



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:53 pm BST

PDB ID : 5VYE  
Title : Crystal Structure of L-Threonine Aldolase from Pseudomonas putida  
Authors : Beaudoin, S.F.; Burg, M.J.; Stewart, J.D.  
Deposited on : 2017-05-25  
Resolution : 2.27 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](mailto: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.

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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 : 2.11  
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) : 2.11

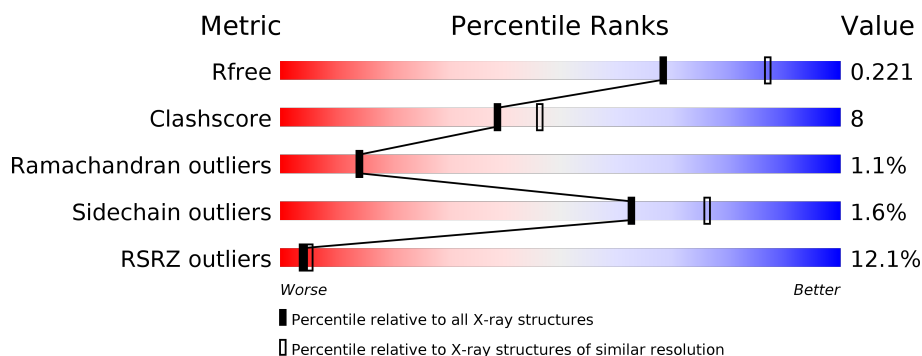
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	346	<div> <div>12%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	B	346	<div> <div>14%</div> <div>84%</div> <div>15%</div> <div>..</div> </div>
1	C	346	<div> <div>11%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	D	346	<div> <div>11%</div> <div>87%</div> <div>11%</div> <div>..</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLR	A	401	-	X	X	X
2	PLR	B	401	-	X	X	X
2	PLR	C	401	-	-	X	X
2	PLR	D	401	-	X	-	X

## 2 Entry composition [i](#)

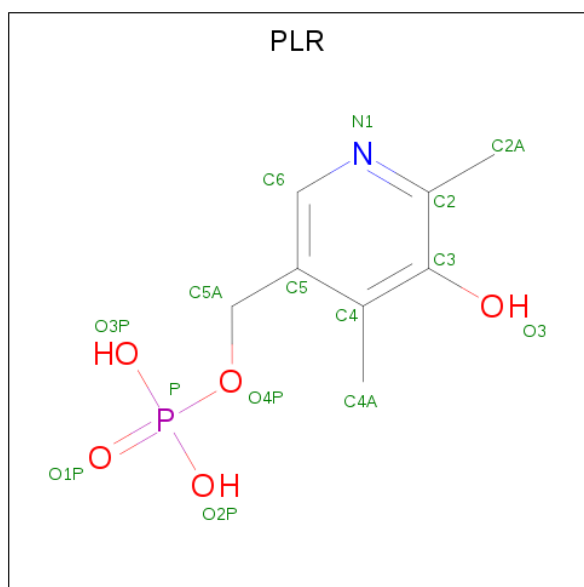
There are 4 unique types of molecules in this entry. The entry contains 21529 atoms, of which 10299 are hydrogens and 0 are deuteriums.

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 L-threonine aldolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	H	N	O	S	0	4	0
			5239	1683	2566	467	504	19			
1	B	344	Total	C	H	N	O	S	0	4	0
			5251	1688	2569	466	509	19			
1	C	342	Total	C	H	N	O	S	0	2	0
			5202	1674	2546	462	501	19			
1	D	342	Total	C	H	N	O	S	0	2	0
			5202	1674	2546	462	501	19			

- Molecule 2 is (5-HYDROXY-4,6-DIMETHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (three-letter code: PLR) (formula: C<sub>8</sub>H<sub>12</sub>NO<sub>5</sub>P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			25	8	10	1	5	1		
2	B	1	Total	C	H	N	O	P	0	0
			25	8	10	1	5	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	P	0	0
			25	8	10	1	5	1		
2	D	1	Total	C	H	N	O	P	0	0
			25	8	10	1	5	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total	O	0	0
			134	134		
4	B	109	Total	O	0	0
			109	109		
4	C	124	Total	O	0	0
			124	124		

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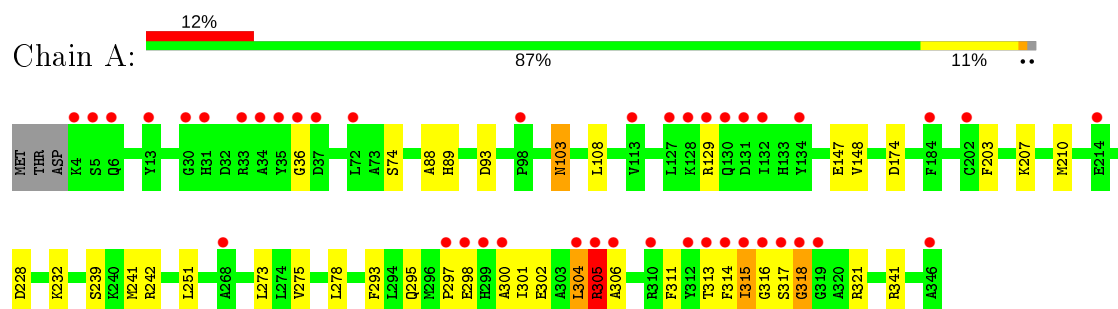
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	112	Total	O	0	0
			112	112		

