



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 02:38 PM EST

PDB ID : 1JG8  
Title : Crystal Structure of Threonine Aldolase (Low-specificity)  
Authors : Kielkopf, C.L.; Bonanno, J.; Ray, S.; Burley, S.K.; New York SGX Research  
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Deposited on : 2001-06-23  
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

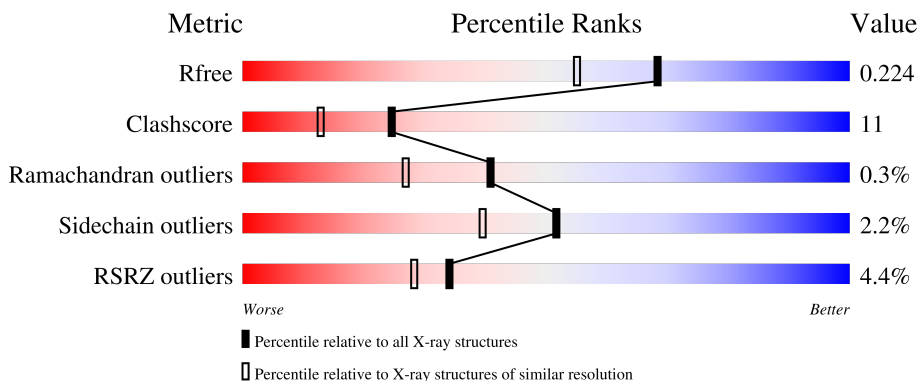
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

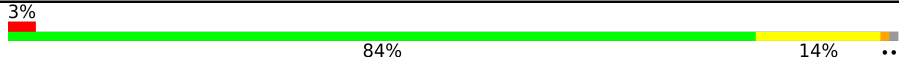



The reported resolution of this entry is 1.80 Å.

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	 3% 84% 14% ..
1	B	347	 3% 83% 14% ..
1	C	347	 4% 84% 12% ..
1	D	347	 7% 80% 18% ..

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11435 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	Total 2639	C 1648	N 472	O 502	P 1	S 16	0	0	0
1	B	343	Total 2649	C 1654	N 476	O 502	P 1	S 16	0	0	0
1	C	340	Total 2641	C 1649	N 476	O 499	P 1	S 16	0	1	0
1	D	344	Total 2657	C 1659	N 477	O 503	P 1	S 17	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9X266
A	2	PRO	-	cloning artifact	UNP Q9X266
A	3	HIS	-	cloning artifact	UNP Q9X266
A	4	MET	-	cloning artifact	UNP Q9X266
A	203	LLP	LYS	modified residue	UNP Q9X266
B	1	GLY	-	cloning artifact	UNP Q9X266
B	2	PRO	-	cloning artifact	UNP Q9X266
B	3	HIS	-	cloning artifact	UNP Q9X266
B	4	MET	-	cloning artifact	UNP Q9X266
B	203	LLP	LYS	modified residue	UNP Q9X266
C	1	GLY	-	cloning artifact	UNP Q9X266
C	2	PRO	-	cloning artifact	UNP Q9X266
C	3	HIS	-	cloning artifact	UNP Q9X266
C	4	MET	-	cloning artifact	UNP Q9X266
C	203	LLP	LYS	modified residue	UNP Q9X266
D	1	GLY	-	cloning artifact	UNP Q9X266
D	2	PRO	-	cloning artifact	UNP Q9X266
D	3	HIS	-	cloning artifact	UNP Q9X266
D	4	MET	-	cloning artifact	UNP Q9X266
D	203	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	1	Total Ca 1 1	0	0
2	D	2	Total Ca 2 2	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0

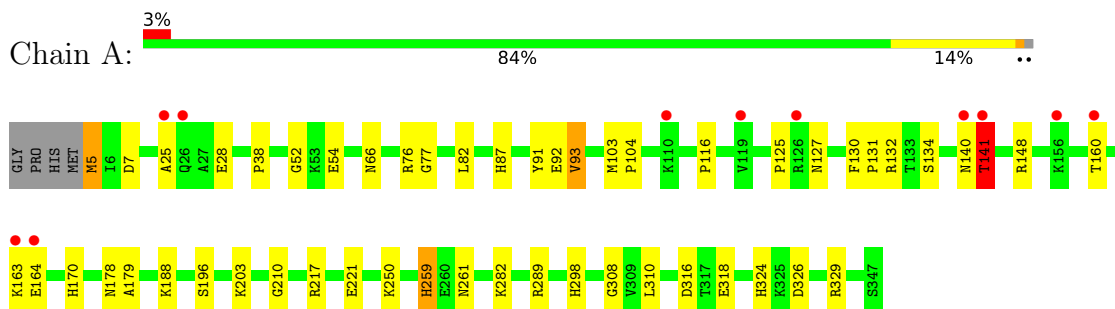
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	229	Total O 229 229	0	0
4	B	211	Total O 211 211	0	0
4	C	197	Total O 197 197	0	0
4	D	204	Total O 204 204	0	0

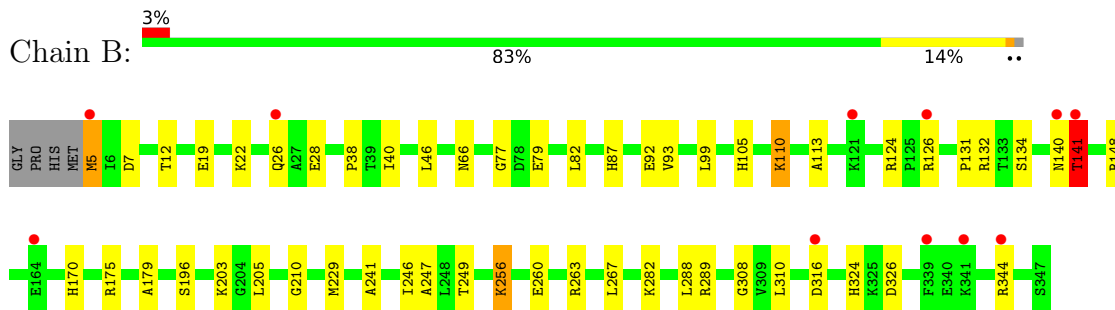
### 3 Residue-property plots [i](#)

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.

