA:O	2:E:748:SER:HA	2.18	0.43
2:E:817:VAL:HG22	2:E:907:LEU:HD22	2.01	0.43
3:C:1343:VAL:HG21	3:C:1455:VAL:HB	2.00	0.43
3:F:1485:ARG:HD2	5:F:707:GOL:O3	2.18	0.43
4:A:644:NDG:H6C1	4:A:645:NDG:C7	2.48	0.43
1:D:236:ARG:HH12	1:D:240:GLY:HA2	1.83	0.43
1:D:292:LEU:H	1:D:292:LEU:HD22	1.63	0.43
1:A:160:SER:CA	1:A:167:LEU:HD21	2.49	0.43
1:D:154:LYS:HD2	1:D:171:TRP:CD1	2.54	0.43
1:D:39:ASP:OD1	1:D:39:ASP:N	2.51	0.43
1:A:50:GLU:OE2	1:A:50:GLU:HA	2.18	0.43
1:A:177:VAL:CG2	1:A:182:TRP:CZ2	3.02	0.43
1:D:14:LEU:HD21	1:D:101:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:THR:HA	1:D:274:GLY:O	2.18	0.43
1:D:193:GLN:H	1:D:193:GLN:CD	2.22	0.43
1:A:21:VAL:HG23	1:A:478:LEU:HD13	2.01	0.43
1:D:160:SER:CB	1:D:167:LEU:CD1	2.85	0.43
1:A:443:LEU:HD11	1:A:449:LEU:HD22	2.00	0.43
1:A:10:ASN:HB3	1:A:635:ARG:HD3	2.00	0.43
2:B:731:GLU:H	2:B:731:GLU:CD	2.20	0.43
1:A:241:LYS:HG3	2:B:832:TYR:CE2	2.54	0.43
3:C:1472:HIS:HB3	3:C:1475:LYS:HB2	2.00	0.43
1:D:427:VAL:HG12	1:D:521:GLN:NE2	2.34	0.43
1:A:151:ILE:HA	1:A:152:PRO:HD3	1.93	0.43
1:A:432:ASN:OD1	1:A:457:MET:CB	2.67	0.42
2:E:907:LEU:HD12	2:E:907:LEU:N	2.32	0.42
3:F:1385:MET:HE2	3:F:1389:PHE:C	2.39	0.42
1:D:89:THR:HB	1:D:94:VAL:HG22	2.02	0.42
3:C:1387:THR:CG2	3:C:1451:GLN:N	2.72	0.42
1:D:126:ARG:CZ	1:D:572:VAL:HB	2.49	0.42
1:D:6:ILE:HG13	1:D:20:MET:SD	2.57	0.42
1:A:24:ALA:HB3	1:A:60:HIS:HB3	2.01	0.42
3:C:1359:LYS:HZ2	3:C:1446:ASN:HB2	1.84	0.42
1:A:552:GLN:HA	1:A:553:PRO:HD2	1.86	0.42
3:C:1414:LYS:HB3	3:C:1415:ALA:H	1.76	0.42
1:A:127:ILE:CD1	1:A:169:LEU:HD12	2.50	0.42
2:E:742:ARG:HB3	2:E:775:ASP:HB3	2.02	0.42
2:E:739:ILE:HB	2:E:891:LYS:HD3	2.01	0.42
3:F:1450:ILE:HG13	3:F:1450:ILE:O	2.16	0.42
1:D:509:LEU:C	1:D:509:LEU:CD1	2.88	0.42
1:D:177:VAL:CG2	1:D:182:TRP:HZ2	2.32	0.42
1:D:279:VAL:HG12	1:D:280:LEU:C	2.40	0.42
1:A:105:SER:O	1:A:131:ASN:HA	2.20	0.42
1:D:469:THR:O	1:D:511:ALA:HA	2.19	0.42
1:A:390:ASN:HD22	1:A:391:THR:H	1.66	0.42
1:A:342:PHE:HD1	1:A:391:THR:HG21	1.83	0.42
5:E:705:GOL:H32	7:E:510:HOH:O	2.20	0.42
1:A:214:VAL:CG2	1:A:214:VAL:O	2.68	0.42
3:C:1387:THR:HG21	3:C:1451:GLN:H	1.79	0.42
1:A:191:SER:HA	1:A:193:GLN:NE2	2.28	0.42
2:E:746:PRO:CD	2:E:774:LYS:HG2	2.50	0.42
1:A:307:THR:OG1	1:A:318:GLN:NE2	2.47	0.42
3:C:1504:LYS:CG	3:C:1506:THR:HG23	2.50	0.41
1:A:465:ILE:HD12	1:A:513:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:HIS:HA	1:A:393:PRO:HD3	1.91	0.41
3:F:1335:THR:O	3:F:1336:CYS:C	2.57	0.41
1:D:236:ARG:NH1	1:D:240:GLY:HA2	2.35	0.41
1:A:146:GLU:OE1	1:A:185:ARG:HD3	2.20	0.41
3:C:1341:LEU:HD22	3:C:1457:VAL:CG2	2.43	0.41
