



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 02:48 PM EST

PDB ID : 1M6S  
Title : Crystal Structure Of Threonine Aldolase  
Authors : Burley, S.K.; Kielkopf, C.L.  
Deposited on : 2002-07-17  
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](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 : 2.16  
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) : 2.16

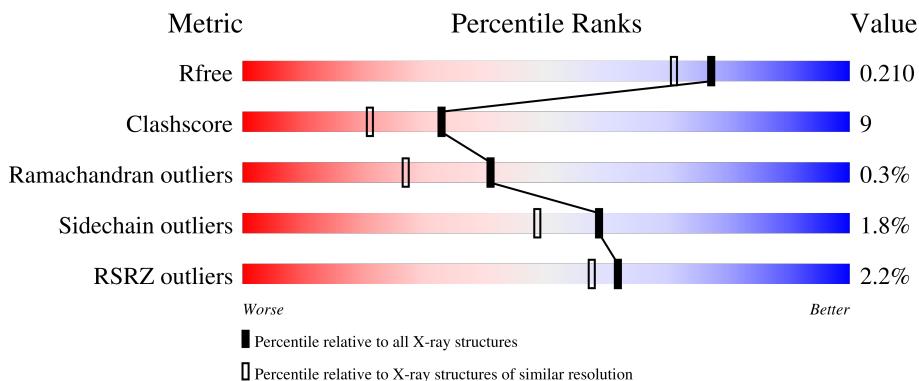
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


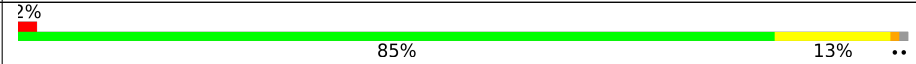
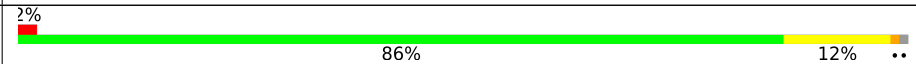

The reported resolution of this entry is 1.80 Å.

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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 of 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	347	 85% 12% ...
1	B	347	 85% 13% ..
1	C	347	 86% 12% ..
1	D	347	 83% 15% ..

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11566 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 L-allo-threonine aldolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	343	2569	1606	456	490	1	16	0	0	0
1	B	343	2590	1619	463	491	1	16	0	0	0
1	C	343	2572	1611	464	480	1	16	0	1	0
1	D	344	2568	1609	456	485	1	17	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	cloning artifact	UNP Q9X266
A	-2	PRO	-	cloning artifact	UNP Q9X266
A	-1	HIS	-	cloning artifact	UNP Q9X266
A	0	MET	-	cloning artifact	UNP Q9X266
A	199	LLP	LYS	modified residue	UNP Q9X266
B	-3	GLY	-	cloning artifact	UNP Q9X266
B	-2	PRO	-	cloning artifact	UNP Q9X266
B	-1	HIS	-	cloning artifact	UNP Q9X266
B	0	MET	-	cloning artifact	UNP Q9X266
B	199	LLP	LYS	modified residue	UNP Q9X266
C	-3	GLY	-	cloning artifact	UNP Q9X266
C	-2	PRO	-	cloning artifact	UNP Q9X266
C	-1	HIS	-	cloning artifact	UNP Q9X266
C	0	MET	-	cloning artifact	UNP Q9X266
C	199	LLP	LYS	modified residue	UNP Q9X266
D	-3	GLY	-	cloning artifact	UNP Q9X266
D	-2	PRO	-	cloning artifact	UNP Q9X266
D	-1	HIS	-	cloning artifact	UNP Q9X266
D	0	MET	-	cloning artifact	UNP Q9X266
D	199	LLP	LYS	modified residue	UNP Q9X266

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

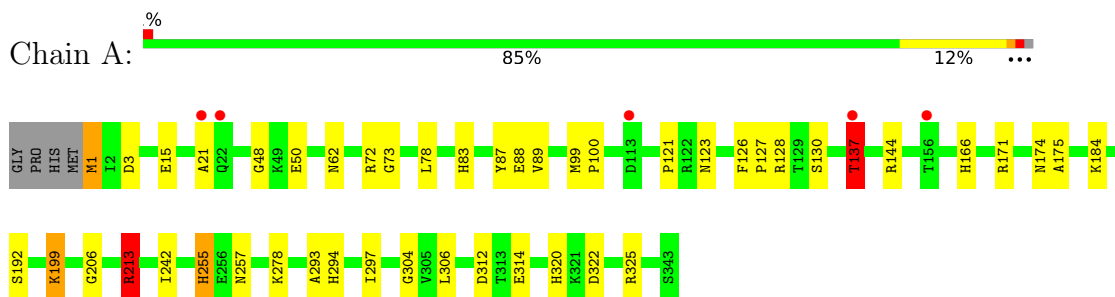
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	327	Total O 327 327	0	0
4	B	319	Total O 319 319	0	0
4	C	312	Total O 312 312	0	0
4	D	297	Total O 297 297	0	0