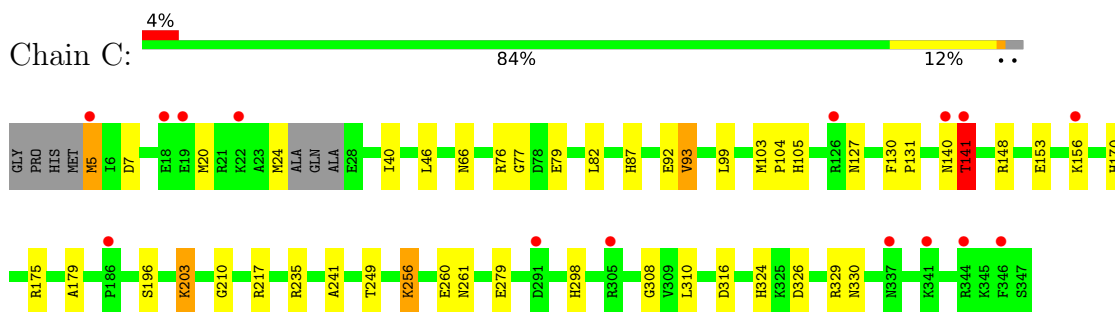
- Molecule 1: L-allo-threonine aldolase



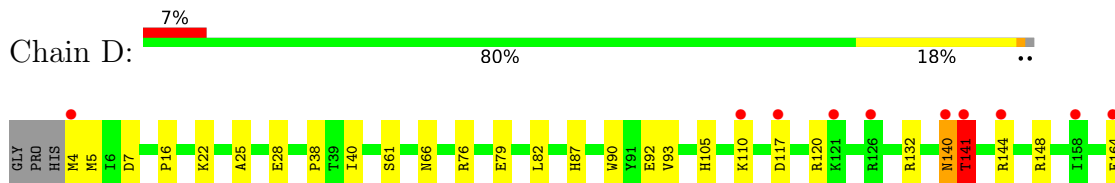
- Molecule 1: L-allo-threonine aldolase

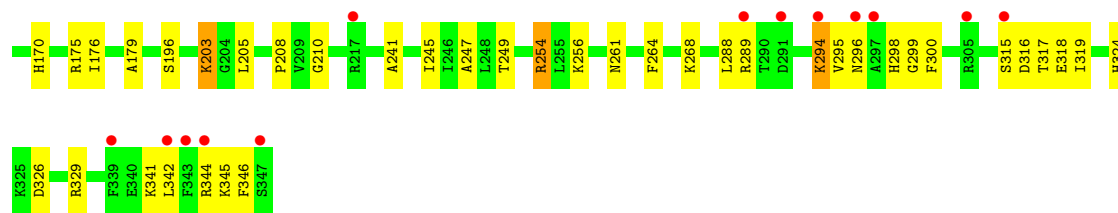


- Molecule 1: L-allo-threonine aldolase



- 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)	100.0 (20.00-1.80) 98.5 (19.94-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.87 (at 1.80Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.207 , 0.222 0.208 , 0.224	Depositor DCC
$R_{free}$ test set	9326 reflections (7.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.1	Xtrriage
Anisotropy	0.011	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.56 , 68.4	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	11435	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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, LLP