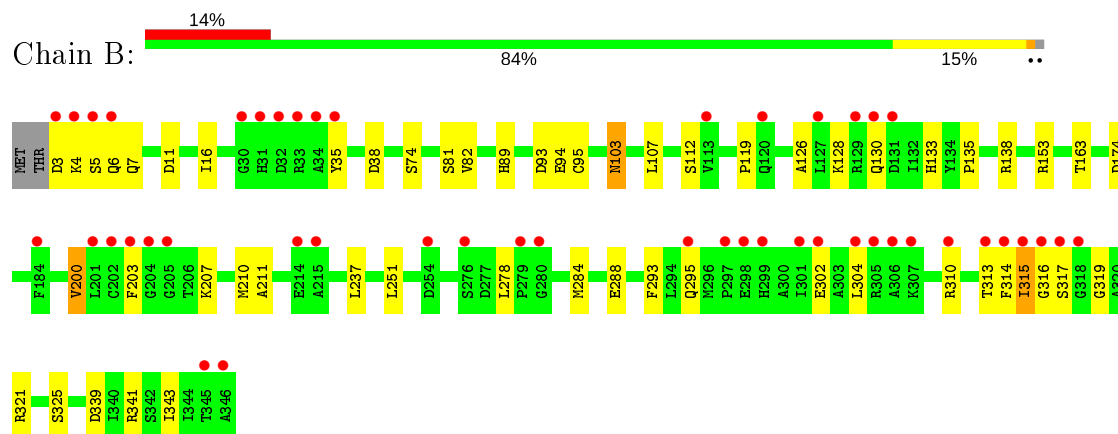
### 3 Residue-property plots [i](#)

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

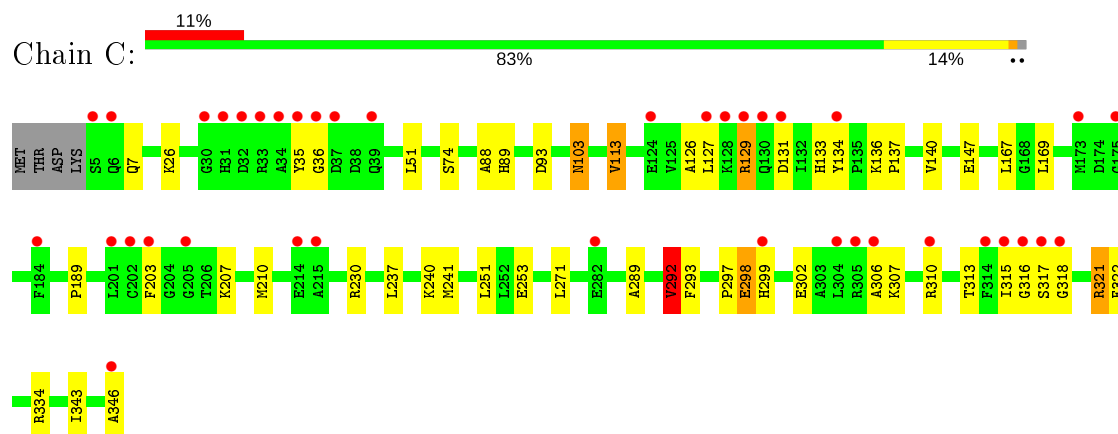
- Molecule 1: L-threonine aldolase



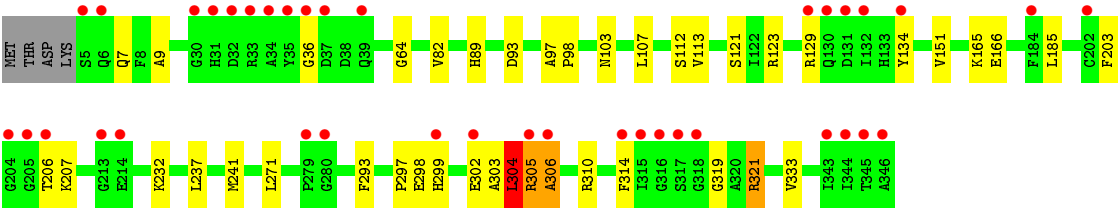
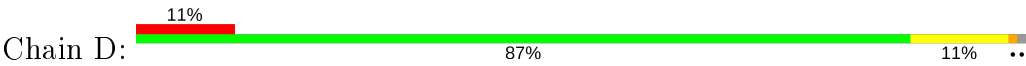
- Molecule 1: L-threonine aldolase



- Molecule 1: L-threonine aldolase



● Molecule 1: L-threonine aldolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.17Å 186.96Å 53.27Å 90.00° 98.92° 90.00°	Depositor
Resolution (Å)	26.75 – 2.27 26.81 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.3 (26.75-2.27) 94.5 (26.81-2.28)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.180 , 0.219 0.180 , 0.221	Depositor DCC
$R_{free}$ test set	1996 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, PLR