1:A:345:GLY:O	1:A:456:ARG:NH2	2.53	0.41
1:D:10:ASN:HB3	1:D:635:ARG:HD3	2.02	0.41
1:A:221:TYR:O	1:A:326:ILE:HA	2.20	0.41
1:D:63:ASN:O	1:D:64:VAL:HG22	2.20	0.41
2:E:866:ILE:HA	2:E:867:PRO:HD2	1.90	0.41
1:D:128:PHE:CD1	2:E:787:MET:HE1	2.55	0.41
1:D:142:MET:O	1:D:186:ALA:HA	2.20	0.41
3:C:1387:THR:HG23	3:C:1451:GLN:N	2.34	0.41
2:B:897:HIS:N	2:B:897:HIS:HD1	2.17	0.41
1:A:154:LYS:HD2	1:A:171:TRP:HD1	1.81	0.41
1:A:223:ILE:HG12	1:A:298:VAL:HG22	2.02	0.41
1:D:49:SER:CB	1:D:50:GLU:OE2	2.68	0.41
2:E:758:GLU:CD	2:E:758:GLU:H	2.24	0.41
3:C:1412:LEU:HD12	3:C:1412:LEU:HA	1.89	0.41
3:C:1392:ASP:HB2	3:C:1442:HIS:HE2	1.86	0.41
1:D:147:ASN:HB2	1:D:148:PRO:HD2	2.01	0.41
3:F:1336:CYS:HB3	3:F:1467:CYS:HB2	1.89	0.41
2:E:833:ARG:O	2:E:834:GLN:C	2.59	0.41
1:A:39:ASP:OD1	1:A:44:LYS:N	2.53	0.41
1:D:241:LYS:HD3	1:D:241:LYS:HA	1.88	0.41
3:C:1576:GLU:O	3:C:1577:LYS:HB2	2.21	0.41
1:A:164:LEU:O	2:B:787:MET:HG2	2.21	0.41
1:D:3:MET:CE	1:D:522:ARG:CD	2.99	0.41
2:B:837:GLU:CB	2:B:868:PRO:HD3	2.44	0.41
1:A:592:SER:HB2	7:A:724:HOH:O	2.20	0.41
1:A:148:PRO:HD3	1:A:182:TRP:CE2	2.55	0.41
1:D:362:ALA:O	1:D:383:GLY:HA2	2.20	0.41
1:D:114:LYS:HE3	1:D:117:TYR:CE1	2.56	0.41
1:A:407:GLN:C	1:A:408:GLU:HG3	2.41	0.41
2:E:877:VAL:HG13	3:F:1451:GLN:CD	2.41	0.41
3:F:1385:MET:CE	3:F:1389:PHE:HB3	2.52	0.41
1:A:10:ASN:HA	1:A:10:ASN:HD22	1.69	0.40
1:D:459:ARG:HG2	1:D:459:ARG:H	1.62	0.40
1:A:15:GLU:CG	1:A:70:ALA:HB2	2.52	0.40
3:C:1337:ASN:N	3:C:1337:ASN:ND2	2.67	0.40
1:A:47:LEU:HD21	1:A:50:GLU:CG	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:850:PHE:CE1	2:E:878:ILE:HD11	2.56	0.40
3:F:1377:THR:HB	3:F:1378:MET:H	1.70	0.40
3:C:1437:LEU:HD12	3:C:1437:LEU:C	2.41	0.40
2:B:889:GLU:OE2	2:B:891:LYS:HE3	2.22	0.40
3:C:1450:ILE:HG13	3:C:1450:ILE:O	2.22	0.40
1:A:45:LEU:HD21	1:A:48:SER:CB	2.50	0.40
1:D:31:VAL:HA	1:D:32:PRO:HD2	1.98	0.40
3:F:1560:ARG:HD3	3:F:1560:ARG:HA	1.92	0.40
1:D:42:GLY:O	1:D:43:LYS:HG3	2.22	0.40
3:C:1541:MET:O	3:C:1559:GLN:HA	2.21	0.40
1:D:45:LEU:HG	1:D:48:SER:OG	2.21	0.40
3:F:1380:ILE:HG23	3:F:1423:ILE:HG23	2.04	0.40
3:F:1380:ILE:O	3:F:1457:VAL:HA	2.21	0.40
1:D:343:LYS:HD2	1:D:343:LYS:N	2.36	0.40
3:C:1403:VAL:HA	7:C:499:HOH:O	2.21	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	624/643 (97%)	582 (93%)	27 (4%)	15 (2%)	7	7
1	D	629/643 (98%)	593 (94%)	21 (3%)	15 (2%)	7	7
2	B	181/188 (96%)	172 (95%)	8 (4%)	1 (1%)	30	43
2	E	182/188 (97%)	167 (92%)	13 (7%)	2 (1%)	17	25
3	C	290/343 (84%)	270 (93%)	9 (3%)	11 (4%)	4	3
3	F	294/343 (86%)	274 (93%)	11 (4%)	9 (3%)	5	4
All	All	2200/2348 (94%)	2058 (94%)	89 (4%)	53 (2%)	7	7