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	0.38	0/2655	0.71	4/3583 (0.1%)
1	B	0.38	0/2665	0.72	4/3594 (0.1%)
1	C	0.37	0/2656	0.71	5/3579 (0.1%)
1	D	0.39	0/2673	0.73	5/3604 (0.1%)
All	All	0.38	0/10649	0.72	18/14360 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	THR	N-CA-C	-11.49	79.97	111.00
1	A	141	THR	N-CA-C	-11.43	80.15	111.00
1	D	141	THR	N-CA-C	-11.25	80.62	111.00
1	C	141	THR	N-CA-C	-11.22	80.71	111.00
1	A	141	THR	N-CA-CB	7.75	125.03	110.30
1	B	141	THR	N-CA-CB	7.46	124.48	110.30
1	D	141	THR	N-CA-CB	7.43	124.42	110.30
1	C	141	THR	N-CA-CB	7.38	124.32	110.30
1	D	140	ASN	C-N-CA	6.60	138.19	121.70
1	B	140	ASN	C-N-CA	6.58	138.14	121.70
1	C	140	ASN	C-N-CA	6.53	138.03	121.70
1	A	140	ASN	C-N-CA	6.26	137.35	121.70
1	A	210	GLY	N-CA-C	5.47	126.77	113.10
1	D	140	ASN	CA-C-N	-5.30	105.54	117.20
1	C	140	ASN	CA-C-N	-5.24	105.67	117.20
1	D	210	GLY	N-CA-C	5.13	125.91	113.10
1	C	210	GLY	N-CA-C	5.11	125.89	113.10
1	B	210	GLY	N-CA-C	5.06	125.76	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	2639	0	2639	50	0
1	B	2649	0	2661	66	0
1	C	2641	0	2654	64	0
1	D	2657	0	2670	73	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	229	0	0	1	0
4	B	211	0	0	10	0
4	C	197	0	0	6	0
4	D	204	0	0	10	0
All	All	11435	0	10624	231	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (231) 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:ARG:NH1	1:D:254:ARG:O	1.98	0.97
1:B:110:LYS:HE3	1:B:113:ALA:HB3	1.47	0.95
1:A:178:ASN:HD22	1:A:259:HIS:HE1	1.15	0.94
1:D:254:ARG:HG3	1:D:254:ARG:HH11	1.34	0.92
1:B:263:ARG:NH1	1:B:267:LEU:HD11	1.85	0.91
1:D:254:ARG:CG	1:D:254:ARG:HH11	1.86	0.88
1:C:256:LYS:HB2	1:C:256:LYS:NZ	1.87	0.87
1:A:289:ARG:HD2	1:A:318:GLU:HG2	1.56	0.86
1:D:341:LYS:HD3	1:D:344:ARG:NH1	1.91	0.85
1:D:4:MET:HG3	1:D:5:MET:H	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:LYS:HD3	1:D:344:ARG:HH12	1.43	0.83
1:B:110:LYS:HE2	4:B:1107:HOH:O	1.78	0.82
1:A:104:PRO:HG3	1:C:103:MET:CE	2.12	0.79
1:D:341:LYS:CD	1:D:344:ARG:HH12	1.95	0.79
1:A:103:MET:HE2	1:C:104:PRO:HG3	1.64	0.78
1:B:229:MET:CB	1:C:93:VAL:HG11	2.12	0.78
1:D:144:ARG:O	1:D:144:ARG:HD2	1.85	0.76
1:A:141:THR:HA	1:A:148:ARG:O	1.85	0.76
1:B:110:LYS:CE	4:B:1107:HOH:O	2.31	0.76
1:C:279:GLU:N	1:C:279:GLU:OE1	2.15	0.75
1:B:46:LEU:HD21	1:B:249:THR:CG2	2.17	0.74
1:A:103:MET:CE	1:C:104:PRO:HG3	2.17	0.74
1:A:5:MET:HE2	1:A:310:LEU:HG	1.69	0.74
1:D:16:PRO:HG3	1:D:208:PRO:HG3	1.67	0.74
1:B:256:LYS:HE3	1:B:260:GLU:OE2	1.88	0.73
1:D:28:GLU:HG2	1:D:38:PRO:HG2	1.69	0.73
1:D:341:LYS:CE	1:D:344:ARG:HH12	2.02	0.72
1:B:229:MET:CA	1:C:93:VAL:HG11	2.20	0.72
1:B:5:MET:HE3	1:B:308:GLY:C	2.10	0.72
1:B:229:MET:HB2	1:C:93:VAL:HG11	1.72	0.71
1:A:324:HIS:HD2	1:A:326:ASP:H	1.37	0.70
1:B:256:LYS:NZ	1:B:256:LYS:HB2	2.06	0.69
1:C:46:LEU:HD21	1:C:249:THR:CG2	2.23	0.69
1:A:104:PRO:HG3	1:C:103:MET:HE2	1.74	0.68
1:A:66:ASN:ND2	1:A:170:HIS:HE1	1.91	0.68
1:B:77:GLY:O	1:B:131:PRO:HB3	1.93	0.68
1:C:153:GLU:OE1	1:C:156:LYS:HE2	1.94	0.68
1:C:256:LYS:HB2	1:C:256:LYS:HZ3	1.57	0.68
1:A:289:ARG:CD	1:A:318:GLU:HG2	2.23	0.67
1:B:324:HIS:HD2	1:B:326:ASP:H	1.42	0.67
1:B:229:MET:HA	1:C:93:VAL:HG11	1.75	0.67
1:C:93:VAL:HG13	1:C:93:VAL:O	1.94	0.67
1:D:324:HIS:HD2	1:D:326:ASP:H	1.41	0.67
1:A:5:MET:HE3	1:A:308:GLY:C	2.15	0.66
1:B:110:LYS:HE3	1:B:113:ALA:CB	2.23	0.65
1:D:4:MET:HG3	1:D:5:MET:N	2.10	0.65
1:C:261:ASN:ND2	1:C:329:ARG:HE	1.94	0.65
1:B:66:ASN:HD22	1:B:170:HIS:HE1	1.45	0.65
1:C:79:GLU:OE2	1:C:105:HIS:HD2	1.80	0.65
1:D:4:MET:N	4:D:997:HOH:O	2.30	0.64
1:B:66:ASN:ND2	1:B:170:HIS:HE1	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PRO:HG3	1:C:103:MET:HE3	1.78	0.63
1:A:66:ASN:HD22	1:A:170:HIS:HE1	1.45	0.63
1:D:254:ARG:NH1	1:D:254:ARG:C	2.52	0.63
1:D:254:ARG:CB	1:D:254:ARG:HH11	2.11	0.63