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	0.68	1/2749 (0.0%)	0.77	3/3724 (0.1%)
1	B	0.75	2/2753 (0.1%)	0.71	1/3729 (0.0%)
1	C	0.72	1/2723 (0.0%)	0.75	5/3690 (0.1%)
1	D	0.68	0/2723	0.71	1/3690 (0.0%)
All	All	0.71	4/10948 (0.0%)	0.73	10/14833 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	200	VAL	CB-CG1	-11.26	1.29	1.52
1	C	292	VAL	CB-CG1	-8.70	1.34	1.52
1	B	200	VAL	CB-CG2	-6.89	1.38	1.52
1	A	103	ASN	CB-CG	5.01	1.62	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	VAL	CG1-CB-CG2	7.14	122.33	110.90
1	C	334	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	B	200	VAL	CG1-CB-CG2	6.32	121.01	110.90
1	C	113	VAL	CA-CB-CG2	6.11	120.06	110.90
1	A	228	ASP	CB-CG-OD1	5.96	123.67	118.30
1	C	292	VAL	CG1-CB-CG2	5.82	120.22	110.90
1	C	321	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	242	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	273	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	D	304	LEU	CA-CB-CG	5.19	127.23	115.30

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	2673	2566	2548	34	2
1	B	2682	2569	2559	51	0
1	C	2656	2546	2538	46	2
1	D	2656	2546	2538	33	0
2	A	15	10	10	6	0
2	B	15	10	10	6	0
2	C	15	10	10	6	0
2	D	15	10	10	5	0
3	A	6	8	8	1	0
3	B	6	8	8	1	0
3	C	6	8	8	2	0
3	D	6	8	8	0	0
4	A	134	0	0	0	0
4	B	109	0	0	8	0
4	C	124	0	0	10	0
4	D	112	0	0	4	0
All	All	11230	10299	10255	158	2

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 8.

