Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 04:20 PM EDT

PDB ID	:	6P4W
Title	:	XPB helicase in a complex with truncated Bax1 from Sulfurisphaera tokodaii at 2.96 Angstrom resolution
Authors	:	Fan, L.; He, F.; DuPrez, K.T.
Deposited on	:	2019-05-28
Resolution	:	2.96 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

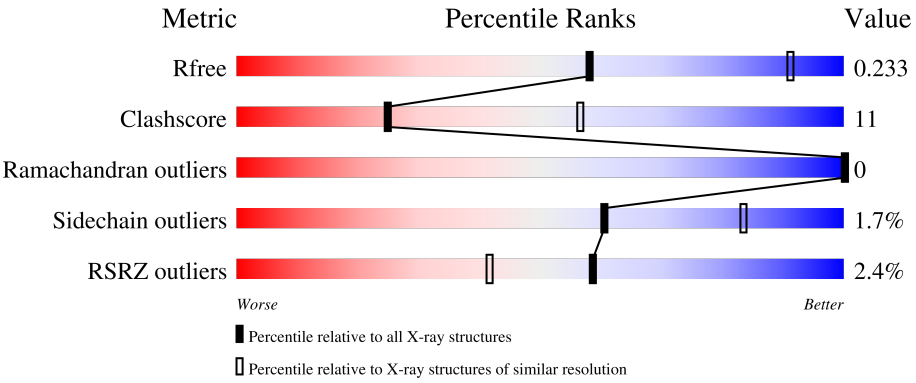
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	440	82% 16%
1	C	440	78% 20%
2	B	374	3% 71% 28%
2	D	374	6% 72% 28%

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
6	CL	C	505	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13068 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-dependent ATPase XPBII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3468	2250	578	636	4			
1	C	435	Total	C	N	O	S	0	1	0
			3485	2262	580	639	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q970I2
A	1	SER	-	expression tag	UNP Q970I2
C	0	GLY	-	expression tag	UNP Q970I2
C	1	SER	-	expression tag	UNP Q970I2

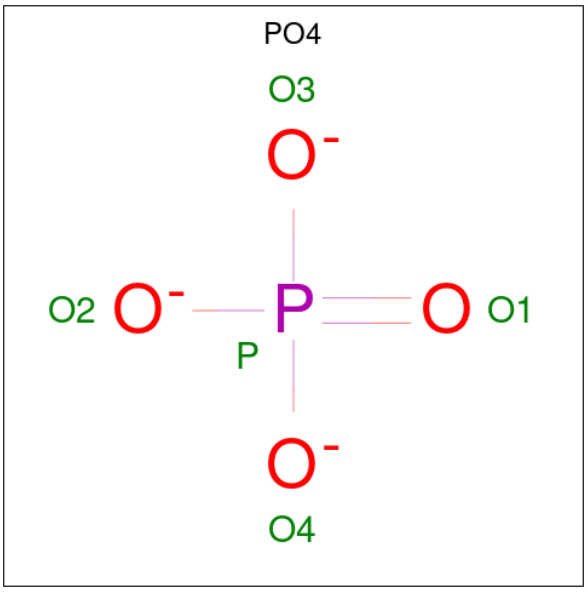
- Molecule 2 is a protein called Endonuclease Bax1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	374	Total	C	N	O	S	0	1	0
			3028	2004	480	540	4			
2	D	373	Total	C	N	O	S	0	1	0
			2949	1950	474	522	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP Q970I1
B	1	GLY	-	expression tag	UNP Q970I1
D	0	MET	-	expression tag	UNP Q970I1
D	1	GLY	-	expression tag	UNP Q970I1

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

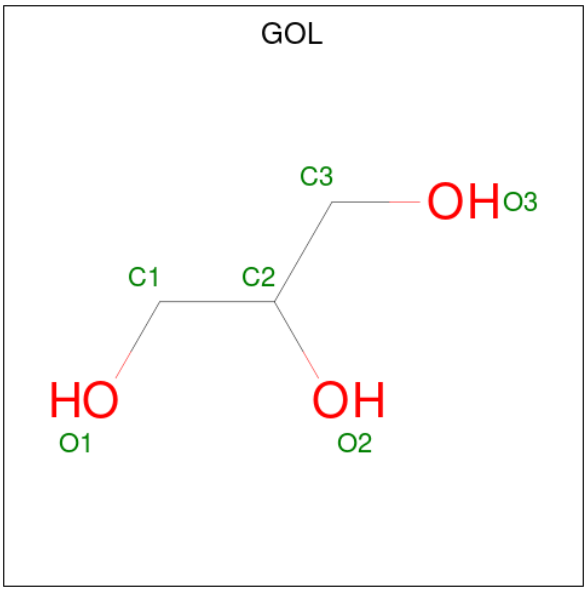


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- 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 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total Cl 8 8	0	0
6	B	2	Total Cl 2 2	0	0
6	C	7	Total Cl 7 7	0	0
6	D	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	32	Total O 32 32	0	0
7	B	27	Total O 27 27	0	0
7	C	26	Total O 26 26	0	0

