Full wwPDB X-ray Structure Validation Report (i)

Jul 31, 2016 – 11:58 PM EDT

PDB ID	:	5ETZ
Title	:	Structure of the all-trans isomer of pharaonis halorhodopsin in the absence of halide ions
Authors	:	Kouyama, T.
Deposited on	:	2015-11-18
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

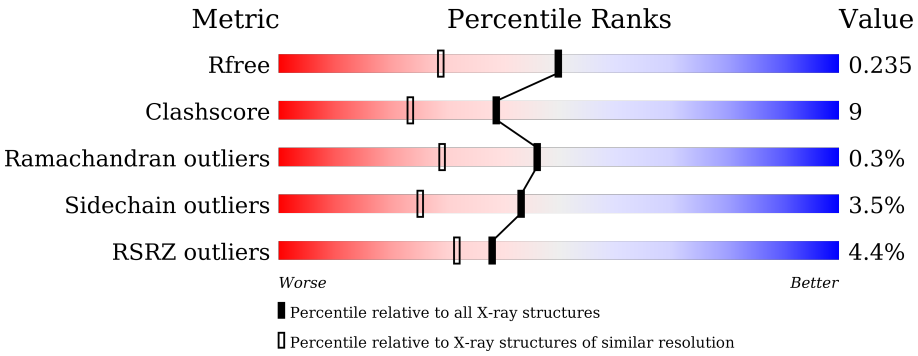
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	291	3% 74% 15% • 10%
1	B	291	3% 74% 14% • 11%
1	D	291	5% 70% 18% • 11%

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
3	22B	A	302	-	-	-	X
4	L3P	A	303	-	-	-	X
4	L3P	A	304	-	-	-	X
4	L3P	B	302	-	-	-	X
4	L3P	B	303	-	-	-	X
4	L3P	D	302	-	-	-	X
4	L3P	D	303	-	-	-	X
5	BNG	A	305	-	-	-	X
5	BNG	A	306	-	-	-	X
5	BNG	A	307	-	-	-	X
5	BNG	B	305	-	-	-	X
5	BNG	D	304	-	-	-	X

2 Entry composition

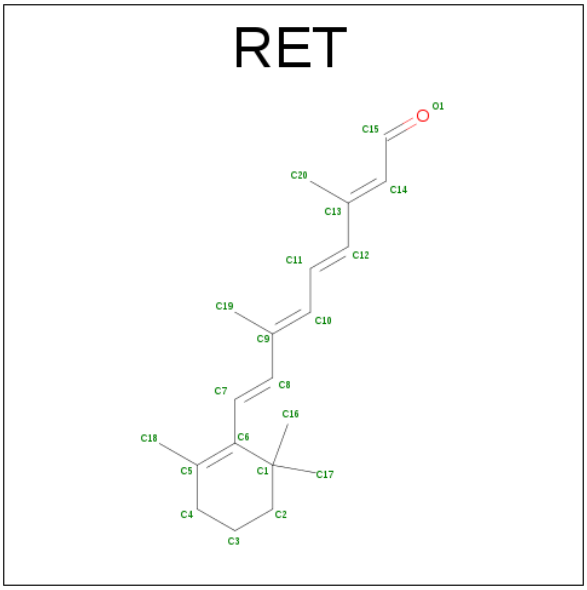
There are 6 unique types of molecules in this entry. The entry contains 6467 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Halorhodopsin.

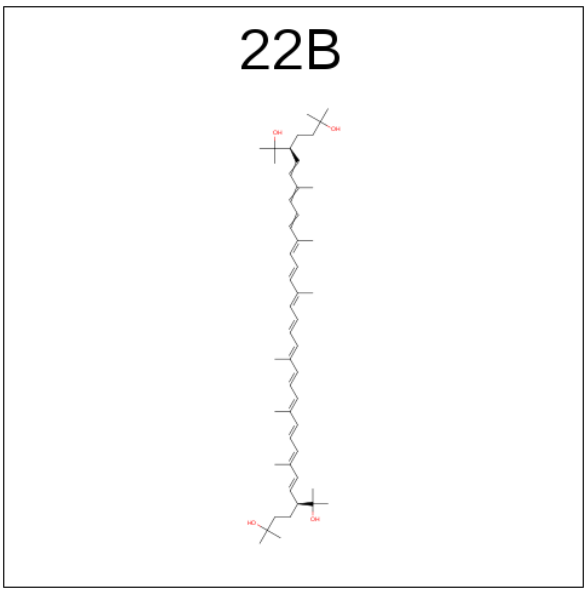
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			1971	1308	300	352	11			
1	B	260	Total	C	N	O	S	0	0	0
			1963	1302	299	351	11			
1	D	260	Total	C	N	O	S	0	0	0
			1963	1302	299	351	11			