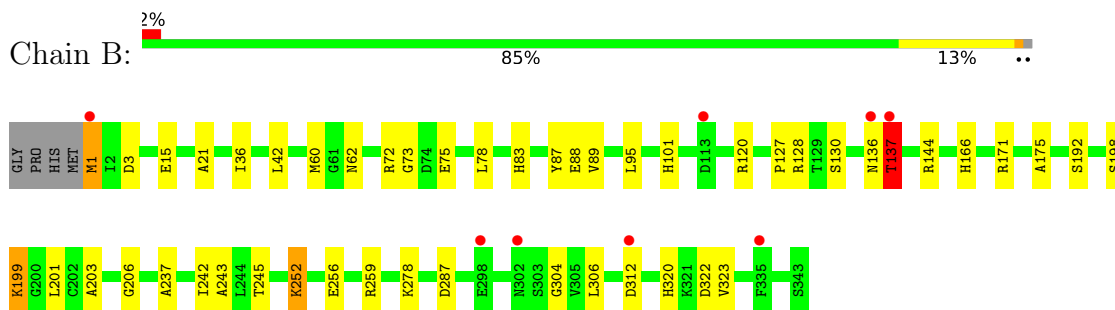
### 3 Residue-property plots [i](#)

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.

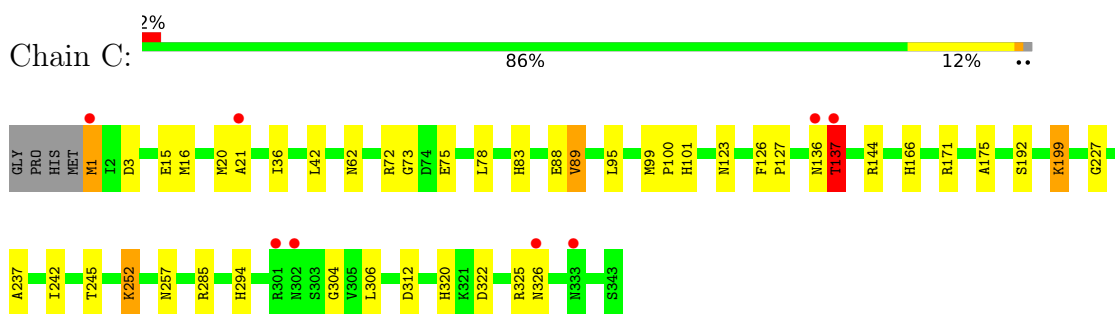
- Molecule 1: L-*allo*-threonine aldolase



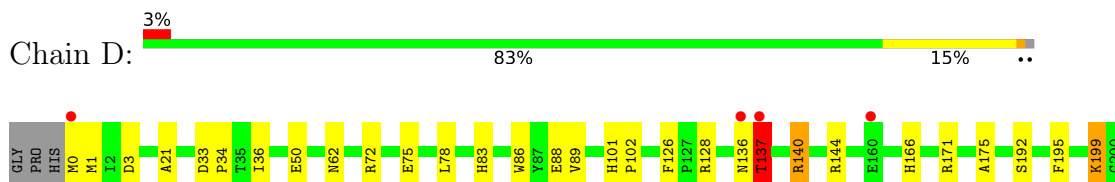
- Molecule 1: L-*allo*-threonine aldolase



- Molecule 1: L-*allo*-threonine aldolase



- Molecule 1: L-*allo*-threonine aldolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.89Å 100.60Å 149.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 19.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.80) 98.5 (19.94-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.87 (at 1.80Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.200 , 0.213 0.199 , 0.210	Depositor DCC
$R_{free}$ test set	6294 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.1	Xtrriage
Anisotropy	0.022	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.52 , 74.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.006 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.14% 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: CA, LLP, 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	0.30	0/2585	0.68	4/3504 (0.1%)
1	B	0.30	0/2606	0.67	4/3527 (0.1%)
1	C	0.31	0/2588	0.67	3/3505 (0.1%)
1	D	0.32	0/2584	0.68	5/3501 (0.1%)
All	All	0.31	0/10363	0.67	16/14037 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	THR	N-CA-C	-10.71	82.09	111.00
1	D	137	THR	N-CA-C	-10.49	82.68	111.00
1	A	137	THR	N-CA-C	-10.46	82.77	111.00
1	C	137	THR	N-CA-C	-10.31	83.16	111.00
1	A	213	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	A	137	THR	N-CA-CB	6.35	122.37	110.30
1	D	137	THR	N-CA-CB	6.27	122.21	110.30
1	B	137	THR	N-CA-CB	6.27	122.20	110.30
1	C	137	THR	N-CA-CB	6.10	121.89	110.30
1	D	259	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	D	136	ASN	C-N-CA	5.52	135.51	121.70
1	A	206	GLY	N-CA-C	5.36	126.51	113.10
1	C	136	ASN	C-N-CA	5.34	135.04	121.70
1	B	136	ASN	C-N-CA	5.28	134.91	121.70
1	B	206	GLY	N-CA-C	5.09	125.83	113.10
1	D	206	GLY	N-CA-C	5.01	125.63	113.10

