



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2017 – 10:02 PM EDT

PDB ID : 5UZE  
Title : Crystal Structure of Inosine 5'-monophosphate Dehydrogenase from *Clostridium perfringens* Complexed with IMP and P182  
Authors : Maltseva, N.; Kim, Y.; Mulligan, R.; Makowska-Grzyska, M.; Gu, M.; Gollapalli, D.R.; Hedstrom, L.; Joachimiak, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2017-02-26  
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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

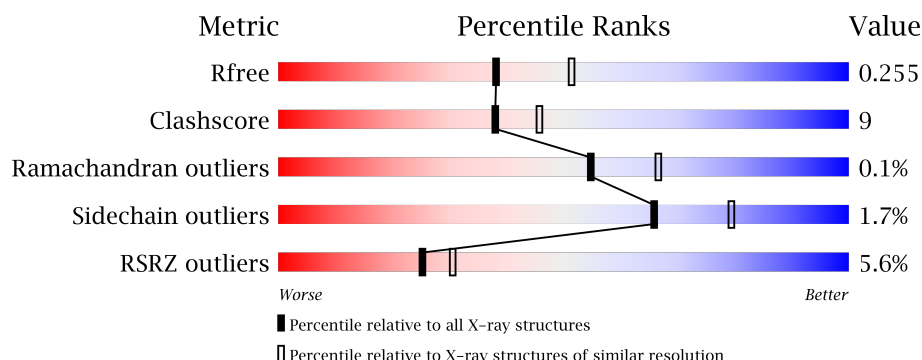
# 1 Overall quality at a glance

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))
$R_{free}$	100719	5609 (2.30-2.26)
Clashscore	112137	6364 (2.30-2.26)
Ramachandran outliers	110173	6281 (2.30-2.26)
Sidechain outliers	110143	6281 (2.30-2.26)
RSRZ outliers	101464	5639 (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. 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	363	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• 6%</div> </div> </div>
1	B	363	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>6%</div> </div> </div>
1	C	363	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• 6%</div> </div> </div>
1	D	363	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• 6%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10463 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 Inosine-5'-monophosphate dehydrogenase, Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2512	1580	432	481	19			
1	B	343	Total	C	N	O	S	0	0	0
			2532	1592	438	483	19			
1	C	341	Total	C	N	O	S	1	0	0
			2508	1574	434	481	19			
1	D	342	Total	C	N	O	S	0	0	0
			2523	1586	436	482	19			

There are 24 discrepancies between the modelled and reference sequences:

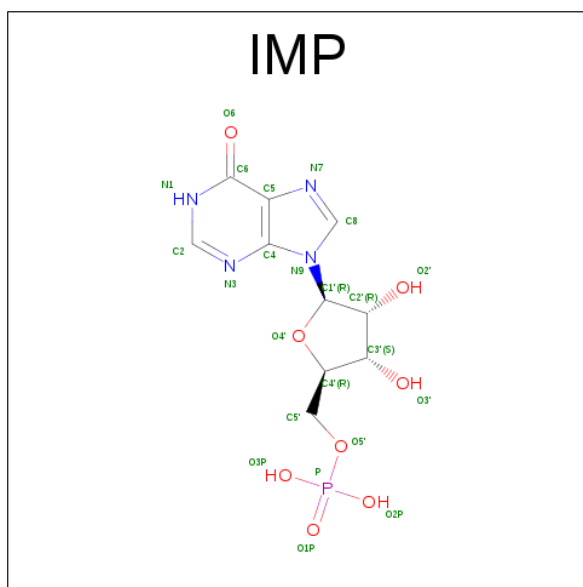
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A0H2YRZ7
A	-1	ASN	-	expression tag	UNP A0A0H2YRZ7
A	0	ALA	-	expression tag	UNP A0A0H2YRZ7
A	89	SER	-	linker	UNP A0A0H2YRZ7
A	90	GLY	-	linker	UNP A0A0H2YRZ7
A	91	GLY	-	linker	UNP A0A0H2YRZ7
B	-2	SER	-	expression tag	UNP A0A0H2YRZ7
B	-1	ASN	-	expression tag	UNP A0A0H2YRZ7
B	0	ALA	-	expression tag	UNP A0A0H2YRZ7
B	89	SER	-	linker	UNP A0A0H2YRZ7
B	90	GLY	-	linker	UNP A0A0H2YRZ7
B	91	GLY	-	linker	UNP A0A0H2YRZ7
C	-2	SER	-	expression tag	UNP A0A0H2YRZ7
C	-1	ASN	-	expression tag	UNP A0A0H2YRZ7
C	0	ALA	-	expression tag	UNP A0A0H2YRZ7
C	89	SER	-	linker	UNP A0A0H2YRZ7
C	90	GLY	-	linker	UNP A0A0H2YRZ7
C	91	GLY	-	linker	UNP A0A0H2YRZ7
D	-2	SER	-	expression tag	UNP A0A0H2YRZ7
D	-1	ASN	-	expression tag	UNP A0A0H2YRZ7