1:A:261:ASN:ND2	1:A:329:ARG:HE	1.98	0.62
1:C:5:MET:HE2	1:C:310:LEU:HG	1.82	0.62
1:B:229:MET:HG3	1:C:93:VAL:CG1	2.30	0.61
1:D:261:ASN:ND2	1:D:329:ARG:HE	1.97	0.61
1:D:141:THR:HA	1:D:148:ARG:O	1.99	0.61
1:B:110:LYS:HD2	1:B:110:LYS:O	1.99	0.61
1:A:221:GLU:OE2	1:B:126:ARG:NH2	2.33	0.61
1:B:132:ARG:NH1	1:B:134:SER:HB3	2.16	0.61
1:D:254:ARG:C	1:D:254:ARG:HH11	2.04	0.60
1:D:298:HIS:HD2	4:D:1062:HOH:O	1.83	0.60
1:D:295:VAL:HG11	1:D:346:PHE:CD1	2.36	0.60
1:B:141:THR:HA	1:B:148:ARG:O	2.01	0.60
1:B:170:HIS:HD2	1:B:196:SER:OG	1.84	0.60
1:C:66:ASN:ND2	1:C:170:HIS:HE1	1.99	0.60
1:C:5:MET:HE3	1:C:308:GLY:C	2.21	0.60
1:A:160:THR:O	1:A:164:GLU:HG3	2.01	0.60
1:C:170:HIS:HD2	1:C:196:SER:OG	1.85	0.60
1:B:132:ARG:HH11	1:B:134:SER:HB3	1.67	0.59
1:C:298:HIS:HE1	1:C:316:ASP:OD1	1.86	0.59
1:A:76:ARG:NH1	4:B:995:HOH:O	2.33	0.59
1:D:105:HIS:HE1	4:D:1075:HOH:O	1.85	0.59
1:C:77:GLY:O	1:C:131:PRO:HB3	2.04	0.58
1:D:87:HIS:HD2	1:D:92:GLU:OE2	1.86	0.58
1:C:66:ASN:HD22	1:C:170:HIS:HE1	1.51	0.58
1:A:5:MET:HE3	1:A:308:GLY:O	2.04	0.58
1:B:87:HIS:HD2	1:B:92:GLU:OE2	1.85	0.58
1:D:295:VAL:CG1	1:D:346:PHE:CD1	2.87	0.58
1:C:40:ILE:HD13	1:C:241:ALA:HB2	1.85	0.57
1:A:178:ASN:HD22	1:A:259:HIS:CE1	2.07	0.57
1:B:5:MET:N	4:B:1105:HOH:O	2.37	0.57
1:D:144:ARG:C	1:D:144:ARG:HD2	2.25	0.57
1:B:141:THR:OG1	1:B:175:ARG:HB2	2.04	0.56
1:C:141:THR:OG1	1:C:175:ARG:HB2	2.04	0.56
1:C:141:THR:CG2	1:C:179:ALA:HB2	2.35	0.56
1:C:175:ARG:NH2	1:C:203:LLP:HE3	2.21	0.56
1:D:254:ARG:NH1	1:D:254:ARG:HG3	2.10	0.56
1:D:264:PHE:CZ	1:D:268:LYS:HE3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:GLU:HG3	4:D:1074:HOH:O	2.05	0.56
1:B:5:MET:CA	4:B:1105:HOH:O	2.52	0.56
1:D:295:VAL:HG11	1:D:346:PHE:CE1	2.40	0.56
1:A:141:THR:HG23	1:A:179:ALA:HB2	1.87	0.56
1:A:170:HIS:HD2	1:A:196:SER:OG	1.89	0.56
1:D:298:HIS:HE1	1:D:316:ASP:OD1	1.89	0.56
1:C:279:GLU:H	1:C:279:GLU:CD	2.04	0.56
1:A:25:ALA:HB2	1:D:25:ALA:HB2	1.89	0.55
1:D:295:VAL:HG13	1:D:346:PHE:HD1	1.71	0.55
1:C:141:THR:HA	1:C:148:ARG:O	2.05	0.55
1:B:229:MET:HA	1:C:93:VAL:CG1	2.36	0.55
1:D:141:THR:OG1	1:D:175:ARG:HB2	2.06	0.55
1:B:229:MET:HG3	1:C:93:VAL:HG13	1.88	0.54
1:A:28:GLU:HG2	1:A:38:PRO:HG2	1.90	0.54
1:C:324:HIS:HD2	1:C:326:ASP:H	1.56	0.54
1:D:120:ARG:HD2	4:D:1101:HOH:O	2.07	0.54
1:A:87:HIS:HD2	1:A:92:GLU:OE2	1.91	0.53
1:A:132:ARG:HH11	1:A:134:SER:HB3	1.74	0.52
1:C:141:THR:HG23	1:C:179:ALA:HB2	1.89	0.52
1:C:76[A]:ARG:HG2	1:C:76[A]:ARG:HH11	1.73	0.52
1:C:76[B]:ARG:HG2	1:C:76[B]:ARG:HH11	1.73	0.52
1:A:77:GLY:O	1:A:131:PRO:HB3	2.10	0.52
1:D:342:LEU:O	1:D:346:PHE:HD2	1.93	0.52
1:B:99:LEU:HD22	1:C:99:LEU:HD22	1.92	0.52
1:C:92:GLU:O	1:C:93:VAL:HG12	2.10	0.51
1:D:120:ARG:NE	4:D:1101:HOH:O	2.41	0.51
1:D:324:HIS:CD2	1:D:326:ASP:H	2.26	0.51
1:D:170:HIS:HD2	1:D:196:SER:OG	1.93	0.51
1:C:87:HIS:HD2	1:C:92:GLU:OE2	1.93	0.51
1:A:91:TYR:CD1	1:C:130:PHE:HE1	2.28	0.51
1:A:298:HIS:HE1	1:A:316:ASP:OD1	1.94	0.51
1:A:324:HIS:CD2	1:A:326:ASP:H	2.24	0.51
1:C:256:LYS:HB2	1:C:256:LYS:HZ2	1.72	0.50
1:D:132:ARG:NH1	4:D:1027:HOH:O	2.43	0.50
1:A:289:ARG:HD2	1:A:318:GLU:CG	2.35	0.50
1:B:344:ARG:HG3	4:B:1080:HOH:O	2.11	0.50
1:C:5:MET:HE3	1:C:308:GLY:O	2.12	0.50
1:B:110:LYS:O	1:B:110:LYS:CD	2.60	0.49
1:B:66:ASN:HD22	1:B:170:HIS:CE1	2.30	0.49
1:D:66:ASN:OD1	1:D:170:HIS:HE1	1.94	0.49
1:B:282:LYS:HE3	4:B:1074:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:970:HOH:O	1:D:76:ARG:NH1	2.37	0.49
1:A:52:GLY:HA3	1:A:188:LYS:HE3	1.95	0.49
1:A:125:PRO:HG2	1:A:130:PHE:CE2	2.48	0.48
1:C:76[A]:ARG:HG2	1:C:76[A]:ARG:NH1	2.28	0.48
1:C:76[B]:ARG:NH1	1:C:76[B]:ARG:HG2	2.28	0.48
1:A:25:ALA:HB2	1:D:25:ALA:CB	2.44	0.48
1:B:40:ILE:HD13	1:B:241:ALA:HB2	1.96	0.48
1:D:205:LEU:HB3	1:D:247:ALA:HB1	1.94	0.48
1:B:5:MET:CE	1:B:308:GLY:C	2.82	0.48
1:D:7:ASP:O	1:D:324:HIS:HE1	1.97	0.48