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	SER
1	A	550	ASP
3	C	1361	THR
1	D	41	PRO
1	D	372	GLU
1	D	549	GLU
1	D	550	ASP
2	E	834	GLN
3	F	1336	CYS
3	F	1500	LYS
1	A	91	GLY
1	A	375	VAL
1	A	518	ALA
2	B	732	ASP
3	C	1414	LYS
3	C	1504	LYS
3	C	1505	VAL
1	D	50	GLU
1	D	64	VAL
1	D	256	GLY
1	D	375	VAL
1	D	518	ALA
1	D	551	ARG
1	D	609	SER
2	E	833	ARG
3	F	1449	LEU
3	F	1499	GLN
3	F	1618	GLU
3	F	1619	GLU
1	A	50	GLU
1	A	64	VAL
1	A	372	GLU
1	A	404	THR
1	A	407	GLN
1	A	548	SER
1	A	549	GLU
3	C	1477	ASP
3	C	1499	GLN
3	C	1619	GLU
1	D	410	SER
1	D	376	GLN
3	F	1504	LYS
3	F	1505	VAL

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Mol	Chain	Res	Type
1	A	81	ASN
1	A	609	SER
3	C	1416	PHE
3	C	1417	SER
3	C	1573	LYS
3	C	1618	GLU
1	D	552	GLN
3	F	1377	THR
1	A	376	GLN
1	D	91	GLY

5.3.2 Protein sidechains [i](#)

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	555/567 (98%)	498 (90%)	57 (10%)	9	13
1	D	558/567 (98%)	487 (87%)	71 (13%)	5	6
2	B	171/175 (98%)	156 (91%)	15 (9%)	12	18
2	E	171/175 (98%)	155 (91%)	16 (9%)	11	16
3	C	270/309 (87%)	232 (86%)	38 (14%)	4	5
3	F	272/309 (88%)	242 (89%)	30 (11%)	8	10
All	All	1997/2102 (95%)	1770 (89%)	227 (11%)	7	9

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	10	ASN
1	A	36	THR
1	A	45	LEU
1	A	46	VAL
1	A	47	LEU
1	A	51	LYS
1	A	55	THR

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Mol	Chain	Res	Type
1	A	61	MET
1	A	64	VAL
1	A	92	THR
1	A	137	VAL
1	A	155	GLN
1	A	161	GLN
1	A	163	GLN
1	A	179	MET
1	A	183	LYS
1	A	193	GLN
1	A	207	LEU
1	A	223	ILE
1	A	227	LYS
1	A	236	ARG
1	A	249	VAL
1	A	275	SER
1	A	277	GLU
1	A	293	ARG
1	A	311	HIS
1	A	350	LEU
1	A	364	ARG
1	A	372	GLU
1	A	379	THR
1	A	386	LYS
1	A	390	ASN
1	A	391	THR
1	A	396	LYS
1	A	398	LEU
1	A	408	GLU
1	A	410	SER
1	A	417	ARG
1	A	438	VAL
1	A	444	ARG
1	A	448	THR
1	A	456	ARG
1	A	477	ARG
1	A	487	GLU
1	A	509	LEU
1	A	516	ILE
1	A	521	GLN
1	A	529	VAL
1	A	550	ASP