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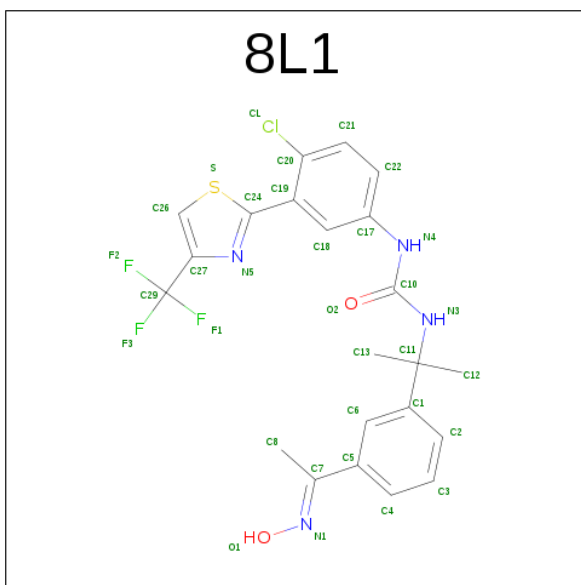
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ALA	-	expression tag	UNP A0A0H2YRZ7
D	89	SER	-	linker	UNP A0A0H2YRZ7
D	90	GLY	-	linker	UNP A0A0H2YRZ7
D	91	GLY	-	linker	UNP A0A0H2YRZ7

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula:  $C_{10}H_{13}N_4O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is N-{4-chloro-3-[4-(trifluoromethyl)-1,3-thiazol-2-yl]phenyl}-N'-(2-{3-[(1E)-N-hydroxyethanimidoyl]phenyl}propan-2-yl)urea (three-letter code: 8L1) (formula:  $C_{22}H_{20}ClF_3N_4O_2S$ ).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	0	0
			33	22	1	3	4	2	1		
3	B	1	Total	C	Cl	F	N	O	S	0	0
			33	22	1	3	4	2	1		
3	C	1	Total	C	Cl	F	N	O	S	0	0
			33	22	1	3	4	2	1		
3	D	1	Total	C	Cl	F	N	O	S	0	0
			33	22	1	3	4	2	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

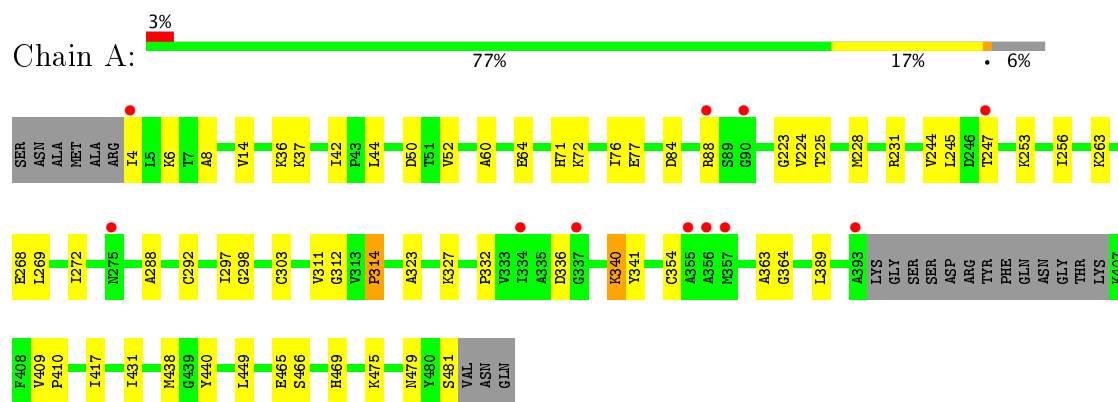
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total	O	0	0
			39	39		
6	B	41	Total	O	0	0
			41	41		
6	C	37	Total	O	0	0
			37	37		
6	D	39	Total	O	0	0
			39	39		

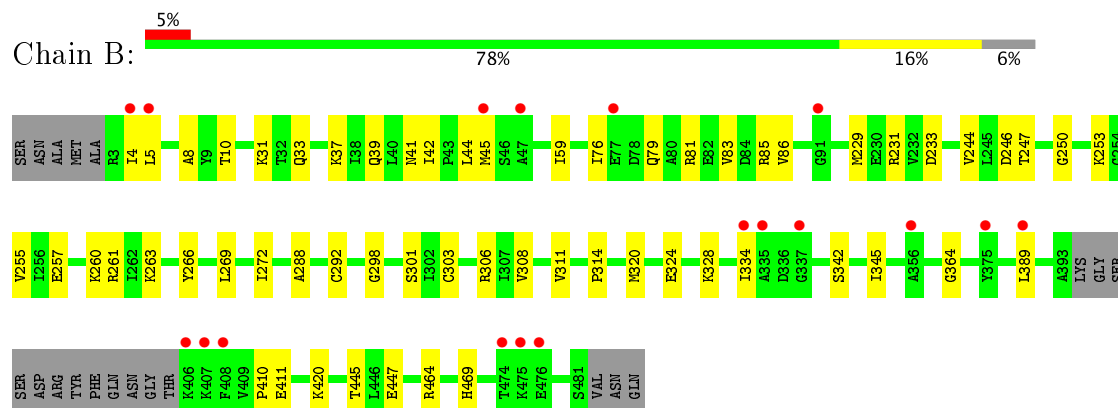
### 3 Residue-property plots [i](#)

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.

