



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:09 AM GMT

PDB ID : 1ZXN
Title : Human DNA topoisomerase IIa ATPase/ADP
Authors : Wei, H.; Ruthenburg, A.J.; Bechis, S.K.; Verdine, G.L.
Deposited on : 2005-06-08
Resolution : 2.51 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

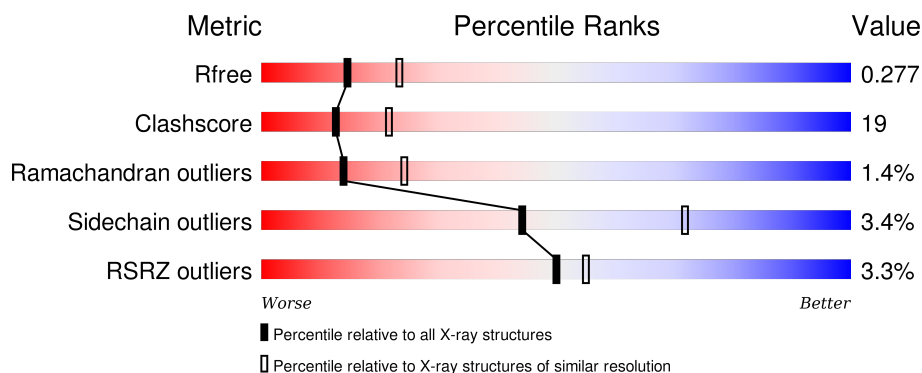
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	400	<div> <div>4%</div> <div>60% 30% 9%</div> </div>
1	B	400	<div> <div>3%</div> <div>62% 30% 5%</div> </div>
1	C	400	<div> <div>0%</div> <div>68% 26% 6%</div> </div>
1	D	400	<div> <div>5%</div> <div>58% 34% 7%</div> </div>

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
5	GOL	A	599	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11646 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 DNA topoisomerase II, alpha isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2736	1748	455	515	18			
1	B	379	Total	C	N	O	S	0	0	0
			2886	1844	481	543	18			
1	C	384	Total	C	N	O	S	0	0	0
			2897	1850	485	543	19			
1	D	371	Total	C	N	O	S	0	0	0
			2761	1766	458	518	19			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

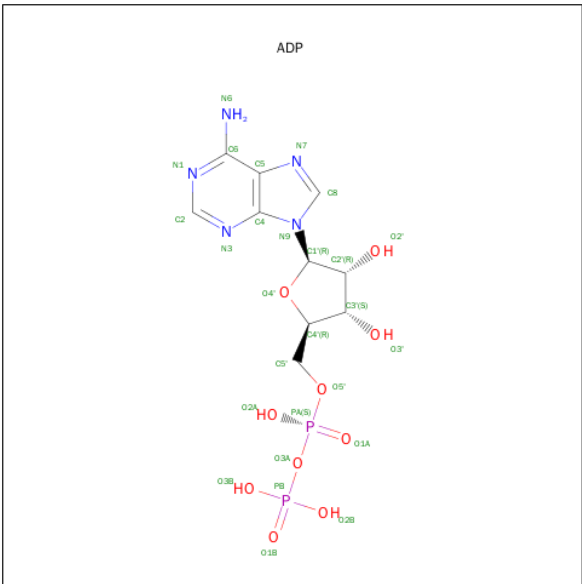
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

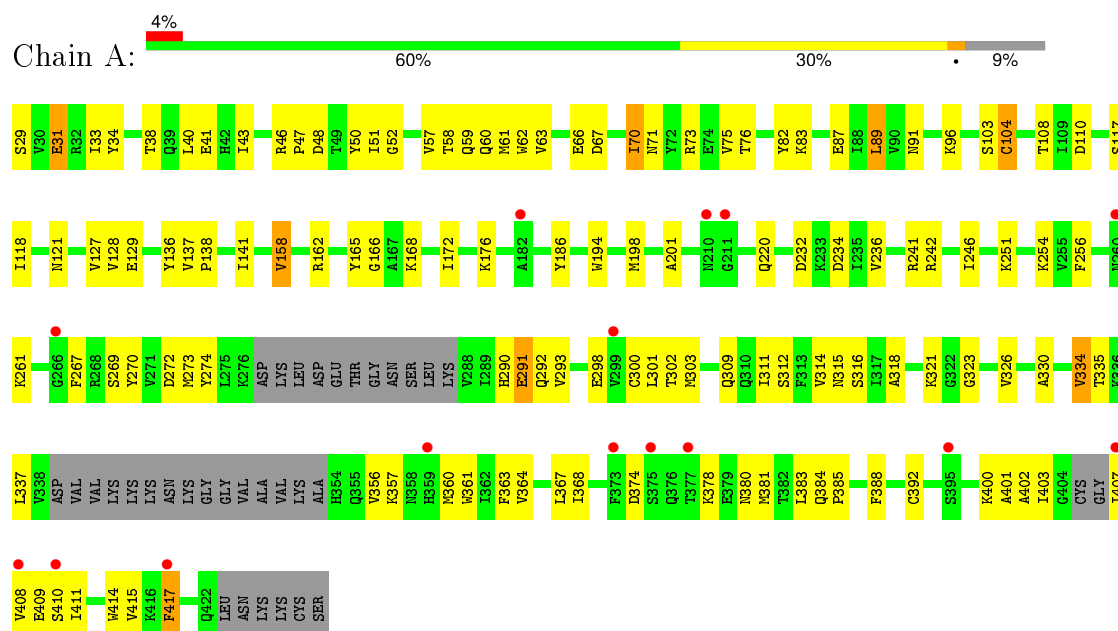
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	59	Total	O	0	0
			59	59		
6	B	72	Total	O	0	0
			72	72		
6	C	72	Total	O	0	0
			72	72		
6	D	35	Total	O	0	0
			35	35		

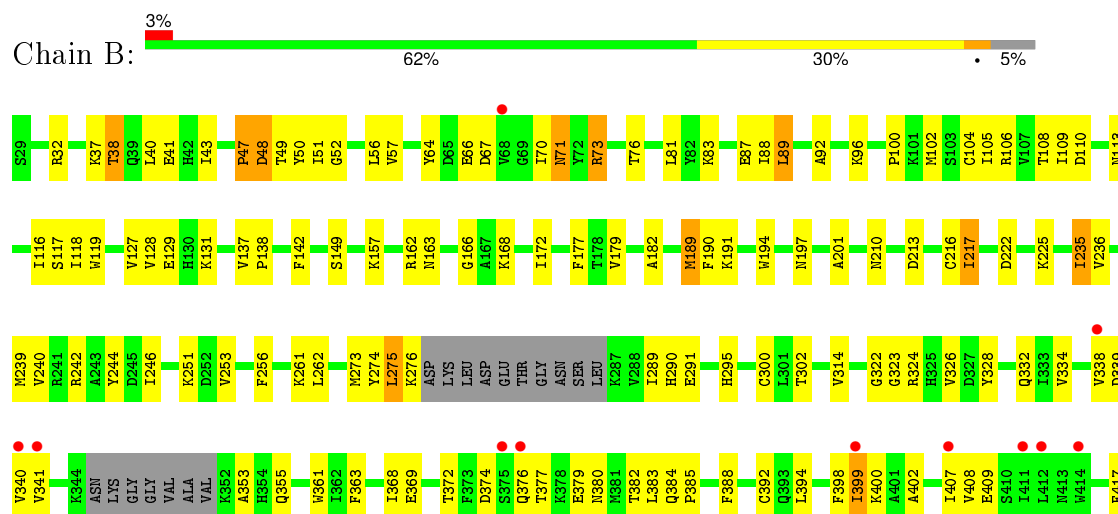
3 Residue-property plots

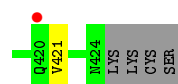
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: DNA topoisomerase II, alpha isozyme

