



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:33 PM UTC

PDB ID : 8DH2 / pdb_00008dh2
Title : T7 RNA polymerase elongation complex with unnatural base dDs-ATP mismatch
Authors : Oh, J.; Wang, D.
Deposited on : 2022-06-24
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

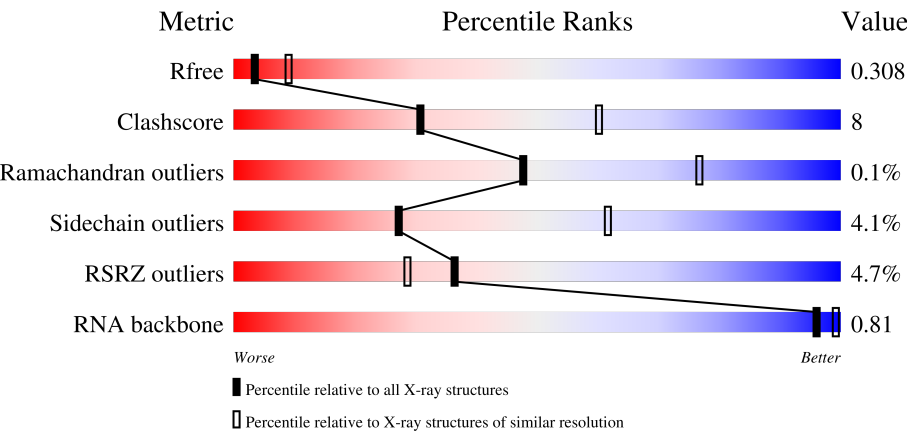
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



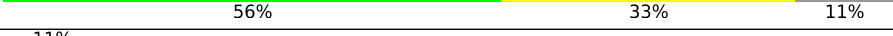
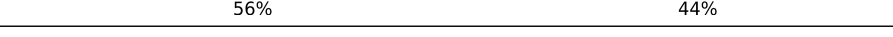
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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 ≥ 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	B	883	
1	E	883	
1	I	883	
1	L	883	

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Mol	Chain	Length	Quality of chain
2	A	18	 72%22%6%
2	F	18	 78%17%6%
2	J	18	 61%6%33%
2	M	18	 56%22%22%
3	C	12	 58%8%33%
3	G	12	 67%33%
3	K	12	 58%8%33%
3	N	12	 67%33%
4	D	9	 56%33%11%
4	H	9	 11%89%11%
4	O	9	 56%44%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27806 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 T7 RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	856	Total	C	N	O	S	0	0	0
			6706	4270	1165	1236	35			
1	E	841	Total	C	N	O	S	0	0	0
			6622	4222	1151	1214	35			
1	I	833	Total	C	N	O	S	0	0	0
			6518	4151	1124	1209	34			
1	L	741	Total	C	N	O	S	0	0	0
			5536	3517	967	1022	30			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	17	Total	C	N	O	P	S	0	0
			351	170	67	97	16	1		
2	F	17	Total	C	N	O	P	S	0	0
			351	170	67	97	16	1		
2	J	12	Total	C	N	O	P	S	0	0
			248	120	45	70	12	1		
2	M	14	Total	C	N	O	P	S	0	0
			289	140	52	82	14	1		

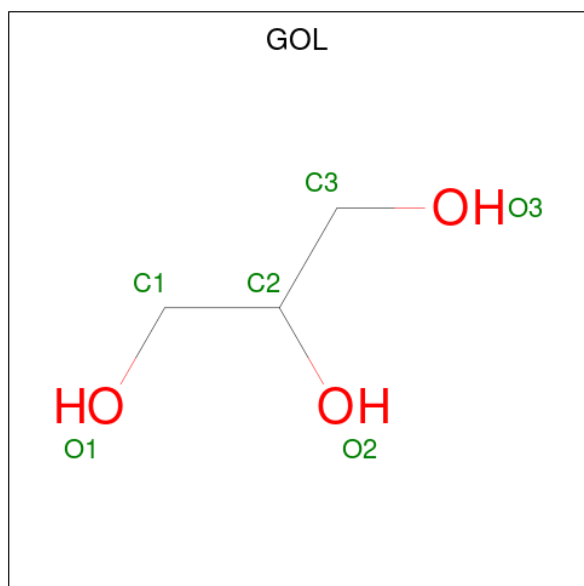
- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	P	0	0
			173	77	33	55	8		
3	G	8	Total	C	N	O	P	0	0
			173	77	33	55	8		
3	K	8	Total	C	N	O	P	0	0
			173	77	33	55	8		
3	N	8	Total	C	N	O	P	0	0
			170	77	33	53	7		