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



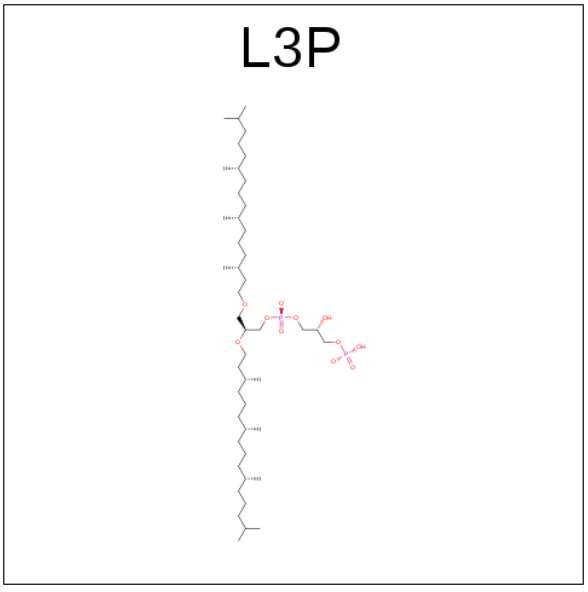
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		
2	B	1	Total	C	0	0
			20	20		
2	D	1	Total	C	0	0
			20	20		

- Molecule 3 is BACTERIORUBERIN (three-letter code: 22B) (formula: $C_{50}H_{76}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	37	35	2	0	0

- Molecule 4 is 2,3-DI-O-PHYTANLY-3-SN-GLYCERO-1-PHOSPHORYL-3'-SN-GLYCEROL-1'-PHOSPHATE (three-letter code: L3P) (formula: $C_{46}H_{94}O_{11}P_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
4	A	1	20	20	0	0

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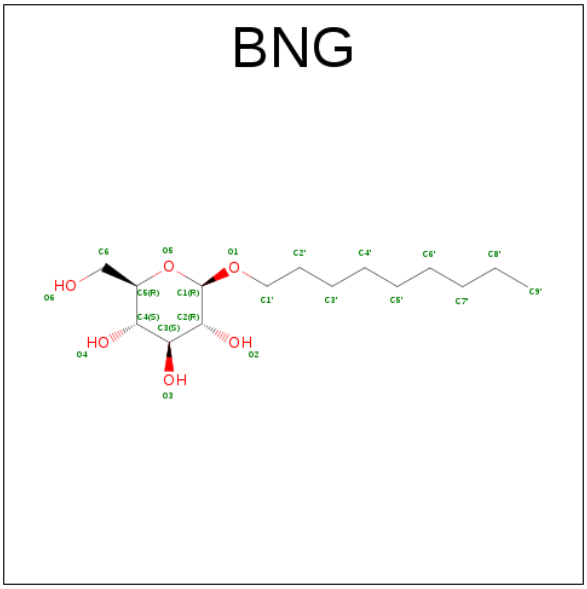
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 20 20	0	0
4	B	1	Total C 20 20	0	0
4	B	1	Total C 20 20	0	0
4	D	1	Total C 20 20	0	0
4	D	1	Total C 20 20	0	0

- Molecule 5 is B-NONYLGLUCOSIDE (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 21 15 6	0	0
5	A	1	Total C O 21 15 6	0	0
5	A	1	Total C O 21 15 6	0	0
5	B	1	Total C O 21 15 6	0	0
5	B	1	Total C O 21 15 6	0	0
5	D	1	Total C O 21 15 6	0	0

- Molecule 6 is water.

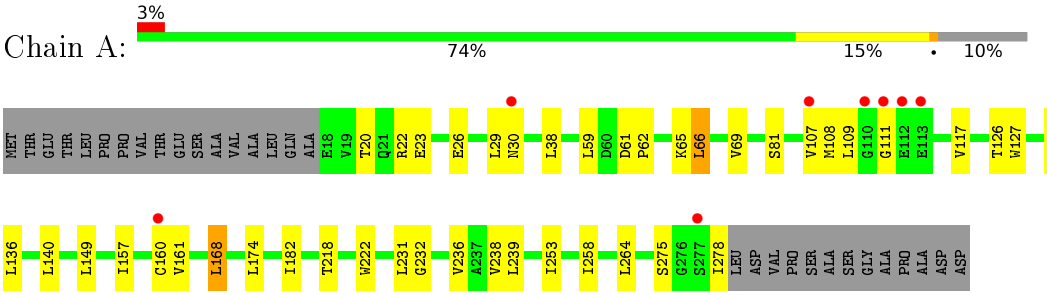
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	76	Total O 76 76	0	0
6	B	76	Total O 76 76	0	0
6	D	75	Total O 75 75	0	0

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.

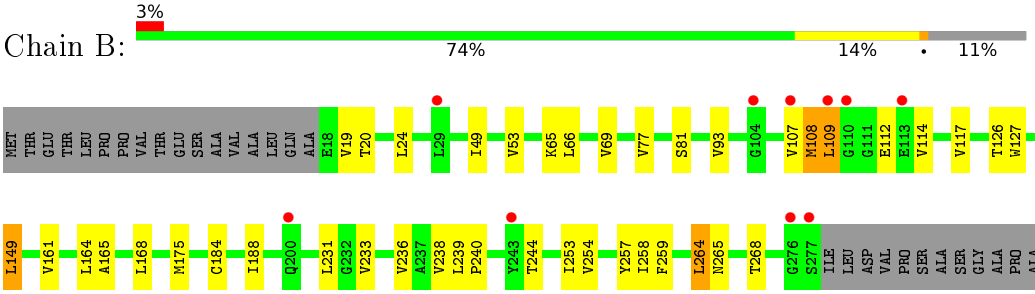
- Molecule 1: Halorhodopsin

Chain A:



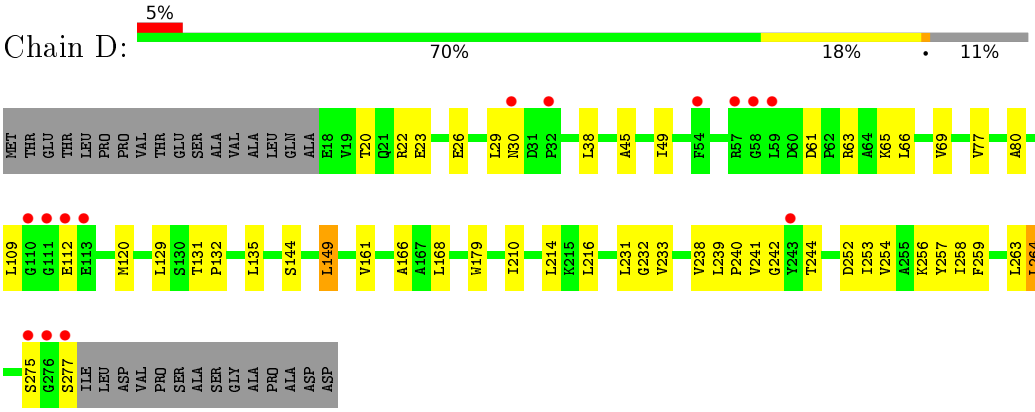
- Molecule 1: Halorhodopsin

Chain B:



- Molecule 1: Halorhodopsin

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.40Å 97.77Å 101.62Å 90.00° 128.81° 90.00°	Depositor
Resolution (Å)	15.00 – 1.80 50.77 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (15.00-1.80) 91.1 (50.77-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.236 0.219 , 0.235	Depositor DCC
R_{free} test set	5001 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 65.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.019 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6467	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: BNG, RET, L3P, 22B

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	0.36	0/2017	0.57	0/2762
1	B	0.32	0/2009	0.54	0/2751
1	D	0.32	0/2009	0.53	0/2751
All	All	0.33	0/6035	0.55	0/8264

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

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	1971	0	2025	38	0
1	B	1963	0	2014	34	0
1	D	1963	0	2014	40	0
2	A	20	0	27	1	0
2	B	20	0	27	2	0
2	D	20	0	27	0	0
3	A	37	0	49	6	0
4	A	40	0	78	2	0
4	B	40	0	78	2	0
4	D	40	0	78	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	63	0	90	0	0
5	B	42	0	60	1	0
5	D	21	0	30	0	0
6	A	76	0	0	2	1
6	B	76	0	0	4	0
6	D	75	0	0	3	0
All	All	6467	0	6597	115	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 9.