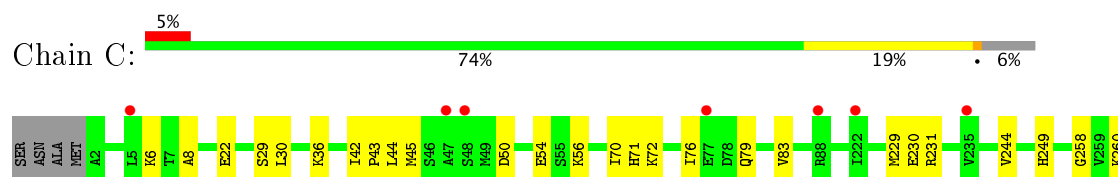
- Molecule 1: Inosine-5'-monophosphate dehydrogenase, Inosine-5'-monophosphate dehydrogenase

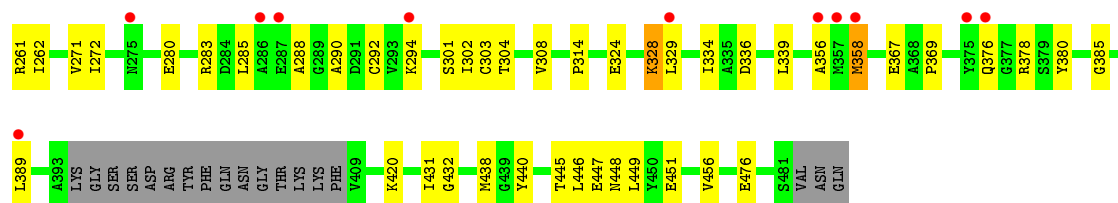


- Molecule 1: Inosine-5'-monophosphate dehydrogenase, Inosine-5'-monophosphate dehydrogenase

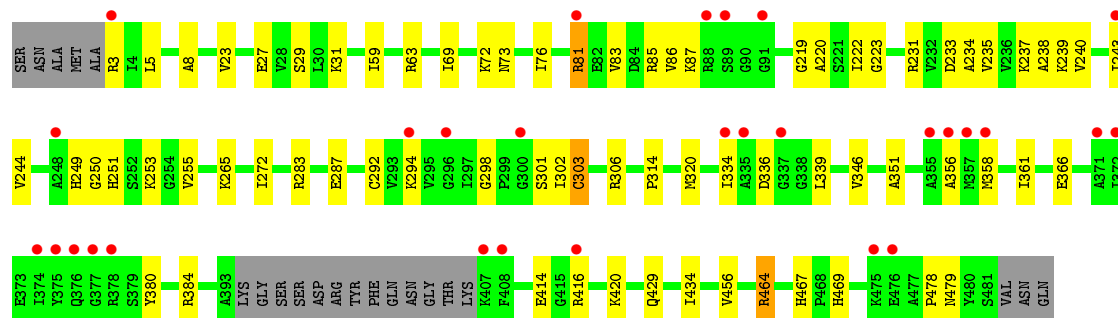
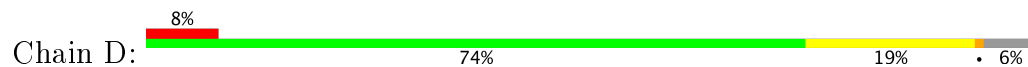


- Molecule 1: Inosine-5'-monophosphate dehydrogenase, Inosine-5'-monophosphate dehydrogenase





- Molecule 1: Inosine-5'-monophosphate dehydrogenase, Inosine-5'-monophosphate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.78Å 77.66Å 80.32Å 110.03° 103.99° 105.46°	Depositor
Resolution (Å)	31.39 – 2.27 31.39 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.1 (31.39-2.27) 81.5 (31.39-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.194 , 0.255 0.192 , 0.255	Depositor DCC
$R_{free}$ test set	2822 reflections (4.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.001 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10463	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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, K, 8L1, IMP

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	0.44	0/2545	0.62	0/3434
1	B	0.43	0/2565	0.60	0/3459
1	C	0.42	0/2540	0.60	0/3428
1	D	0.42	0/2556	0.58	0/3448
All	All	0.43	0/10206	0.60	0/13769