1:B:141:THR:CG2	1:B:179:ALA:HB2	2.44	0.47
1:B:46:LEU:HD21	1:B:249:THR:HG22	1.93	0.47
1:C:217:ARG:NH2	4:C:1074:HOH:O	2.46	0.47
1:A:261:ASN:HD22	1:A:329:ARG:HH21	1.61	0.47
1:A:5:MET:CE	1:A:308:GLY:C	2.83	0.47
1:D:79:GLU:OE2	1:D:105:HIS:HD2	1.97	0.47
1:A:132:ARG:NH1	1:A:134:SER:CB	2.77	0.47
1:A:7:ASP:O	1:A:324:HIS:HE1	1.97	0.47
1:D:256:LYS:HE3	1:D:256:LYS:HB3	1.56	0.47
1:D:141:THR:CG2	1:D:179:ALA:HB2	2.45	0.47
1:A:103:MET:HE3	1:C:104:PRO:HG3	1.96	0.47
1:B:256:LYS:HZ1	1:B:256:LYS:HB2	1.80	0.47
1:C:5:MET:HB3	1:C:5:MET:HE3	1.76	0.46
1:B:124:ARG:HH22	1:D:90:TRP:HA	1.80	0.46
1:A:282:LYS:HG3	4:A:988:HOH:O	2.15	0.46
1:B:229:MET:CB	1:C:93:VAL:CG1	2.91	0.46
1:C:298:HIS:HD2	4:C:1024:HOH:O	1.97	0.46
1:D:295:VAL:CG1	1:D:346:PHE:HD1	2.23	0.46
1:B:28:GLU:HG2	1:B:38:PRO:HG2	1.98	0.46
1:D:296:ASN:ND2	1:D:299:GLY:H	2.13	0.46
1:D:144:ARG:NH2	4:D:1050:HOH:O	2.47	0.46
1:D:254:ARG:NH1	1:D:254:ARG:CB	2.77	0.46
1:B:19:GLU:HG2	1:B:246:ILE:HD13	1.98	0.46
4:C:956:HOH:O	1:D:76:ARG:HD3	2.15	0.45
1:A:127:ASN:HB3	1:A:130:PHE:CD2	2.52	0.45
1:B:5:MET:HA	4:B:1105:HOH:O	2.14	0.45
1:C:261:ASN:HD22	1:C:329:ARG:HE	1.62	0.45
1:C:7:ASP:O	1:C:324:HIS:HE1	2.00	0.45
1:D:296:ASN:ND2	1:D:298:HIS:H	2.15	0.45
1:D:296:ASN:HD22	1:D:298:HIS:H	1.64	0.45
1:A:5:MET:HB3	1:A:5:MET:HE3	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76[A]:ARG:HD3	4:C:1097:HOH:O	2.15	0.45
1:C:76[B]:ARG:HD3	4:C:1097:HOH:O	2.15	0.45
1:B:141:THR:HG23	1:B:179:ALA:HB2	1.99	0.44
1:D:300:PHE:HD2	1:D:319:ILE:CD1	2.31	0.44
1:D:40:ILE:HD13	1:D:241:ALA:HB2	1.99	0.44
1:B:324:HIS:CD2	1:B:326:ASP:H	2.28	0.44
1:A:132:ARG:NH1	1:A:134:SER:HB3	2.32	0.44
1:D:141:THR:HG23	1:D:179:ALA:HB2	1.99	0.44
1:D:144:ARG:CD	1:D:144:ARG:C	2.86	0.44
1:D:120:ARG:CD	4:D:1101:HOH:O	2.64	0.44
1:D:140:ASN:HB3	1:D:176:ILE:HD13	2.00	0.44
1:B:5:MET:HE3	1:B:308:GLY:CA	2.48	0.44
1:D:315:SER:OG	1:D:318:GLU:N	2.51	0.44
1:D:261:ASN:HD22	1:D:329:ARG:HE	1.62	0.44
1:B:5:MET:HE3	1:B:308:GLY:HA2	2.00	0.43
1:B:132:ARG:NH1	1:B:134:SER:CB	2.81	0.43
1:D:140:ASN:HB3	1:D:176:ILE:CD1	2.48	0.43
1:A:66:ASN:HD22	1:A:170:HIS:CE1	2.29	0.43
1:B:205:LEU:HB3	1:B:247:ALA:HB1	1.99	0.43
1:D:164:GLU:HG3	4:D:1064:HOH:O	2.17	0.43
1:D:294:LYS:HD3	1:D:294:LYS:HA	1.38	0.43
1:B:5:MET:HB3	1:B:5:MET:HE3	1.74	0.43
1:A:141:THR:CA	1:A:148:ARG:O	2.62	0.42
1:A:141:THR:CG2	1:A:179:ALA:HB2	2.49	0.42
1:B:22:LYS:O	1:B:26:GLN:HG3	2.19	0.42
1:B:5:MET:HE2	1:B:310:LEU:CD2	2.50	0.42
1:B:7:ASP:O	1:B:324:HIS:HE1	2.02	0.42
1:A:54:GLU:HB3	1:A:217:ARG:HG3	2.01	0.42
1:C:170:HIS:CD2	1:C:196:SER:OG	2.69	0.42
1:B:79:GLU:OE1	1:B:105:HIS:HD2	2.02	0.42
1:D:61:SER:HB2	1:D:203:LLP:OP1	2.19	0.42
1:C:256:LYS:O	1:C:260:GLU:HG3	2.20	0.42
1:C:5:MET:CE	1:C:308:GLY:C	2.86	0.42
1:B:263:ARG:HG3	4:B:1049:HOH:O	2.20	0.42
1:D:345:LYS:HD2	1:D:346:PHE:CE2	2.55	0.42
1:B:289:ARG:HG3	1:B:289:ARG:NH1	2.35	0.42
1:B:289:ARG:HG3	1:B:289:ARG:HH11	1.84	0.42
1:B:12:THR:HB	1:C:235:ARG:HD2	2.02	0.42
1:B:256:LYS:CB	1:B:256:LYS:NZ	2.81	0.41
1:A:261:ASN:ND2	1:A:329:ARG:HH21	2.19	0.41
1:C:20:MET:O	1:C:24:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:C	1:A:93:VAL:HG23	2.41	0.41
1:B:170:HIS:CD2	1:B:196:SER:OG	2.71	0.41
1:D:245:ILE:O	1:D:249:THR:HG23	2.21	0.41
1:B:288:LEU:C	1:B:288:LEU:HD23	2.41	0.41
1:C:46:LEU:HD21	1:C:249:THR:HG22	1.99	0.41
1:D:296:ASN:HD21	1:D:298:HIS:HB2	1.85	0.41
1:A:217:ARG:HB2	1:A:217:ARG:HE	1.78	0.40
1:B:263:ARG:HH12	1:B:267:LEU:HD11	1.80	0.40
1:C:127:ASN:HB3	1:C:130:PHE:CD2	2.56	0.40
1:C:261:ASN:HD22	1:C:329:ARG:HH21	1.69	0.40
1:B:229:MET:CG	1:C:93:VAL:CG1	2.99	0.40
1:D:261:ASN:HA	1:D:261:ASN:HD22	1.70	0.40
1:D:288:LEU:HD23	1:D:288:LEU:C	2.41	0.40
1:D:289:ARG:HA	1:D:317:THR:O	2.21	0.40
1:B:110:LYS:NZ	4:B:1107:HOH:O	2.48	0.40
1:C:79:GLU:HG2	1:C:105:HIS:HB2	2.03	0.40