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	2569	0	2508	46	0
1	B	2590	0	2552	47	0
1	C	2572	0	2531	46	0
1	D	2568	0	2514	52	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	327	0	0	4	1
4	B	319	0	0	7	1
4	C	312	0	0	4	0
4	D	297	0	0	9	0
All	All	11566	0	10105	177	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 (177) 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:250:ARG:HG3	1:D:250:ARG:HH11	1.24	1.01
1:C:285:ARG:NH1	4:C:1614:HOH:O	2.01	0.92
1:A:174:ASN:HD22	1:A:255:HIS:HE1	1.18	0.91
1:D:0:MET:HG3	1:D:1:MET:H	1.41	0.85
1:C:15:GLU:HG2	1:C:242:ILE:HD13	1.60	0.84
1:D:250:ARG:CG	1:D:250:ARG:HH11	1.91	0.84
1:A:1:MET:HE2	1:A:306:LEU:HG	1.60	0.83
1:A:100:PRO:HG3	1:C:99:MET:HE2	1.64	0.80
1:A:99:MET:HE2	1:C:100:PRO:HG3	1.64	0.79
1:B:72:ARG:NH1	4:B:1588:HOH:O	2.12	0.79
1:D:250:ARG:NH1	1:D:250:ARG:O	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PRO:HG3	1:C:99:MET:CE	2.14	0.78
1:C:252:LYS:NZ	1:C:252:LYS:HB2	1.99	0.77
1:A:99:MET:CE	1:C:100:PRO:HG3	2.17	0.74
1:C:72[B]:ARG:NH1	4:C:1493:HOH:O	2.20	0.74
1:C:83:HIS:HE1	4:C:1505:HOH:O	1.69	0.73
1:A:137:THR:HA	1:A:144:ARG:O	1.88	0.72
1:B:42:LEU:HD21	1:B:245:THR:CG2	2.20	0.71
1:B:252:LYS:HE3	1:B:256:GLU:OE2	1.91	0.71
1:B:1:MET:HE3	1:B:304:GLY:C	2.10	0.70
1:B:21:ALA:HB2	1:C:21:ALA:HB2	1.72	0.69
1:C:1:MET:HE2	1:C:306:LEU:HG	1.73	0.69
1:B:252:LYS:NZ	1:B:252:LYS:HB2	2.05	0.69
1:A:320:HIS:HD2	1:A:322:ASP:H	1.40	0.68
1:D:0:MET:HG3	1:D:1:MET:N	2.09	0.68
1:B:73:GLY:O	1:B:127:PRO:HB3	1.93	0.67
1:C:42:LEU:HD21	1:C:245:THR:CG2	2.24	0.67
1:C:75:GLU:OE2	1:C:101:HIS:HD2	1.78	0.67
1:B:320:HIS:HD2	1:B:322:ASP:H	1.43	0.67
1:D:320:HIS:HD2	1:D:322:ASP:H	1.42	0.66
1:C:257:ASN:ND2	1:C:325:ARG:HE	1.94	0.65
1:A:294:HIS:HD2	4:A:1546:HOH:O	1.81	0.64
1:D:137:THR:HA	1:D:144:ARG:O	1.98	0.62
1:A:62:ASN:ND2	1:A:166:HIS:HE1	1.96	0.62
1:B:128:ARG:NH1	1:B:130:SER:HB3	2.15	0.62
1:B:62:ASN:ND2	1:B:166:HIS:HE1	1.98	0.62
1:C:36:ILE:HD13	1:C:237:ALA:HB2	1.81	0.62
1:B:137:THR:HA	1:B:144:ARG:O	2.00	0.61
1:D:257:ASN:ND2	1:D:325:ARG:HE	1.97	0.61
1:C:73:GLY:O	1:C:127:PRO:HB3	2.01	0.61
1:A:72:ARG:NH1	4:A:1385:HOH:O	2.32	0.60
1:C:137:THR:OG1	1:C:171:ARG:HB2	2.01	0.60
1:B:128:ARG:HH11	1:B:130:SER:HB3	1.66	0.60
1:D:250:ARG:NH1	1:D:250:ARG:CG	2.61	0.60
1:B:15:GLU:HG2	1:B:242:ILE:HD13	1.84	0.59
1:A:21:ALA:HB2	1:D:21:ALA:HB2	1.85	0.59
1:C:294:HIS:HE1	1:C:312:ASP:OD1	1.86	0.59
1:C:137:THR:CG2	1:C:175:ALA:HB2	2.33	0.59
1:C:62:ASN:ND2	1:C:166:HIS:HE1	2.01	0.58
1:A:257:ASN:ND2	1:A:325:ARG:HE	2.02	0.58
1:D:72:ARG:NH1	4:D:1383:HOH:O	2.30	0.58
1:D:308:ASN:ND2	4:D:1544:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:THR:OG1	1:B:171:ARG:HB2	2.04	0.57
1:A:1:MET:HE3	1:A:304:GLY:C	2.24	0.57