All (115) 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:254:VAL:HG13	1:D:258:ILE:HD11	1.63	0.81
3:A:302:22B:H15	3:A:302:22B:H42	1.62	0.80
1:D:210:ILE:HA	6:D:467:HOH:O	1.86	0.75
1:B:254:VAL:HG13	1:B:258:ILE:HD11	1.70	0.73
1:D:20:THR:OG1	1:D:22:ARG:HG2	1.89	0.72
1:D:240:PRO:O	1:D:244:THR:HG23	1.93	0.69
1:B:19:VAL:HG11	1:B:109:LEU:HD13	1.74	0.69
1:A:22:ARG:HD2	6:A:440:HOH:O	1.93	0.69
1:B:108:MET:HA	1:B:112:GLU:O	1.93	0.68
1:A:253:ILE:O	1:A:258:ILE:HD13	1.95	0.67
1:D:129:LEU:HD13	4:D:302:L3P:H23	1.77	0.67
1:A:238:VAL:HG23	1:A:239:LEU:HD13	1.76	0.66
1:D:254:VAL:HG13	1:D:258:ILE:CD1	2.25	0.66
1:D:233:VAL:H	1:D:244:THR:HG21	1.62	0.65
1:B:254:VAL:HG13	1:B:258:ILE:CD1	2.27	0.64
1:B:240:PRO:O	1:B:244:THR:HG23	1.99	0.63
1:D:120:MET:HG2	6:D:434:HOH:O	1.97	0.62
1:A:81:SER:HB3	1:A:126:THR:OG1	1.99	0.62
1:A:107:VAL:HG23	1:A:109:LEU:HD13	1.81	0.62
1:B:236:VAL:HG13	1:B:238:VAL:HG13	1.82	0.62
1:B:109:LEU:HD12	1:B:114:VAL:HB	1.83	0.61
1:D:254:VAL:HA	1:D:258:ILE:HG12	1.83	0.61
1:B:254:VAL:HA	1:B:258:ILE:HG12	1.82	0.60
1:A:29:LEU:O	1:A:30:ASN:HB2	2.02	0.60
1:A:231:LEU:O	1:A:238:VAL:HG22	2.02	0.60
1:A:182:ILE:HG23	3:A:302:22B:H14	1.85	0.58
1:D:80:ALA:HB3	4:D:302:L3P:H241	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:CYS:O	1:B:188:ILE:HD13	2.04	0.58
1:B:258:ILE:HG13	1:B:259:PHE:N	2.19	0.57
1:D:77:VAL:HG13	4:D:302:L3P:H243	1.86	0.57
1:A:161:VAL:HG11	4:B:303:L3P:H222	1.85	0.57
1:A:174:LEU:HD23	5:B:304:BNG:H4'1	1.87	0.56
1:D:20:THR:OG1	1:D:23:GLU:HG3	2.06	0.56
1:B:49:ILE:O	1:B:53:VAL:HG23	2.05	0.56
1:B:164:LEU:O	1:B:168:LEU:HD13	2.06	0.56
1:B:161:VAL:HG11	4:D:302:L3P:H221	1.87	0.55
1:A:69:VAL:HG22	6:D:463:HOH:O	2.07	0.55
1:D:264:LEU:O	1:D:268:THR:HG22	2.07	0.55
1:B:233:VAL:H	1:B:244:THR:HG21	1.71	0.55
6:B:407:HOH:O	1:D:65:LYS:HE2	2.07	0.55
1:D:94:LEU:HD21	4:D:303:L3P:H192	1.89	0.54
1:A:66:LEU:HD13	1:A:140:LEU:HD11	1.89	0.54
1:B:20:THR:O	1:B:24:LEU:HD23	2.08	0.53
1:B:264:LEU:O	1:B:268:THR:HG22	2.09	0.53
1:A:65:LYS:O	1:A:69:VAL:HG23	2.09	0.53
1:A:22:ARG:O	1:A:26:GLU:HG3	2.09	0.53
1:A:61:ASP:O	1:A:65:LYS:HG3	2.09	0.53
1:A:168:LEU:HD21	4:A:303:L3P:H242	1.91	0.52
1:D:65:LYS:O	1:D:69:VAL:HG23	2.09	0.52
1:D:238:VAL:HG23	1:D:239:LEU:CD1	2.40	0.51
1:A:26:GLU:O	1:A:29:LEU:O	2.29	0.51
1:A:157:ILE:O	1:A:160:CYS:SG	2.60	0.51
1:B:117:VAL:HG21	6:B:420:HOH:O	2.10	0.51
1:D:29:LEU:O	1:D:30:ASN:HB2	2.11	0.51
4:A:304:L3P:H201	1:D:161:VAL:HG12	1.91	0.50
1:B:93:VAL:HG21	1:B:109:LEU:HD11	1.94	0.50
1:B:107:VAL:O	1:B:108:MET:HB3	2.11	0.50
1:A:232:GLY:HA2	1:A:239:LEU:HB2	1.93	0.50
1:D:61:ASP:OD2	1:D:275:SER:HA	2.11	0.50
1:D:258:ILE:HG13	1:D:259:PHE:N	2.27	0.49
1:A:107:VAL:CG2	1:A:109:LEU:HD13	2.43	0.49
1:A:236:VAL:HG22	1:A:236:VAL:O	2.12	0.49
1:D:63:ARG:HD2	1:D:277:SER:O	2.11	0.49
1:B:165:ALA:HB2	4:D:302:L3P:H172	1.94	0.49
1:A:108:MET:O	1:A:109:LEU:HD12	2.14	0.48
1:B:144:SER:OG	1:B:149:LEU:HD22	2.14	0.48
1:A:20:THR:OG1	1:A:23:GLU:HG3	2.14	0.47
1:B:109:LEU:HA	6:B:466:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:HB3	1:A:22:ARG:NH1	2.28	0.47
1:B:65:LYS:O	1:B:69:VAL:HG23	2.14	0.47
1:A:182:ILE:HA	3:A:302:22B:H14	1.96	0.47
1:B:231:LEU:O	1:B:238:VAL:HG22	2.15	0.47
1:D:107:VAL:HG22	1:D:109:LEU:HD13	1.97	0.47
1:B:81:SER:HB2	1:B:126:THR:OG1	2.16	0.46
1:A:117:VAL:HG21	6:A:425:HOH:O	2.15	0.46
1:B:253:ILE:HA	1:B:257:TYR:CD2	2.50	0.46
1:A:258:ILE:HD12	1:A:258:ILE:N	2.30	0.46
1:B:127:TRP:CD1	2:B:301:RET:H14	2.51	0.45
1:D:131:THR:OG1	1:D:132:PRO:HD3	2.16	0.45
1:D:232:GLY:HA2	1:D:239:LEU:HB2	1.99	0.45
3:A:302:22B:C12	3:A:302:22B:H191	2.46	0.45
1:D:238:VAL:HG23	1:D:239:LEU:HD13	1.99	0.45
1:A:29:LEU:O	1:A:30:ASN:CB	2.65	0.45
1:D:214:LEU:CD1	1:D:263:LEU:HD13	2.48	0.44
1:B:161:VAL:CG1	4:D:302:L3P:H221	2.47	0.44
1:A:236:VAL:HG13	1:A:238:VAL:HG13	1.99	0.44
1:D:216:LEU:HD13	1:D:216:LEU:C	2.38	0.44
1:B:238:VAL:HG23	1:B:239:LEU:CD1	2.48	0.44
1:B:238:VAL:HG23	1:B:239:LEU:HD13	1.99	0.44
1:A:62:PRO:HB2	1:A:278:ILE:HD11	1.98	0.43
1:D:253:ILE:HA	1:D:257:TYR:CD2	2.54	0.43
1:B:77:VAL:HG22	4:B:303:L3P:H262	2.00	0.43
1:D:45:ALA:O	1:D:49:ILE:HG13	2.19	0.43
1:B:254:VAL:O	1:B:258:ILE:HG12	2.19	0.42
2:B:301:RET:H7	2:B:301:RET:H181	1.84	0.42
1:A:258:ILE:N	1:A:258:ILE:CD1	2.82	0.42
1:D:129:LEU:CD1	4:D:302:L3P:H23	2.45	0.42
1:D:20:THR:HG1	1:D:23:GLU:HG3	1.84	0.42
1:A:66:LEU:HD13	1:A:140:LEU:CD1	2.50	0.42
1:D:166:ALA:HB2	1:D:179:TRP:HB3	2.01	0.42
1:A:127:TRP:CD1	2:A:301:RET:H14	2.55	0.42
1:A:182:ILE:HG23	3:A:302:22B:C14	2.50	0.41
1:A:218:THR:HG23	1:A:222:TRP:NE1	2.35	0.41
1:A:61:ASP:OD2	1:A:275:SER:HA	2.20	0.41
1:D:61:ASP:O	1:D:65:LYS:HG3	2.20	0.41
1:A:157:ILE:HA	1:A:160:CYS:SG	2.60	0.41
1:B:109:LEU:HG	6:B:466:HOH:O	2.20	0.41
1:D:252:ASP:O	1:D:256:LYS:HB2	2.20	0.41
1:D:144:SER:OG	1:D:149:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:VAL:HG13	1:D:242:GLY:N	2.35	0.41
3:A:302:22B:H202	1:B:49:ILE:HD13	2.03	0.41
1:D:131:THR:N	1:D:132:PRO:CD	2.83	0.41
1:D:22:ARG:O	1:D:26:GLU:HG3	2.21	0.40
1:D:231:LEU:O	1:D:238:VAL:HG22	2.22	0.40
1:A:131:THR:N	1:A:132:PRO:CD	2.84	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)
6:A:418:HOH:O	6:A:418:HOH:O[2_656]	0.94	1.26