- Molecule 4 is a DNA chain called Non-template strand DNA.

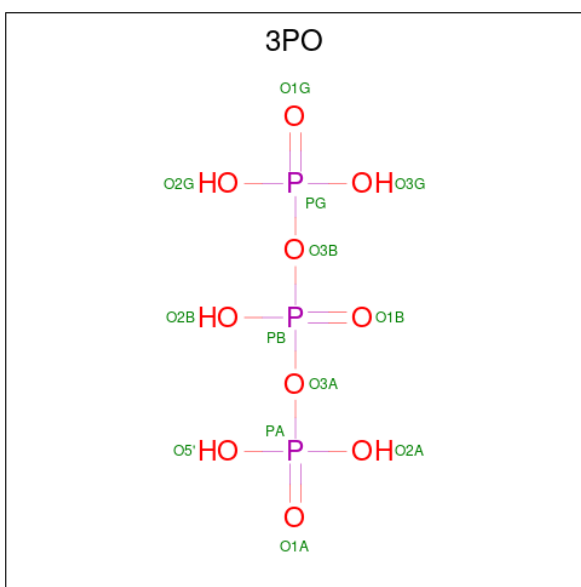
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			
4	H	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			
4	O	5	Total	C	N	O	P	0	0	0
			102	49	17	31	5			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is TRIPHOSPHATE (CCD ID: 3PO) (formula: $H_5O_{10}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			13	10	3		
6	E	1	Total	O	P	0	0
			13	10	3		
6	I	1	Total	O	P	0	0
			13	10	3		
6	L	1	Total	O	P	0	0
			13	10	3		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	E	1	Total	Mg	0	0
			1	1		
7	I	1	Total	Mg	0	0
			1	1		
7	L	1	Total	Mg	0	0
			1	1		