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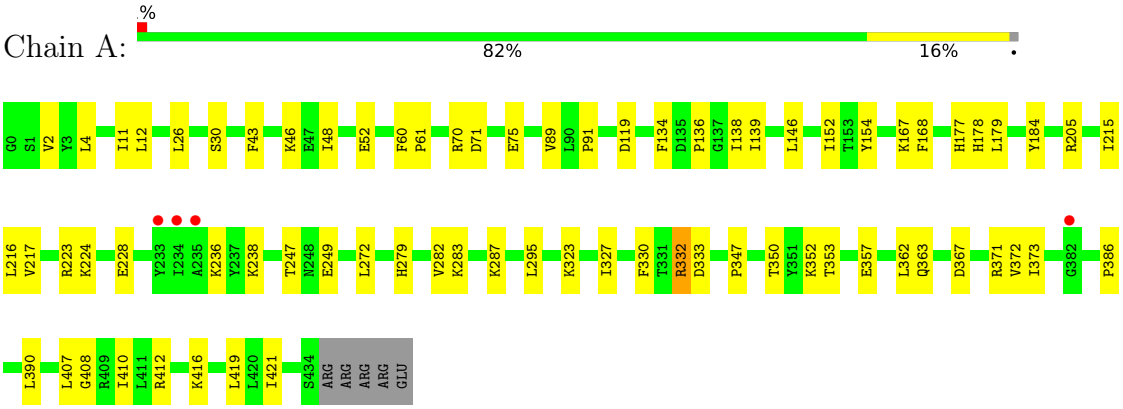
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	11	Total	O	0	0
			11	11		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

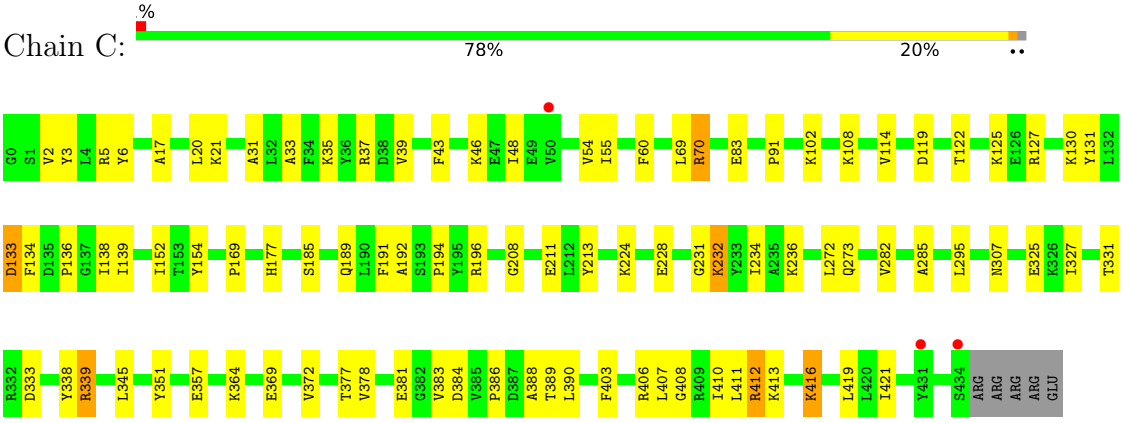
• Molecule 1: DNA-dependent ATPase XPBII

Chain A:



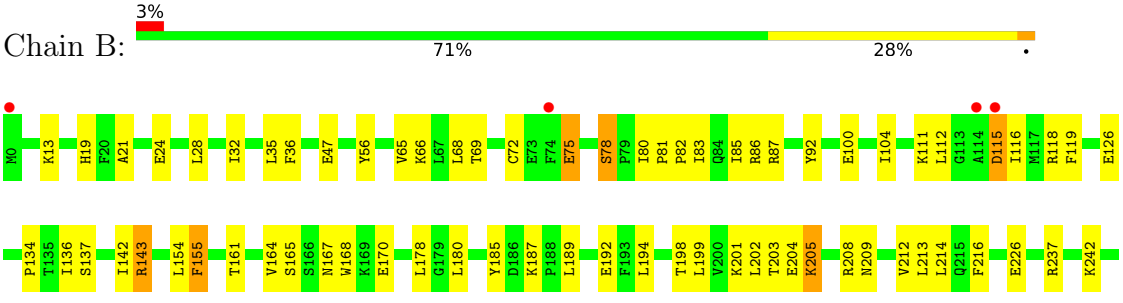
• Molecule 1: DNA-dependent ATPase XPBII

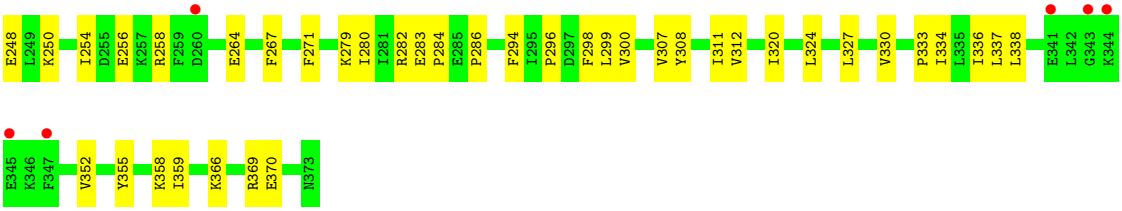
Chain C:



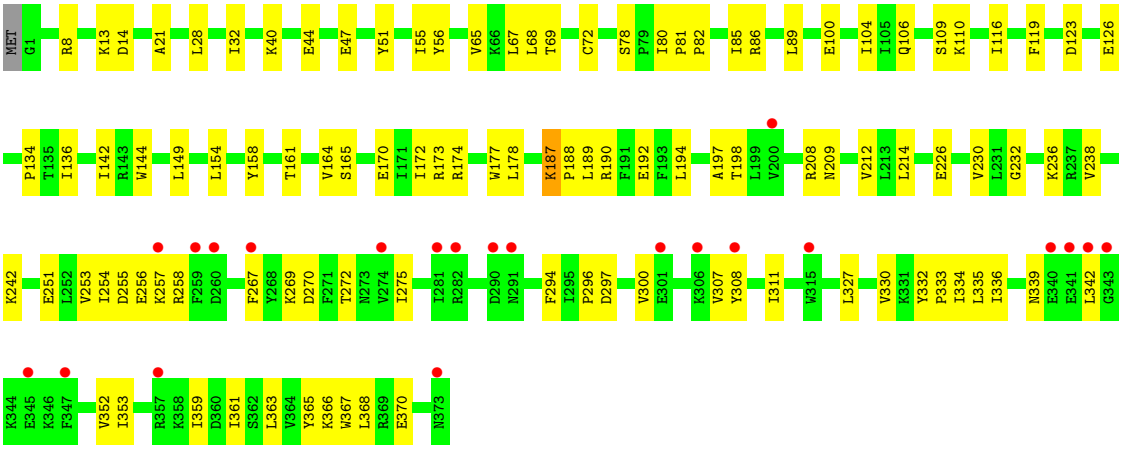
• Molecule 2: Endonuclease Bax1

Chain B:





• Molecule 2: Endonuclease Bax1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.41Å 101.37Å 114.48Å 83.09° 81.15° 90.17°	Depositor
Resolution (Å)	29.28 – 2.96 29.26 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.28-2.96) 98.4 (29.26-2.96)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.183 , 0.233 0.183 , 0.233	Depositor DCC
R_{free} test set	2513 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	75.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13068	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, MG, CL

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	0.47	0/3532	0.64	0/4766
1	C	0.53	0/3552	0.71	4/4792 (0.1%)
2	B	0.52	0/3097	0.68	0/4198
2	D	0.48	0/3018	0.67	1/4094 (0.0%)
All	All	0.50	0/13199	0.68	5/17850 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	413	LYS	CD-CE-NZ	-8.21	92.81	111.70
2	D	368	LEU	CA-CB-CG	6.87	131.11	115.30
1	C	413	LYS	CA-CB-CG	6.17	126.97	113.40
1	C	339	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	133	ASP	CB-CG-OD1	-5.36	113.48	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	187	LYS	Peptide
2	D	187	LYS	Peptide

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	3468	0	3556	49	1
1	C	3485	0	3591	74	0
2	B	3028	0	3000	83	0
2	D	2949	0	2894	87	1
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	6	0	8	1	0
5	C	6	0	8	1	0
6	A	8	0	0	0	0
6	B	2	0	0	0	0
6	C	7	0	0	2	0
6	D	1	0	0	0	0
7	A	32	0	0	2	0
7	B	27	0	0	2	0
7	C	26	0	0	5	0
7	D	11	0	0	0	0
All	All	13068	0	13057	282	1

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 11.