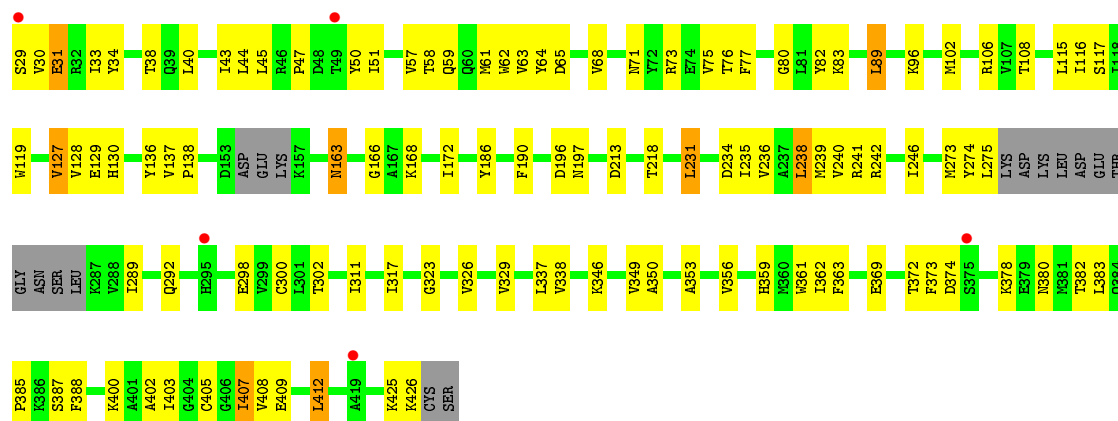


- Molecule 1: DNA topoisomerase II, alpha isozyme

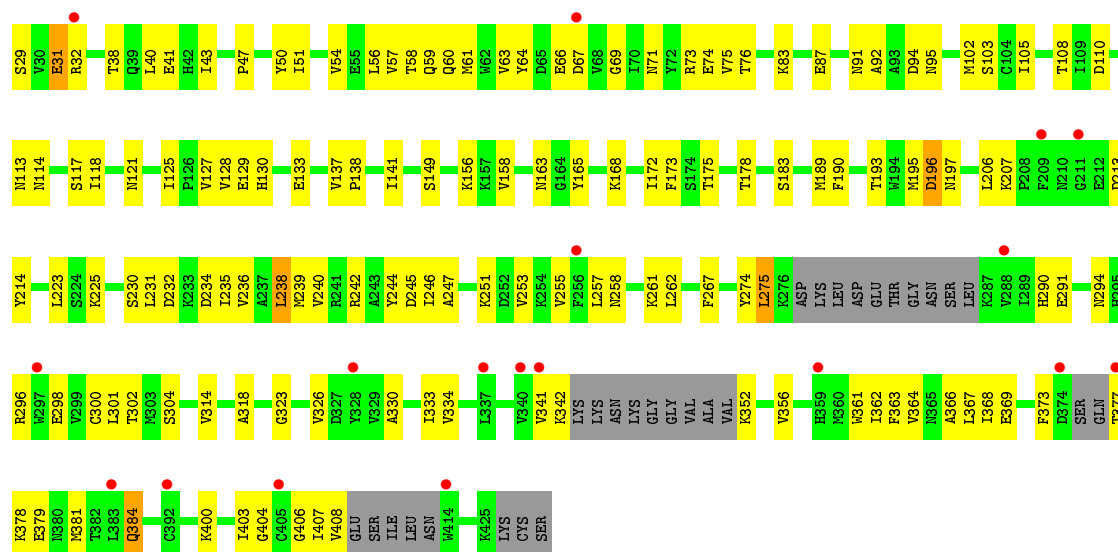




- Molecule 1: DNA topoisomerase II, alpha isozyme



- Molecule 1: DNA topoisomerase II, alpha isozyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.02Å 90.49Å 148.29Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	50.00 – 2.51 40.58 – 2.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.51) 94.9 (40.58-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.281 0.231 , 0.277	Depositor DCC
R_{free} test set	4648 reflections (7.61%)	DCC
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.6	EDS
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 63748 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11646	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, SO4, ADP

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	0.39	0/2790	0.64	0/3793
1	B	0.41	0/2944	0.64	0/4003
1	C	0.39	0/2956	0.64	0/4025
1	D	0.35	0/2816	0.58	0/3832
All	All	0.39	0/11506	0.62	0/15653