There are no symmetry-related clashes.

## 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%)	334 (98%)	5 (2%)	1 (0%)	41 27
1	B	340/347 (98%)	333 (98%)	6 (2%)	1 (0%)	41 27
1	C	336/347 (97%)	330 (98%)	5 (2%)	1 (0%)	41 27
1	D	341/347 (98%)	335 (98%)	5 (2%)	1 (0%)	41 27
All	All	1357/1388 (98%)	1332 (98%)	21 (2%)	4 (0%)	41 27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	THR
1	B	141	THR
1	C	141	THR
1	D	141	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	278/283 (98%)	271 (98%)	7 (2%)	47 34
1	B	280/283 (99%)	274 (98%)	6 (2%)	53 42
1	C	280/283 (99%)	275 (98%)	5 (2%)	59 48
1	D	281/283 (99%)	274 (98%)	7 (2%)	47 34
All	All	1119/1132 (99%)	1094 (98%)	25 (2%)	52 39

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	82	LEU
1	A	93	VAL
1	A	116	PRO
1	A	163	LYS
1	A	250	LYS
1	A	259	HIS
1	B	5	MET
1	B	82	LEU
1	B	93	VAL
1	B	110	LYS
1	B	256	LYS
1	B	316	ASP
1	C	5	MET
1	C	82	LEU
1	C	93	VAL
1	C	256	LYS
1	C	330	ASN

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Mol	Chain	Res	Type
1	D	22	LYS
1	D	82	LEU
1	D	93	VAL
1	D	110	LYS
1	D	117	ASP
1	D	254	ARG
1	D	294	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	87	HIS
1	A	165	HIS
1	A	170	HIS
1	A	259	HIS
1	A	261	ASN
1	A	298	HIS
1	A	324	HIS
1	B	66	ASN
1	B	87	HIS
1	B	105	HIS
1	B	165	HIS
1	B	170	HIS
1	B	324	HIS
1	C	66	ASN
1	C	67	GLN
1	C	87	HIS
1	C	105	HIS
1	C	111	ASN
1	C	165	HIS
1	C	170	HIS
1	C	261	ASN
1	C	298	HIS
1	C	324	HIS
1	C	330	ASN
1	D	75	GLN
1	D	87	HIS
1	D	105	HIS
1	D	111	ASN
1	D	129	HIS
1	D	154	ASN

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Mol	Chain	Res	Type
1	D	170	HIS
1	D	261	ASN
1	D	296	ASN
1	D	298	HIS
1	D	312	ASN
1	D	324	HIS
1	D	337	ASN

### 5.3.3 RNA [i](#)

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	B	203	1	23,24,25	3.15	9 (39%)	25,32,34	2.99	12 (48%)
1	LLP	D	203	1	23,24,25	3.70	11 (47%)	25,32,34	2.98	11 (44%)
1	LLP	A	203	1	23,24,25	3.33	9 (39%)	25,32,34	2.72	13 (52%)
1	LLP	C	203	1	23,24,25	3.17	8 (34%)	25,32,34	2.83	14 (56%)