All (282) 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:C:70:ARG:NH2	1:C:412:ARG:CD	1.72	1.52
1:C:70:ARG:NH2	1:C:412:ARG:HD2	0.84	1.16
2:D:254:ILE:HD12	2:D:255:ASP:N	1.60	1.14
2:B:115:ASP:OD1	2:B:118:ARG:HB2	1.56	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:LYS:HD2	1:C:369:GLU:OE1	1.59	0.99
1:C:236[B]:LYS:HE2	1:C:412:ARG:HA	1.43	0.96
2:B:201:LYS:HB3	2:B:202:LEU:HD22	1.48	0.95
2:B:13:LYS:NZ	7:B:501:HOH:O	1.99	0.92
2:D:254:ILE:HD12	2:D:255:ASP:H	1.19	0.92
2:B:205:LYS:H	2:B:205:LYS:HD2	1.36	0.90
1:C:364:LYS:HD2	1:C:369:GLU:CD	1.91	0.89
2:B:178:LEU:HD23	2:B:209:ASN:HB3	1.55	0.86
1:C:295:LEU:HD23	2:D:55:ILE:HD11	1.58	0.84
2:D:254:ILE:HD13	2:D:256:GLU:H	1.42	0.81
2:B:194:LEU:HB3	2:B:198:THR:HG21	1.64	0.79
2:D:109:SER:HB3	2:D:116:ILE:HG12	1.65	0.78
1:C:351:TYR:HB3	1:C:381:GLU:HG2	1.66	0.77
1:C:70:ARG:NH2	1:C:412:ARG:CG	2.47	0.75
2:D:194:LEU:HB3	2:D:198:THR:HG21	1.67	0.75
2:D:254:ILE:CD1	2:D:255:ASP:N	2.46	0.74
1:C:364:LYS:HB3	1:C:369:GLU:HG3	1.67	0.74
2:B:85:ILE:HG23	2:B:116:ILE:HG23	1.68	0.74
1:C:17:ALA:HB3	1:C:20:LEU:HD22	1.69	0.73
1:C:282:VAL:HG13	2:D:55:ILE:HD13	1.70	0.73
2:B:264:GLU:HG3	2:B:311:ILE:HD12	1.69	0.73
2:B:327:LEU:O	2:B:330:VAL:HG12	1.89	0.73
2:D:256:GLU:OE2	2:D:257:LYS:N	2.21	0.72
2:B:254:ILE:HD12	2:B:256:GLU:H	1.53	0.72
2:D:230:VAL:HG12	2:D:238:VAL:HG22	1.71	0.71
1:C:70:ARG:NH2	1:C:412:ARG:HH11	1.89	0.70
2:D:294:PHE:CE2	2:D:296:PRO:HG3	2.28	0.69
2:D:251:GLU:OE2	2:D:253:VAL:HG12	1.93	0.68
2:D:335:LEU:HD11	2:D:353:ILE:HG12	1.76	0.68
2:B:115:ASP:OD1	2:B:118:ARG:CB	2.40	0.67
2:B:83:ILE:O	2:B:87:ARG:HG3	1.95	0.67
2:B:366:LYS:O	2:B:370:GLU:HG3	1.95	0.67
2:D:300:VAL:CG2	2:D:307:VAL:HG12	2.25	0.67
2:D:161:THR:HG23	2:D:192:GLU:HG2	1.77	0.67
2:D:154:LEU:HD12	2:D:214:LEU:HD11	1.77	0.66
2:D:21:ALA:HB3	2:D:142:ILE:HG23	1.78	0.66
1:C:232:LYS:H	1:C:232:LYS:HD2	1.62	0.65
2:B:337:LEU:HD13	2:B:359:ILE:HD13	1.77	0.65
1:A:247:THR:HG22	1:A:249:GLU:H	1.62	0.65
1:C:364:LYS:HB3	1:C:369:GLU:CG	2.27	0.64
2:B:312:VAL:HG21	2:B:338:LEU:HD23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:PHE:CD1	2:B:280:ILE:HD12	2.34	0.62
1:C:2:VAL:HG11	1:C:43:PHE:CE2	2.34	0.62
2:D:173:ARG:HD2	2:D:177:TRP:CZ2	2.34	0.62
2:D:187:LYS:HE3	2:D:190:ARG:HH22	1.63	0.62
1:A:347:PRO:HB2	1:A:373:ILE:HG22	1.82	0.62
2:B:85:ILE:CG2	2:B:116:ILE:HG23	2.30	0.62
2:B:164:VAL:HG21	2:B:189:LEU:HD23	1.80	0.62
2:B:80:ILE:HD12	2:B:81:PRO:HD2	1.81	0.61
1:C:285:ALA:HB3	2:D:55:ILE:HD12	1.82	0.61
2:D:327:LEU:HD23	2:D:330:VAL:HG21	1.83	0.61
1:A:89:VAL:HB	1:A:223:ARG:HG3	1.81	0.61
2:B:312:VAL:CG2	2:B:338:LEU:HD23	2.29	0.61
2:D:85:ILE:HG23	2:D:116:ILE:HG23	1.81	0.61
1:A:167:LYS:NZ	7:A:601:HOH:O	2.32	0.61
2:B:294[B]:PHE:CE2	2:B:296:PRO:HG3	2.36	0.61
2:D:300:VAL:HG23	2:D:307:VAL:HG12	1.83	0.61
1:C:70:ARG:NH2	1:C:412:ARG:NH1	2.49	0.60
1:A:70:ARG:HE	1:A:236:LYS:NZ	1.99	0.60
2:D:300:VAL:CG2	2:D:307:VAL:CG1	2.80	0.59
1:C:70:ARG:NH2	1:C:412:ARG:NE	2.49	0.59
2:B:155:PHE:HD1	2:B:155:PHE:O	1.86	0.59
2:B:202:LEU:HB3	2:B:205:LYS:HD3	1.84	0.58
1:C:20:LEU:HD11	1:C:39:VAL:HG21	1.84	0.58
1:C:169:PRO:HA	1:C:194:PRO:HD2	1.85	0.58