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Mol	Chain	Res	Type
1	A	554	VAL
1	A	583	LEU
1	A	590	THR
1	A	592	SER
1	A	628	SER
1	A	637	GLU
1	A	639	GLN
2	B	730	ASP
2	B	731	GLU
2	B	788	SER
2	B	812	ARG
2	B	813	LEU
2	B	819	ARG
2	B	826	ARG
2	B	834	GLN
2	B	841	ARG
2	B	870	SER
2	B	872	LEU
2	B	894	VAL
2	B	897	HIS
2	B	907	LEU
2	B	912	GLU
3	C	1335	THR
3	C	1337	ASN
3	C	1338	LYS
3	C	1342	LYS
3	C	1344	THR
3	C	1361	THR
3	C	1387	THR
3	C	1393	THR
3	C	1401	ASN
3	C	1411	GLU
3	C	1412	LEU
3	C	1414	LYS
3	C	1416	PHE
3	C	1418	ASP
3	C	1428	LYS
3	C	1432	SER
3	C	1433	GLU
3	C	1440	LYS
3	C	1450	ILE
3	C	1457	VAL

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Mol	Chain	Res	Type
3	C	1462	ASN
3	C	1469	ARG
3	C	1474	GLU
3	C	1479	LYS
3	C	1483	LEU
3	C	1503	ASP
3	C	1504	LYS
3	C	1505	VAL
3	C	1507	LEU
3	C	1532	LEU
3	C	1555	GLN
3	C	1558	GLN
3	C	1566	ILE
3	C	1573	LYS
3	C	1602	LYS
3	C	1611	GLU
3	C	1619	GLU
3	C	1623	GLN
1	D	3	MET
1	D	6	ILE
1	D	10	ASN
1	D	20	MET
1	D	31	VAL
1	D	34	THR
1	D	46	VAL
1	D	47	LEU
1	D	50	GLU
1	D	51	LYS
1	D	52	THR
1	D	63	ASN
1	D	64	VAL
1	D	81	ASN
1	D	82	LYS
1	D	87	GLN
1	D	89	THR
1	D	98	VAL
1	D	103	LEU
1	D	126	ARG
1	D	133	LYS
1	D	140	THR
1	D	153	VAL
1	D	155	GLN

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Mol	Chain	Res	Type
1	D	158	LEU
1	D	189	GLU
1	D	190	ASN
1	D	191	SER
1	D	194	GLN
1	D	217	THR
1	D	232	THR
1	D	236	ARG
1	D	292	LEU
1	D	297	LEU
1	D	300	LYS
1	D	302	LEU
1	D	304	VAL
1	D	316	MET
1	D	364	ARG
1	D	372	GLU
1	D	373	ASP
1	D	376	GLN
1	D	384	VAL
1	D	389	ILE
1	D	396	LYS
1	D	400	ILE
1	D	407	GLN
1	D	408	GLU
1	D	410	SER
1	D	411	GLU
1	D	425	SER
1	D	437	SER
1	D	440	ARG
1	D	443	LEU
1	D	459	ARG
1	D	471	LEU
1	D	477	ARG
1	D	483	ARG
1	D	509	LEU
1	D	510	VAL
1	D	516	ILE
1	D	529	VAL
1	D	547	GLN
1	D	549	GLU
1	D	550	ASP
1	D	551	ARG

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Mol	Chain	Res	Type
1	D	554	VAL
1	D	564	GLU
1	D	574	VAL
1	D	592	SER
1	D	639	GLN
2	E	731	GLU
2	E	753	VAL
2	E	757	LYS
2	E	759	PRO
2	E	761	LYS
2	E	778	THR
2	E	795	VAL
2	E	833	ARG
2	E	834	GLN
2	E	840	VAL
2	E	842	VAL
2	E	865	THR
2	E	872	LEU
2	E	877	VAL
2	E	878	ILE
2	E	907	LEU
3	F	1335	THR
3	F	1336	CYS
3	F	1342	LYS
3	F	1359	LYS
3	F	1360	ASN
3	F	1369	ARG
3	F	1373	ASP
3	F	1374	GLN
3	F	1377	THR
3	F	1393	THR
3	F	1411	GLU
3	F	1418	ASP
3	F	1449	LEU
3	F	1450	ILE
3	F	1487	GLU
3	F	1499	GLN
3	F	1501	SER
3	F	1504	LYS
3	F	1506	THR
3	F	1507	LEU
3	F	1511	LEU