1:B:252:LYS:HZ1	1:B:252:LYS:HB2	1.69	0.56
1:C:252:LYS:HZ3	1:C:252:LYS:HB2	1.68	0.56
1:B:62:ASN:HD22	1:B:166:HIS:HE1	1.53	0.56
1:D:291:VAL:HG11	1:D:342:PHE:CD1	2.40	0.56
1:C:166:HIS:HD2	1:C:192:SER:OG	1.88	0.56
1:D:101:HIS:HE1	4:D:1477:HOH:O	1.88	0.56
1:D:294:HIS:HD2	4:D:1463:HOH:O	1.88	0.56
1:C:1:MET:HE3	1:C:304:GLY:C	2.27	0.55
1:D:137:THR:OG1	1:D:171:ARG:HB2	2.06	0.55
1:A:314:GLU:OE2	4:A:1610:HOH:O	2.17	0.55
1:C:137:THR:HA	1:C:144:ARG:O	2.06	0.54
1:A:174:ASN:HD22	1:A:255:HIS:CE1	2.11	0.54
1:B:36:ILE:HD13	1:B:237:ALA:HB2	1.90	0.54
1:D:250:ARG:NH1	1:D:250:ARG:HG3	2.05	0.54
1:B:95:LEU:HD22	1:C:95:LEU:HD22	1.90	0.54
1:D:83:HIS:HD2	1:D:88:GLU:OE2	1.90	0.54
1:C:320:HIS:HD2	1:C:322:ASP:H	1.56	0.53
1:B:83:HIS:HE1	4:B:1529:HOH:O	1.90	0.53
1:C:62:ASN:HD22	1:C:166:HIS:HE1	1.56	0.53
1:A:73:GLY:O	1:A:127:PRO:HB3	2.09	0.53
1:A:137:THR:HG23	1:A:175:ALA:HB2	1.89	0.53
1:A:62:ASN:HD22	1:A:166:HIS:HE1	1.55	0.53
1:B:166:HIS:HD2	1:B:192:SER:OG	1.91	0.53
1:A:294:HIS:HE1	1:A:312:ASP:OD1	1.93	0.52
1:A:166:HIS:HD2	1:A:192:SER:OG	1.93	0.52
1:D:291:VAL:HG11	1:D:342:PHE:CE1	2.45	0.52
1:B:83:HIS:HD2	1:B:88:GLU:OE2	1.92	0.52
1:D:260:PHE:CZ	1:D:264:LYS:HE3	2.45	0.51
1:D:291:VAL:CG1	1:D:342:PHE:CD1	2.94	0.51
1:D:294:HIS:HE1	1:D:312:ASP:OD1	1.94	0.51
1:A:50:GLU:HB3	1:A:213:ARG:HG3	1.93	0.51
1:A:21:ALA:HB2	1:D:21:ALA:CB	2.42	0.50
1:C:72[A]:ARG:HG2	1:C:72[A]:ARG:HH11	1.76	0.50
1:D:320:HIS:CD2	1:D:322:ASP:H	2.27	0.50
1:B:137:THR:CG2	1:B:175:ALA:HB2	2.41	0.50
1:D:201:LEU:HB3	1:D:243:ALA:HB1	1.92	0.50
1:D:62:ASN:OD1	1:D:166:HIS:HE1	1.94	0.50
1:A:48:GLY:HA3	1:A:184:LYS:HE3	1.94	0.50
1:D:140:ARG:HD2	1:D:140:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ARG:NH1	1:D:250:ARG:C	2.64	0.49
1:C:137:THR:HG23	1:C:175:ALA:HB2	1.95	0.49
1:A:100:PRO:HG3	1:C:99:MET:HE3	1.92	0.49
1:D:50:GLU:HG3	4:D:1331:HOH:O	2.13	0.49
1:A:137:THR:OG1	1:A:171:ARG:HB2	2.12	0.49
1:A:87:TYR:CD1	1:C:126:PHE:HE1	2.30	0.49
1:D:137:THR:CG2	1:D:175:ALA:HB2	2.43	0.49
1:D:3:ASP:O	1:D:320:HIS:HE1	1.96	0.48
1:A:137:THR:CG2	1:A:175:ALA:HB2	2.43	0.48
1:A:320:HIS:CD2	1:A:322:ASP:H	2.27	0.48
1:D:298:GLU:HG2	4:D:1541:HOH:O	2.12	0.48
1:A:83:HIS:HD2	1:A:88:GLU:OE2	1.97	0.48
1:D:0:MET:N	4:D:1401:HOH:O	2.38	0.48
1:B:120:ARG:HH22	1:D:86:TRP:HA	1.78	0.48
1:D:166:HIS:HD2	1:D:192:SER:OG	1.96	0.47
1:A:128:ARG:HH11	1:A:130:SER:HB3	1.79	0.47
1:C:171:ARG:NH1	1:C:199:LLP:O3	2.48	0.47
1:A:3:ASP:O	1:A:320:HIS:HE1	1.97	0.47
1:D:36:ILE:HD13	1:D:237:ALA:HB2	1.96	0.47
1:A:99:MET:HE3	1:C:100:PRO:HG3	1.96	0.47
1:B:201:LEU:HB3	1:B:243:ALA:HB1	1.96	0.47
1:B:323:VAL:O	1:B:323:VAL:HG23	2.15	0.46
1:A:278:LYS:HG3	4:A:1391:HOH:O	2.15	0.46
1:B:278:LYS:HE3	4:B:1477:HOH:O	2.15	0.46