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	259/291 (89%)	251 (97%)	7 (3%)	1 (0%)	39 23
1	B	258/291 (89%)	253 (98%)	4 (2%)	1 (0%)	39 23
1	D	258/291 (89%)	255 (99%)	3 (1%)	0	100 100
All	All	775/873 (89%)	759 (98%)	14 (2%)	2 (0%)	46 29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	MET
1	A	111	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	209/233 (90%)	201 (96%)	8 (4%)	40	22
1	B	208/233 (89%)	201 (97%)	7 (3%)	44	26
1	D	208/233 (89%)	201 (97%)	7 (3%)	44	26
All	All	625/699 (89%)	603 (96%)	22 (4%)	43	25

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	59	LEU
1	A	66	LEU
1	A	135	LEU
1	A	136	LEU
1	A	149	LEU
1	A	168	LEU
1	A	264	LEU
1	B	66	LEU
1	B	109	LEU
1	B	135	LEU
1	B	149	LEU
1	B	175	MET
1	B	264	LEU
1	B	265	ASN
1	D	38	LEU
1	D	66	LEU
1	D	112	GLU
1	D	135	LEU
1	D	149	LEU
1	D	168	LEU
1	D	264	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	B	41	ASN
1	B	265	ASN
1	B	270	ASN
1	D	41	ASN
1	D	265	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
2	RET	A	301	1	19,20,21	2.06	4 (21%)	27,27,28	1.51	5 (18%)
3	22B	A	302	-	35,36,53	3.61	24 (68%)	38,47,72	1.52	5 (13%)
4	L3P	A	303	-	19,19,58	1.87	8 (42%)	21,22,73	1.26	3 (14%)
4	L3P	A	304	-	19,19,58	1.87	7 (36%)	21,22,73	1.31	3 (14%)
5	BNG	A	305	-	21,21,21	1.63	6 (28%)	26,26,26	0.71	0
5	BNG	A	306	-	21,21,21	1.63	5 (23%)	26,26,26	0.71	0
5	BNG	A	307	-	21,21,21	1.64	5 (23%)	26,26,26	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	RET	B	301	1	19,20,21	2.03	4 (21%)	27,27,28	1.69	7 (25%)
4	L3P	B	302	-	19,19,58	1.89	8 (42%)	21,22,73	1.34	3 (14%)
4	L3P	B	303	-	19,19,58	1.87	8 (42%)	21,22,73	1.33	3 (14%)
5	BNG	B	304	-	21,21,21	1.54	4 (19%)	26,26,26	0.71	0
5	BNG	B	305	-	21,21,21	1.67	6 (28%)	26,26,26	0.71	0
2	RET	D	301	1	19,20,21	1.96	4 (21%)	27,27,28	1.52	5 (18%)
4	L3P	D	302	-	19,19,58	1.86	8 (42%)	21,22,73	1.24	3 (14%)
4	L3P	D	303	-	19,19,58	1.87	8 (42%)	21,22,73	1.29	3 (14%)
5	BNG	D	304	-	21,21,21	1.67	5 (23%)	26,26,26	0.70	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
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
3	22B	A	302	-	-	2/42/42/65	0/0/0/0
4	L3P	A	303	-	-	0/20/20/67	0/0/0/0
4	L3P	A	304	-	-	0/20/20/67	0/0/0/0
5	BNG	A	305	-	-	0/12/32/32	0/1/1/1
5	BNG	A	306	-	-	0/12/32/32	0/1/1/1
5	BNG	A	307	-	-	0/12/32/32	0/1/1/1
2	RET	B	301	1	-	0/13/30/31	0/1/1/1
4	L3P	B	302	-	-	0/20/20/67	0/0/0/0
4	L3P	B	303	-	-	0/20/20/67	0/0/0/0
5	BNG	B	304	-	-	0/12/32/32	0/1/1/1
5	BNG	B	305	-	-	0/12/32/32	0/1/1/1
2	RET	D	301	1	-	0/13/30/31	0/1/1/1
4	L3P	D	302	-	-	0/20/20/67	0/0/0/0
4	L3P	D	303	-	-	0/20/20/67	0/0/0/0
5	BNG	D	304	-	-	0/12/32/32	0/1/1/1