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2736	0	2520	125	0
1	B	2886	0	2715	102	0
1	C	2897	0	2706	95	0
1	D	2761	0	2531	108	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	5	0	0	1	0
4	A	27	0	12	3	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	2	0
5	A	6	0	8	1	0
6	A	59	0	0	0	0
6	B	72	0	0	2	0
6	C	72	0	0	1	0
6	D	35	0	0	0	0
All	All	11646	0	10528	426	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 (426) 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:108:THR:HB	1:D:117:SER:HB3	1.32	1.07
1:B:38:THR:HG22	1:B:41:GLU:H	1.27	1.00
1:B:407:ILE:HG23	1:B:408:VAL:H	1.31	0.95
1:B:182:ALA:O	1:B:213:ASP:HB2	1.74	0.88
1:D:38:THR:HG22	1:D:40:LEU:H	1.43	0.84
1:A:89:LEU:HD22	1:A:246:ILE:HG13	1.61	0.82
1:D:168:LYS:O	1:D:172:ILE:HG12	1.80	0.81
1:B:48:ASP:HA	1:B:52:GLY:O	1.80	0.81
1:D:400:LYS:O	1:D:403:ILE:HG12	1.81	0.80
1:A:71:ASN:OD1	1:A:73:ARG:HG3	1.82	0.80
1:A:293:VAL:HG21	1:A:392:CYS:SG	2.22	0.79
1:D:38:THR:HB	1:D:41:GLU:HG3	1.64	0.77
1:C:289:ILE:HD11	1:C:405:CYS:HB3	1.66	0.77
1:A:290:HIS:ND1	1:A:291:GLU:N	2.32	0.77
1:D:206:LEU:O	1:D:207:LYS:HG3	1.86	0.75
1:C:89:LEU:CD2	1:C:246:ILE:HG13	2.17	0.75
1:B:40:LEU:HD13	1:B:172:ILE:HD12	1.68	0.75
1:B:407:ILE:HG23	1:B:408:VAL:N	2.01	0.74
1:C:346:LYS:HA	1:C:346:LYS:HE2	1.70	0.74
1:D:314:VAL:HG21	1:D:381:MET:HG3	1.68	0.73
1:D:173:PHE:HE1	1:D:225:LYS:HE2	1.52	0.73
1:A:168:LYS:O	1:A:172:ILE:HG12	1.88	0.73
1:D:38:THR:HG22	1:D:40:LEU:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LYS:O	1:B:172:ILE:HG12	1.90	0.72
1:D:314:VAL:HG13	1:D:368:ILE:HD13	1.70	0.72
1:D:56:LEU:HD22	1:D:76:THR:HG22	1.70	0.72
1:A:104:CYS:HB2	1:A:254:LYS:O	1.89	0.72
1:D:173:PHE:CE1	1:D:225:LYS:HE2	2.26	0.71
1:A:62:TRP:CE3	1:A:70:ILE:HD11	2.27	0.70
1:A:29:SER:O	1:A:33:ILE:HG22	1.93	0.69
1:A:38:THR:HG23	1:A:41:GLU:H	1.57	0.69
1:C:289:ILE:CD1	1:C:402:ALA:HA	2.22	0.69
1:D:231:LEU:HD12	1:D:231:LEU:N	2.08	0.69
1:C:127:VAL:HG12	1:C:127:VAL:O	1.93	0.69
1:D:75:VAL:HG13	1:D:234:ASP:HB3	1.75	0.68
1:B:289:ILE:HD13	1:B:402:ALA:HA	1.75	0.68
1:A:321:LYS:NZ	1:A:380:ASN:HB2	2.09	0.67
1:A:269:SER:O	1:A:272:ASP:HB2	1.94	0.67
1:C:33:ILE:HG23	1:C:34:TYR:CD2	2.30	0.67
1:C:89:LEU:HD21	1:C:246:ILE:HG13	1.76	0.67
1:B:40:LEU:CD1	1:B:172:ILE:HD12	2.25	0.66
1:B:377:THR:HB	1:B:379:GLU:HG3	1.78	0.66
1:D:236:VAL:O	1:D:240:VAL:HG23	1.95	0.66
1:D:235:ILE:O	1:D:239:MET:HG3	1.95	0.66
1:C:61:MET:SD	1:C:238:LEU:HD21	2.35	0.66
1:B:81:LEU:HD23	1:B:235:ILE:HG13	1.78	0.66
1:D:301:LEU:HD22	1:D:333:ILE:HD13	1.78	0.66
1:D:172:ILE:O	1:D:197:ASN:HA	1.96	0.65
1:D:368:ILE:HD12	1:D:368:ILE:N	2.11	0.65
1:A:104:CYS:H	1:A:121:ASN:HD21	1.44	0.65
1:A:108:THR:HB	1:A:117:SER:OG	1.96	0.65
1:B:289:ILE:CD1	1:B:402:ALA:HA	2.26	0.65
1:A:400:LYS:C	1:A:402:ALA:H	2.00	0.64
1:B:251:LYS:O	1:B:253:VAL:HG23	1.98	0.64
1:A:314:VAL:HG13	1:A:368:ILE:HD13	1.80	0.64
1:D:384:GLN:NE2	1:D:384:GLN:H	1.94	0.64
1:A:62:TRP:HE3	1:A:70:ILE:HD11	1.63	0.63
1:A:38:THR:HG22	1:A:41:GLU:CG	2.28	0.63
1:C:168:LYS:O	1:C:172:ILE:HG12	1.98	0.63
1:A:403:ILE:O	1:A:408:VAL:HG22	1.99	0.63
1:D:323:GLY:O	1:D:326:VAL:HG12	1.99	0.63
1:C:302:THR:CG2	1:C:361:TRP:HB3	2.29	0.63
1:B:38:THR:CG2	1:B:41:GLU:H	2.09	0.63
1:C:63:VAL:HG12	1:C:238:LEU:HD22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ILE:HA	1:B:83:LYS:HD3	1.81	0.63
1:A:40:LEU:CD1	1:A:172:ILE:HD12	2.29	0.62
1:D:58:THR:HA	1:D:75:VAL:O	1.98	0.62
1:D:137:VAL:HB	1:D:138:PRO:HD3	1.80	0.62
1:D:274:TYR:O	1:D:275:LEU:HD13	1.99	0.62
1:C:57:VAL:O	1:C:76:THR:HA	1.99	0.62
1:C:300:CYS:HB2	1:C:363:PHE:HB2	1.82	0.62
1:A:321:LYS:HZ2	1:A:380:ASN:HB2	1.64	0.61
1:A:368:ILE:HG12	1:A:381:MET:HE1	1.82	0.61
1:D:156:LYS:HB3	1:D:369:GLU:OE1	2.00	0.61
1:D:275:LEU:HD22	1:D:275:LEU:N	2.15	0.61
1:C:29:SER:O	1:C:33:ILE:HG22	2.00	0.61
1:B:314:VAL:HG13	1:B:368:ILE:HD13	1.82	0.61
1:C:71:ASN:OD1	1:C:73:ARG:HG3	2.01	0.60
1:B:106:ARG:HG3	1:B:119:TRP:CE3	2.35	0.60
1:B:71:ASN:OD1	1:B:73:ARG:HG2	2.01	0.60
1:A:383:LEU:HD12	1:A:384:GLN:H	1.67	0.60
1:D:114:ASN:OD1	1:D:231:LEU:HD11	2.02	0.60
1:D:127:VAL:HG13	1:D:190:PHE:HB2	1.83	0.60
1:B:302:THR:HG22	1:B:361:TRP:HB3	1.84	0.60
1:D:300:CYS:HB2	1:D:363:PHE:HB2	1.83	0.60
1:C:236:VAL:O	1:C:240:VAL:HG23	2.02	0.59
1:C:412:LEU:CD2	1:C:412:LEU:H	2.16	0.59
1:B:372:THR:HG22	1:B:383:LEU:HB2	1.84	0.59
1:B:83:LYS:O	1:B:87:GLU:HG2	2.03	0.59
1:B:338:VAL:O	1:B:341:VAL:HB	2.03	0.59
1:A:256:PHE:CZ	1:A:261:LYS:HB2	2.37	0.59
1:D:47:PRO:HB2	1:D:54:VAL:HG11	1.85	0.58
1:D:92:ALA:HB1	1:D:105:ILE:HD12	1.85	0.58
1:A:38:THR:CG2	1:A:41:GLU:H	2.14	0.58
1:A:274:TYR:CE1	1:A:311:ILE:HD13	2.39	0.58
1:B:89:LEU:HD22	1:B:246:ILE:HG13	1.86	0.58
1:A:66:GLU:O	1:A:67:ASP:HB2	2.04	0.58
1:D:232:ASP:O	1:D:236:VAL:HG23	2.04	0.58
1:A:368:ILE:HD12	1:A:368:ILE:N	2.18	0.58