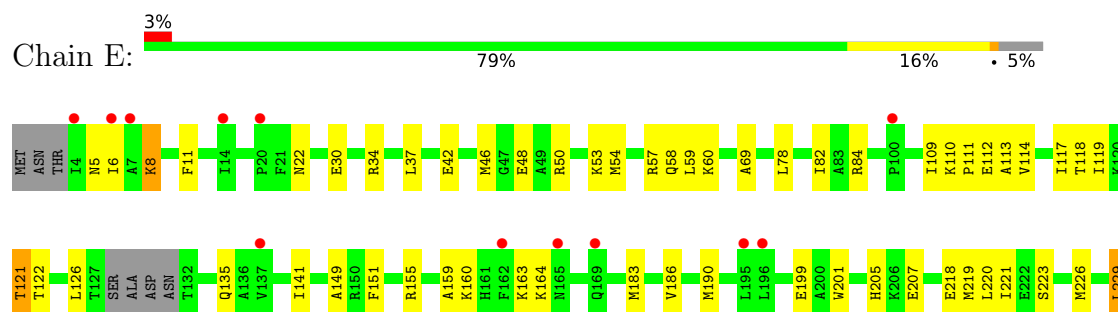
3 Residue-property plots

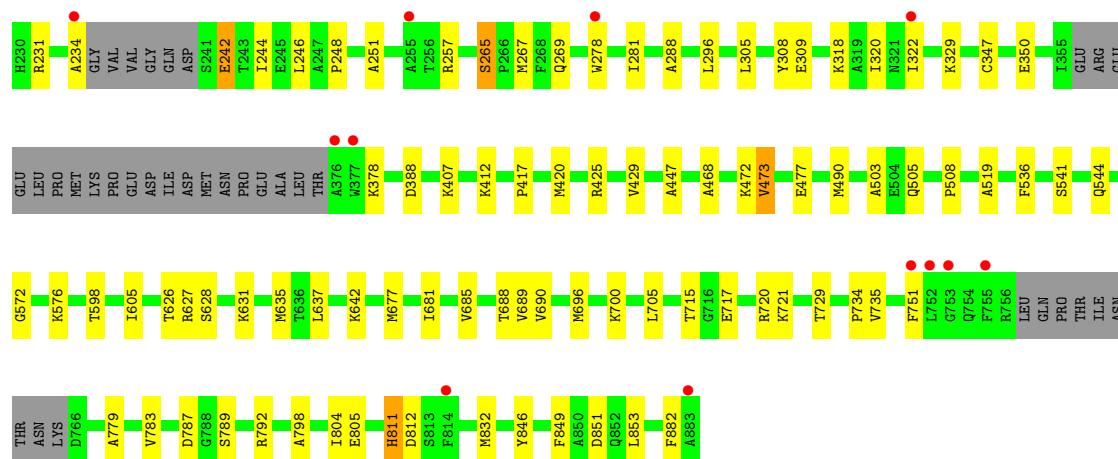
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: T7 RNA polymerase