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2512	0	2578	46	1
1	B	2532	0	2604	45	0
1	C	2508	0	2574	55	0
1	D	2523	0	2591	47	1
2	A	23	0	11	2	0
2	B	23	0	11	1	0
2	C	23	0	11	2	0
2	D	23	0	11	0	0
3	A	33	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	0	1	0
3	C	33	0	0	1	0
3	D	33	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	6	0	8	0	0
6	A	39	0	0	0	0
6	B	41	0	0	0	0
6	C	37	0	0	0	0
6	D	39	0	0	1	0
All	All	10463	0	10399	179	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 (179) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:CYS:SG	2:C:500:IMP:H2	2.31	0.70
1:C:30:LEU:HD12	1:C:431:ILE:HD12	1.76	0.66
1:C:272:ILE:HG12	1:C:292:CYS:HB3	1.77	0.65
1:C:324:GLU:O	1:C:328:LYS:HG2	1.96	0.64
1:C:30:LEU:CD1	1:C:431:ILE:HD12	2.29	0.63
1:C:283:ARG:HG2	1:C:329:LEU:HD11	1.80	0.63
1:A:42:ILE:HD12	1:A:44:LEU:HD12	1.81	0.62
1:C:445:THR:HG23	1:C:448:ASN:H	1.64	0.62
1:A:479:ASN:HD22	1:B:410:PRO:HG2	1.65	0.61
1:C:230:GLU:OE1	1:C:230:GLU:N	2.31	0.61
1:D:29:SER:OG	1:D:31:LYS:HE3	2.02	0.60
1:B:8:ALA:HB3	1:B:314:PRO:HD2	1.83	0.60
3:D:501:8L1:S	3:D:501:8L1:CL	2.97	0.60
1:D:233:ASP:OD1	1:D:265:LYS:NZ	2.35	0.60
1:C:447:GLU:O	1:C:451:GLU:HG2	2.01	0.60
1:C:8:ALA:HB3	1:C:314:PRO:HD2	1.85	0.59
1:B:389:LEU:HD21	1:B:410:PRO:HG3	1.84	0.59
1:A:37:LYS:NZ	1:A:268:GLU:OE2	2.34	0.59
1:B:42:ILE:HD12	1:B:44:LEU:HD12	1.84	0.59
1:C:79:GLN:O	1:C:83:VAL:HG23	2.02	0.59
1:D:244:VAL:HG22	1:D:272:ILE:HB	1.84	0.59
1:C:72:LYS:HA	1:C:79:GLN:NE2	2.18	0.58
1:B:260:LYS:NZ	1:B:288:ALA:HA	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LYS:HG3	1:D:239:LYS:HB2	1.86	0.57
1:A:409:VAL:HG21	1:C:432:GLY:HA3	1.86	0.57
1:D:298:GLY:HA2	1:D:303:CYS:SG	2.43	0.57
1:D:380:TYR:CG	1:D:416:ARG:HD3	2.39	0.57
1:C:438:MET:HG2	1:C:449:LEU:HD13	1.87	0.57
1:D:69:ILE:HD13	1:D:219:GLY:HA3	1.87	0.57
1:C:8:ALA:CB	1:C:314:PRO:HD2	2.35	0.56
1:C:43:PRO:HG3	1:C:446:LEU:HD11	1.86	0.56
1:A:14:VAL:HG11	1:B:4:ILE:HD11	1.87	0.56
1:B:260:LYS:HZ3	1:B:288:ALA:HA	1.71	0.56
1:C:304:THR:O	1:C:308:VAL:HG22	2.06	0.55
1:D:250:GLY:HA2	1:D:255:VAL:HG21	1.89	0.55
1:C:56:LYS:HE3	1:C:367:GLU:HA	1.88	0.55
1:A:440:TYR:HB3	1:B:311:VAL:HG11	1.89	0.55
1:B:76:ILE:HG12	1:B:231:ARG:HG3	1.88	0.55
1:B:298:GLY:HA2	1:B:303:CYS:SG	2.46	0.55
1:D:72:LYS:HE2	1:D:223:GLY:N	2.22	0.55
1:A:256:ILE:HG23	1:A:288:ALA:HB2	1.89	0.54
1:C:389:LEU:HD11	1:D:478:PRO:HD3	1.88	0.54
1:D:235:VAL:HG13	1:D:240:VAL:HG11	1.90	0.54
1:D:81:ARG:O	1:D:85:ARG:HG2	2.07	0.54
1:C:336:ASP:OD1	2:C:500:IMP:O2'	2.24	0.54
1:B:31:LYS:HE3	1:B:41:ASN:ND2	2.23	0.54
1:C:50:ASP:HA	1:C:71:HIS:CD2	2.43	0.54
1:A:60:ALA:O	1:A:64:GLU:HG2	2.08	0.53
1:A:303:CYS:SG	2:A:500:IMP:H2	2.49	0.53
1:C:229:MET:HE2	1:C:261:ARG:HG2	1.90	0.52
1:C:54:GLU:HB2	1:C:369:PRO:HG3	1.91	0.52
1:D:320:MET:HG3	1:D:351:ALA:HB1	1.90	0.52