2:D:300:VAL:HG22	2:D:307:VAL:CG1	2.34	0.58
2:B:237:ARG:NH1	7:B:502:HOH:O	2.34	0.58
1:C:378:VAL:O	1:C:381:GLU:HG3	2.04	0.58
2:D:254:ILE:CD1	2:D:256:GLU:H	2.15	0.57
1:A:350:THR:H	1:A:353:THR:HG23	1.68	0.57
2:B:168:TRP:HH2	2:B:286:PRO:HG2	1.69	0.57
2:D:178:LEU:HD23	2:D:209:ASN:HB3	1.87	0.57
2:D:164:VAL:HG21	2:D:189:LEU:HD23	1.86	0.57
1:C:3:TYR:CE2	1:C:5:ARG:HD3	2.40	0.57
1:C:333:ASP:HB3	2:D:47:GLU:OE1	2.04	0.57
1:A:287:LYS:NZ	2:B:24:GLU:OE1	2.34	0.56
2:B:336:ILE:HB	2:B:352:VAL:HG22	1.87	0.56
2:B:205:LYS:O	2:B:209:ASN:ND2	2.38	0.56
1:C:325:GLU:OE1	1:C:389:THR:HG21	2.05	0.56
1:C:327:ILE:HG12	1:C:390:LEU:HD23	1.86	0.56
1:C:388:ALA:O	1:C:411:LEU:HD23	2.04	0.56
2:B:204:GLU:OE2	2:B:208:ARG:HD2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:366:LYS:O	2:D:370:GLU:HG3	2.05	0.56
1:A:419:LEU:HD21	1:A:421:ILE:HD11	1.88	0.56
1:A:363:GLN:NE2	1:A:367:ASP:OD1	2.39	0.55
1:A:52:GLU:O	1:A:52:GLU:HG3	2.06	0.55
1:A:386:PRO:O	1:A:410:ILE:HG23	2.07	0.55
2:D:327:LEU:HA	2:D:330:VAL:HG23	1.89	0.54
1:C:236[A]:LYS:NZ	1:C:416:LYS:HA	2.23	0.54
2:D:100:GLU:O	2:D:104:ILE:HG12	2.08	0.54
2:D:51:TYR:O	2:D:55:ILE:HG12	2.07	0.54
2:B:205:LYS:HD2	2:B:205:LYS:N	2.17	0.53
2:D:170:GLU:HB3	2:D:174:ARG:NH1	2.24	0.53
2:D:8:ARG:H	2:D:149:LEU:HD11	1.73	0.53
1:C:383:VAL:HG23	1:C:383:VAL:O	2.08	0.53
2:D:78:SER:HB2	2:D:119:PHE:CD1	2.44	0.53
2:B:111:LYS:HG2	2:B:112:LEU:HD23	1.90	0.52
1:C:345:LEU:HD22	2:D:89:LEU:HG	1.91	0.52
2:D:307:VAL:HG23	2:D:333:PRO:O	2.09	0.52
1:A:4:LEU:HG	1:A:11:ILE:HD11	1.92	0.52
1:A:247:THR:HG22	1:A:249:GLU:N	2.23	0.52
1:A:408:GLY:O	1:A:412:ARG:HB2	2.09	0.52
2:D:269:LYS:O	2:D:272:THR:HG22	2.09	0.52
1:A:70:ARG:HE	1:A:236:LYS:HZ3	1.57	0.52
2:D:267:PHE:HA	2:D:359:ILE:HD11	1.92	0.52
1:A:350:THR:H	1:A:353:THR:CG2	2.23	0.51
2:B:226:GLU:HG3	2:B:242:LYS:HG2	1.92	0.51
5:C:503:GOL:H11	7:C:614:HOH:O	2.09	0.51
1:A:352:LYS:HD3	2:B:126:GLU:OE1	2.11	0.51
2:B:92:TYR:CD1	2:B:104:ILE:HD12	2.46	0.51
1:C:419:LEU:HD21	1:C:421:ILE:HD11	1.93	0.51
2:D:14:ASP:OD1	2:D:14:ASP:N	2.31	0.51
2:B:154:LEU:HD12	2:B:214:LEU:HD11	1.92	0.51
2:B:167:ASN:HB2	2:B:170:GLU:HB2	1.93	0.51
1:A:327:ILE:HB	1:A:372:VAL:HG22	1.92	0.51
1:A:12:LEU:HD21	1:A:26:LEU:HD12	1.93	0.50
1:C:46:LYS:HB2	1:C:48:ILE:CD1	2.42	0.50
1:C:273:GLN:HG3	7:C:622:HOH:O	2.11	0.50
2:B:205:LYS:HA	2:B:208:ARG:HD3	1.92	0.50
1:A:178:HIS:ND1	5:A:503:GOL:H12	2.26	0.50
2:B:282:ARG:HG3	2:B:298:PHE:CE1	2.46	0.50
1:C:3:TYR:HD2	6:C:505:CL:CL	2.32	0.50
1:C:331:THR:O	1:C:377:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:109:SER:HA	2:D:116:ILE:HD11	1.94	0.50
1:A:362:LEU:HD23	1:A:386:PRO:HD3	1.93	0.49
2:B:21:ALA:HB3	2:B:142:ILE:HG23	1.95	0.49
1:A:357:GLU:OE2	2:B:86:ARG:HD2	2.12	0.49
2:B:100:GLU:O	2:B:104:ILE:HG12	2.13	0.49
2:B:264:GLU:HG3	2:B:311:ILE:CD1	2.41	0.49
2:D:333:PRO:O	2:D:334:ILE:HG13	2.12	0.49
1:A:332:ARG:HG3	1:A:333:ASP:OD2	2.11	0.49
1:A:146:LEU:HD11	1:A:168:PHE:HZ	1.77	0.49
2:B:32:ILE:HG22	2:B:68:LEU:HD12	1.95	0.48
2:B:143:ARG:HB3	2:B:250:LYS:HB3	1.95	0.48
2:B:202:LEU:HA	2:B:205:LYS:HZ2	1.78	0.48
2:B:299:LEU:HD13	2:B:308:TYR:CZ	2.49	0.48