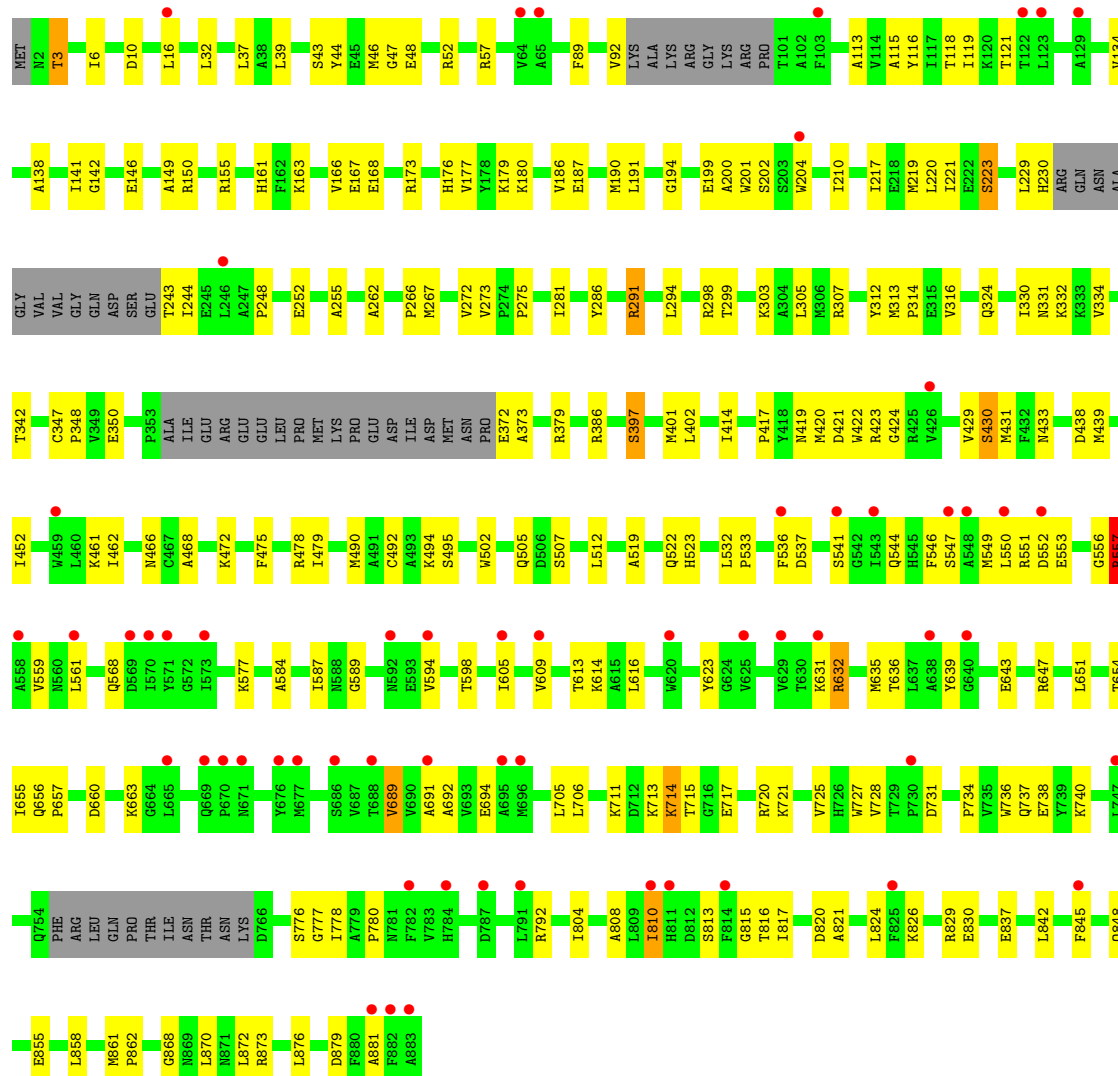


• Molecule 1: T7 RNA polymerase

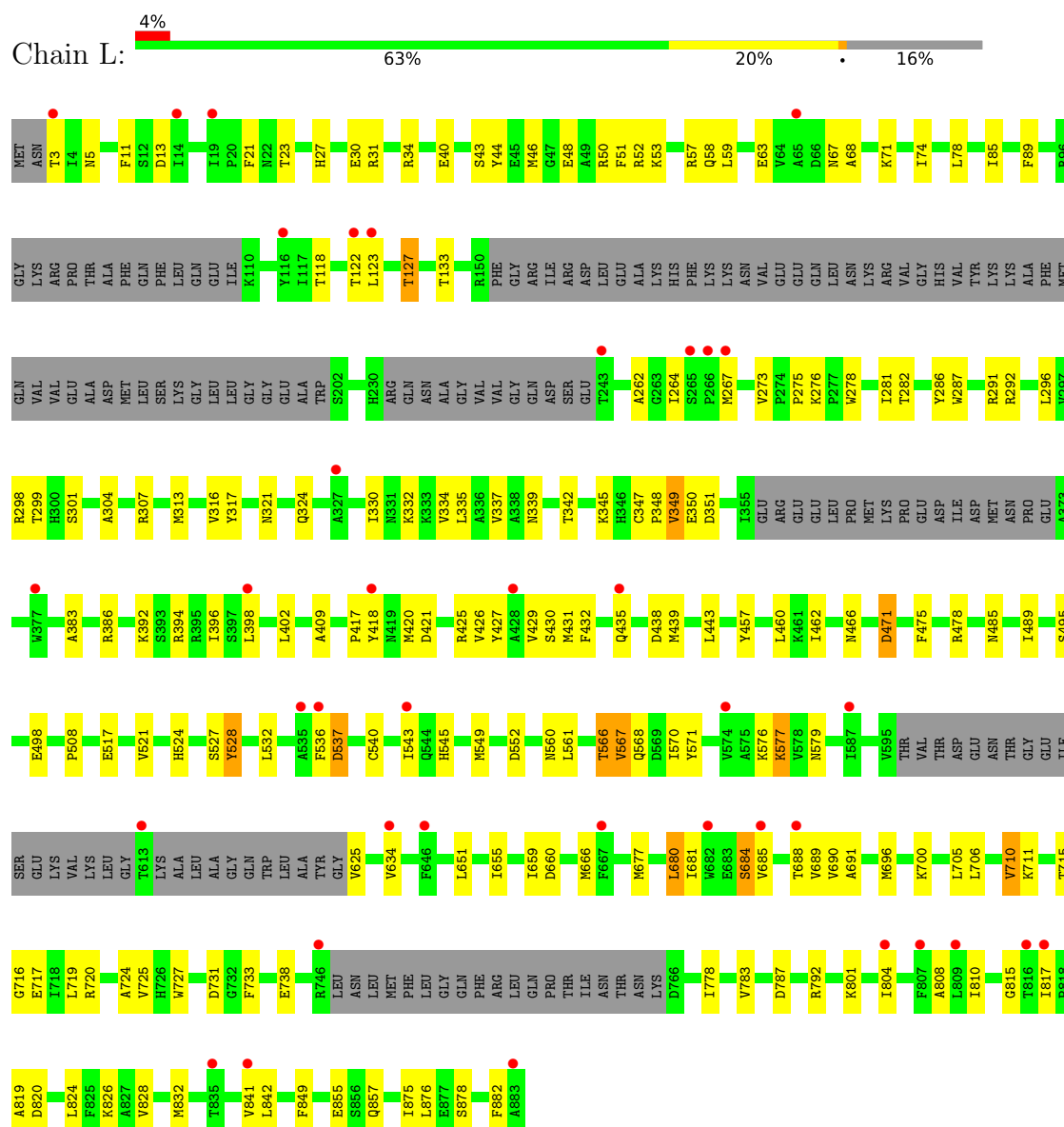




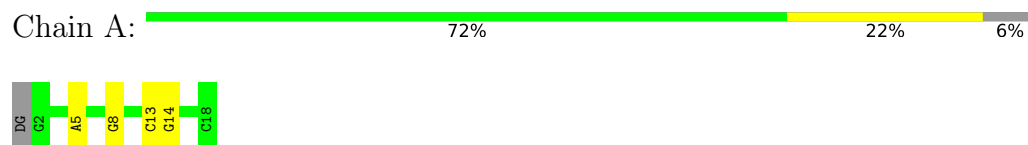
• Molecule 1: T7 RNA polymerase



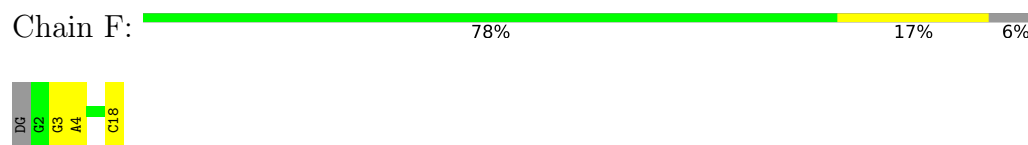
• Molecule 1: T7 RNA polymerase



• Molecule 2: Template strand DNA

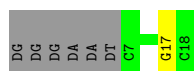


• Molecule 2: Template strand DNA



• Molecule 2: Template strand DNA

Chain J:  61% 6% 33%



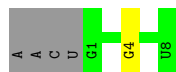
• Molecule 2: Template strand DNA

Chain M:  56% 22% 22%



• Molecule 3: RNA

Chain C:  58% 8% 33%



• Molecule 3: RNA

Chain G:  67% 33%



• Molecule 3: RNA

Chain K:  58% 8% 33%



• Molecule 3: RNA

Chain N:  67% 33%



• Molecule 4: Non-template strand DNA

Chain D:  56% 33% 11%



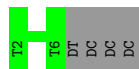
• Molecule 4: Non-template strand DNA

Chain H:  11% 89% 11%



- Molecule 4: Non-template strand DNA

Chain O:  56% 44%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.70Å 85.05Å 200.48Å 89.87° 85.38° 69.51°	Depositor
Resolution (Å)	47.37 – 2.90 47.37 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.37-2.90) 97.9 (47.37-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.260 , 0.307 0.261 , 0.308	Depositor DCC
R_{free} test set	2005 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 84.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27806	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, 91N, 3PO, GOL