1:A:389:LEU:CD1	1:A:410:PRO:HG3	2.38	0.52
3:A:501:8L1:S	3:A:501:8L1:CL	3.04	0.52
1:D:235:VAL:HG22	1:D:240:VAL:HB	1.90	0.52
1:C:42:ILE:CG2	1:C:431:ILE:HD11	2.40	0.52
1:D:298:GLY:HA3	1:D:306:ARG:HE	1.76	0.51
1:A:224:VAL:HG23	1:A:224:VAL:O	2.10	0.51
1:D:235:VAL:HG11	1:D:243:ILE:HD11	1.91	0.51
1:C:76:ILE:HD11	1:C:230:GLU:C	2.30	0.51
1:C:376:GLN:O	1:C:378:ARG:HG3	2.10	0.51
1:D:294:LYS:HG3	1:D:334:ILE:HB	1.93	0.51
1:C:258:GLY:O	1:C:262:ILE:HG13	2.11	0.51
1:C:476:GLU:CD	1:C:476:GLU:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ARG:O	1:D:287:GLU:HG3	2.11	0.51
1:A:244:VAL:HG22	1:A:272:ILE:HB	1.93	0.51
1:D:8:ALA:CB	1:D:314:PRO:HD2	2.40	0.51
1:B:445:THR:OG1	1:B:447:GLU:HG2	2.12	0.50
1:D:429:GLN:HE21	1:D:479:ASN:HB3	1.76	0.50
1:D:23:VAL:HA	1:D:27:GLU:OE2	2.10	0.50
1:B:8:ALA:CB	1:B:314:PRO:HD2	2.41	0.50
1:C:76:ILE:HD11	1:C:230:GLU:O	2.10	0.50
1:C:42:ILE:HG21	1:C:431:ILE:HD11	1.93	0.50
1:B:244:VAL:HG22	1:B:272:ILE:HB	1.94	0.50
1:A:389:LEU:HD13	1:A:410:PRO:HG3	1.94	0.49
1:D:272:ILE:HG12	1:D:292:CYS:HB3	1.94	0.49
1:A:77:GLU:H	1:A:77:GLU:CD	2.16	0.49
1:D:302:ILE:HD12	1:D:302:ILE:C	2.32	0.49
1:A:223:GLY:O	1:A:228:MET:HG3	2.13	0.49
1:B:45:MET:HE1	1:B:334:ILE:HG12	1.96	0.48
1:A:323:ALA:O	1:A:327:LYS:HG3	2.14	0.48
1:A:50:ASP:HA	1:A:71:HIS:CD2	2.48	0.48
1:C:280:GLU:HA	1:C:283:ARG:NH1	2.28	0.48
3:B:502:8L1:CL	3:B:502:8L1:S	3.09	0.47
1:D:294:LYS:NZ	1:D:336:ASP:OD2	2.34	0.47
1:C:6:LYS:HG2	1:D:456:VAL:HG23	1.96	0.47
1:A:8:ALA:CB	1:A:314:PRO:HD2	2.45	0.47
1:B:253:LYS:HE2	1:B:257:GLU:OE2	2.15	0.47
1:B:324:GLU:O	1:B:328:LYS:HG3	2.14	0.47
1:B:33:GLN:HE22	1:B:39:GLN:HE21	1.61	0.47
1:A:272:ILE:HG12	1:A:292:CYS:HB3	1.96	0.47
1:A:42:ILE:HG21	1:A:431:ILE:HD11	1.97	0.47
1:A:52:VAL:HG22	1:A:363:ALA:HB2	1.96	0.47
1:D:8:ALA:HB3	1:D:314:PRO:HD2	1.95	0.47
1:C:324:GLU:O	1:C:328:LYS:CG	2.60	0.47
1:D:272:ILE:HA	1:D:292:CYS:O	2.15	0.47
1:A:4:ILE:HG13	1:A:4:ILE:O	2.14	0.47
1:B:342:SER:HA	1:B:345:ILE:HD12	1.97	0.47
1:A:469:HIS:O	1:B:301:SER:HB2	2.15	0.47
1:A:72:LYS:HE3	1:A:223:GLY:H	1.80	0.47
1:C:271:VAL:HG13	1:C:290:ALA:HA	1.98	0.46
1:C:260:LYS:HZ2	1:C:288:ALA:HA	1.79	0.46
1:A:253:LYS:HD3	1:C:22:GLU:HG2	1.98	0.46
1:A:8:ALA:HB3	1:A:314:PRO:HD2	1.98	0.46
1:C:378:ARG:HD3	1:C:380:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ILE:HG12	1:D:231:ARG:HG3	1.98	0.46
1:B:244:VAL:HG12	1:B:246:ASP:HB3	1.97	0.46
1:B:247:THR:HG21	1:B:255:VAL:HG22	1.96	0.46
1:A:336:ASP:OD1	2:A:500:IMP:O3'	2.29	0.46
1:A:42:ILE:HD13	1:A:431:ILE:HD11	1.97	0.46
1:B:229:MET:HG2	1:B:261:ARG:HD3	1.98	0.45
1:B:303:CYS:SG	2:B:501:IMP:H2	2.57	0.45
1:A:225:THR:H	1:A:228:MET:HE2	1.82	0.45
1:A:479:ASN:HD22	1:B:410:PRO:CG	2.27	0.45
1:A:479:ASN:HD22	1:B:410:PRO:CD	2.30	0.45
1:C:244:VAL:HG22	1:C:272:ILE:HB	1.98	0.45