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Mol	Chain	Res	Type
3	F	1525	THR
3	F	1528	VAL
3	F	1545	GLN
3	F	1553	GLU
3	F	1554	VAL
3	F	1566	ILE
3	F	1602	LYS
3	F	1613	ASP
3	F	1619	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	38	HIS
1	A	60	HIS
1	A	87	GLN
1	A	104	GLN
1	A	155	GLN
1	A	163	GLN
1	A	193	GLN
1	A	318	GLN
1	A	332	GLN
1	A	334	HIS
1	A	390	ASN
1	A	490	GLN
1	A	639	GLN
2	B	738	ASN
2	B	820	ASN
2	B	834	GLN
2	B	836	GLN
3	C	1337	ASN
3	C	1401	ASN
3	C	1431	HIS
3	C	1451	GLN
3	C	1462	ASN
3	C	1531	GLN
3	C	1579	HIS
3	C	1616	GLN
3	C	1620	ASN
1	D	10	ASN
1	D	38	HIS

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Mol	Chain	Res	Type
1	D	81	ASN
1	D	132	HIS
1	D	144	ASN
1	D	155	GLN
1	D	190	ASN
1	D	291	ASN
1	D	318	GLN
1	D	356	ASN
1	D	376	GLN
1	D	521	GLN
1	D	547	GLN
1	D	558	GLN
1	D	591	GLN
2	E	770	ASN
2	E	805	GLN
2	E	822	GLN
2	E	834	GLN
3	F	1431	HIS
3	F	1620	ASN
3	F	1641	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 carbohydrates are modelled in this entry.

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
4	NDG	A	644	4	14,14,15	0.59	0	15,19,21	0.64	0
4	NDG	A	645	4	14,14,15	0.53	0	15,19,21	0.82	0
4	NDG	D	644	4	14,14,15	0.53	0	15,19,21	1.04	1 (6%)
4	NDG	D	645	4	14,14,15	0.92	1 (7%)	15,19,21	0.75	0

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
4	NDG	A	644	4	-	0/6/23/26	0/1/1/1
4	NDG	A	645	4	1/1/5/7	0/6/23/26	0/1/1/1
4	NDG	D	644	4	-	0/6/23/26	0/1/1/1
4	NDG	D	645	4	1/1/5/7	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	645	NDG	C1-C2	-2.94	1.48	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	644	NDG	O4-C4-C5	2.55	116.00	109.24

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	645	NDG	C1
4	D	645	NDG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	644	NDG	2	0
4	A	645	NDG	1	0
4	D	644	NDG	1	0

5.6 Ligand geometry

16 ligands are modelled in this entry.

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	GOL	A	703	-	5,5,5	0.30	0	5,5,5	0.25	0
5	GOL	A	712	-	5,5,5	0.30	0	5,5,5	0.34	0
5	GOL	A	713	-	5,5,5	0.40	0	5,5,5	0.36	0
5	GOL	B	701	-	5,5,5	0.40	0	5,5,5	0.47	0
5	GOL	B	702	-	5,5,5	0.36	0	5,5,5	0.23	0
5	GOL	C	708	-	5,5,5	0.26	0	5,5,5	0.38	0
5	GOL	C	709	-	5,5,5	0.30	0	5,5,5	0.38	0
6	NO3	C	801	-	3,3,3	3.38	3 (100%)	3,3,3	0.19	0
5	GOL	D	711	-	5,5,5	0.38	0	5,5,5	0.32	0
5	GOL	E	704	-	5,5,5	0.40	0	5,5,5	0.44	0
5	GOL	E	705	-	5,5,5	0.35	0	5,5,5	0.32	0
5	GOL	E	706	-	5,5,5	0.31	0	5,5,5	0.48	0
5	GOL	F	707	-	5,5,5	0.33	0	5,5,5	0.26	0
5	GOL	F	710	-	5,5,5	0.33	0	5,5,5	0.18	0
6	NO3	F	802	-	3,3,3	3.36	3 (100%)	3,3,3	0.17	0
6	NO3	F	803	-	3,3,3	3.34	3 (100%)	3,3,3	0.27	0