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	B	0.18	0/6856	0.42	2/9277 (0.0%)
1	E	0.19	0/6770	0.44	4/9153 (0.0%)
1	I	0.22	0/6664	0.51	1/9020 (0.0%)
1	L	0.20	0/5653	0.48	1/7668 (0.0%)
2	A	0.18	0/365	0.31	0/559
2	F	0.18	0/365	0.32	0/559
2	J	0.19	0/248	0.34	0/377
2	M	0.18	0/294	0.36	0/448
3	C	0.11	0/193	0.28	0/299
3	G	0.10	0/193	0.23	0/299
3	K	0.08	0/193	0.21	0/299
3	N	0.10	0/190	0.22	0/295
4	D	0.21	0/177	0.48	0/270
4	H	0.19	0/177	0.39	0/270
4	O	0.20	0/113	0.44	0/172
All	All	0.20	0/28451	0.45	8/38965 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	714	LYS	CD-CE-NZ	-6.47	91.21	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	811	HIS	CA-C-N	6.01	133.03	121.54
1	E	811	HIS	C-N-CA	6.01	133.03	121.54
1	L	577	LYS	CB-CG-CD	5.95	124.98	111.30
1	E	219	MET	CA-CB-CG	5.37	124.83	114.10
1	B	18	ALA	CA-C-N	5.10	125.33	120.43
1	B	18	ALA	C-N-CA	5.10	125.33	120.43
1	E	218	GLU	CA-C-O	-5.02	115.73	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	557	ARG	Sidechain
1	I	777	GLY	Peptide
1	I	810	ILE	Peptide

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	B	6706	0	6650	95	0
1	E	6622	0	6583	85	0
1	I	6518	0	6414	141	0
1	L	5536	0	5251	118	0
2	A	351	0	180	3	0
2	F	351	0	180	2	0
2	J	248	0	123	1	0
2	M	289	0	146	3	0
3	C	173	0	86	1	0
3	G	173	0	86	0	0
3	K	173	0	86	1	0
3	N	170	0	87	0	0
4	D	160	0	92	2	0
4	H	160	0	92	0	0
4	O	102	0	58	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	6	0	8	0	0
6	B	13	0	0	0	0
6	E	13	0	0	2	0
6	I	13	0	0	0	0
6	L	13	0	0	0	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
7	L	1	0	0	0	0
All	All	27806	0	26138	444	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 8.