1:D:358:MET:HG2	1:D:361:ILE:HD12	1.99	0.45
1:D:346:VAL:HG22	1:D:434:ILE:HA	1.98	0.44
1:D:467:HIS:O	1:D:469:HIS:HD2	2.01	0.44
1:C:302:ILE:HD13	1:C:385:GLY:HA2	1.99	0.44
1:C:56:LYS:CE	1:C:367:GLU:HA	2.47	0.44
1:A:475:LYS:HD3	1:A:475:LYS:HA	1.77	0.44
1:A:263:LYS:NZ	1:A:269:LEU:O	2.45	0.44
1:B:45:MET:HE1	1:B:334:ILE:CG1	2.48	0.44
1:C:301:SER:HB2	1:D:469:HIS:O	2.17	0.44
1:B:320:MET:HE1	1:D:3:ARG:HB2	2.00	0.44
1:D:220:ALA:CB	1:D:235:VAL:HG21	2.47	0.44
1:A:84:ASP:O	1:A:88:ARG:HG3	2.19	0.43
1:D:83:VAL:HG21	1:D:235:VAL:CG2	2.48	0.43
1:B:389:LEU:HD23	1:B:410:PRO:HB3	1.99	0.43
1:C:445:THR:OG1	1:C:446:LEU:N	2.51	0.43
1:A:6:LYS:HG2	1:C:456:VAL:HG23	1.99	0.43
1:D:59:ILE:HG13	1:D:86:VAL:HG22	2.00	0.43
1:B:389:LEU:HD21	1:B:410:PRO:CG	2.47	0.43
1:C:431:ILE:HD13	1:C:431:ILE:HA	1.93	0.43
1:C:249:HIS:HB3	3:C:501:8L1:S	2.59	0.43
1:C:76:ILE:CD1	1:C:231:ARG:HA	2.49	0.43
1:B:81:ARG:HD2	1:B:85:ARG:NH1	2.34	0.42
1:B:59:ILE:HG12	1:B:86:VAL:HG13	2.01	0.42
1:C:36:LYS:HD3	1:C:36:LYS:N	2.34	0.42
1:A:297:ILE:HG22	1:A:312:GLY:HA2	2.02	0.42
1:B:250:GLY:HA2	1:B:255:VAL:HG21	2.00	0.42
1:D:234:ALA:HA	1:D:237:LYS:NZ	2.35	0.42
1:D:339:LEU:CD1	1:D:356:ALA:HB1	2.50	0.42
1:A:438:MET:HG2	1:A:449:LEU:HD13	2.01	0.42
1:B:308:VAL:HG21	1:B:411:GLU:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:LYS:HE2	1:C:420:LYS:HB2	1.87	0.42
1:B:469:HIS:O	1:D:301:SER:HB2	2.19	0.42
1:C:294:LYS:HG3	1:C:334:ILE:HB	2.01	0.42
1:B:364:GLY:HA3	1:B:420:LYS:HE3	2.01	0.42
1:A:224:VAL:HG12	1:A:245:LEU:HD11	2.02	0.41
1:A:298:GLY:HA2	1:A:303:CYS:SG	2.60	0.41
1:B:389:LEU:CD2	1:B:410:PRO:HG3	2.49	0.41
1:C:339:LEU:CD1	1:C:356:ALA:HB1	2.51	0.41
1:D:464:ARG:NH1	6:D:604:HOH:O	2.52	0.41
1:A:364:GLY:N	1:A:417:ILE:HD11	2.35	0.41
1:A:466:SER:HA	1:B:306:ARG:HD2	2.02	0.41
1:D:384:ARG:HA	1:D:414:GLU:HA	2.03	0.41
1:B:79:GLN:O	1:B:83:VAL:HG12	2.20	0.41
1:C:45:MET:SD	1:C:334:ILE:HD13	2.61	0.41
1:A:311:VAL:HG11	1:C:440:TYR:HB3	2.02	0.41
1:C:356:ALA:HB3	1:C:358:MET:CE	2.51	0.41
1:D:233:ASP:O	1:D:237:LYS:HG3	2.21	0.41
1:D:238:ALA:O	1:D:239:LYS:HB2	2.21	0.41
1:A:76:ILE:HG23	1:A:231:ARG:HA	2.03	0.41
1:C:285:LEU:HA	1:C:285:LEU:HD23	1.83	0.41
1:A:332:PRO:HB2	1:A:354:CYS:SG	2.61	0.41
1:B:263:LYS:NZ	1:B:269:LEU:O	2.51	0.41
1:D:302:ILE:CD1	1:D:302:ILE:C	2.90	0.41
1:D:59:ILE:O	1:D:63:ARG:HG2	2.21	0.41
1:C:302:ILE:HD13	1:C:385:GLY:CA	2.51	0.41
1:D:222:ILE:HG13	1:D:243:ILE:HD12	2.03	0.40
1:A:465:GLU:OE2	1:B:10:THR:OG1	2.39	0.40
1:B:233:ASP:OD2	1:B:266:TYR:OH	2.29	0.40
1:B:45:MET:HE1	1:B:334:ILE:HD13	2.03	0.40
1:B:81:ARG:O	1:B:85:ARG:HG3	2.21	0.40
1:B:272:ILE:HA	1:B:292:CYS:O	2.21	0.40
1:D:249:HIS:CE1	1:D:251:HIS:HB3	2.57	0.40
1:A:340:LYS:HG3	1:A:341:TYR:CD2	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LYS:O	1:D:366:GLU:OE2[1_444]	2.00	0.20