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	GOL	A	703	-	-	0/4/4/4	0/0/0/0
5	GOL	A	712	-	-	0/4/4/4	0/0/0/0
5	GOL	A	713	-	-	0/4/4/4	0/0/0/0
5	GOL	B	701	-	-	0/4/4/4	0/0/0/0
5	GOL	B	702	-	-	0/4/4/4	0/0/0/0
5	GOL	C	708	-	-	0/4/4/4	0/0/0/0
5	GOL	C	709	-	-	0/4/4/4	0/0/0/0
6	NO3	C	801	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	D	711	-	-	0/4/4/4	0/0/0/0
5	GOL	E	704	-	-	0/4/4/4	0/0/0/0
5	GOL	E	705	-	-	0/4/4/4	0/0/0/0
5	GOL	E	706	-	-	0/4/4/4	0/0/0/0
5	GOL	F	707	-	-	0/4/4/4	0/0/0/0
5	GOL	F	710	-	-	0/4/4/4	0/0/0/0
6	NO3	F	802	-	-	0/0/0/0	0/0/0/0
6	NO3	F	803	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	803	NO3	O3-N	2.94	1.40	1.25
6	C	801	NO3	O2-N	2.97	1.40	1.25
6	F	802	NO3	O2-N	2.99	1.40	1.25
6	F	802	NO3	O3-N	3.00	1.40	1.25
6	C	801	NO3	O3-N	3.08	1.41	1.25
6	F	803	NO3	O2-N	3.09	1.41	1.25
6	F	803	NO3	O1-N	3.90	1.40	1.24
6	F	802	NO3	O1-N	3.98	1.40	1.24
6	C	801	NO3	O1-N	3.98	1.40	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703	GOL	2	0
5	A	712	GOL	4	0
5	B	701	GOL	2	0
5	D	711	GOL	5	0
5	E	705	GOL	2	0
5	F	707	GOL	3	0
5	F	710	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	630/643 (97%)	0.56	59 (9%)	11 10	30, 44, 55, 73	0
1	D	633/643 (98%)	0.64	73 (11%)	6 6	33, 44, 56, 78	0
2	B	183/188 (97%)	0.55	18 (9%)	10 9	32, 44, 52, 59	0
2	E	184/188 (97%)	1.24	47 (25%)	1 1	37, 44, 51, 71	0
3	C	296/343 (86%)	0.72	37 (12%)	5 5	33, 45, 56, 65	0
3	F	298/343 (86%)	0.81	37 (12%)	5 5	30, 45, 57, 68	0
All	All	2224/2348 (94%)	0.69	271 (12%)	5 5	30, 44, 55, 78	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1502	ASP	11.8
3	C	1416	PHE	11.3
3	F	1501	SER	10.3
2	E	899	ILE	8.3
1	A	374	THR	7.9
1	D	551	ARG	7.9
3	F	1503	ASP	7.9
2	E	913	GLY	7.4
2	E	759	PRO	7.4
1	D	550	ASP	7.4
1	D	549	GLU	7.0
1	D	373	ASP	6.9
1	A	548	SER	6.8
3	C	1503	ASP	6.7
2	E	896	HIS	6.5
3	F	1335	THR	6.4
1	D	643	PRO	6.3
3	F	1641	ASN	6.2
2	E	914	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
2	E	834	GLN	6.1
3	C	1641	ASN	5.9
2	E	763	GLY	5.9
1	A	550	ASP	5.8
3	C	1417	SER	5.8
1	D	642	GLN	5.7
3	F	1499	GLN	5.7
2	E	835	ASN	5.3
1	D	440	ARG	4.9
1	D	545	SER	4.9
1	A	642	GLN	4.8
1	D	548	SER	4.8
2	E	768	LEU	4.7
3	F	1504	LYS	4.7
1	D	257	GLU	4.7
1	D	80	ARG	4.5
1	A	442	GLU	4.5
1	D	162	ASN	4.4
1	A	549	GLU	4.4
1	A	297	LEU	4.4
1	D	371	GLY	4.3
1	A	373	ASP	4.3
1	A	551	ARG	4.3
2	E	868	PRO	4.2
2	E	731	GLU	4.2
1	A	6	ILE	4.2
1	A	622	LEU	4.2
3	F	1373	ASP	4.1
1	A	1	SER	4.1
3	C	1372	GLY	4.1
1	A	510	VAL	4.0
3	C	1499	GLN	4.0
1	D	190	ASN	3.9
1	A	371	GLY	3.9
2	B	731	GLU	3.9
1	D	427	VAL	3.9
3	F	1445	PHE	3.9
2	E	869	LYS	3.8
2	B	898	PHE	3.8
3	F	1534	ASN	3.8
3	F	1464	GLU	3.8
1	D	471	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	732	ASP	3.7
1	D	622	LEU	3.7
2	E	790	LYS	3.7
3	C	1335	THR	3.7
1	D	57	ALA	3.7
1	A	157	SER	3.6
1	D	164	LEU	3.6
2	E	876	TYR	3.6
2	E	825	ILE	3.6
3	C	1445	PHE	3.5
3	F	1416	PHE	3.5
2	B	836	GLN	3.4
1	D	48	SER	3.4
1	A	469	THR	3.4
2	E	738	ASN	3.4
3	F	1447	VAL	3.4
1	A	470	TYR	3.4
3	C	1410	TYR	3.4
2	E	895	TYR	3.4
1	A	44	LYS	3.4
3	C	1522	VAL	3.4
1	D	512	TYR	3.4
2	E	783	LEU	3.3
3	C	1418	ASP	3.4
1	D	469	THR	3.3
1	D	519	SER	3.3
2	E	875	PRO	3.3
1	A	7	ILE	3.2
1	A	471	LEU	3.2
2	E	811	LEU	3.2
2	E	870	SER	3.2
1	A	511	ALA	3.2
2	B	873	SER	3.2
1	D	510	VAL	3.2
1	A	472	ILE	3.2
1	D	7	ILE	3.2