All (158) 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:207:LYS:HZ1	2:D:401:PLR:H4A2	1.33	0.91
1:A:301:ILE:O	1:A:305:ARG:HB2	1.78	0.83
1:D:207:LYS:NZ	2:D:401:PLR:H4A2	1.96	0.79
1:A:301:ILE:HG22	1:A:305:ARG:HD2	1.66	0.77
1:B:103:ASN:OD1	1:D:103:ASN:HB2	1.84	0.77
1:C:207:LYS:HZ1	2:C:401:PLR:H4A2	1.51	0.76
1:B:103:ASN:HB2	1:D:103:ASN:ND2	2.01	0.75
1:B:153:ARG:NH2	1:B:288:GLU:OE2	2.21	0.74
1:C:207:LYS:NZ	2:C:401:PLR:H4A2	2.03	0.73
1:B:126:ALA:O	1:B:130:GLN:NE2	2.24	0.69
1:D:304:LEU:O	1:D:306:ALA:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLU:HA	1:A:305:ARG:HB2	1.79	0.64
1:C:210:MET:HE2	1:C:251:LEU:HD22	1.80	0.64
1:C:297:PRO:O	1:C:299:HIS:N	2.34	0.61
1:B:304:LEU:HD22	4:B:609:HOH:O	2.01	0.61
1:C:237:LEU:HD13	4:C:509:HOH:O	2.00	0.60
2:C:401:PLR:H4A1	2:C:401:PLR:O4P	2.01	0.60
1:B:89:HIS:CE1	2:B:401:PLR:H5A1	2.37	0.60
1:A:103:ASN:ND2	1:C:103:ASN:HB2	2.16	0.60
1:D:297:PRO:O	1:D:299:HIS:N	2.35	0.60
1:B:207:LYS:HZ1	2:B:401:PLR:H4A2	1.65	0.60
1:B:302:GLU:HG2	1:B:343:ILE:HG23	1.85	0.59
1:D:165:LYS:NZ	4:D:502:HOH:O	2.31	0.58
1:B:284:MET:HG2	1:B:295:GLN:HG3	1.84	0.58
1:B:210:MET:HE2	1:B:251:LEU:HD22	1.85	0.57
1:D:123:ARG:NH2	1:D:166:GLU:OE1	2.38	0.57
1:A:293:PHE:CZ	1:A:321:ARG:HD2	2.40	0.57
1:C:271:LEU:HD23	1:C:292:VAL:HG11	1.86	0.56
2:D:401:PLR:H4A1	2:D:401:PLR:O4P	2.06	0.56
1:D:7:GLN:HG2	1:D:9:ALA:H	1.71	0.55
1:A:210:MET:HE2	1:A:251:LEU:HD22	1.88	0.55
1:B:5:SER:HB2	4:B:588:HOH:O	2.06	0.55
1:C:306:ALA:O	1:C:307:LYS:HB3	2.06	0.55
1:C:298:GLU:O	1:C:302:GLU:HG2	2.07	0.54
1:D:89:HIS:CD2	1:D:93:ASP:HB2	2.42	0.54
1:C:127:LEU:HD12	1:C:127:LEU:N	2.23	0.54
1:C:26:LYS:NZ	4:C:507:HOH:O	2.39	0.54
1:D:314:PHE:N	1:D:319:GLY:O	2.41	0.53
1:A:207:LYS:HZ1	2:A:401:PLR:H4A2	1.73	0.53
1:C:316:GLY:O	1:C:318:GLY:N	2.40	0.53
1:D:113:VAL:HG23	4:D:556:HOH:O	2.09	0.53
1:B:315:ILE:CG2	4:C:615:HOH:O	2.56	0.53
1:A:304:LEU:HG	1:A:311:PHE:CZ	2.44	0.53
1:B:313:THR:HG21	4:B:609:HOH:O	2.08	0.53
1:C:293:PHE:CZ	1:C:321:ARG:HD2	2.43	0.53
1:D:304:LEU:HD23	1:D:305:ARG:HG3	1.91	0.53
1:C:133:HIS:CE1	4:C:553:HOH:O	2.62	0.52
1:B:138:ARG:CG	4:B:602:HOH:O	2.58	0.52
1:C:297:PRO:C	1:C:299:HIS:H	2.12	0.52
1:A:301:ILE:O	1:A:305:ARG:N	2.39	0.52
1:B:207:LYS:NZ	2:B:401:PLR:H4A2	2.25	0.52
1:C:129:ARG:HD3	1:C:134:TYR:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:ARG:HG3	1:D:129:ARG:O	2.10	0.51
1:A:298:GLU:C	1:A:300:ALA:H	2.13	0.51
1:B:89:HIS:CD2	1:B:93:ASP:HB2	2.46	0.51
1:B:313:THR:CG2	4:B:609:HOH:O	2.59	0.51
1:C:292:VAL:HG13	1:C:322:PHE:HB2	1.93	0.51
1:D:129:ARG:NH1	1:D:134:TYR:CD1	2.79	0.51
1:B:133:HIS:CE1	4:B:594:HOH:O	2.63	0.51
1:A:298:GLU:C	1:A:300:ALA:N	2.62	0.50
1:B:314:PHE:C	1:B:316:GLY:H	2.14	0.50
1:B:35:TYR:CD1	1:B:237:LEU:HD23	2.47	0.50
1:A:103:ASN:HB2	1:C:103:ASN:OD1	2.13	0.49
1:D:36:GLY:HA2	1:D:241:MET:HG2	1.93	0.49
1:B:138:ARG:HG2	4:B:602:HOH:O	2.11	0.49
1:C:89:HIS:CD2	1:C:93:ASP:HB2	2.46	0.49
1:C:237:LEU:CD1	4:C:509:HOH:O	2.58	0.49
1:B:3:ASP:CB	1:B:4:LYS:HB2	2.43	0.49
1:D:232:LYS:HD3	1:D:237:LEU:HD22	1.94	0.49
1:D:302:GLU:O	1:D:306:ALA:HB3	2.13	0.48
1:B:278:LEU:HD11	1:B:341:ARG:CZ	2.43	0.48
1:B:4:LYS:HG3	1:B:6:GLN:H	1.79	0.48
1:A:36:GLY:HA2	1:A:241:MET:HG2	1.96	0.48
1:A:301:ILE:HG22	1:A:305:ARG:CD	2.41	0.47
1:A:316:GLY:HA2	1:A:317:SER:HA	1.70	0.47
1:B:7:GLN:HB3	1:B:310:ARG:HB2	1.97	0.47
1:B:302:GLU:HG2	1:B:343:ILE:CG2	2.44	0.47
1:A:89:HIS:CE1	2:A:401:PLR:C5	2.97	0.47