1:C:83:HIS:HD2	1:C:88:GLU:OE2	1.98	0.46
1:A:121:PRO:HG2	1:A:126:PHE:CE2	2.50	0.46
1:B:1:MET:HE3	1:B:304:GLY:CA	2.45	0.46
1:A:257:ASN:HD22	1:A:325:ARG:HH21	1.63	0.46
1:B:1:MET:HE2	1:B:306:LEU:HG	1.97	0.46
1:C:72[A]:ARG:HG2	1:C:72[A]:ARG:NH1	2.32	0.45
1:D:296:PHE:HD2	1:D:315:ILE:CD1	2.30	0.45
1:C:257:ASN:HD22	1:C:325:ARG:HE	1.61	0.45
1:C:3:ASP:O	1:C:320:HIS:HE1	2.00	0.45
1:D:250:ARG:C	1:D:250:ARG:HH11	2.20	0.45
1:C:88:GLU:C	1:C:89:VAL:HG23	2.36	0.45
1:D:128:ARG:NH1	4:D:1429:HOH:O	2.48	0.45
1:D:171:ARG:NH1	1:D:199:LLP:O3	2.50	0.45
1:A:171:ARG:NH1	1:A:199:LLP:O3	2.49	0.45
1:B:128:ARG:NH1	1:B:130:SER:CB	2.79	0.45
1:B:1:MET:HE3	1:B:304:GLY:HA2	1.98	0.45
1:C:1:MET:HE3	1:C:1:MET:HB3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:HIS:HD2	4:C:1422:HOH:O	1.99	0.45
1:B:1:MET:HE2	1:B:306:LEU:CD2	2.48	0.44
1:C:252:LYS:NZ	1:C:252:LYS:CB	2.74	0.44
1:A:123:ASN:HB3	1:A:126:PHE:CD2	2.53	0.44
1:B:1:MET:CA	4:B:1507:HOH:O	2.65	0.44
1:B:320:HIS:CD2	1:B:322:ASP:H	2.28	0.44
1:D:291:VAL:HG13	1:D:342:PHE:HD1	1.82	0.44
1:D:102:PRO:HD2	4:D:1512:HOH:O	2.16	0.44
1:D:257:ASN:HD22	1:D:325:ARG:HE	1.63	0.44
1:B:171:ARG:NH1	1:B:199:LLP:O3	2.51	0.44
1:C:137:THR:HG22	1:C:175:ALA:HB2	1.98	0.43
1:B:62:ASN:HD22	1:B:166:HIS:CE1	2.35	0.43
1:A:15:GLU:HG2	1:A:242:ILE:HD13	2.01	0.43
1:D:311:SER:OG	1:D:314:GLU:N	2.51	0.43
1:A:128:ARG:NH1	1:A:130:SER:CB	2.81	0.43
1:A:62:ASN:HD22	1:A:166:HIS:CE1	2.37	0.43
1:A:126:PHE:HA	1:A:127:PRO:HD3	1.93	0.42
1:A:128:ARG:NH1	1:A:130:SER:HB3	2.34	0.42
1:B:320:HIS:H	1:B:323:VAL:CG2	2.32	0.42
1:D:338:LEU:O	1:D:342:PHE:HD2	2.02	0.42
1:B:259:ARG:HG3	4:B:1452:HOH:O	2.19	0.42
1:B:75:GLU:OE1	1:B:101:HIS:HD2	2.01	0.42
1:A:1:MET:HE3	1:A:304:GLY:O	2.19	0.42
1:B:198:SER:HA	1:B:203:ALA:O	2.20	0.42
1:C:126:PHE:HA	1:C:127:PRO:HD3	1.94	0.42
1:B:287:ASP:CB	4:B:1616:HOH:O	2.67	0.42
1:C:16:MET:O	1:C:20:MET:HG3	2.20	0.42
1:D:75:GLU:OE2	1:D:101:HIS:HD2	2.02	0.42
1:A:137:THR:CA	1:A:144:ARG:O	2.62	0.41
1:A:293:ALA:O	1:A:297:ILE:HG12	2.20	0.41
1:B:3:ASP:O	1:B:320:HIS:HE1	2.04	0.41
1:B:42:LEU:HD21	1:B:245:THR:HG22	2.01	0.41
1:B:83:HIS:CD2	1:B:88:GLU:HG3	2.56	0.41
1:D:257:ASN:HA	1:D:257:ASN:HD22	1.69	0.41
1:B:1:MET:HA	4:B:1507:HOH:O	2.20	0.41
1:B:137:THR:HG22	1:B:175:ALA:HB2	2.03	0.41
1:D:286:THR:HG22	1:D:289:LEU:HD12	2.03	0.41
1:D:291:VAL:CG1	1:D:342:PHE:HD1	2.32	0.41
1:B:87:TYR:CD1	1:D:126:PHE:HE1	2.38	0.41
1:D:195:PHE:CE1	1:D:208:VAL:HB	2.56	0.41
1:C:123:ASN:HB3	1:C:126:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:MET:HB2	1:C:227:GLY:HA3	2.03	0.40
1:D:33:ASP:HA	1:D:34:PRO:HD3	1.92	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)
4:A:1563:HOH:O	4:B:1587:HOH:O[1_455]	2.17	0.03