1:C:65:ASP:OD1	1:C:73:ARG:NH1	2.37	0.58
1:A:51:ILE:HA	1:A:83:LYS:HD3	1.84	0.58
1:C:89:LEU:HD22	1:C:246:ILE:HG13	1.86	0.58
1:B:104:CYS:HG	1:B:256:PHE:HE1	1.51	0.58
1:B:106:ARG:HB2	1:B:119:TRP:HB3	1.86	0.57
1:A:51:ILE:CA	1:A:83:LYS:HD3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:NH1	1:A:318:ALA:HB2	2.19	0.57
1:A:323:GLY:O	1:A:326:VAL:HG12	2.04	0.57
1:B:189:MET:HE3	1:B:190:PHE:C	2.24	0.57
1:C:292:GLN:HG3	1:C:298:GLU:HG3	1.86	0.57
1:B:289:ILE:HG22	1:B:398:PHE:CE2	2.39	0.57
1:B:256:PHE:CE2	1:B:261:LYS:HB2	2.40	0.57
1:C:235:ILE:HG13	1:C:239:MET:CE	2.34	0.57
1:A:71:ASN:OD1	1:A:73:ARG:CG	2.53	0.56
1:A:172:ILE:HD13	1:A:198:MET:HB3	1.86	0.56
1:B:182:ALA:O	1:B:213:ASP:CB	2.50	0.56
1:A:300:CYS:HB2	1:A:363:PHE:HB2	1.87	0.56
1:C:235:ILE:O	1:C:239:MET:HG3	2.06	0.56
1:C:82:TYR:CD1	1:C:238:LEU:HD12	2.41	0.56
1:B:302:THR:CG2	1:B:361:TRP:HB3	2.35	0.56
1:B:66:GLU:O	1:B:67:ASP:HB2	2.04	0.56
1:D:117:SER:C	1:D:118:ILE:HD12	2.26	0.56
1:A:172:ILE:HD11	1:A:198:MET:CE	2.35	0.56
1:A:33:ILE:HG23	1:A:34:TYR:CD2	2.41	0.56
1:C:408:VAL:O	1:C:412:LEU:HD22	2.06	0.56
1:B:407:ILE:CG2	1:B:408:VAL:H	2.12	0.56
1:A:302:THR:HG23	1:A:361:TRP:HB3	1.88	0.56
1:A:302:THR:CG2	1:A:361:TRP:HB3	2.36	0.55
1:C:323:GLY:O	1:C:326:VAL:HG22	2.05	0.55
1:A:385:PRO:HA	1:A:388:PHE:CE2	2.42	0.55
1:B:47:PRO:O	1:B:49:THR:N	2.39	0.55
1:A:407:ILE:N	1:A:407:ILE:HD12	2.21	0.55
1:B:88:ILE:HB	1:B:118:ILE:HD12	1.89	0.55
1:D:373:PHE:CD2	1:D:378:LYS:HG2	2.41	0.55
1:B:376:GLN:HE21	1:B:376:GLN:HA	1.71	0.55
1:A:83:LYS:O	1:A:87:GLU:HG2	2.07	0.55
1:D:231:LEU:HD12	1:D:231:LEU:H	1.70	0.55
1:B:96:LYS:HE2	1:B:100:PRO:O	2.07	0.55
1:D:29:SER:HB3	1:D:32:ARG:HB3	1.89	0.55
1:A:104:CYS:H	1:A:121:ASN:ND2	2.04	0.55
1:A:172:ILE:HD13	1:A:198:MET:CB	2.37	0.54
1:D:91:ASN:O	1:D:94:ASP:HB2	2.05	0.54
1:A:337:LEU:CD1	1:A:356:VAL:HG11	2.37	0.54
1:B:89:LEU:CD2	1:B:246:ILE:HG13	2.37	0.54
1:A:176:LYS:HD3	1:A:220:GLN:HE21	1.71	0.54
1:A:59:GLN:HE21	1:A:61:MET:CE	2.20	0.54
1:A:400:LYS:O	1:A:403:ILE:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:THR:HG23	1:C:361:TRP:HB3	1.90	0.54
1:A:104:CYS:N	1:A:121:ASN:HD21	2.04	0.54
1:A:267:PHE:HB3	1:A:298:GLU:OE2	2.08	0.54
1:B:172:ILE:O	1:B:197:ASN:HB3	2.08	0.53
1:A:117:SER:C	1:A:118:ILE:HD12	2.29	0.53
1:C:59:GLN:HE21	1:C:61:MET:HE2	1.73	0.53
1:B:96:LYS:NZ	1:B:251:LYS:O	2.40	0.53
1:D:290:HIS:ND1	1:D:291:GLU:N	2.56	0.53
1:D:128:VAL:HG22	1:D:129:GLU:N	2.22	0.53
1:D:141:ILE:HD12	4:D:907:ADP:H1'	1.91	0.53
1:B:244:TYR:CZ	1:B:262:LEU:HD22	2.44	0.53
1:D:59:GLN:HE21	1:D:61:MET:CE	2.20	0.53
1:B:417:PHE:O	1:B:421:VAL:HG23	2.09	0.53
1:A:118:ILE:HD12	1:A:118:ILE:N	2.23	0.53
1:D:367:LEU:C	1:D:368:ILE:HD12	2.28	0.53
1:A:337:LEU:HD12	1:A:337:LEU:O	2.09	0.52
1:C:163:ASN:H	1:C:163:ASN:ND2	2.07	0.52
1:B:323:GLY:O	1:B:326:VAL:HG12	2.08	0.52
1:C:372:THR:HG23	1:C:382:THR:OG1	2.09	0.52
1:D:352:LYS:O	1:D:356:VAL:HG23	2.09	0.52
1:D:302:THR:HG23	1:D:361:TRP:HB3	1.91	0.52
1:D:257:LEU:HG	1:D:258:ASN:HD22	1.75	0.52
1:D:183:SER:HA	1:D:213:ASP:OD1	2.10	0.52
1:B:108:THR:HB	1:B:117:SER:OG	2.09	0.52
1:A:417:PHE:HD1	1:A:417:PHE:H	1.56	0.52
1:B:137:VAL:HB	1:B:138:PRO:HD3	1.92	0.51
1:C:385:PRO:HA	1:C:388:PHE:CZ	2.46	0.51
1:B:399:ILE:HG23	1:B:400:LYS:N	2.26	0.51
1:C:163:ASN:ND2	6:C:977:HOH:O	2.43	0.51
1:A:38:THR:HG22	1:A:41:GLU:HB2	1.93	0.51
1:A:70:ILE:O	1:A:70:ILE:HG13	2.10	0.51
1:C:40:LEU:HD13	1:C:172:ILE:HD12	1.91	0.51
1:A:176:LYS:HD3	1:A:220:GLN:NE2	2.26	0.51
1:C:302:THR:HG22	1:C:361:TRP:HB3	1.92	0.51
1:A:321:LYS:HZ2	1:A:380:ASN:HD22	1.59	0.50
1:D:290:HIS:CG	1:D:291:GLU:N	2.79	0.50
1:B:38:THR:HG22	1:B:41:GLU:N	2.11	0.50
1:A:400:LYS:O	1:A:402:ALA:N	2.45	0.50
1:C:412:LEU:HD23	1:C:412:LEU:H	1.76	0.50
1:A:128:VAL:HB	1:A:186:TYR:CD2	2.45	0.50
1:B:56:LEU:HD22	1:B:76:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:GLU:O	1:D:67:ASP:HB2	2.11	0.50
1:A:409:GLU:C	1:A:411:ILE:H	2.14	0.50
1:D:342:LYS:N	1:D:342:LYS:HD2	2.26	0.50
1:C:374:ASP:HB2	1:C:380:ASN:HB3	1.94	0.50
1:B:300:CYS:HB2	1:B:363:PHE:HB2	1.93	0.50
1:A:63:VAL:HG11	1:A:75:VAL:HG21	1.93	0.50
1:A:303:MET:HG3	1:A:407:ILE:HG13	1.94	0.50
1:C:338:VAL:HG21	1:C:353:ALA:HA	1.93	0.50
1:B:328:TYR:HE2	1:B:392:CYS:HB3	1.76	0.50
1:C:40:LEU:CD1	1:C:172:ILE:HD12	2.41	0.50
1:B:163:ASN:HB2	3:B:909:SO4:O2	2.11	0.50
1:C:128:VAL:HB	1:C:186:TYR:CD2	2.47	0.49
1:C:289:ILE:HD13	1:C:402:ALA:HA	1.92	0.49
1:A:357:LYS:HA	1:A:360:MET:SD	2.52	0.49
1:C:108:THR:HB	1:C:117:SER:OG	2.13	0.49
1:A:367:LEU:C	1:A:368:ILE:HD12	2.32	0.49
1:C:82:TYR:CE1	1:C:238:LEU:HD12	2.48	0.49
1:A:165:TYR:HB2	5:A:599:GOL:H11	1.95	0.49
1:C:337:LEU:HD23	1:C:403:ILE:HG22	1.94	0.49
1:A:38:THR:HG22	1:A:41:GLU:CB	2.43	0.49
1:C:329:VAL:HG12	1:C:362:ILE:HD11	1.93	0.49
1:B:394:LEU:HD23	1:B:398:PHE:CD1	2.48	0.49