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	RET	C2-C3	-2.52	1.45	1.52
2	D	301	RET	C2-C3	-2.43	1.46	1.52
2	A	301	RET	C2-C3	-2.32	1.46	1.52
5	B	305	BNG	C3-C2	2.00	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	L3P	C16-C15	2.01	1.61	1.52
5	A	305	BNG	C3-C2	2.01	1.57	1.52
4	D	302	L3P	C16-C15	2.01	1.61	1.52
4	D	303	L3P	C16-C15	2.02	1.61	1.52
5	B	304	BNG	O5-C5	2.02	1.49	1.44
4	A	303	L3P	C16-C15	2.02	1.61	1.52
4	B	303	L3P	C16-C15	2.03	1.61	1.52
3	A	302	22B	C22-C23	2.04	1.60	1.53
3	A	302	22B	C41-C40	2.06	1.49	1.43
5	D	304	BNG	C1-C2	2.12	1.58	1.52
5	A	305	BNG	O5-C5	2.13	1.49	1.44
5	A	306	BNG	C1-C2	2.16	1.58	1.52
5	A	307	BNG	C1-C2	2.16	1.58	1.52
3	A	302	22B	C12-C13	2.17	1.50	1.45
5	A	307	BNG	O5-C5	2.20	1.49	1.44
5	A	306	BNG	O5-C5	2.21	1.49	1.44
5	B	305	BNG	C1-C2	2.21	1.59	1.52
3	A	302	22B	C15-C14	2.22	1.50	1.43
5	A	305	BNG	C1-C2	2.23	1.59	1.52
4	B	303	L3P	C26-C25	2.26	1.62	1.52
4	A	304	L3P	C26-C25	2.27	1.62	1.52
4	D	303	L3P	C26-C25	2.27	1.62	1.52
5	D	304	BNG	O5-C5	2.28	1.50	1.44
5	B	305	BNG	O5-C5	2.28	1.50	1.44
4	D	302	L3P	C19-C18	2.31	1.60	1.52
4	B	302	L3P	C26-C25	2.32	1.62	1.52
4	A	303	L3P	C26-C25	2.33	1.62	1.52
4	D	302	L3P	C26-C25	2.33	1.62	1.52
3	A	302	22B	C8-C9	2.33	1.51	1.45
4	B	303	L3P	C19-C18	2.33	1.60	1.52
4	A	303	L3P	C19-C18	2.36	1.60	1.52
4	D	303	L3P	C19-C18	2.38	1.60	1.52
4	B	303	L3P	C14-C13	2.39	1.60	1.52
4	B	302	L3P	C14-C13	2.39	1.60	1.52
4	D	303	L3P	C14-C13	2.40	1.60	1.52
4	A	303	L3P	C14-C13	2.40	1.60	1.52
4	D	302	L3P	C14-C13	2.41	1.60	1.52
4	A	304	L3P	C19-C18	2.41	1.61	1.52
4	A	304	L3P	C14-C13	2.41	1.61	1.52
3	A	302	22B	C40-C39	2.45	1.40	1.34
4	B	302	L3P	C19-C18	2.45	1.61	1.52
4	A	303	L3P	C17-C18	2.47	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	303	L3P	C17-C18	2.48	1.65	1.52
4	D	302	L3P	C26-C27	2.50	1.63	1.52
4	B	303	L3P	C17-C18	2.50	1.65	1.52
4	A	304	L3P	C26-C27	2.51	1.63	1.52
4	A	304	L3P	C17-C18	2.52	1.65	1.52
4	B	302	L3P	C17-C18	2.52	1.65	1.52
2	D	301	RET	C7-C6	2.52	1.55	1.45
4	D	302	L3P	C17-C18	2.53	1.65	1.52
2	A	301	RET	C7-C6	2.53	1.55	1.45
4	B	303	L3P	C26-C27	2.54	1.63	1.52
4	D	303	L3P	C26-C27	2.55	1.63	1.52
5	A	305	BNG	C4-C5	2.56	1.58	1.53
4	A	303	L3P	C26-C27	2.56	1.63	1.52
5	A	306	BNG	C4-C5	2.57	1.58	1.53
4	A	304	L3P	C25-C23	2.58	1.66	1.52
2	B	301	RET	C7-C6	2.58	1.55	1.45
4	D	303	L3P	C25-C23	2.59	1.66	1.52
4	B	302	L3P	C26-C27	2.61	1.63	1.52
4	A	303	L3P	C25-C23	2.61	1.66	1.52
4	B	303	L3P	C25-C23	2.62	1.66	1.52
4	B	302	L3P	C25-C23	2.64	1.66	1.52
4	D	302	L3P	C25-C23	2.66	1.66	1.52
5	B	305	BNG	C4-C5	2.67	1.58	1.53
5	A	307	BNG	C4-C5	2.67	1.58	1.53
5	B	304	BNG	C4-C5	2.68	1.58	1.53
5	D	304	BNG	C4-C5	2.73	1.59	1.53
3	A	302	22B	C21-C2	2.75	1.57	1.53
3	A	302	22B	C38-C39	2.86	1.58	1.50
4	A	303	L3P	C15-C13	2.89	1.67	1.52
4	B	303	L3P	C15-C13	2.89	1.67	1.52
4	D	303	L3P	C15-C13	2.90	1.67	1.52
4	B	302	L3P	C15-C13	2.91	1.67	1.52
4	A	304	L3P	C15-C13	2.91	1.67	1.52
4	D	302	L3P	C15-C13	2.92	1.67	1.52
3	A	302	22B	C45-C44	3.15	1.52	1.43
3	A	302	22B	C11-C10	3.17	1.52	1.43
5	B	304	BNG	O1-C1	3.58	1.46	1.40
3	A	302	22B	C18-C5	3.60	1.57	1.50
3	A	302	22B	C17-C1	3.68	1.58	1.52
3	A	302	22B	C42-C43	3.68	1.54	1.45
3	A	302	22B	O27-C23	3.71	1.54	1.44
5	B	304	BNG	O5-C1	3.72	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	306	BNG	O1-C1	3.80	1.47	1.40
3	A	302	22B	C20-C13	3.80	1.58	1.50
5	A	305	BNG	O1-C1	3.83	1.47	1.40
5	A	307	BNG	O1-C1	3.83	1.47	1.40
5	A	305	BNG	O5-C1	3.92	1.51	1.41
5	D	304	BNG	O1-C1	3.95	1.47	1.40
5	B	305	BNG	O1-C1	3.97	1.47	1.40
5	A	307	BNG	O5-C1	3.98	1.52	1.41
5	A	306	BNG	O5-C1	4.02	1.52	1.41
3	A	302	22B	C50-C43	4.03	1.58	1.50
5	B	305	BNG	O5-C1	4.04	1.52	1.41
5	D	304	BNG	O5-C1	4.06	1.52	1.41
2	D	301	RET	C5-C6	4.09	1.41	1.34
2	B	301	RET	C5-C6	4.16	1.41	1.34
2	A	301	RET	C5-C6	4.23	1.42	1.34
3	A	302	22B	C44-C43	4.79	1.42	1.35
3	A	302	22B	C4-C5	4.88	1.56	1.45
3	A	302	22B	C16-C1	5.04	1.61	1.52
3	A	302	22B	C19-C9	5.18	1.60	1.50
3	A	302	22B	C22-C21	5.28	1.64	1.53
2	D	301	RET	C1-C6	5.69	1.61	1.53
2	B	301	RET	C1-C6	5.96	1.62	1.53
2	A	301	RET	C1-C6	6.15	1.62	1.53
3	A	302	22B	C2-C3	6.19	1.56	1.50
3	A	302	22B	C10-C9	7.27	1.45	1.35
3	A	302	22B	C4-C3	9.09	1.56	1.32