1:D:304:LEU:HD23	1:D:305:ARG:H	1.80	0.47
1:A:207:LYS:NZ	2:A:401:PLR:H4A2	2.30	0.46
1:B:315:ILE:HG22	4:C:615:HOH:O	2.15	0.46
1:D:303:ALA:O	1:D:304:LEU:O	2.33	0.46
1:B:103:ASN:OD1	1:D:103:ASN:CB	2.58	0.46
1:A:174:ASP:OD2	2:A:401:PLR:N1	2.49	0.46
1:A:297:PRO:O	1:A:300:ALA:N	2.43	0.46
1:C:89:HIS:CE1	2:C:401:PLR:H5A1	2.50	0.46
1:C:89:HIS:CD2	2:C:401:PLR:C3	2.98	0.46
1:C:298:GLU:O	1:C:298:GLU:HG3	2.16	0.45
1:C:297:PRO:HD2	1:C:299:HIS:ND1	2.31	0.45
1:A:304:LEU:HD11	1:A:313:THR:CG2	2.47	0.45
1:B:11:ASP:HA	1:B:325:SER:OG	2.16	0.45
1:B:7:GLN:CG	1:B:310:ARG:HB2	2.45	0.45
1:A:278:LEU:HD21	1:A:341:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ARG:HB2	1:C:134:TYR:CD1	2.51	0.45
1:C:240:LYS:HE3	1:D:206:THR:HG22	1.98	0.45
1:C:292:VAL:CG1	1:C:322:PHE:HB2	2.46	0.45
1:A:232:LYS:HG2	1:B:95:CYS:HB2	1.99	0.45
1:A:108:LEU:HD13	1:A:129:ARG:HD3	1.98	0.45
1:A:298:GLU:O	1:A:301:ILE:HG13	2.17	0.45
1:B:293:PHE:CZ	1:B:321:ARG:HD2	2.51	0.45
1:C:230:ARG:HH21	3:C:402:GOL:C3	2.29	0.45
2:A:401:PLR:O4P	2:A:401:PLR:H4A1	2.16	0.45
1:C:88:ALA:HA	1:C:147:GLU:OE2	2.16	0.45
1:C:129:ARG:HG3	1:C:129:ARG:O	2.18	0.44
1:B:74:SER:O	3:B:402:GOL:H32	2.17	0.44
1:B:4:LYS:HD2	4:B:588:HOH:O	2.16	0.44
1:C:127:LEU:HD11	1:C:167:LEU:CD2	2.48	0.44
1:B:313:THR:O	1:B:314:PHE:HB2	2.18	0.44
1:B:119:PRO:HB3	1:B:163:THR:OG1	2.18	0.44
1:B:174:ASP:OD2	2:B:401:PLR:N1	2.51	0.44
1:B:3:ASP:HB3	1:B:4:LYS:HB2	2.00	0.44
1:A:295:GLN:OE1	1:A:318:GLY:HA2	2.18	0.44
1:A:89:HIS:CD2	1:A:93:ASP:HB2	2.53	0.43
1:C:126:ALA:HA	1:C:137:PRO:HG2	2.00	0.43
1:C:7:GLN:HG3	1:C:310:ARG:HB2	2.01	0.43
1:A:210:MET:CE	1:A:251:LEU:HD22	2.49	0.43
1:B:82:VAL:HB	1:B:107:LEU:HD23	2.00	0.43
1:A:148:VAL:HA	1:A:293:PHE:CZ	2.54	0.43
1:B:93:ASP:HA	1:C:133:HIS:HB3	2.00	0.43
1:C:35:TYR:HE1	4:C:545:HOH:O	2.02	0.43
1:B:314:PHE:CB	1:B:316:GLY:H	2.32	0.43
1:C:140:VAL:HG23	1:C:169:LEU:HD13	2.01	0.43
1:A:88:ALA:HA	1:A:147:GLU:OE2	2.19	0.42
1:B:284:MET:HE1	1:B:319:GLY:HA3	2.01	0.42
1:D:113:VAL:O	1:D:113:VAL:CG2	2.68	0.42
1:C:127:LEU:N	1:C:127:LEU:CD1	2.82	0.42
1:C:51:LEU:HG	1:C:189:PRO:HG2	2.02	0.42
1:D:97:ALA:HB3	1:D:98:PRO:HD3	2.02	0.42
1:D:151:VAL:CG1	1:D:185:LEU:HD11	2.49	0.42
1:C:299:HIS:HB3	1:C:343:ILE:CG2	2.50	0.42
1:C:89:HIS:CE1	2:C:401:PLR:C5	3.03	0.42
1:D:310:ARG:HD3	1:D:310:ARG:HA	1.86	0.42
1:D:82:VAL:HB	1:D:107:LEU:HD23	2.02	0.42
1:A:305:ARG:HB3	1:A:306:ALA:H	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:SER:O	4:D:501:HOH:O	2.21	0.41
1:D:293:PHE:CZ	1:D:321:ARG:HD2	2.55	0.41
1:A:207:LYS:NZ	2:A:401:PLR:O3	2.53	0.41
1:B:339:ASP:O	1:B:343:ILE:HD12	2.21	0.41
1:B:16:ILE:HD11	1:B:211:ALA:HB2	2.01	0.41
1:C:74:SER:HA	3:C:402:GOL:H31	2.03	0.41
1:B:89:HIS:CE1	2:B:401:PLR:C5A	3.03	0.41
1:B:89:HIS:CE1	1:B:94:GLU:HG2	2.56	0.41
1:C:136:LYS:CE	4:C:510:HOH:O	2.68	0.41
1:B:7:GLN:HG3	1:B:310:ARG:HB2	2.03	0.41
1:C:253:GLU:OE2	4:C:501:HOH:O	2.22	0.41
1:D:237:LEU:HD13	4:D:513:HOH:O	2.20	0.41
1:A:298:GLU:O	1:A:300:ALA:N	2.54	0.41
1:A:74:SER:O	3:A:402:GOL:H32	2.21	0.41
1:C:131:ASP:HB2	4:C:597:HOH:O	2.20	0.41
1:C:36:GLY:HA2	1:C:241:MET:HG2	2.02	0.41
1:B:89:HIS:CE1	2:B:401:PLR:C5	3.04	0.40
1:A:314:PHE:CG	1:A:315:ILE:N	2.89	0.40
1:D:64:GLY:HA3	2:D:401:PLR:H5A2	2.03	0.40
1:D:271:LEU:HB2	1:D:333:VAL:HG13	2.03	0.40
1:B:278:LEU:HD11	1:B:341:ARG:NH1	2.37	0.40
1:B:128:LYS:HG3	1:C:315:ILE:HD13	2.03	0.40
1:D:89:HIS:CE1	2:D:401:PLR:H5A1	2.57	0.40
1:B:81:SER:HB3	1:B:135:PRO:HB2	2.03	0.40