## 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	337/363 (93%)	324 (96%)	13 (4%)	0	100	100
1	B	339/363 (93%)	326 (96%)	13 (4%)	0	100	100
1	C	337/363 (93%)	324 (96%)	13 (4%)	0	100	100
1	D	338/363 (93%)	323 (96%)	14 (4%)	1 (0%)	44	54
All	All	1351/1452 (93%)	1297 (96%)	53 (4%)	1 (0%)	55	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	5	LEU

### 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	264/282 (94%)	260 (98%)	4 (2%)	70	82
1	B	266/282 (94%)	263 (99%)	3 (1%)	78	88
1	C	263/282 (93%)	258 (98%)	5 (2%)	62	77
1	D	265/282 (94%)	259 (98%)	6 (2%)	56	71
All	All	1058/1128 (94%)	1040 (98%)	18 (2%)	66	79

All (18) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	247	THR
1	A	314	PRO
1	A	340	LYS
1	A	481	SER
1	B	5	LEU
1	B	37	LYS
1	B	464	ARG
1	C	29	SER
1	C	44	LEU
1	C	70	ILE
1	C	328	LYS
1	C	358	MET
1	D	73	ASN
1	D	81	ARG
1	D	253	LYS
1	D	303	CYS
1	D	420	LYS
1	D	464	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	448	ASN
1	A	479	ASN
1	B	33	GLN
1	B	41	ASN
1	C	33	GLN
1	D	19	ASN
1	D	429	GLN
1	D	448	ASN
1	D	452	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](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	IMP	A	500	-	21,25,25	1.11	0	22,38,38	2.19	5 (22%)
3	8L1	A	501	-	32,35,35	2.01	6 (18%)	43,52,52	2.21	6 (13%)
2	IMP	B	501	-	21,25,25	0.97	0	22,38,38	2.25	4 (18%)
3	8L1	B	502	-	32,35,35	2.08	6 (18%)	43,52,52	2.14	8 (18%)
5	GOL	B	504	-	5,5,5	0.24	0	5,5,5	0.30	0
2	IMP	C	500	-	21,25,25	0.92	0	22,38,38	2.23	4 (18%)
3	8L1	C	501	-	32,35,35	2.01	5 (15%)	43,52,52	2.03	6 (13%)
2	IMP	D	500	-	21,25,25	0.99	0	22,38,38	2.34	4 (18%)
3	8L1	D	501	-	32,35,35	2.25	7 (21%)	43,52,52	2.05	7 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	A	500	-	-	0/6/26/26	0/3/3/3
3	8L1	A	501	-	-	0/29/31/31	0/3/3/3
2	IMP	B	501	-	-	0/6/26/26	0/3/3/3
3	8L1	B	502	-	-	0/29/31/31	0/3/3/3
5	GOL	B	504	-	-	0/4/4/4	0/0/0/0
2	IMP	C	500	-	-	0/6/26/26	0/3/3/3
3	8L1	C	501	-	-	0/29/31/31	0/3/3/3
2	IMP	D	500	-	-	0/6/26/26	0/3/3/3
3	8L1	D	501	-	-	0/29/31/31	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	8L1	C8-C7	-9.72	1.31	1.50
3	B	502	8L1	C8-C7	-9.22	1.32	1.50
3	A	501	8L1	C8-C7	-9.13	1.33	1.50
3	C	501	8L1	C8-C7	-9.05	1.33	1.50
3	D	501	8L1	C11-C1	-3.51	1.48	1.53
3	D	501	8L1	C17-N4	-3.26	1.35	1.41
3	D	501	8L1	C11-N3	-2.75	1.44	1.48
3	B	502	8L1	C17-N4	-2.57	1.36	1.41
3	A	501	8L1	C17-N4	-2.38	1.37	1.41
3	C	501	8L1	C17-N4	-2.26	1.37	1.41
3	B	502	8L1	C11-C1	-2.19	1.50	1.53
3	A	501	8L1	C11-C1	-2.09	1.50	1.53
3	D	501	8L1	C24-N5	2.11	1.34	1.31
3	D	501	8L1	C7-N1	2.14	1.32	1.28
3	D	501	8L1	C20-CL	2.17	1.78	1.73
3	C	501	8L1	C20-CL	2.64	1.79	1.73
3	A	501	8L1	C20-CL	2.68	1.80	1.73
3	B	502	8L1	C20-CL	2.72	1.80	1.73
3	B	502	8L1	C7-N1	2.73	1.33	1.28
3	A	501	8L1	C24-N5	2.74	1.35	1.31
3	A	501	8L1	C7-N1	2.90	1.33	1.28
3	C	501	8L1	C7-N1	2.98	1.34	1.28
3	C	501	8L1	C24-N5	3.12	1.36	1.31
3	B	502	8L1	C24-N5	3.54	1.36	1.31