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	22B	C50-C43-C44	-4.40	116.49	122.89
3	A	302	22B	C21-C2-C3	-3.47	106.45	111.21
2	B	301	RET	C1-C6-C5	-3.23	118.17	122.50
2	D	301	RET	C1-C6-C5	-3.22	118.19	122.50
3	A	302	22B	C7-C6-C5	-2.88	123.04	127.22
2	A	301	RET	C1-C6-C5	-2.73	118.85	122.50
3	A	302	22B	C20-C13-C14	-2.67	119.00	122.89
2	B	301	RET	C8-C9-C10	-2.21	115.40	118.95
2	A	301	RET	C8-C9-C10	-2.06	115.63	118.95
4	D	302	L3P	C21-C20-C18	2.05	121.80	115.46
4	A	303	L3P	C21-C20-C18	2.16	122.14	115.46
2	D	301	RET	C20-C13-C12	2.17	121.63	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	303	L3P	C16-C17-C18	2.25	122.43	115.46
2	B	301	RET	C20-C13-C12	2.26	121.77	118.08
4	A	303	L3P	C16-C17-C18	2.28	122.50	115.46
2	B	301	RET	C19-C9-C8	2.28	121.82	118.08
2	D	301	RET	C2-C1-C6	2.33	113.94	110.48
2	A	301	RET	C20-C13-C12	2.35	121.92	118.08
4	B	302	L3P	C21-C20-C18	2.37	122.79	115.46
4	D	303	L3P	C21-C20-C18	2.37	122.80	115.46
4	B	303	L3P	C16-C17-C18	2.41	122.91	115.46
4	D	302	L3P	C16-C17-C18	2.42	122.96	115.46
2	B	301	RET	C2-C1-C6	2.46	114.14	110.48
4	B	302	L3P	C16-C17-C18	2.50	123.19	115.46
4	A	304	L3P	C21-C20-C18	2.53	123.29	115.46
4	A	304	L3P	C16-C17-C18	2.59	123.47	115.46
4	B	303	L3P	C21-C20-C18	2.60	123.50	115.46
2	D	301	RET	C17-C1-C6	2.61	114.32	110.33
2	A	301	RET	C1-C6-C7	2.69	123.65	115.96
2	B	301	RET	C17-C1-C6	2.80	114.61	110.33
2	D	301	RET	C1-C6-C7	2.82	124.02	115.96
3	A	302	22B	C42-C43-C44	3.17	124.07	118.95
2	B	301	RET	C1-C6-C7	3.18	125.06	115.96
2	A	301	RET	C17-C1-C6	3.20	115.22	110.33
4	D	302	L3P	C26-C25-C23	3.44	126.09	115.46
4	A	304	L3P	C26-C25-C23	3.61	126.61	115.46
4	A	303	L3P	C26-C25-C23	3.78	127.17	115.46
4	D	303	L3P	C26-C25-C23	3.87	127.43	115.46
4	B	303	L3P	C26-C25-C23	3.89	127.49	115.46
4	B	302	L3P	C26-C25-C23	3.95	127.69	115.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	22B	C15-C14-C13-C12
3	A	302	22B	C15-C14-C13-C20