## 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	340/347 (98%)	335 (98%)	4 (1%)	1 (0%)	41 27
1	B	340/347 (98%)	333 (98%)	6 (2%)	1 (0%)	41 27
1	C	341/347 (98%)	335 (98%)	5 (2%)	1 (0%)	41 27
1	D	341/347 (98%)	334 (98%)	6 (2%)	1 (0%)	41 27
All	All	1362/1388 (98%)	1337 (98%)	21 (2%)	4 (0%)	41 27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	137	THR
1	C	137	THR
1	D	137	THR
1	A	137	THR

### 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	262/283 (93%)	257 (98%)	5 (2%)	57	46
1	B	266/283 (94%)	261 (98%)	5 (2%)	57	46
1	C	260/283 (92%)	255 (98%)	5 (2%)	57	46
1	D	260/283 (92%)	256 (98%)	4 (2%)	65	56
All	All	1048/1132 (93%)	1029 (98%)	19 (2%)	59	48

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	78	LEU
1	A	89	VAL
1	A	213	ARG
1	A	255	HIS
1	B	1	MET
1	B	78	LEU
1	B	89	VAL
1	B	252	LYS
1	B	312	ASP
1	C	1	MET
1	C	78	LEU
1	C	89	VAL
1	C	252	LYS
1	C	326	ASN
1	D	78	LEU
1	D	89	VAL
1	D	140	ARG
1	D	250	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	83	HIS
1	A	161	HIS
1	A	166	HIS
1	A	255	HIS
1	A	257	ASN
1	A	294	HIS
1	A	320	HIS
1	B	62	ASN
1	B	83	HIS
1	B	101	HIS
1	B	161	HIS
1	B	166	HIS
1	B	320	HIS
1	C	62	ASN
1	C	63	GLN
1	C	71	GLN
1	C	83	HIS
1	C	101	HIS
1	C	161	HIS
1	C	166	HIS
1	C	257	ASN
1	C	294	HIS
1	C	320	HIS
1	C	326	ASN
1	D	71	GLN
1	D	83	HIS
1	D	101	HIS
1	D	107	ASN
1	D	125	HIS
1	D	166	HIS
1	D	257	ASN
1	D	294	HIS
1	D	308	ASN
1	D	320	HIS
1	D	333	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.



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

4 non-standard protein/DNA/RNA residues 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
1	LLP	C	199	1	23,24,25	3.41	6 (26%)	25,32,34	2.51	11 (44%)
1	LLP	D	199	1	23,24,25	3.50	7 (30%)	25,32,34	2.51	10 (40%)
1	LLP	A	199	1	23,24,25	3.45	8 (34%)	25,32,34	2.51	11 (44%)
1	LLP	B	199	1	23,24,25	3.47	7 (30%)	25,32,34	2.54	10 (40%)