1:A:321:LYS:NZ	1:A:380:ASN:HD22	2.10	0.49
1:B:88:ILE:HG21	1:B:217:ILE:CG1	2.43	0.49
1:A:400:LYS:C	1:A:402:ALA:N	2.66	0.49
1:A:128:VAL:O	1:A:137:VAL:HG23	2.13	0.49
1:D:60:GLN:HA	1:D:73:ARG:O	2.12	0.48
1:D:247:ALA:HA	1:D:255:VAL:HG21	1.94	0.48
1:D:130:HIS:HB3	1:D:133:GLU:HB2	1.96	0.48
1:D:102:MET:CE	1:D:105:ILE:HD11	2.44	0.48
1:C:129:GLU:HA	1:C:136:TYR:HA	1.95	0.48
1:D:51:ILE:HA	1:D:83:LYS:HD3	1.96	0.48
1:B:275:LEU:N	1:B:275:LEU:CD1	2.75	0.48
1:A:91:ASN:HB3	4:A:901:ADP:N7	2.28	0.48
1:C:274:TYR:CE1	1:C:311:ILE:HD13	2.48	0.48
1:A:383:LEU:HD12	1:A:384:GLN:N	2.29	0.48
1:A:62:TRP:O	1:A:241:ARG:HD3	2.14	0.47
1:B:374:ASP:HB3	1:B:382:THR:HG21	1.96	0.47
1:B:334:VAL:O	1:B:338:VAL:HG23	2.13	0.47
1:C:235:ILE:HG13	1:C:239:MET:HE2	1.96	0.47
1:C:373:PHE:CG	1:C:378:LYS:HG2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:GLY:C	1:D:408:VAL:H	2.17	0.47
1:A:129:GLU:HA	1:A:136:TYR:HA	1.96	0.47
1:C:38:THR:HG22	1:C:40:LEU:H	1.79	0.47
1:C:130:HIS:NE2	1:D:31:GLU:HA	2.29	0.47
1:B:408:VAL:HG23	1:B:409:GLU:N	2.29	0.47
1:A:137:VAL:HB	1:A:138:PRO:HD3	1.96	0.47
1:C:383:LEU:HD11	1:C:387:SER:HB2	1.97	0.47
1:D:43:ILE:HA	1:D:50:TYR:CE2	2.49	0.47
1:D:110:ASP:OD1	1:D:113:ASN:ND2	2.45	0.47
1:C:44:LEU:HD21	1:C:172:ILE:HG22	1.97	0.47
1:A:292:GLN:HA	1:A:298:GLU:HG3	1.95	0.47
1:D:294:ASN:OD1	1:D:296:ARG:N	2.45	0.47
1:B:57:VAL:O	1:B:76:THR:HA	2.15	0.47
1:D:330:ALA:O	1:D:334:VAL:HG23	2.15	0.47
1:C:115:LEU:HD13	1:C:116:ILE:N	2.30	0.47
1:B:372:THR:HG23	1:B:382:THR:OG1	2.15	0.47
1:A:70:ILE:HG21	1:A:273:MET:HB3	1.97	0.47
1:C:359:HIS:HB2	1:C:407:ILE:HD13	1.96	0.47
1:C:116:ILE:HD11	1:C:231:LEU:HD21	1.96	0.46
1:D:261:LYS:HG2	1:D:262:LEU:N	2.30	0.46
1:A:57:VAL:O	1:A:76:THR:HA	2.15	0.46
1:D:362:ILE:HG12	1:D:364:VAL:HG23	1.96	0.46
1:A:48:ASP:HA	1:A:52:GLY:O	2.15	0.46
1:D:377:THR:OG1	1:D:379:GLU:HG3	2.16	0.46
1:A:60:GLN:HA	1:A:73:ARG:O	2.16	0.46
1:B:149:SER:O	1:B:157:LYS:NZ	2.48	0.46
1:B:322:GLY:O	1:B:380:ASN:HA	2.16	0.46
1:D:267:PHE:HB3	1:D:298:GLU:OE2	2.15	0.46
1:A:58:THR:HA	1:A:75:VAL:O	2.16	0.46
1:C:75:VAL:HG13	1:C:234:ASP:HB3	1.98	0.46
1:D:223:LEU:HD13	1:D:230:SER:HA	1.97	0.46
1:D:63:VAL:HG12	1:D:238:LEU:HD22	1.97	0.46
1:A:43:ILE:HA	1:A:50:TYR:CE2	2.51	0.46
1:D:163:ASN:HB2	3:D:908:SO4:O1	2.16	0.46
1:B:70:ILE:HG23	1:B:70:ILE:O	2.16	0.46
1:B:88:ILE:CG2	1:B:217:ILE:HG12	2.47	0.46
1:C:292:GLN:HA	1:C:298:GLU:HG3	1.98	0.45
1:A:40:LEU:HD13	1:A:172:ILE:HD12	1.99	0.45
1:C:235:ILE:HG13	1:C:239:MET:HE3	1.96	0.45
1:B:177:PHE:CE1	1:B:217:ILE:HD13	2.51	0.45
1:A:141:ILE:HD12	4:A:901:ADP:HI'	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:VAL:CG1	1:C:350:ALA:N	2.78	0.45
1:D:274:TYR:C	1:D:275:LEU:HD13	2.37	0.45
1:A:256:PHE:CE2	1:A:261:LYS:HB2	2.51	0.45
1:B:64:TYR:HE2	1:B:273:MET:CE	2.28	0.45
1:A:301:LEU:HD12	1:A:302:THR:H	1.82	0.45
1:B:368:ILE:HD12	1:B:368:ILE:N	2.31	0.45
1:C:31:GLU:HA	1:D:130:HIS:CE1	2.52	0.45
1:D:103:SER:H	1:D:121:ASN:HD21	1.64	0.45
1:B:110:ASP:CG	1:B:113:ASN:HD22	2.19	0.45
1:A:290:HIS:CG	1:A:291:GLU:N	2.85	0.45
1:B:394:LEU:HD23	1:B:398:PHE:CE1	2.52	0.45
1:B:194:TRP:CD1	1:B:201:ALA:HB2	2.52	0.45
1:A:110:ASP:C	1:A:110:ASP:OD2	2.55	0.45
1:A:232:ASP:O	1:A:236:VAL:HG23	2.17	0.45
1:C:65:ASP:CG	1:C:73:ARG:HH11	2.20	0.45
1:A:415:VAL:HA	1:A:417:PHE:CE1	2.51	0.45
1:B:274:TYR:C	1:B:275:LEU:HD12	2.37	0.45
1:C:96:LYS:NZ	1:C:102:MET:O	2.50	0.45
1:B:92:ALA:HB1	1:B:105:ILE:HD12	1.97	0.45
1:D:406:GLY:C	1:D:408:VAL:N	2.71	0.45
1:D:57:VAL:O	1:D:76:THR:HA	2.17	0.45
1:C:59:GLN:NE2	1:C:61:MET:CE	2.80	0.45
1:A:51:ILE:HA	1:A:83:LYS:CD	2.47	0.45
1:C:338:VAL:HG22	1:C:356:VAL:HG21	1.99	0.44
1:D:73:ARG:HB3	1:D:74:GLU:H	1.52	0.44
1:B:225:LYS:HB3	1:B:225:LYS:HE3	1.80	0.44
1:A:337:LEU:HD13	1:A:356:VAL:HG11	1.99	0.44
1:A:311:ILE:HD12	1:A:363:PHE:CE2	2.52	0.44
1:D:304:SER:HB2	1:D:361:TRP:HB2	2.00	0.44
1:A:62:TRP:HE3	1:A:70:ILE:CD1	2.30	0.44
1:C:59:GLN:CG	1:C:61:MET:HE3	2.48	0.44
1:C:58:THR:HA	1:C:75:VAL:O	2.17	0.44
1:A:312:SER:HA	1:A:364:VAL:O	2.17	0.44
1:B:353:ALA:C	1:B:355:GLN:N	2.71	0.44
1:B:52:GLY:HA3	6:B:937:HOH:O	2.18	0.44
1:D:223:LEU:CD1	1:D:230:SER:HA	2.48	0.44
1:D:251:LYS:O	1:D:253:VAL:HG23	2.17	0.44
1:C:62:TRP:O	1:C:241:ARG:HD3	2.18	0.44
1:A:46:ARG:N	1:A:47:PRO:HD3	2.33	0.44
1:D:206:LEU:C	1:D:207:LYS:HG3	2.38	0.44
1:A:267:PHE:O	1:A:270:TYR:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:GLU:HB2	1:C:388:PHE:O	2.18	0.44
1:B:235:ILE:O	1:B:239:MET:HG3	2.18	0.43
1:A:33:ILE:O	1:B:149:SER:HA	2.19	0.43
1:C:33:ILE:HG23	1:C:34:TYR:HD2	1.83	0.43
1:B:236:VAL:O	1:B:240:VAL:HG23	2.17	0.43
1:A:103:SER:OG	1:A:121:ASN:ND2	2.51	0.43
1:B:290:HIS:ND1	1:B:291:GLU:N	2.66	0.43
1:A:31:GLU:OE1	1:B:131:LYS:N	2.50	0.43
1:A:321:LYS:HZ2	1:A:321:LYS:HB2	1.83	0.43
1:C:33:ILE:O	1:D:149:SER:HA	2.19	0.43