All (2) 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:305:ARG:NH2	1:C:346:ALA:O[4_548]	2.11	0.09
1:A:305:ARG:HH22	1:C:346:ALA:O[4_548]	1.59	0.01

## 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	345/346 (100%)	320 (93%)	20 (6%)	5 (1%)	11	10
1	B	346/346 (100%)	320 (92%)	24 (7%)	2 (1%)	25	29
1	C	342/346 (99%)	322 (94%)	16 (5%)	4 (1%)	13	12
1	D	342/346 (99%)	324 (95%)	14 (4%)	4 (1%)	13	12
All	All	1375/1384 (99%)	1286 (94%)	74 (5%)	15 (1%)	14	14

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	ARG
1	C	298	GLU
1	D	298	GLU
1	D	304	LEU
1	D	305	ARG
1	A	318	GLY
1	D	306	ALA
1	C	129	ARG
1	B	317	SER
1	A	304	LEU
1	A	315	ILE
1	C	289	ALA
1	C	317	SER
1	B	315	ILE
1	A	275	VAL

### 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	276/277 (100%)	273 (99%)	3 (1%)	73	84
1	B	277/277 (100%)	272 (98%)	5 (2%)	59	72
1	C	273/277 (99%)	268 (98%)	5 (2%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	273/277 (99%)	269 (98%)	4 (2%)	65	77
All	All	1099/1108 (99%)	1082 (98%)	17 (2%)	62	77

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	PHE
1	A	239	SER
1	A	305	ARG
1	B	38	ASP
1	B	103	ASN
1	B	112	SER
1	B	200	VAL
1	B	203	PHE
1	C	103	ASN
1	C	113	VAL
1	C	203	PHE
1	C	292	VAL
1	C	313	THR
1	D	112	SER
1	D	203	PHE
1	D	304	LEU
1	D	321	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	C	68	ASN
1	D	103	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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$
3	GOL	C	402	-	5,5,5	0.61	0	5,5,5	0.87	0
2	PLR	A	401	-	15,15,15	2.17	7 (46%)	20,22,22	2.25	9 (45%)
3	GOL	A	402	-	5,5,5	0.47	0	5,5,5	1.19	0
2	PLR	C	401	-	15,15,15	2.13	6 (40%)	20,22,22	1.61	3 (15%)
2	PLR	D	401	-	15,15,15	1.96	7 (46%)	20,22,22	2.03	6 (30%)
3	GOL	D	402	-	5,5,5	0.47	0	5,5,5	0.61	0
3	GOL	B	402	-	5,5,5	0.66	0	5,5,5	1.15	0
2	PLR	B	401	-	15,15,15	2.13	6 (40%)	20,22,22	2.21	10 (50%)

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
3	GOL	C	402	-	-	2/4/4/4	-
2	PLR	A	401	-	-	3/6/6/6	0/1/1/1
3	GOL	A	402	-	-	2/4/4/4	-
2	PLR	C	401	-	-	5/6/6/6	0/1/1/1
2	PLR	D	401	-	-	5/6/6/6	0/1/1/1
3	GOL	D	402	-	-	0/4/4/4	-
3	GOL	B	402	-	-	2/4/4/4	-
2	PLR	B	401	-	-	3/6/6/6	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	PLR	P-O1P	4.18	1.64	1.50
2	A	401	PLR	P-O1P	4.14	1.63	1.50
2	B	401	PLR	P-O4P	3.78	1.72	1.60
2	A	401	PLR	C2-N1	3.15	1.39	1.33
2	B	401	PLR	C2-N1	3.15	1.39	1.33
2	D	401	PLR	C2-N1	2.97	1.39	1.33
2	B	401	PLR	O3-C3	2.97	1.43	1.37
2	A	401	PLR	C4A-C4	2.96	1.57	1.51
2	D	401	PLR	P-O4P	2.93	1.69	1.60
2	C	401	PLR	P-O4P	2.87	1.69	1.60
2	C	401	PLR	C4A-C4	2.84	1.57	1.51
2	B	401	PLR	C2A-C2	2.78	1.55	1.50
2	A	401	PLR	C2A-C2	2.76	1.55	1.50
2	C	401	PLR	C2-N1	2.75	1.39	1.33
2	A	401	PLR	P-O4P	2.73	1.69	1.60
2	C	401	PLR	O3-C3	2.70	1.43	1.37
2	A	401	PLR	C3-C2	2.64	1.43	1.40
2	D	401	PLR	C2A-C2	2.63	1.54	1.50
2	D	401	PLR	C4A-C4	2.40	1.56	1.51
2	D	401	PLR	O3-C3	2.35	1.42	1.37
2	D	401	PLR	P-O3P	2.33	1.63	1.54
2	B	401	PLR	P-O3P	2.31	1.63	1.54
2	A	401	PLR	O3-C3	2.23	1.42	1.37
2	D	401	PLR	P-O1P	2.17	1.57	1.50
2	C	401	PLR	C6-C5	2.09	1.42	1.37
2	B	401	PLR	C4A-C4	2.04	1.55	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLR	C6-C5-C4	6.34	123.15	118.16
2	D	401	PLR	C6-C5-C4	5.15	122.21	118.16
2	C	401	PLR	C6-C5-C4	4.55	121.74	118.16
2	D	401	PLR	O2P-P-O4P	4.39	118.42	106.73
2	B	401	PLR	O2P-P-O4P	4.26	118.08	106.73
2	B	401	PLR	C2A-C2-C3	-3.70	116.32	120.89
2	D	401	PLR	C5-C6-N1	-3.39	118.17	123.82
2	B	401	PLR	C4A-C4-C5	3.38	124.42	120.94
2	B	401	PLR	C6-C5-C4	3.13	120.62	118.16
2	C	401	PLR	C2A-C2-C3	-3.05	117.12	120.89
2	B	401	PLR	O3P-P-O4P	-2.99	98.77	106.73
2	A	401	PLR	C4A-C4-C5	2.97	123.99	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	PLR	C2A-C2-N1	2.96	123.45	117.67
2	A	401	PLR	O2P-P-O4P	2.93	114.54	106.73
2	B	401	PLR	O4P-C5A-C5	2.87	114.82	109.35
2	A	401	PLR	C2A-C2-C3	-2.70	117.55	120.89
2	A	401	PLR	C5-C6-N1	-2.68	119.35	123.82
2	A	401	PLR	O2P-P-O1P	2.62	120.94	110.68
2	A	401	PLR	C2A-C2-N1	2.50	122.54	117.67
2	D	401	PLR	O4P-P-O1P	-2.49	99.50	106.47
2	D	401	PLR	O3P-P-O4P	-2.40	100.35	106.73
2	B	401	PLR	C4A-C4-C3	-2.39	116.44	120.50
2	B	401	PLR	O3P-P-O2P	2.14	115.82	107.64
2	A	401	PLR	C3-C4-C5	-2.11	116.46	118.74
2	A	401	PLR	O3P-P-O4P	-2.08	101.20	106.73
2	D	401	PLR	O3P-P-O2P	2.06	115.51	107.64
2	C	401	PLR	O2P-P-O1P	2.05	118.72	110.68
2	B	401	PLR	C5-C6-N1	-2.05	120.41	123.82