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	IMP	N3-C2-N1	-9.45	120.63	128.86
3	A	501	8L1	C26-C27-C29	-9.08	117.87	128.09
2	B	501	IMP	N3-C2-N1	-8.60	121.37	128.86
3	B	502	8L1	C26-C27-C29	-8.44	118.59	128.09
3	C	501	8L1	C26-C27-C29	-8.31	118.74	128.09
2	C	500	IMP	N3-C2-N1	-8.17	121.74	128.86
2	A	500	IMP	N3-C2-N1	-8.07	121.83	128.86
3	D	501	8L1	C26-C27-C29	-8.02	119.06	128.09
3	A	501	8L1	F3-C29-C27	-5.13	103.79	112.46
3	B	502	8L1	C6-C5-C7	-3.88	117.37	120.55
3	B	502	8L1	F3-C29-C27	-3.56	106.45	112.46
3	D	501	8L1	C6-C5-C7	-3.54	117.65	120.55
3	C	501	8L1	F3-C29-C27	-2.96	107.45	112.46
3	A	501	8L1	C6-C5-C7	-2.96	118.12	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	IMP	C4-C5-N7	-2.83	106.67	109.41
2	B	501	IMP	C4-C5-N7	-2.71	106.79	109.41
2	A	500	IMP	C4-C5-N7	-2.61	106.89	109.41
3	B	502	8L1	C13-C11-C1	-2.60	103.15	110.68
3	D	501	8L1	F3-C29-C27	-2.56	108.14	112.46
3	A	501	8L1	F1-C29-C27	-2.48	108.28	112.46
2	D	500	IMP	C6-C5-C4	-2.39	118.47	120.84
3	D	501	8L1	F2-C29-C27	-2.37	108.45	112.46
2	B	501	IMP	C6-C5-C4	-2.15	118.71	120.84
2	D	500	IMP	C4-C5-N7	-2.12	107.36	109.41
2	A	500	IMP	P-O5'-C5'	2.04	123.91	118.30
2	C	500	IMP	P-O5'-C5'	2.17	124.28	118.30
3	B	502	8L1	C19-C20-CL	2.20	123.54	120.46
3	B	502	8L1	C8-C7-C5	2.23	122.93	119.67
3	C	501	8L1	C11-N3-C10	2.23	129.16	123.37
3	A	501	8L1	C19-C18-C17	2.37	122.16	119.12
2	A	500	IMP	O3P-P-O5'	2.47	113.32	106.73
3	C	501	8L1	C19-C18-C17	2.49	122.31	119.12
2	C	500	IMP	C2-N1-C6	2.54	120.15	115.91
2	B	501	IMP	C2-N1-C6	2.68	120.37	115.91
3	D	501	8L1	C19-C20-CL	2.77	124.34	120.46
2	A	500	IMP	C2-N1-C6	2.78	120.55	115.91
3	C	501	8L1	C8-C7-C5	2.84	123.83	119.67
2	D	500	IMP	C2-N1-C6	3.01	120.94	115.91
3	B	502	8L1	C19-C18-C17	3.04	123.02	119.12
3	D	501	8L1	C1-C11-N3	3.62	115.79	110.35
3	D	501	8L1	O1-N1-C7	5.72	121.19	112.82
3	C	501	8L1	O1-N1-C7	5.97	121.56	112.82
3	B	502	8L1	O1-N1-C7	6.19	121.88	112.82
3	A	501	8L1	O1-N1-C7	6.37	122.15	112.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	IMP	2	0
3	A	501	8L1	1	0
2	B	501	IMP	1	0
3	B	502	8L1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	IMP	2	0
3	C	501	8L1	1	0
3	D	501	8L1	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	341/363 (93%)	-0.07	11 (3%) 48 54	28, 44, 65, 87	0
1	B	343/363 (94%)	0.06	18 (5%) 28 34	28, 45, 70, 98	0
1	C	341/363 (93%)	0.21	18 (5%) 27 33	30, 54, 82, 100	1 (0%)
1	D	342/363 (94%)	0.24	29 (8%) 11 15	29, 51, 83, 115	0
All	All	1367/1452 (94%)	0.11	76 (5%) 25 30	28, 48, 77, 115	1 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	375	TYR	6.6
1	D	408	PHE	5.7
1	B	375	TYR	5.1
1	D	372	ILE	4.3
1	D	371	ALA	4.0
1	D	355	ALA	4.0
1	D	374	ILE	3.8
1	D	334	ILE	3.6
1	C	48	SER	3.6
1	C	389	LEU	3.5
1	C	375	TYR	3.5
1	D	376	GLN	3.5
1	C	222	ILE	3.4
1	B	408	PHE	3.3
1	B	389	LEU	3.3
1	C	5	LEU	3.1
1	C	329	LEU	2.9
1	B	406	LYS	2.9
1	C	358	MET	2.9
1	D	357	MET	2.9
1	D	88	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	337	GLY	2.8
1	C	275	ASN	2.8
1	A	4	ILE	2.8
1	D	356	ALA	2.8
1	D	294	LYS	2.7
1	A	357	MET	2.7
1	C	287	GLU	2.7
1	D	475	LYS	2.7
1	C	356	ALA	2.7
1	D	243	ILE	2.7
1	D	377	GLY	2.6
1	A	275	ASN	2.6
1	A	356	ALA	2.6
1	D	81	ARG	2.6
1	D	407	LYS	2.6
1	C	286	ALA	2.5
1	A	355	ALA	2.5
1	D	358	MET	2.5
1	B	47	ALA	2.5
1	C	47	ALA	2.5
1	B	4	ILE	2.5
1	D	378	ARG	2.4
1	B	474	THR	2.4
1	D	89	SER	2.4
1	B	356	ALA	2.3
1	B	475	LYS	2.3
1	B	5	LEU	2.3
1	B	335	ALA	2.3
1	B	337	GLY	2.3
1	D	296	GLY	2.3
1	D	335	ALA	2.3
1	A	90	GLY	2.2
1	B	91	GLY	2.2
1	A	88	ARG	2.2
1	D	248	ALA	2.2
1	D	337	GLY	2.2
1	B	77	GLU	2.2
1	A	334	ILE	2.2
1	C	357	MET	2.2
1	C	294	LYS	2.1
1	D	476	GLU	2.1
1	B	334	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	45	MET	2.1
1	C	88	ARG	2.1
1	C	77	GLU	2.1
1	B	476	GLU	2.1
1	D	416	ARG	2.1
1	D	91	GLY	2.1
1	A	247	THR	2.1
1	A	393	ALA	2.1
1	C	376	GLN	2.1
1	C	235	VAL	2.1
1	D	300	GLY	2.1
1	D	3	ARG	2.0
1	B	407	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	B	504	6/6	0.83	0.30	1.84	63,70,73,76	0
3	8L1	B	502	33/33	0.92	0.13	0.78	28,43,78,81	0
2	IMP	D	500	23/23	0.97	0.20	0.31	29,40,46,46	0
2	IMP	A	500	23/23	0.96	0.17	0.24	27,35,42,43	0
2	IMP	B	501	23/23	0.97	0.17	0.19	30,40,45,49	0
3	8L1	C	501	33/33	0.91	0.13	0.01	34,61,94,95	0
2	IMP	C	500	23/23	0.94	0.17	-0.00	29,39,44,45	0
3	8L1	D	501	33/33	0.93	0.12	-0.21	37,50,74,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	8L1	A	501	33/33	0.95	0.10	-0.65	34,48,75,81	0
4	K	B	503	1/1	0.98	0.04	-1.85	46,46,46,46	0
4	K	A	502	1/1	0.99	0.03	-2.55	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.