2	E	865	THR	3.2
1	A	48	SER	3.2
3	C	1374	GLN	3.2
2	E	867	PRO	3.1
1	D	228	GLY	3.1
1	D	110	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	574	VAL	3.1
2	E	898	PHE	3.0
3	F	1570	GLU	3.0
3	F	1487	GLU	3.0
3	F	1618	GLU	3.0
1	A	512	TYR	3.0
3	F	1384	SER	3.0
1	A	12	LEU	3.0
2	B	730	ASP	3.0
2	E	827	ALA	3.0
2	E	874	VAL	2.9
2	E	785	VAL	2.9
1	D	511	ALA	2.9
2	B	876	TYR	2.9
3	C	1448	GLU	2.9
1	D	476	GLY	2.9
2	E	795	VAL	2.9
1	D	547	GLN	2.9
3	F	1500	LYS	2.9
1	A	80	ARG	2.9
3	C	1547	ILE	2.9
1	D	572	VAL	2.8
1	D	397	PRO	2.8
1	D	125	TYR	2.8
2	B	842	VAL	2.8
3	F	1431	HIS	2.8
2	E	762	ASN	2.8
2	E	877	VAL	2.8
2	B	875	PRO	2.8
3	F	1420	ASN	2.8
2	E	789	ASP	2.8
2	E	782	ILE	2.7
1	D	470	TYR	2.7
3	F	1403	VAL	2.7
3	F	1417	SER	2.7
1	D	375	VAL	2.7
3	F	1404	ASP	2.7
1	D	574	VAL	2.7
3	C	1383	ILE	2.7
1	D	312	SER	2.7
3	C	1384	SER	2.7
2	E	758	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	144	ASN	2.7
1	A	287	ASP	2.7
2	E	897	HIS	2.7
1	A	226	GLU	2.7
1	D	53	VAL	2.7
1	D	639	GLN	2.7
3	C	1616	GLN	2.7
2	E	837	GLU	2.7
1	A	518	ALA	2.7
1	A	9	PRO	2.6
2	E	754	GLU	2.6
3	F	1448	GLU	2.6
3	C	1613	ASP	2.6
1	A	189	GLU	2.6
2	B	890	VAL	2.6
1	D	442	GLU	2.6
1	D	15	GLU	2.6
2	B	825	ILE	2.6
2	E	836	GLN	2.6
3	C	1359	LYS	2.6
1	A	573	LEU	2.6
1	D	489	GLY	2.5
1	A	110	ILE	2.5
3	F	1385	MET	2.5
3	F	1600	ILE	2.5
1	D	491	ASP	2.5
3	F	1640	PRO	2.5
3	C	1581	LEU	2.5
3	C	1562	PHE	2.5
1	A	193	GLN	2.5
1	A	616	VAL	2.5
1	A	21	VAL	2.5
1	A	436	LEU	2.5
2	E	878	ILE	2.5
1	A	313	GLY	2.5
1	A	526	ALA	2.5
3	F	1454	ALA	2.5
1	A	40	PHE	2.4
1	A	108	LEU	2.4
1	D	623	THR	2.4
1	A	575	ALA	2.4
1	D	69	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	2.4
2	E	809	ILE	2.4
2	B	784	ALA	2.4
3	F	1581	LEU	2.4
3	C	1504	LYS	2.4
2	E	753	VAL	2.4
1	A	617	PHE	2.4
1	A	509	LEU	2.4
1	D	103	LEU	2.4
3	C	1639	CYS	2.3
1	A	372	GLU	2.3
3	C	1617	ASP	2.3
3	F	1383	ILE	2.3
1	D	396	LYS	2.3
3	F	1599	ILE	2.3
1	D	436	LEU	2.3
2	E	829	LEU	2.3
3	C	1487	GLU	2.3
1	D	395	GLN	2.3
3	C	1431	HIS	2.3
1	A	99	VAL	2.3
2	B	789	ASP	2.3
2	E	873	SER	2.3
3	F	1521	TYR	2.3
1	D	127	ILE	2.2
1	D	226	GLU	2.2
2	E	769	MET	2.2
1	A	375	VAL	2.2
2	B	826	ARG	2.2
2	B	877	VAL	2.2
3	C	1433	GLU	2.2
1	A	621	GLY	2.2
1	D	229	LEU	2.2
1	D	256	GLY	2.2
1	A	41	PRO	2.2
2	E	872	LEU	2.2
1	D	473	MET	2.2
1	D	372	GLU	2.2
3	C	1373	ASP	2.2
3	F	1337	ASN	2.2
1	A	185	ARG	2.1
2	E	808	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	1412	LEU	2.1
3	C	1413	ASP	2.1
1	D	10	ASN	2.1
2	B	785	VAL	2.1
1	A	513	TYR	2.1
3	C	1486	ASP	2.1
1	A	128	PHE	2.1
1	D	28	GLN	2.1
1	D	520	GLY	2.1
3	F	1582	MET	2.1
1	D	6	ILE	2.1
1	D	44	LYS	2.1
1	D	472	ILE	2.1
3	C	1600	ILE	2.1
1	A	407	GLN	2.1
3	F	1555	GLN	2.1
2	E	765	SER	2.1
3	C	1618	GLU	2.1
1	D	82	LYS	2.1
1	D	143	VAL	2.1
1	D	186	ALA	2.1
2	B	809	ILE	2.1
1	D	126	ARG	2.1
1	D	108	LEU	2.1
2	B	811	LEU	2.1
3	C	1500	LYS	2.1
1	A	273	ASP	2.1
2	B	828	VAL	2.1
3	C	1534	ASN	2.1
3	C	1599	ILE	2.0
3	C	1615	CYS	2.0
1	A	293	ARG	2.0
1	D	56	PRO	2.0
1	D	111	GLN	2.0
1	D	194	GLN	2.0
1	D	558	GLN	2.0
3	C	1621	GLN	2.0
1	D	464	LYS	2.0
1	D	543	VAL	2.0
1	A	11	ILE	2.0
1	D	9	PRO	2.0
3	F	1613	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
4	NDG	D	644	14/15	0.69	0.30	3.20	61,66,70,73	0
4	NDG	A	644	14/15	0.83	0.21	-0.05	54,57,59,62	0
4	NDG	A	645	14/15	0.63	0.39	-	64,66,69,69	0
4	NDG	D	645	14/15	0.72	0.43	-	75,76,78,79	0