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	GOL	O1-C1-C2-C3
2	A	401	PLR	C5A-O4P-P-O2P
2	A	401	PLR	C5A-O4P-P-O3P
3	A	402	GOL	C1-C2-C3-O3
2	C	401	PLR	C5A-O4P-P-O1P
2	C	401	PLR	C5A-O4P-P-O2P
2	C	401	PLR	C5A-O4P-P-O3P
2	D	401	PLR	C4-C5-C5A-O4P
2	D	401	PLR	C6-C5-C5A-O4P
2	D	401	PLR	C5A-O4P-P-O2P
2	D	401	PLR	C5A-O4P-P-O3P
3	B	402	GOL	C1-C2-C3-O3
2	B	401	PLR	C5A-O4P-P-O2P
2	B	401	PLR	C5A-O4P-P-O3P
3	A	402	GOL	O2-C2-C3-O3
3	B	402	GOL	O2-C2-C3-O3
3	C	402	GOL	O1-C1-C2-O2
2	D	401	PLR	C5A-O4P-P-O1P
2	B	401	PLR	C5A-O4P-P-O1P
2	C	401	PLR	C6-C5-C5A-O4P
2	C	401	PLR	C4-C5-C5A-O4P

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Mol	Chain	Res	Type	Atoms
2	A	401	PLR	C5A-O4P-P-O1P

There are no ring outliers.