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RET	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	22B	6	0
4	A	303	L3P	1	0
4	A	304	L3P	1	0
2	B	301	RET	2	0
4	B	303	L3P	2	0
5	B	304	BNG	1	0
4	D	302	L3P	7	0
4	D	303	L3P	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, 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	261/291 (89%)	-0.01	8 (3%)	52	47	15, 16, 34, 50	0
1	B	260/291 (89%)	0.04	10 (3%)	44	38	15, 23, 37, 56	0
1	D	260/291 (89%)	0.00	16 (6%)	24	19	15, 20, 38, 54	0
All	All	781/873 (89%)	0.01	34 (4%)	38	32	15, 20, 37, 56	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	SER	9.2
1	D	276	GLY	8.6
1	D	30	ASN	6.0
1	A	111	GLY	5.9
1	B	110	GLY	5.5
1	D	111	GLY	5.2
1	D	277	SER	5.1
1	A	107	VAL	5.1
1	B	276	GLY	5.0
1	B	107	VAL	4.8
1	A	160	CYS	4.4
1	B	109	LEU	4.2
1	A	110	GLY	4.0
1	B	104	GLY	3.9
1	A	277	SER	3.8
1	D	57	ARG	3.7
1	B	243	TYR	3.6
1	D	243	TYR	3.3
1	A	112	GLU	2.9
1	D	58	GLY	2.6
1	D	272	GLY	2.5
1	D	59	LEU	2.5
1	D	268	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	113	GLU	2.5
1	D	54	PHE	2.4
1	D	275	SER	2.4
1	B	200	GLN	2.4
1	B	29	LEU	2.4
1	A	30	ASN	2.4
1	D	110	GLY	2.3
1	D	112	GLU	2.2
1	D	113	GLU	2.2
1	B	113	GLU	2.1
1	D	32	PRO	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
4	L3P	D	303	20/59	0.56	0.62	48.79	92,92,95,95	0
4	L3P	A	304	20/59	0.64	0.67	42.67	78,80,82,82	0
4	L3P	D	302	20/59	0.60	0.61	24.31	77,79,81,81	0
4	L3P	B	303	20/59	0.55	0.72	21.20	87,89,89,89	0
4	L3P	B	302	20/59	0.46	0.72	20.32	82,83,83,84	0
3	22B	A	302	37/54	0.48	0.48	20.14	24,52,64,65	0
4	L3P	A	303	20/59	0.53	0.66	18.59	90,91,94,94	0
5	BNG	D	304	21/21	0.59	0.29	15.24	74,77,78,79	0
5	BNG	B	305	21/21	0.47	0.30	8.43	79,81,81,81	0
5	BNG	A	306	21/21	0.43	0.34	5.16	85,86,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	BNG	A	305	21/21	0.72	0.26	3.78	81,82,87,88	0
5	BNG	A	307	21/21	0.76	0.21	2.76	78,79,85,86	0
2	RET	D	301	20/21	0.93	0.10	1.23	14,15,19,19	0
2	RET	B	301	20/21	0.95	0.10	0.97	18,19,21,22	0
5	BNG	B	304	21/21	0.92	0.14	0.76	26,30,58,61	0
2	RET	A	301	20/21	0.93	0.12	0.26	14,14,18,18	0

6.5 Other polymers

There are no such residues in this entry.