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	B	203	1	-	5/16/17/19	0/1/1/1
1	LLP	D	203	1	-	4/16/17/19	0/1/1/1
1	LLP	A	203	1	-	5/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	C	203	1	-	6/16/17/19	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	203	LLP	C3-C2	10.15	1.51	1.40
1	D	203	LLP	C4-C5	9.15	1.53	1.42
1	B	203	LLP	C3-C2	8.58	1.49	1.40
1	C	203	LLP	C3-C2	8.19	1.49	1.40
1	A	203	LLP	C4-C5	7.72	1.51	1.42
1	A	203	LLP	C3-C2	6.96	1.47	1.40
1	C	203	LLP	C4-C5	6.92	1.50	1.42
1	B	203	LLP	C4-C5	6.79	1.50	1.42
1	A	203	LLP	C2-N1	6.40	1.45	1.33
1	C	203	LLP	C2-N1	6.35	1.45	1.33
1	D	203	LLP	P-OP3	-6.02	1.31	1.54
1	B	203	LLP	C2-N1	5.86	1.44	1.33
1	A	203	LLP	C4-C3	-5.15	1.33	1.40
1	D	203	LLP	C2-N1	5.09	1.43	1.33
1	B	203	LLP	C6-N1	4.96	1.44	1.34
1	A	203	LLP	OP4-C5'	-4.38	1.28	1.45
1	C	203	LLP	C6-N1	4.13	1.43	1.34
1	D	203	LLP	P-OP4	3.80	1.72	1.60
1	C	203	LLP	OP4-C5'	-3.78	1.30	1.45
1	B	203	LLP	OP4-C5'	-3.76	1.31	1.45
1	A	203	LLP	C6-N1	3.73	1.42	1.34
1	A	203	LLP	O3-C3	-3.50	1.28	1.37
1	D	203	LLP	C6-N1	3.42	1.41	1.34
1	C	203	LLP	CE-NZ	-3.17	1.39	1.46
1	C	203	LLP	C4-C3	-3.08	1.36	1.40
1	A	203	LLP	C2'-C2	-2.84	1.45	1.50
1	C	203	LLP	O3-C3	-2.81	1.30	1.37
1	A	203	LLP	CE-NZ	-2.72	1.40	1.46
1	B	203	LLP	P-OP4	2.59	1.68	1.60
1	D	203	LLP	C6-C5	-2.59	1.32	1.37
1	D	203	LLP	O3-C3	-2.49	1.31	1.37
1	B	203	LLP	CE-NZ	-2.33	1.41	1.46
1	D	203	LLP	P-OP1	2.24	1.57	1.50
1	B	203	LLP	P-OP3	-2.17	1.46	1.54
1	D	203	LLP	OP4-C5'	-2.15	1.37	1.45
1	D	203	LLP	C4-C4'	-2.13	1.42	1.46
1	B	203	LLP	C5'-C5	2.01	1.56	1.50

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	LLP	OP4-C5'-C5	8.71	125.95	109.35
1	D	203	LLP	C5'-C5-C6	8.53	133.41	119.37
1	A	203	LLP	OP4-C5'-C5	8.03	124.66	109.35
1	C	203	LLP	OP4-C5'-C5	7.35	123.36	109.35
1	B	203	LLP	C5'-C5-C6	6.58	130.19	119.37
1	C	203	LLP	C5'-C5-C6	6.17	129.51	119.37
1	D	203	LLP	OP4-C5'-C5	5.86	120.52	109.35
1	A	203	LLP	C5'-C5-C6	5.52	128.46	119.37
1	D	203	LLP	OP4-P-OP1	-4.31	94.40	106.47
1	C	203	LLP	C2'-C2-C3	3.99	125.82	120.89
1	D	203	LLP	C3-C2-N1	-3.91	115.72	120.77
1	B	203	LLP	C2'-C2-C3	3.70	125.46	120.89
1	B	203	LLP	C5-C6-N1	-3.68	117.68	123.82
1	D	203	LLP	CE-NZ-C4'	3.56	129.84	118.90
1	C	203	LLP	C3-C2-N1	-3.45	116.31	120.77
1	A	203	LLP	C5-C6-N1	-3.42	118.12	123.82
1	C	203	LLP	CE-NZ-C4'	3.35	129.18	118.90
1	B	203	LLP	CE-NZ-C4'	3.29	128.99	118.90
1	C	203	LLP	C5-C6-N1	-3.25	118.40	123.82
1	D	203	LLP	C2'-C2-C3	3.21	124.85	120.89
1	A	203	LLP	CE-NZ-C4'	3.20	128.73	118.90
1	B	203	LLP	C3-C2-N1	-3.19	116.65	120.77
1	A	203	LLP	OP4-P-OP1	-3.17	97.57	106.47
1	B	203	LLP	CD-CE-NZ	-3.13	103.26	110.93
1	D	203	LLP	C3-C4-C4'	-3.08	114.67	120.41
1	C	203	LLP	OP4-P-OP1	-3.04	97.95	106.47
1	A	203	LLP	C2'-C2-C3	2.95	124.53	120.89
1	B	203	LLP	OP4-P-OP1	-2.94	98.24	106.47
1	C	203	LLP	C4-C4'-NZ	-2.85	111.21	124.31
1	D	203	LLP	OP2-P-OP4	2.82	114.25	106.73
1	D	203	LLP	C4-C4'-NZ	-2.81	111.40	124.31
1	A	203	LLP	C4-C4'-NZ	-2.77	111.59	124.31
1	D	203	LLP	OP3-P-OP1	2.72	121.33	110.68
1	D	203	LLP	C5-C4-C4'	2.67	125.95	121.56
1	B	203	LLP	C3-C4-C5	2.64	120.29	118.26
1	A	203	LLP	C3-C2-N1	-2.60	117.41	120.77
1	B	203	LLP	OP2-P-OP4	2.54	113.48	106.73
1	A	203	LLP	C3-C4-C5	2.50	120.18	118.26
1	C	203	LLP	C4-C3-C2	2.47	121.72	120.19
1	B	203	LLP	C6-N1-C2	2.42	123.64	119.17
1	B	203	LLP	C4-C4'-NZ	-2.31	113.68	124.31
1	A	203	LLP	CD-CE-NZ	-2.25	105.41	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	LLP	C3-C4-C5	2.14	119.90	118.26
1	C	203	LLP	CG-CD-CE	-2.13	106.14	113.57
1	C	203	LLP	OP2-P-OP4	2.13	112.40	106.73
1	A	203	LLP	OP2-P-OP4	2.11	112.36	106.73
1	C	203	LLP	C6-N1-C2	2.11	123.07	119.17
1	A	203	LLP	C4-C3-C2	2.10	121.49	120.19
1	A	203	LLP	CG-CD-CE	-2.10	106.25	113.57
1	C	203	LLP	OP3-P-OP1	2.09	118.88	110.68