1:C:406:ARG:O	1:C:410:ILE:HG12	2.12	0.48
2:B:267:PHE:C	2:B:267:PHE:CD2	2.86	0.48
1:A:390:LEU:HD13	1:A:419:LEU:HD23	1.96	0.48
2:B:185:TYR:O	2:B:189:LEU:HD12	2.12	0.48
1:C:134:PHE:CE2	1:C:136:PRO:HA	2.48	0.48
2:B:294[A]:PHE:O	2:B:296:PRO:HD3	2.14	0.48
1:C:191:PHE:O	1:C:196:ARG:NH1	2.47	0.48
2:B:78:SER:OG	2:B:80:ILE:O	2.31	0.48
1:C:295:LEU:CD2	2:D:55:ILE:HD11	2.37	0.48
1:C:338:TYR:HE2	2:D:126:GLU:HG3	1.78	0.47
2:B:75:GLU:OE1	2:B:75:GLU:HA	2.14	0.47
2:D:40:LYS:HG2	2:D:44:GLU:OE1	2.13	0.47
1:C:6:TYR:HB2	1:C:54:VAL:HG13	1.97	0.47
2:D:106:GLN:HA	2:D:109:SER:OG	2.14	0.47
2:D:275:ILE:HD11	2:D:365:TYR:CB	2.45	0.47
2:D:256:GLU:CD	2:D:257:LYS:H	2.16	0.47
1:A:2:VAL:HG21	1:A:43:PHE:CE2	2.49	0.47
1:C:231:GLY:HA3	1:C:234:ILE:HD12	1.95	0.47
2:D:158[B]:TYR:HD1	2:D:197:ALA:HB3	1.79	0.47
2:D:172:ILE:HG13	2:D:173:ARG:N	2.29	0.47
2:B:65:VAL:O	2:B:69:THR:HG23	2.14	0.47
2:B:143:ARG:NH1	2:B:248:GLU:OE1	2.47	0.47
1:A:238:LYS:HB2	1:A:419:LEU:HD12	1.97	0.47
2:D:308:TYR:HE2	2:D:332:TYR:CE2	2.33	0.47
1:C:177:HIS:HA	1:C:213:TYR:OH	2.15	0.46
1:A:327:ILE:HG12	1:A:390:LEU:HD23	1.97	0.46
2:B:68:LEU:HD21	2:B:136:ILE:HG21	1.97	0.46
2:D:21:ALA:CB	2:D:142:ILE:HG23	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:VAL:O	2:D:69:THR:HG23	2.15	0.46
2:B:161:THR:HG23	2:B:192:GLU:HG2	1.96	0.46
2:B:330:VAL:CG1	2:B:334:ILE:HD11	2.46	0.46
2:D:308:TYR:HB2	2:D:334:ILE:HG12	1.97	0.46
2:D:339:ASN:OD1	2:D:342:LEU:HD13	2.15	0.46
1:C:3:TYR:CD2	6:C:505:CL:CL	3.06	0.46
1:C:130:LYS:HD3	1:C:131:TYR:CZ	2.50	0.46
1:A:71:ASP:O	1:A:75:GLU:HG3	2.15	0.46
2:D:251:GLU:CD	2:D:253:VAL:HG12	2.35	0.46
1:A:177:HIS:O	1:A:205:ARG:NH2	2.45	0.46
2:B:294[B]:PHE:O	2:B:296:PRO:HD3	2.16	0.46
1:A:224:LYS:HA	1:A:228:GLU:OE1	2.15	0.46
2:B:280:ILE:O	2:B:280:ILE:HG23	2.15	0.45
1:C:208:GLY:O	1:C:211:GLU:HG2	2.16	0.45
1:C:327:ILE:HB	1:C:372:VAL:HG22	1.98	0.45
1:C:357:GLU:OE2	2:D:86:ARG:HD2	2.16	0.45
2:D:170:GLU:HB3	2:D:174:ARG:HH12	1.80	0.45
2:D:226:GLU:HG3	2:D:242:LYS:HG2	1.98	0.45
2:D:297:ASP:OD2	2:D:311:ILE:HG22	2.17	0.45
2:B:282:ARG:HG3	2:B:298:PHE:HE1	1.81	0.45
1:C:70:ARG:NH2	1:C:412:ARG:CZ	2.80	0.45
2:D:80:ILE:HG13	2:D:81:PRO:HD2	1.99	0.45
2:D:173:ARG:HD3	2:D:173:ARG:HA	1.83	0.45
1:A:12:LEU:HD23	1:A:30:SER:HB2	1.99	0.45
2:D:208:ARG:CB	2:D:258:ARG:HH22	2.30	0.45
2:D:353:ILE:HD11	2:D:367:TRP:CD1	2.52	0.45
1:C:185:SER:O	1:C:189:GLN:HG3	2.17	0.45
2:D:28:LEU:HD13	2:D:56:TYR:CD2	2.52	0.44
1:C:122:THR:HG22	7:C:626:HOH:O	2.17	0.44
2:D:72:CYS:SG	2:D:134:PRO:HD3	2.57	0.44
2:D:178:LEU:HD21	2:D:212:VAL:HB	1.99	0.44
2:B:279:LYS:O	2:B:300:VAL:HA	2.17	0.44
1:A:134:PHE:CE2	1:A:136:PRO:HA	2.52	0.44
1:C:60:PHE:CE2	1:C:108:LYS:HA	2.53	0.44
1:C:403:PHE:CZ	1:C:407:LEU:HD12	2.53	0.44
2:B:36:PHE:HE2	2:B:69:THR:HG22	1.83	0.44
2:B:334:ILE:N	2:B:334:ILE:HD12	2.33	0.44
2:D:300:VAL:HG22	2:D:307:VAL:HG13	1.99	0.44
2:B:28:LEU:HD13	2:B:56:TYR:CD2	2.52	0.44
2:D:336:ILE:HB	2:D:352:VAL:HG12	1.99	0.44
1:C:21:LYS:HE3	7:C:608:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:HIS:HB3	7:C:623:HOH:O	2.18	0.43
1:A:279:HIS:HB3	7:A:630:HOH:O	2.18	0.43
2:D:254:ILE:HD12	2:D:255:ASP:CA	2.44	0.43