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
1	LLP	C	199	1	-	7/16/17/19	0/1/1/1
1	LLP	D	199	1	-	8/16/17/19	0/1/1/1
1	LLP	A	199	1	-	7/16/17/19	0/1/1/1
1	LLP	B	199	1	-	7/16/17/19	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	199	LLP	C4-C5	12.50	1.57	1.42
1	B	199	LLP	C4-C5	12.38	1.57	1.42
1	A	199	LLP	C4-C5	12.24	1.57	1.42
1	C	199	LLP	C4-C5	12.14	1.57	1.42
1	D	199	LLP	C3-C2	7.81	1.48	1.40
1	A	199	LLP	C3-C2	7.76	1.48	1.40
1	B	199	LLP	C3-C2	7.74	1.48	1.40
1	C	199	LLP	C3-C2	7.44	1.48	1.40
1	B	199	LLP	C2-N1	4.12	1.41	1.33
1	A	199	LLP	C2-N1	4.08	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	199	LLP	C2-N1	4.05	1.41	1.33
1	D	199	LLP	C2-N1	4.02	1.41	1.33
1	C	199	LLP	C4'-NZ	3.48	1.39	1.27
1	B	199	LLP	C6-N1	3.35	1.41	1.34
1	A	199	LLP	C6-N1	3.33	1.41	1.34
1	C	199	LLP	C6-N1	3.33	1.41	1.34
1	D	199	LLP	C6-N1	3.28	1.41	1.34
1	B	199	LLP	C4'-NZ	3.24	1.38	1.27
1	D	199	LLP	C4'-NZ	3.23	1.38	1.27
1	A	199	LLP	C4'-NZ	3.17	1.37	1.27
1	C	199	LLP	P-OP3	-2.15	1.46	1.54
1	D	199	LLP	C5'-C5	2.15	1.56	1.50
1	A	199	LLP	C4-C3	2.14	1.44	1.40
1	B	199	LLP	P-OP3	-2.08	1.46	1.54
1	A	199	LLP	C5'-C5	2.08	1.56	1.50
1	D	199	LLP	P-OP3	-2.08	1.46	1.54
1	B	199	LLP	C4-C3	2.07	1.43	1.40
1	A	199	LLP	P-OP3	-2.05	1.46	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	LLP	C2'-C2-C3	6.21	128.56	120.89
1	A	199	LLP	C2'-C2-C3	6.20	128.54	120.89
1	D	199	LLP	C2'-C2-C3	6.16	128.49	120.89
1	C	199	LLP	C2'-C2-C3	6.10	128.43	120.89
1	B	199	LLP	CE-NZ-C4'	4.44	132.54	118.90
1	D	199	LLP	CE-NZ-C4'	4.42	132.47	118.90
1	A	199	LLP	CE-NZ-C4'	4.41	132.44	118.90
1	C	199	LLP	CE-NZ-C4'	4.34	132.22	118.90
1	D	199	LLP	C6-N1-C2	4.22	126.98	119.17
1	A	199	LLP	C6-N1-C2	4.20	126.95	119.17
1	B	199	LLP	C6-N1-C2	4.20	126.94	119.17
1	C	199	LLP	C6-N1-C2	4.13	126.81	119.17
1	B	199	LLP	OP4-C5'-C5	3.67	116.35	109.35
1	D	199	LLP	OP4-C5'-C5	3.67	116.34	109.35
1	A	199	LLP	OP4-C5'-C5	3.63	116.28	109.35
1	B	199	LLP	C3-C2-N1	-3.62	116.09	120.77
1	A	199	LLP	C3-C2-N1	-3.62	116.09	120.77
1	D	199	LLP	C3-C2-N1	-3.61	116.10	120.77
1	C	199	LLP	C3-C2-N1	-3.57	116.16	120.77
1	D	199	LLP	C4-C4'-NZ	-3.56	107.99	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	LLP	OP4-C5'-C5	3.51	116.03	109.35
1	C	199	LLP	C4-C4'-NZ	-3.41	108.65	124.31
1	A	199	LLP	C4-C4'-NZ	-3.39	108.73	124.31
1	B	199	LLP	C4-C4'-NZ	-3.39	108.77	124.31
1	B	199	LLP	C5-C4-C4'	3.36	127.08	121.56
1	C	199	LLP	C5-C4-C4'	3.36	127.08	121.56
1	D	199	LLP	C5-C4-C4'	3.23	126.88	121.56
1	A	199	LLP	C5-C4-C4'	3.12	126.68	121.56
1	C	199	LLP	C5-C6-N1	-2.90	118.99	123.82
1	C	199	LLP	C3-C4-C4'	-2.89	115.02	120.41
1	B	199	LLP	C3-C4-C4'	-2.89	115.03	120.41
1	D	199	LLP	C5-C6-N1	-2.87	119.03	123.82
1	B	199	LLP	C5-C6-N1	-2.87	119.04	123.82
1	A	199	LLP	C5-C6-N1	-2.86	119.06	123.82
1	D	199	LLP	C3-C4-C4'	-2.81	115.17	120.41
1	A	199	LLP	C3-C4-C4'	-2.70	115.39	120.41
1	A	199	LLP	O3-C3-C4	2.26	125.68	119.60
1	C	199	LLP	O3-C3-C4	2.24	125.61	119.60
1	B	199	LLP	O3-C3-C4	2.23	125.59	119.60
1	D	199	LLP	O3-C3-C4	2.10	125.24	119.60
1	C	199	LLP	O3-C3-C2	-2.04	113.05	117.49
1	A	199	LLP	O3-C3-C2	-2.03	113.08	117.49