4:D:907:ADP:H5'1	4:D:907:ADP:PB	2.59	0.43
1:C:57:VAL:HG22	1:C:77:PHE:O	2.18	0.43
1:C:409:GLU:O	1:C:412:LEU:HD23	2.18	0.43
1:D:66:GLU:O	1:D:67:ASP:CB	2.66	0.43
1:D:242:ARG:O	1:D:245:ASP:HB2	2.18	0.43
1:A:194:TRP:CD1	1:A:201:ALA:HB2	2.53	0.43
1:B:385:PRO:HA	1:B:388:PHE:CD2	2.53	0.43
1:A:158:VAL:C	1:A:315:ASN:ND2	2.71	0.43
1:C:51:ILE:HA	1:C:83:LYS:HD3	1.99	0.43
1:D:47:PRO:CB	1:D:54:VAL:HG11	2.47	0.43
1:B:168:LYS:N	1:B:168:LYS:HD3	2.33	0.43
1:B:109:ILE:HG23	1:B:116:ILE:CD1	2.49	0.43
1:C:409:GLU:HA	1:C:412:LEU:HD21	2.00	0.43
1:A:51:ILE:HA	1:A:83:LYS:HE2	2.01	0.43
1:B:189:MET:HG2	1:B:190:PHE:N	2.34	0.43
1:D:83:LYS:O	1:D:87:GLU:HG2	2.18	0.43
1:C:65:ASP:HB2	1:C:68:VAL:HB	2.00	0.43
1:D:244:TYR:HA	1:D:247:ALA:HB3	2.01	0.43
1:C:115:LEU:HD11	1:C:218:THR:HG23	2.00	0.43
1:A:96:LYS:HE3	1:A:251:LYS:O	2.19	0.43
1:D:368:ILE:CD1	1:D:368:ILE:N	2.80	0.43
1:B:64:TYR:HE2	1:B:273:MET:HE1	1.83	0.43
1:C:137:VAL:HB	1:C:138:PRO:HD3	2.01	0.43
1:B:328:TYR:CE2	1:B:392:CYS:HB3	2.54	0.42
1:C:106:ARG:HB2	1:C:119:TRP:HB3	2.00	0.42
1:B:128:VAL:HG22	1:B:129:GLU:N	2.32	0.42
1:A:75:VAL:HG13	1:A:234:ASP:HB3	2.00	0.42
1:A:172:ILE:HD11	1:A:198:MET:HE2	2.01	0.42
1:C:30:VAL:HA	1:C:33:ILE:HG22	2.01	0.42
1:D:178:THR:HG23	1:D:193:THR:OG1	2.19	0.42
1:A:315:ASN:O	1:A:316:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:ILE:HG13	1:D:404:GLY:N	2.35	0.42
1:A:409:GLU:HG3	1:A:409:GLU:O	2.19	0.42
1:D:242:ARG:HD2	1:D:245:ASP:OD1	2.19	0.42
1:B:385:PRO:HA	1:B:388:PHE:CG	2.54	0.42
1:B:376:GLN:CA	1:B:376:GLN:HE21	2.31	0.42
1:D:242:ARG:NH1	1:D:318:ALA:HB2	2.35	0.42
1:D:175:THR:O	1:D:196:ASP:N	2.36	0.42
1:C:242:ARG:O	1:C:246:ILE:HG12	2.20	0.42
1:D:56:LEU:HD22	1:D:76:THR:CG2	2.45	0.42
1:B:222:ASP:OD1	1:B:225:LYS:HG2	2.20	0.42
1:B:47:PRO:O	1:B:48:ASP:C	2.58	0.42
1:A:40:LEU:HD11	1:A:172:ILE:HD12	2.02	0.42
1:C:59:GLN:NE2	1:C:61:MET:HE2	2.33	0.42
1:B:43:ILE:HA	1:B:50:TYR:CE2	2.54	0.42
1:D:240:VAL:HG13	1:D:257:LEU:CD2	2.50	0.42
1:C:38:THR:HG22	1:C:40:LEU:N	2.34	0.42
1:B:242:ARG:HA	1:B:242:ARG:HD2	1.84	0.42
1:A:415:VAL:C	1:A:417:PHE:H	2.22	0.42
1:A:33:ILE:HG23	1:A:34:TYR:N	2.34	0.41
1:D:102:MET:HE3	1:D:105:ILE:HD11	2.01	0.41
1:A:51:ILE:HA	1:A:83:LYS:CE	2.50	0.41
1:D:373:PHE:CG	1:D:378:LYS:HG2	2.55	0.41
1:A:141:ILE:HD12	4:A:901:ADP:C1'	2.50	0.41
1:C:317:ILE:HD13	1:C:378:LYS:HD2	2.02	0.41
1:C:349:VAL:HG12	1:C:350:ALA:N	2.35	0.41
1:D:373:PHE:HB3	1:D:378:LYS:HA	2.02	0.41
1:B:102:MET:CE	1:B:105:ILE:HD11	2.50	0.41
1:A:290:HIS:ND1	1:A:290:HIS:C	2.74	0.41
1:C:43:ILE:HA	1:C:50:TYR:CE2	2.55	0.41
1:D:64:TYR:CE1	1:D:69:GLY:HA2	2.56	0.41
1:D:231:LEU:CD1	1:D:231:LEU:N	2.78	0.41
1:B:51:ILE:CA	1:B:83:LYS:HD3	2.49	0.41
1:C:128:VAL:HG22	1:C:129:GLU:N	2.35	0.41
1:D:296:ARG:O	1:D:366:ALA:HA	2.21	0.41
1:B:324:ARG:NH1	6:B:946:HOH:O	2.53	0.41
1:A:73:ARG:NH2	1:A:234:ASP:OD2	2.45	0.41
1:A:38:THR:HG22	1:A:41:GLU:HG3	2.00	0.41
1:A:414:TRP:O	1:A:417:PHE:CD1	2.73	0.41
1:D:118:ILE:HD12	1:D:118:ILE:N	2.35	0.41
1:A:321:LYS:HZ1	1:A:380:ASN:HB2	1.84	0.41
1:D:125:ILE:HG21	1:D:141:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ASN:HB3	1:D:102:MET:SD	2.61	0.41
1:B:332:GLN:OE1	1:B:394:LEU:HD13	2.20	0.41
1:D:137:VAL:O	1:D:141:ILE:HG12	2.20	0.41
1:C:407:ILE:HG13	1:C:408:VAL:N	2.35	0.41
1:A:309:GLN:O	1:A:361:TRP:HA	2.20	0.41
1:A:385:PRO:HA	1:A:388:PHE:CD2	2.56	0.41
1:C:385:PRO:HA	1:C:388:PHE:CE1	2.55	0.41
1:A:409:GLU:C	1:A:411:ILE:N	2.73	0.41
1:C:51:ILE:O	1:C:80:GLY:HA2	2.21	0.41
1:A:334:VAL:O	1:A:335:THR:C	2.58	0.41
1:C:425:LYS:O	1:C:426:LYS:CB	2.67	0.41
1:B:323:GLY:O	1:B:326:VAL:CG1	2.69	0.41
1:D:242:ARG:HD2	1:D:242:ARG:HA	1.86	0.41
1:D:69:GLY:O	1:D:71:ASN:ND2	2.54	0.41
1:B:37:LYS:HA	1:B:37:LYS:HD2	1.89	0.41
1:D:75:VAL:HG12	1:D:76:THR:N	2.35	0.40
1:D:128:VAL:CG2	1:D:129:GLU:N	2.84	0.40
1:D:406:GLY:O	1:D:408:VAL:N	2.54	0.40
1:B:142:PHE:CG	1:B:179:VAL:HG21	2.56	0.40
1:D:231:LEU:H	1:D:231:LEU:CD1	2.33	0.40
1:A:410:SER:O	1:A:414:TRP:N	2.41	0.40
1:B:127:VAL:HG12	1:B:127:VAL:O	2.22	0.40
1:C:64:TYR:HE2	1:C:273:MET:CE	2.35	0.40
1:B:190:PHE:CD2	1:B:191:LYS:N	2.89	0.40
1:C:190:PHE:CD2	1:C:190:PHE:C	2.95	0.40
1:C:127:VAL:CG1	1:C:127:VAL:O	2.64	0.40
1:B:106:ARG:HG3	1:B:119:TRP:HE3	1.82	0.40
1:C:45:LEU:C	1:C:47:PRO:HD3	2.41	0.40
1:A:82:TYR:C	1:A:82:TYR:CD2	2.93	0.40
1:C:172:ILE:O	1:C:197:ASN:HB3	2.21	0.40
1:C:400:LYS:O	1:C:403:ILE:HG12	2.21	0.40
1:D:242:ARG:O	1:D:246:ILE:HG12	2.22	0.40
1:B:369:GLU:HG3	1:B:388:PHE:O	2.21	0.40
1:A:127:VAL:HG12	1:A:127:VAL:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	358/400 (90%)	316 (88%)	34 (10%)	8 (2%)	8	13
1	B	373/400 (93%)	343 (92%)	25 (7%)	5 (1%)	15	26
1	C	378/400 (94%)	361 (96%)	14 (4%)	3 (1%)	24	41
1	D	361/400 (90%)	325 (90%)	32 (9%)	4 (1%)	17	31
All	All	1470/1600 (92%)	1345 (92%)	105 (7%)	20 (1%)	14	24