1:A:60:PHE:CD1	1:A:61:PRO:HD2	2.53	0.43
1:A:46:LYS:O	1:A:48:ILE:HD12	2.18	0.43
2:B:199:LEU:HB2	2:B:203:THR:HG22	1.99	0.43
1:C:33:ALA:HB1	1:C:192:ALA:HB2	2.01	0.43
1:C:69:LEU:HD11	1:C:102:LYS:HG2	1.99	0.43
1:C:236[A]:LYS:HZ1	1:C:416:LYS:HA	1.82	0.43
2:D:32:ILE:HG22	2:D:68:LEU:HD12	1.99	0.43
2:D:86:ARG:NH2	2:D:123:ASP:OD1	2.49	0.43
2:D:363:LEU:HA	2:D:366:LYS:HE3	2.00	0.43
2:B:178:LEU:HD21	2:B:212:VAL:HB	2.01	0.43
2:B:72:CYS:SG	2:B:134:PRO:HD3	2.59	0.43
2:B:280:ILE:HG13	2:B:300:VAL:HG12	2.01	0.43
2:B:208:ARG:NH1	2:B:258:ARG:HH12	2.17	0.43
2:B:208:ARG:O	2:B:212:VAL:HG23	2.19	0.43
1:C:272:LEU:HD12	1:C:272:LEU:HA	1.88	0.43
1:C:55:ILE:HD11	1:C:194:PRO:HD3	2.01	0.43
1:C:91:PRO:HD3	1:C:224:LYS:O	2.18	0.43
1:C:307:ASN:HB3	1:C:339:ARG:HH22	1.84	0.43
2:D:187:LYS:HB2	2:D:188:PRO:HD2	2.01	0.43
1:A:91:PRO:HD3	1:A:224:LYS:O	2.19	0.42
2:B:116:ILE:N	2:B:116:ILE:HD13	2.33	0.42
2:D:110:LYS:HD2	2:D:110:LYS:N	2.34	0.42
2:B:78:SER:HB2	2:B:119:PHE:CG	2.54	0.42
1:C:46:LYS:HB2	1:C:48:ILE:HD11	2.01	0.42
1:C:139:ILE:HB	1:C:152:ILE:HG13	2.01	0.42
2:D:366:LYS:HG3	2:D:370:GLU:OE1	2.19	0.42
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.87	0.42
2:B:355:TYR:HB2	2:B:358:LYS:O	2.19	0.42
2:B:283:GLU:N	2:B:284:PRO:CD	2.82	0.42
2:D:300:VAL:HG22	2:D:307:VAL:HG12	1.99	0.42
2:B:307:VAL:HB	2:B:333:PRO:HG2	2.00	0.42
2:B:320:ILE:HG22	2:B:324:LEU:HD12	2.02	0.42
1:C:37:ARG:NH1	1:C:83:GLU:O	2.46	0.42
1:C:114:VAL:HG12	1:C:154:TYR:CD1	2.53	0.42
1:A:238:LYS:HE3	1:A:419:LEU:HD13	2.02	0.42
2:D:267:PHE:HB2	2:D:359:ILE:HG12	2.02	0.42
1:A:136:PRO:O	1:A:138:ILE:HD12	2.19	0.42
1:C:232:LYS:H	1:C:232:LYS:CD	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:HD23	1:A:217:VAL:CG2	2.50	0.42
1:C:55:ILE:CD1	1:C:194:PRO:HD3	2.49	0.42
2:D:85:ILE:CG2	2:D:116:ILE:HG23	2.47	0.42
1:A:215:ILE:HG22	1:A:216:LEU:HD23	2.02	0.42
2:B:35:LEU:HD23	2:B:35:LEU:HA	1.80	0.42
1:C:122:THR:O	1:C:125:LYS:HB3	2.19	0.42
1:C:408:GLY:O	1:C:412:ARG:HB2	2.19	0.42
2:D:67:LEU:HB3	2:D:144:TRP:CZ3	2.55	0.42
1:C:136:PRO:O	1:C:138:ILE:HD12	2.19	0.41
2:D:173:ARG:HD2	2:D:177:TRP:HZ2	1.83	0.41
2:D:270:ASP:HB3	2:D:361:ILE:HG21	2.02	0.41
1:A:70:ARG:NH1	1:A:412:ARG:HD2	2.35	0.41
1:A:416:LYS:HD3	1:A:416:LYS:N	2.35	0.41
1:C:31:ALA:HB1	1:C:35:LYS:HD2	2.01	0.41
2:D:81:PRO:HA	2:D:82:PRO:HD3	1.92	0.41
2:D:232:GLY:O	2:D:236:LYS:HG2	2.19	0.41
1:A:330:PHE:CE2	1:A:407:LEU:HD21	2.55	0.41
1:C:31:ALA:CB	1:C:35:LYS:HD2	2.50	0.41
2:D:68:LEU:HD21	2:D:136:ILE:HG21	2.02	0.41
2:B:167:ASN:ND2	2:B:216:PHE:CE2	2.88	0.41
1:A:139:ILE:O	1:A:152:ILE:HA	2.20	0.41
2:B:180:LEU:CD1	2:B:213:LEU:HD22	2.51	0.41
1:A:333:ASP:HB3	2:B:47:GLU:OE2	2.21	0.41
1:C:386:PRO:O	1:C:410:ILE:HG23	2.21	0.41
2:B:81:PRO:HA	2:B:82:PRO:HD3	1.91	0.41
2:D:154:LEU:HD23	2:D:154:LEU:HA	1.92	0.41
1:A:282:VAL:HG22	1:A:295:LEU:HD21	2.03	0.41
2:B:307:VAL:HG23	2:B:333:PRO:O	2.21	0.41
1:A:154:TYR:HB3	1:A:184:TYR:CE1	2.56	0.40
2:B:299:LEU:HB2	2:B:308:TYR:CE1	2.57	0.40
1:C:224:LYS:HA	1:C:228:GLU:OE1	2.21	0.40
1:C:327:ILE:O	1:C:372:VAL:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LYS:O	2:D:13:LYS:NZ[1_455]	2.19	0.01