7 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	GOL	2	0
2	A	401	PLR	6	0
3	A	402	GOL	1	0
2	C	401	PLR	6	0
2	D	401	PLR	5	0
3	B	402	GOL	1	0
2	B	401	PLR	6	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	343/346 (99%)	0.55	42 (12%) 4 5	28, 47, 93, 133	9 (2%)
1	B	344/346 (99%)	0.50	47 (13%) 3 3	29, 49, 93, 116	6 (1%)
1	C	342/346 (98%)	0.43	39 (11%) 5 6	27, 50, 91, 124	8 (2%)
1	D	342/346 (98%)	0.51	38 (11%) 5 7	30, 50, 93, 111	10 (2%)
All	All	1371/1384 (99%)	0.50	166 (12%) 4 5	27, 49, 93, 133	33 (2%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	SER	9.8
1	A	305	ARG	9.6
1	D	34	ALA	9.2
1	A	316	GLY	9.0
1	C	30	GLY	8.8
1	D	31	HIS	8.6
1	A	315	ILE	8.2
1	B	317	SER	8.0
1	A	306	ALA	7.9
1	D	305	ARG	7.8
1	B	315	ILE	7.7
1	D	315	ILE	7.6
1	D	317	SER	7.6
1	C	306	ALA	7.5
1	C	315	ILE	7.5
1	D	33	ARG	7.2
1	C	34	ALA	7.2
1	C	33	ARG	7.1
1	A	314	PHE	7.0
1	B	127	LEU	6.6
1	B	314	PHE	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	130	GLN	6.4
1	A	318	GLY	6.3
1	B	307	LYS	6.0
1	D	299	HIS	6.0
1	B	3	ASP	5.9
1	D	318	GLY	5.8
1	A	4	LYS	5.5
1	B	279	PRO	5.4
1	D	30	GLY	5.4
1	B	34	ALA	5.4
1	A	31	HIS	5.3
1	A	346	ALA	5.3
1	C	317	SER	5.3
1	D	279	PRO	5.3
1	B	31	HIS	5.3
1	D	316	GLY	5.2
1	A	202	CYS	5.1
1	C	318	GLY	5.0
1	D	36	GLY	5.0
1	C	32	ASP	5.0
1	D	37	ASP	4.8
1	C	36	GLY	4.8
1	D	314	PHE	4.7
1	B	316	GLY	4.7
1	C	31	HIS	4.7
1	B	306	ALA	4.6
1	B	302	GLU	4.6
1	B	298	GLU	4.5
1	C	5	SER	4.5
1	D	302	GLU	4.4
1	B	305	ARG	4.3
1	B	345	THR	4.3
1	A	134	TYR	4.2
1	A	298	GLU	4.2
1	A	33	ARG	4.2
1	D	32	ASP	4.2
1	A	129	ARG	4.1
1	C	305	ARG	4.1
1	C	316	GLY	4.1
1	B	295	GLN	4.1
1	B	33	ARG	4.1
1	A	5	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	5	SER	4.0
1	D	344	ILE	3.9
1	A	34	ALA	3.9
1	D	35	TYR	3.8
1	A	132	ILE	3.8
1	A	30	GLY	3.7
1	B	318	GLY	3.7
1	A	131	ASP	3.6
1	A	310	ARG	3.5
1	C	304	LEU	3.5
1	C	37	ASP	3.5
1	C	299	HIS	3.5
1	B	30	GLY	3.4
1	B	35	TYR	3.4
1	C	346	ALA	3.4
1	D	130	GLN	3.4
1	D	205	GLY	3.4
1	B	130	GLN	3.3
1	A	6	GLN	3.3
1	B	313	THR	3.3
1	B	299	HIS	3.3
1	D	129	ARG	3.3
1	C	6	GLN	3.3
1	D	345	THR	3.3
1	A	127	LEU	3.2
1	C	35	TYR	3.2
1	A	113	VAL	3.1
1	A	37	ASP	3.1
1	B	205	GLY	3.1
1	B	204	GLY	3.1
1	C	131	ASP	3.0
1	A	299	HIS	3.0
1	D	6	GLN	3.0
1	B	276	SER	3.0
1	D	346	ALA	2.9
1	A	36	GLY	2.9
1	C	127	LEU	2.9
1	C	214[A]	GLU	2.8
1	C	129	ARG	2.8
1	B	184	PHE	2.8
1	A	128	LYS	2.7
1	A	13	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	346	ALA	2.7
1	D	280	GLY	2.7
1	B	214[A]	GLU	2.7
1	D	131	ASP	2.7
1	C	134	TYR	2.7
1	D	134	TYR	2.7
1	B	280	GLY	2.7
1	C	202	CYS	2.6
1	B	131	ASP	2.6
1	D	306	ALA	2.6
1	B	202	CYS	2.6
1	B	6	GLN	2.6
1	C	130	GLN	2.6
1	C	215[A]	ALA	2.6
1	B	215[A]	ALA	2.6
1	D	206	THR	2.5
1	A	304	LEU	2.5
1	D	214[A]	GLU	2.5
1	A	319	GLY	2.5
1	B	113	VAL	2.5
1	B	32	ASP	2.5
1	A	72	LEU	2.5
1	B	203	PHE	2.5
1	A	35	TYR	2.5
1	C	128	LYS	2.5
1	D	132	ILE	2.4
1	D	39	GLN	2.4
1	B	5	SER	2.4
1	D	184	PHE	2.4
1	B	129	ARG	2.3
1	C	203	PHE	2.3
1	C	310	ARG	2.3
1	D	343	ILE	2.3
1	B	4	LYS	2.3
1	A	98	PRO	2.3
1	C	39	GLN	2.3
1	A	312	TYR	2.3
1	D	202	CYS	2.3
1	A	184	PHE	2.2
1	A	268	ALA	2.2
1	C	124	GLU	2.2
1	C	175	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	313	THR	2.2
1	A	214[A]	GLU	2.2
1	C	282	GLU	2.2
1	C	173	MET	2.2
1	B	120	GLN	2.2
1	D	204	GLY	2.1
1	A	297	PRO	2.1
1	B	297	PRO	2.1
1	B	254[A]	ASP	2.1
1	C	184	PHE	2.1
1	A	300	ALA	2.1
1	C	314	PHE	2.1
1	B	310	ARG	2.1
1	C	205	GLY	2.1
1	B	201	LEU	2.0
1	B	304	LEU	2.0
1	C	201	LEU	2.0
1	D	213	GLY	2.0
1	B	301	ILE	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 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	PLR	B	401	15/15	0.68	0.47	46,57,72,72	0
2	PLR	C	401	15/15	0.69	0.45	45,58,73,73	0
2	PLR	D	401	15/15	0.71	0.47	48,61,76,76	0
2	PLR	A	401	15/15	0.74	0.42	45,59,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	D	402	6/6	0.86	0.27	39,61,71,73	0
3	GOL	B	402	6/6	0.89	0.34	44,57,69,70	0
3	GOL	C	402	6/6	0.93	0.18	35,58,77,80	0
3	GOL	A	402	6/6	0.95	0.17	35,51,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.