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	GLY
1	A	334	VAL
1	A	401	ALA
1	B	48	ASP
1	B	162	ARG
1	B	166	GLY
1	C	166	GLY
1	A	374	ASP
1	A	378	LYS
1	D	196	ASP
1	A	162	ARG
1	B	210	ASN
1	C	196	ASP
1	D	341	VAL
1	A	291	GLU
1	A	330	ALA
1	D	158	VAL
1	B	47	PRO
1	C	127	VAL
1	D	407	ILE

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	271/358 (76%)	265 (98%)	6 (2%)	60	84
1	B	297/358 (83%)	281 (95%)	16 (5%)	27	49
1	C	295/358 (82%)	286 (97%)	9 (3%)	47	75
1	D	272/358 (76%)	264 (97%)	8 (3%)	50	77
All	All	1135/1432 (79%)	1096 (97%)	39 (3%)	44	72

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	70	ILE
1	A	89	LEU
1	A	104	CYS
1	A	158	VAL
1	A	417	PHE
1	B	32	ARG
1	B	38	THR
1	B	71	ASN
1	B	73	ARG
1	B	89	LEU
1	B	189	MET
1	B	216	CYS
1	B	217	ILE
1	B	235	ILE
1	B	275	LEU
1	B	276	LYS
1	B	295	HIS
1	B	339	ASP
1	B	340	VAL
1	B	384	GLN
1	B	399	ILE
1	C	31	GLU
1	C	89	LEU