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	203	LLP	O-C-CA-CB
1	D	203	LLP	O-C-CA-CB
1	A	203	LLP	O-C-CA-CB
1	C	203	LLP	C5-C4-C4'-NZ
1	C	203	LLP	O-C-CA-CB
1	B	203	LLP	CG-CD-CE-NZ
1	D	203	LLP	CG-CD-CE-NZ
1	B	203	LLP	C3-C4-C4'-NZ
1	D	203	LLP	C3-C4-C4'-NZ
1	C	203	LLP	C3-C4-C4'-NZ
1	A	203	LLP	C3-C4-C4'-NZ
1	A	203	LLP	C5-C4-C4'-NZ
1	B	203	LLP	CD-CE-NZ-C4'
1	A	203	LLP	CD-CE-NZ-C4'
1	C	203	LLP	CD-CE-NZ-C4'
1	C	203	LLP	CG-CD-CE-NZ
1	D	203	LLP	CD-CE-NZ-C4'
1	C	203	LLP	CE-CD-CG-CB
1	B	203	LLP	C5-C4-C4'-NZ
1	A	203	LLP	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	203	LLP	1	0
1	C	203	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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%)	0.16	11 (3%) 47 41	10, 16, 26, 35	0
1	B	342/347 (98%)	0.12	11 (3%) 47 41	9, 15, 28, 36	0
1	C	339/347 (97%)	0.24	15 (4%) 34 28	11, 17, 29, 34	0
1	D	343/347 (98%)	0.24	23 (6%) 17 14	10, 16, 31, 42	0
All	All	1366/1388 (98%)	0.19	60 (4%) 34 28	9, 16, 29, 42	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	141	THR	4.7
1	B	141	THR	4.6
1	C	141	THR	4.3
1	B	344	ARG	4.0
1	D	296	ASN	3.9
1	C	5	MET	3.8
1	D	342	LEU	3.7
1	D	117	ASP	3.6
1	D	344	ARG	3.6
1	D	140	ASN	3.5
1	A	141	THR	3.4
1	D	126	ARG	3.3
1	C	337	ASN	3.3
1	D	291	ASP	3.2
1	B	140	ASN	3.2
1	A	25	ALA	3.1
1	C	291	ASP	3.0
1	B	126	ARG	3.0
1	B	5	MET	3.0
1	D	164	GLU	2.8
1	A	160	THR	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	344	ARG	2.7
1	D	4	MET	2.7
1	B	339	PHE	2.6
1	B	316	ASP	2.6
1	C	140	ASN	2.6
1	D	121	LYS	2.6
1	A	163	LYS	2.6
1	A	164	GLU	2.5
1	D	294	LYS	2.5
1	D	289	ARG	2.5
1	A	140	ASN	2.5
1	D	347	SER	2.5
1	B	164	GLU	2.5
1	C	19	GLU	2.4
1	D	339	PHE	2.4
1	B	26	GLN	2.4
1	A	156	LYS	2.4
1	A	126	ARG	2.3
1	C	186	PRO	2.3
1	B	341	LYS	2.3
1	D	217	ARG	2.3
1	B	121	LYS	2.3
1	C	305	ARG	2.3
1	C	156	LYS	2.2
1	C	346	PHE	2.2
1	D	158	ILE	2.1
1	C	126	ARG	2.1
1	D	305	ARG	2.1
1	A	110	LYS	2.1
1	C	18	GLU	2.1
1	A	119	VAL	2.1
1	D	110	LYS	2.1
1	D	297	ALA	2.1
1	A	26	GLN	2.1
1	C	341	LYS	2.1
1	D	144	ARG	2.0
1	D	315	SER	2.0
1	C	22	LYS	2.0
1	D	343	PHE	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	D	203	24/25	0.87	0.16	13,20,25,29	0
1	LLP	C	203	24/25	0.88	0.16	11,22,24,28	0
1	LLP	A	203	24/25	0.89	0.14	10,19,22,25	0
1	LLP	B	203	24/25	0.90	0.15	11,19,23,27	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
2	CA	B	905	1/1	0.98	0.05	19,19,19,19	0
2	CA	D	906	1/1	0.98	0.05	15,15,15,15	0
2	CA	B	901	1/1	0.98	0.05	15,15,15,15	0
3	NA	C	908	1/1	0.99	0.08	13,13,13,13	0
2	CA	D	903	1/1	0.99	0.04	15,15,15,15	0
3	NA	A	907	1/1	0.99	0.11	11,11,11,11	0
2	CA	A	902	1/1	0.99	0.05	15,15,15,15	0
2	CA	C	904	1/1	1.00	0.06	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.