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	433/440 (98%)	416 (96%)	17 (4%)	0	100	100
1	C	434/440 (99%)	420 (97%)	14 (3%)	0	100	100
2	B	373/374 (100%)	355 (95%)	18 (5%)	0	100	100
2	D	372/374 (100%)	352 (95%)	20 (5%)	0	100	100
All	All	1612/1628 (99%)	1543 (96%)	69 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	363/384 (94%)	359 (99%)	4 (1%)	73	89
1	C	368/384 (96%)	360 (98%)	8 (2%)	52	79
2	B	310/345 (90%)	300 (97%)	10 (3%)	39	71
2	D	293/345 (85%)	292 (100%)	1 (0%)	92	97
All	All	1334/1458 (92%)	1311 (98%)	23 (2%)	60	83

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ASP
1	A	323	LYS

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Mol	Chain	Res	Type
1	A	332	ARG
1	A	371	ARG
2	B	66	LYS
2	B	75	GLU
2	B	78	SER
2	B	115	ASP
2	B	137	SER
2	B	143	ARG
2	B	155	PHE
2	B	165	SER
2	B	205	LYS
2	B	369	ARG
1	C	70	ARG
1	C	119	ASP
1	C	127	ARG
1	C	133	ASP
1	C	232	LYS
1	C	384	ASP
1	C	412	ARG
1	C	416	LYS
2	D	165	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 20 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	PO4	C	501	-	4,4,4	0.78	0	6,6,6	1.17	1 (16%)
5	GOL	A	503	-	5,5,5	1.53	2 (40%)	5,5,5	0.98	0
5	GOL	C	503	-	5,5,5	1.28	1 (20%)	5,5,5	0.83	0
3	PO4	A	501	-	4,4,4	0.82	0	6,6,6	0.95	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	503	-	-	2/4/4/4	-
5	GOL	C	503	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	GOL	C1-C2	2.46	1.61	1.51
5	A	503	GOL	C3-C2	2.34	1.61	1.51
5	C	503	GOL	C3-C2	2.07	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	PO4	O4-P-O3	2.35	115.52	107.97

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	GOL	C1-C2-C3-O3
5	A	503	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	GOL	1	0
5	C	503	GOL	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, 95^{th} 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	435/440 (98%)	-0.30	4 (0%)	84	71	41, 65, 121, 178	0
1	C	435/440 (98%)	-0.35	3 (0%)	87	76	37, 63, 120, 157	0
2	B	374/374 (100%)	-0.20	10 (2%)	54	38	40, 81, 122, 151	0
2	D	373/374 (99%)	0.04	22 (5%)	22	13	47, 88, 170, 191	0
All	All	1617/1628 (99%)	-0.21	39 (2%)	59	42	37, 73, 147, 191	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	200	VAL	5.6
2	D	373	ASN	4.1
2	B	114	ALA	3.7
2	D	267	PHE	3.7
2	D	345	GLU	3.5
2	D	308	TYR	3.4
1	C	434	SER	3.2
2	D	257	LYS	3.2
2	D	274	VAL	3.0
2	D	343	GLY	3.0
2	D	260	ASP	2.9
1	A	233	TYR	2.9
2	D	301	GLU	2.8
2	D	315	TRP	2.8
2	B	345	GLU	2.8
1	A	234	ILE	2.7
2	D	281	ILE	2.7
2	D	259	PHE	2.6
2	D	306	LYS	2.6
2	B	347	PHE	2.5
2	D	282	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	382	GLY	2.4
2	D	347	PHE	2.4
2	D	342	LEU	2.4
1	C	50	VAL	2.4
2	D	291	ASN	2.3
2	D	290	ASP	2.3
2	B	74	PHE	2.3
2	B	344	LYS	2.3
2	B	260	ASP	2.2
2	B	341	GLU	2.2
1	C	431	TYR	2.2
2	D	341	GLU	2.2
2	D	357	ARG	2.2
2	D	340	GLU	2.1
2	B	0	MET	2.1
2	B	343	GLY	2.1
1	A	235	ALA	2.1
2	B	115	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
6	CL	A	509	1/1	0.76	0.24	119,119,119,119	0
6	CL	B	402	1/1	0.81	0.16	110,110,110,110	0
6	CL	A	511	1/1	0.82	0.52	107,107,107,107	0
5	GOL	A	503	6/6	0.82	0.22	71,83,102,103	0
6	CL	C	507	1/1	0.84	0.25	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	C	503	6/6	0.87	0.16	86,95,103,108	0
6	CL	B	401	1/1	0.88	0.39	100,100,100,100	0
4	MG	C	502	1/1	0.89	0.34	79,79,79,79	0
6	CL	C	509	1/1	0.89	0.10	104,104,104,104	0
3	PO4	A	501	5/5	0.90	0.18	94,112,136,138	0
6	CL	A	506	1/1	0.91	0.21	76,76,76,76	0
6	CL	C	506	1/1	0.91	0.20	94,94,94,94	0
3	PO4	C	501	5/5	0.92	0.15	85,106,122,132	0
6	CL	A	504	1/1	0.92	0.20	73,73,73,73	0
6	CL	A	510	1/1	0.92	0.39	119,119,119,119	0
4	MG	A	502	1/1	0.93	0.45	76,76,76,76	0
6	CL	C	510	1/1	0.93	0.21	107,107,107,107	0
6	CL	A	508	1/1	0.95	0.20	93,93,93,93	0
6	CL	D	401	1/1	0.95	0.20	93,93,93,93	0
6	CL	C	508	1/1	0.96	0.20	92,92,92,92	0
6	CL	C	505	1/1	0.96	0.09	90,90,90,90	0
6	CL	A	507	1/1	0.96	0.15	85,85,85,85	0
6	CL	C	504	1/1	0.96	0.24	71,71,71,71	0
6	CL	A	505	1/1	0.98	0.11	87,87,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.