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Mol	Chain	Res	Type
1	C	163	ASN
1	C	213	ASP
1	C	231	LEU
1	C	238	LEU
1	C	275	LEU
1	C	407	ILE
1	C	412	LEU
1	D	31	GLU
1	D	165	TYR
1	D	189	MET
1	D	195	MET
1	D	214	TYR
1	D	238	LEU
1	D	275	LEU
1	D	384	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	97	GLN
1	A	144	GLN
1	A	150	ASN
1	A	220	GLN
1	A	380	ASN
1	B	97	GLN
1	B	113	ASN
1	B	144	GLN
1	B	376	GLN
1	C	59	GLN
1	C	97	GLN
1	C	144	GLN
1	C	358	ASN
1	C	413	ASN
1	C	424	ASN
1	D	59	GLN
1	D	91	ASN
1	D	144	GLN
1	D	258	ASN
1	D	384	GLN

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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	GOL	A	599	-	5,5,5	1.27	0	5,5,5	0.67	0
4	ADP	A	901	2	22,29,29	1.34	2 (9%)	27,45,45	1.96	3 (11%)
4	ADP	B	903	2	22,29,29	1.21	1 (4%)	27,45,45	1.97	3 (11%)
3	SO4	B	909	-	4,4,4	0.29	0	6,6,6	0.16	0
4	ADP	C	905	2	22,29,29	1.25	2 (9%)	27,45,45	1.89	3 (11%)
4	ADP	D	907	2	22,29,29	1.25	2 (9%)	27,45,45	1.99	3 (11%)
3	SO4	D	908	-	4,4,4	0.18	0	6,6,6	0.12	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	599	-	-	0/4/4/4	0/0/0/0
4	ADP	A	901	2	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	B	903	2	-	0/12/32/32	0/3/3/3
3	SO4	B	909	-	-	0/0/0/0	0/0/0/0
4	ADP	C	905	2	-	0/12/32/32	0/3/3/3
4	ADP	D	907	2	-	0/12/32/32	0/3/3/3
3	SO4	D	908	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	905	ADP	C6-N6	-2.02	1.28	1.34
4	A	901	ADP	O4'-C1'	2.12	1.43	1.41
4	D	907	ADP	O4'-C1'	2.49	1.44	1.41
4	B	903	ADP	C2-N1	3.55	1.40	1.33
4	D	907	ADP	C2-N1	3.67	1.40	1.33
4	C	905	ADP	C2-N1	3.85	1.41	1.33
4	A	901	ADP	C2-N1	4.08	1.41	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	907	ADP	N3-C2-N1	-8.18	122.63	128.89
4	B	903	ADP	N3-C2-N1	-8.13	122.67	128.89
4	A	901	ADP	N3-C2-N1	-8.12	122.68	128.89
4	C	905	ADP	N3-C2-N1	-7.81	122.92	128.89
4	A	901	ADP	C4'-O4'-C1'	2.27	112.21	109.72
4	C	905	ADP	C4'-O4'-C1'	2.31	112.26	109.72
4	B	903	ADP	C4'-O4'-C1'	2.36	112.31	109.72
4	D	907	ADP	C4'-O4'-C1'	2.39	112.34	109.72
4	A	901	ADP	C2-N1-C6	2.81	123.78	118.77
4	D	907	ADP	C2-N1-C6	2.84	123.83	118.77
4	C	905	ADP	C2-N1-C6	2.86	123.87	118.77
4	B	903	ADP	C2-N1-C6	3.09	124.28	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	599	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	ADP	3	0
3	B	909	SO4	1	0
4	D	907	ADP	2	0
3	D	908	SO4	1	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	366/400 (91%)	0.21	15 (4%) 41 46	20, 57, 84, 95	0
1	B	379/400 (94%)	0.13	12 (3%) 51 56	26, 51, 76, 94	0
1	C	384/400 (96%)	-0.07	5 (1%) 79 82	32, 52, 67, 83	0
1	D	371/400 (92%)	0.34	18 (4%) 33 38	46, 68, 89, 103	0
All	All	1500/1600 (93%)	0.15	50 (3%) 50 55	20, 57, 83, 103	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	211	GLY	5.0
1	B	341	VAL	3.9
1	A	210	ASN	3.6
1	B	375	SER	3.5
1	D	341	VAL	3.4
1	A	373	PHE	3.4
1	D	337	LEU	3.3
1	B	411	ILE	3.3
1	A	417	PHE	3.3
1	D	340	VAL	3.0
1	A	407	ILE	3.0
1	D	209	PHE	2.9
1	B	414	TRP	2.9
1	D	359	HIS	2.9
1	A	266	GLY	2.9
1	A	211	GLY	2.9
1	D	256	PHE	2.8
1	D	405	CYS	2.8
1	B	412	LEU	2.7
1	A	359	HIS	2.7
1	A	410	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	338	VAL	2.6
1	B	68	VAL	2.6
1	D	374	ASP	2.6
1	B	376	GLN	2.6
1	D	32	ARG	2.5
1	D	414	TRP	2.5
1	C	49	THR	2.5
1	D	392	CYS	2.5
1	B	399	ILE	2.5
1	D	377	THR	2.5
1	A	408	VAL	2.4
1	C	419	ALA	2.4
1	C	29	SER	2.4
1	D	383	LEU	2.3
1	B	420	GLN	2.3
1	A	375	SER	2.3
1	D	328	TYR	2.3
1	B	407	ILE	2.3
1	A	260	ASN	2.2
1	A	377	THR	2.2
1	A	299	VAL	2.2
1	A	395	SER	2.2
1	D	288	VAL	2.1
1	C	295	HIS	2.1
1	A	182	ALA	2.1
1	D	297	TRP	2.1
1	B	340	VAL	2.0
1	C	375	SER	2.0
1	D	67	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 ⓘ

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(Å ²)	Q<0.9
5	GOL	A	599	6/6	0.85	0.35	3.94	56,59,60,61	0
4	ADP	A	901	27/27	0.95	0.19	1.34	37,52,57,57	0
4	ADP	C	905	27/27	0.95	0.20	1.18	42,52,57,57	0
4	ADP	B	903	27/27	0.95	0.21	1.12	28,32,57,57	0
2	MG	A	900	1/1	0.98	0.16	0.87	33,33,33,33	0
2	MG	D	906	1/1	0.97	0.23	0.69	42,42,42,42	0
4	ADP	D	907	27/27	0.95	0.22	0.67	52,57,62,63	0
3	SO4	B	909	5/5	0.93	0.18	-0.35	85,86,87,89	0
3	SO4	D	908	5/5	0.96	0.20	-0.57	103,103,103,104	0
2	MG	B	902	1/1	0.95	0.17	-0.71	36,36,36,36	0
2	MG	C	904	1/1	0.95	0.16	-	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.