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	199	LLP	C4-C5-C5'-OP4
1	C	199	LLP	C6-C5-C5'-OP4
1	C	199	LLP	O-C-CA-CB
1	D	199	LLP	C4-C5-C5'-OP4
1	D	199	LLP	C6-C5-C5'-OP4
1	D	199	LLP	O-C-CA-CB
1	A	199	LLP	C4-C5-C5'-OP4
1	A	199	LLP	C6-C5-C5'-OP4
1	A	199	LLP	O-C-CA-CB
1	B	199	LLP	C4-C5-C5'-OP4
1	B	199	LLP	C6-C5-C5'-OP4
1	B	199	LLP	O-C-CA-CB
1	B	199	LLP	CG-CD-CE-NZ
1	C	199	LLP	C3-C4-C4'-NZ
1	D	199	LLP	C3-C4-C4'-NZ

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Mol	Chain	Res	Type	Atoms
1	A	199	LLP	C3-C4-C4'-NZ
1	B	199	LLP	C3-C4-C4'-NZ
1	D	199	LLP	CD-CE-NZ-C4'
1	C	199	LLP	CG-CD-CE-NZ
1	D	199	LLP	CG-CD-CE-NZ
1	A	199	LLP	CG-CD-CE-NZ
1	A	199	LLP	CD-CE-NZ-C4'
1	C	199	LLP	CD-CE-NZ-C4'
1	B	199	LLP	CD-CE-NZ-C4'
1	D	199	LLP	C5-C4-C4'-NZ
1	D	199	LLP	C5'-OP4-P-OP2
1	C	199	LLP	C5-C4-C4'-NZ
1	A	199	LLP	C5-C4-C4'-NZ
1	B	199	LLP	C5-C4-C4'-NZ

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	199	LLP	1	0
1	D	199	LLP	1	0
1	A	199	LLP	1	0
1	B	199	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	342/347 (98%)	0.03	5 (1%) 73 70	10, 16, 25, 31	0
1	B	342/347 (98%)	-0.01	8 (2%) 60 56	9, 15, 26, 32	0
1	C	342/347 (98%)	0.12	8 (2%) 60 56	11, 17, 27, 35	0
1	D	343/347 (98%)	0.07	9 (2%) 56 51	10, 15, 30, 37	0
All	All	1369/1388 (98%)	0.05	30 (2%) 62 57	9, 16, 27, 37	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	137	THR	5.3
1	D	137	THR	5.1
1	B	137	THR	4.7
1	A	137	THR	4.1
1	C	333	ASN	3.3
1	A	156	THR	3.2
1	C	1	MET	3.1
1	D	293	ALA	2.9
1	A	22	GLN	2.7
1	A	21	ALA	2.6
1	D	343	SER	2.6
1	B	298	GLU	2.5
1	C	326	ASN	2.5
1	B	1	MET	2.5
1	C	302	ASN	2.3
1	A	113	ASP	2.3
1	B	335	PHE	2.3
1	D	136	ASN	2.3
1	D	160	GLU	2.2
1	C	21	ALA	2.2
1	C	136	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	301	ARG	2.2
1	B	113	ASP	2.2
1	D	313	THR	2.2
1	D	338	LEU	2.2
1	D	0	MET	2.2
1	B	136	ASN	2.1
1	B	312	ASP	2.1
1	B	302	ASN	2.1
1	D	311	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	LLP	A	199	24/25	0.92	0.13	11,19,21,21	0
1	LLP	D	199	24/25	0.93	0.12	13,18,22,24	0
1	LLP	C	199	24/25	0.93	0.11	11,19,22,23	0
1	LLP	B	199	24/25	0.94	0.11	11,18,21,21	0

## 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<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(Å <sup>2</sup> )	Q<0.9
3	CL	B	1308	1/1	0.98	0.05	23,23,23,23	0
3	CL	D	1310	1/1	0.99	0.04	25,25,25,25	0
3	CL	A	1306	1/1	0.99	0.04	17,17,17,17	0
3	CL	A	1311	1/1	0.99	0.04	24,24,24,24	0
2	CA	C	1300	1/1	0.99	0.03	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	B	1304	1/1	0.99	0.07	19,19,19,19	0
3	CL	C	1309	1/1	0.99	0.04	21,21,21,21	0
3	CL	C	1307	1/1	0.99	0.06	19,19,19,19	0
2	CA	D	1305	1/1	0.99	0.05	13,13,13,13	0
2	CA	A	1301	1/1	1.00	0.04	15,15,15,15	0
2	CA	A	1302	1/1	1.00	0.04	15,15,15,15	0
2	CA	B	1303	1/1	1.00	0.04	16,16,16,16	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.