All (444) 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:B:278:TRP:H	1:B:321:ASN:HD21	1.19	0.87
1:I:155:ARG:HA	1:I:163:LYS:HD3	1.67	0.77
1:B:6:ILE:HB	1:B:291:ARG:HH22	1.51	0.75
1:I:468:ALA:HA	1:I:505:GLN:HG3	1.69	0.75
1:B:602:THR:HG23	1:B:604:GLU:H	1.53	0.74
1:L:46:MET:HB2	1:L:267:MET:HG3	1.71	0.72
1:L:68:ALA:HA	1:L:71:LYS:HG3	1.73	0.71
1:E:111:PRO:HA	1:E:114:VAL:HB	1.72	0.70
1:I:200:ALA:O	1:I:204:TRP:NE1	2.21	0.68
1:L:264:ILE:HG22	1:L:291:ARG:HD2	1.76	0.67
1:I:430:SER:O	1:I:433:ASN:ND2	2.27	0.67
1:I:16:LEU:HD23	1:I:37:LEU:HD21	1.76	0.67
1:B:84:ARG:HA	1:B:87:ASP:HB2	1.78	0.66
1:B:90:GLU:HA	1:B:93:LYS:HD2	1.78	0.65
1:B:715:THR:HG23	1:B:717:GLU:H	1.61	0.65
1:L:50:ARG:HD3	1:L:267:MET:HE2	1.77	0.65
1:B:92:VAL:HG11	1:B:100:PRO:HD3	1.78	0.65
1:B:35:GLU:HG2	1:B:272:VAL:HG21	1.79	0.65
1:L:552:ASP:HB2	1:L:691:ALA:HB2	1.79	0.64
1:L:50:ARG:HA	1:L:53:LYS:HE2	1.79	0.64
1:I:552:ASP:HB2	1:I:691:ALA:HB3	1.79	0.64
1:L:495:SER:HB3	1:L:498:GLU:HB2	1.79	0.64
1:L:706:LEU:HD11	1:L:849:PHE:HB2	1.80	0.64
1:E:126:LEU:HD21	1:E:244:ILE:HG23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:571:TYR:HE1	1:L:634:VAL:HB	1.64	0.63
1:E:82:ILE:HG12	1:E:112:GLU:HA	1.81	0.62
1:L:40:GLU:HG2	1:L:286:TYR:HD2	1.64	0.62
1:I:837:GLU:HG3	1:I:872:LEU:HD22	1.81	0.62
1:I:386:ARG:HD2	3:K:4:G:H5"	1.81	0.62
1:E:126:LEU:HD13	1:E:246:LEU:HB2	1.82	0.62
1:I:420:MET:HE1	1:I:792:ARG:HD3	1.82	0.62
1:I:705:LEU:O	1:I:720:ARG:NH2	2.32	0.62
1:L:560:ASN:HD21	1:L:568:GLN:H	1.48	0.62
1:I:16:LEU:H	1:I:37:LEU:HD11	1.64	0.62
1:I:810:ILE:HD11	1:I:813:SER:HB3	1.82	0.62
1:L:347:CYS:HB2	1:L:350:GLU:HB2	1.82	0.61
1:E:425:ARG:NH1	1:E:787:ASP:OD2	2.33	0.61
1:I:275:PRO:HG2	1:I:324:GLN:HB3	1.83	0.61
1:E:677:MET:HE2	1:E:681:ILE:HG13	1.81	0.61
1:E:50:ARG:HB2	1:E:267:MET:HE2	1.83	0.60
1:I:422:TRP:CD1	1:I:423:ARG:HD3	2.36	0.60
1:E:69:ALA:HA	1:E:257:ARG:HG2	1.83	0.60
1:I:559:VAL:HG23	1:I:561:LEU:HG	1.84	0.60
1:B:342:THR:HG22	1:B:348:PRO:HG3	1.81	0.60
1:B:565:GLU:HG2	1:B:566:THR:HG22	1.84	0.60
1:L:48:GLU:HG2	1:L:262:ALA:HB1	1.84	0.60
1:I:294:LEU:HD11	1:I:429:VAL:HG11	1.84	0.60
1:L:57:ARG:HH12	2:M:17:DG:H5"	1.64	0.60
1:E:320:ILE:HD11	1:E:420:MET:HE3	1.84	0.60
1:B:154:ILE:HG23	1:B:190:MET:HE1	1.84	0.59
1:B:726:HIS:ND1	1:B:735:VAL:O	2.34	0.59
1:E:347:CYS:HB3	1:E:350:GLU:HB2	1.84	0.59
1:I:594:VAL:HA	1:I:609:VAL:HA	1.83	0.59
1:B:611:LEU:HD11	1:B:669:GLN:HG3	1.83	0.59
1:L:383:ALA:O	1:L:386:ARG:NH1	2.36	0.59
1:B:227:VAL:HG12	1:B:246:LEU:HA	1.85	0.59