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
5	GOL	D	711	6/6	0.73	0.77	30.19	81,83,84,88	0
5	GOL	A	712	6/6	0.64	0.68	26.84	78,81,82,85	0
6	NO3	F	802	4/4	0.68	0.58	11.27	89,89,89,90	0
5	GOL	F	707	6/6	0.58	0.54	10.13	86,88,88,89	0
5	GOL	B	702	6/6	0.67	0.55	7.60	87,88,88,89	0
5	GOL	E	706	6/6	0.49	0.56	4.90	57,60,63,64	0
6	NO3	F	803	4/4	0.68	0.37	4.79	73,73,73,73	0
5	GOL	A	713	6/6	0.44	0.29	4.70	61,65,66,68	0
6	NO3	C	801	4/4	0.81	0.32	4.41	77,77,77,77	0
5	GOL	C	709	6/6	0.80	0.27	4.10	90,90,91,91	0
5	GOL	E	705	6/6	0.64	0.48	4.02	62,66,66,67	0
5	GOL	A	703	6/6	0.73	0.31	1.71	60,62,63,65	0
5	GOL	E	704	6/6	0.86	0.25	1.19	45,49,51,52	0
5	GOL	C	708	6/6	0.78	0.23	0.09	66,72,73,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	F	710	6/6	0.74	0.21	-0.29	72,73,73,74	0
5	GOL	B	701	6/6	0.93	0.12	-1.52	45,46,48,48	0

6.5 Other polymers

There are no such residues in this entry.