1:I:598:THR:HA	1:I:605:ILE:HA	1.85	0.58
1:B:712:ASP:HB3	1:B:715:THR:HG22	1.85	0.58
1:E:417:PRO:HG2	1:E:429:VAL:HB	1.84	0.58
1:L:71:LYS:HA	1:L:74:ILE:HB	1.85	0.58
1:L:5:ASN:HB2	1:L:52:ARG:HE	1.67	0.58
1:L:715:THR:HG23	1:L:717:GLU:H	1.67	0.58
1:L:706:LEU:HD12	1:L:725:VAL:HG12	1.85	0.58
1:B:468:ALA:HA	1:B:505:GLN:HB3	1.86	0.58
1:I:219:MET:O	1:I:223:SER:OG	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:724:ALA:HB2	1:L:738:GLU:HG3	1.85	0.57
1:E:110:LYS:HE2	1:E:111:PRO:HD2	1.87	0.57
1:E:631:LYS:HE3	1:E:635:MET:HE1	1.85	0.57
1:B:221:ILE:HD13	1:B:229:LEU:HB3	1.87	0.57
1:E:536:PHE:HB3	1:E:882:PHE:HB3	1.87	0.57
1:I:553:GLU:O	1:I:557:ARG:NH1	2.38	0.57
1:B:722:ARG:HB3	1:B:769:ILE:HD12	1.86	0.57
1:E:627:ARG:NH2	6:E:901:3PO:O1A	2.37	0.57
1:L:431:MET:HE2	2:M:15:DC:H5"	1.87	0.57
1:L:435:GLN:HA	1:L:810:ILE:HD11	1.87	0.56
1:L:808:ALA:HB3	1:L:815:GLY:HA3	1.85	0.56
1:B:810:ILE:O	1:B:812:ASP:N	2.39	0.56
1:I:46:MET:HB3	1:I:267:MET:HE2	1.87	0.56
1:E:503:ALA:HA	1:E:508:PRO:HB3	1.87	0.56
1:I:826:LYS:HA	1:I:829:ARG:HH11	1.69	0.56
1:L:561:LEU:HB2	1:L:875:ILE:HD12	1.86	0.56
1:B:731:ASP:HB3	1:B:792:ARG:HH21	1.71	0.56
1:L:543:ILE:HD12	1:L:689:VAL:HG11	1.87	0.56
1:B:423:ARG:NH1	1:B:781:ASN:OD1	2.39	0.56
1:B:737:GLN:HE21	1:B:739:TYR:HE2	1.54	0.56
1:E:118:THR:HA	1:E:141:ILE:HD12	1.88	0.56
1:I:715:THR:HB	1:I:717:GLU:HG2	1.89	0.55
1:L:705:LEU:O	1:L:720:ARG:NH2	2.31	0.55
1:B:737:GLN:O	1:B:774:GLN:NE2	2.39	0.55
1:B:738:GLU:HA	1:B:774:GLN:HE22	1.71	0.55
1:I:47:GLY:HA3	1:I:266:PRO:HA	1.88	0.55
1:I:544:GLN:HE22	1:I:881:ALA:HB1	1.70	0.55
1:L:264:ILE:HG13	1:L:292:ARG:NH2	2.21	0.55
1:I:190:MET:O	1:I:194:GLY:N	2.39	0.55
1:B:740:LYS:HD3	1:B:767:SER:HB2	1.88	0.55
1:I:728:VAL:HA	1:I:734:PRO:HA	1.89	0.55
1:E:205:HIS:ND1	1:E:207:GLU:OE1	2.34	0.55
1:E:598:THR:HG22	1:E:605:ILE:HG12	1.88	0.55
1:L:342:THR:HG22	1:L:348:PRO:HG3	1.89	0.55
1:B:117:ILE:O	1:B:121:THR:OG1	2.23	0.55
1:I:547:SER:HA	1:I:552:ASP:HB3	1.89	0.55
1:I:706:LEU:HD22	1:I:725:VAL:HG12	1.89	0.55
1:I:173:ARG:O	1:I:179:LYS:NZ	2.40	0.55
1:I:44:TYR:HA	1:I:266:PRO:HB3	1.89	0.55
1:L:286:TYR:CE1	1:L:417:PRO:HG3	2.42	0.55
1:B:278:TRP:H	1:B:321:ASN:ND2	1.97	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:43:SER:HA	1:L:46:MET:HE3	1.90	0.54
1:B:720:ARG:HH21	1:B:857:GLN:HE22	1.56	0.54
1:I:149:ALA:HB1	1:I:201:TRP:HZ3	1.71	0.54
1:E:57:ARG:NH1	2:F:18:DC:OP2	2.41	0.54
1:I:150:ARG:HD2	1:I:201:TRP:HB2	1.89	0.54
1:I:420:MET:HE2	1:I:424:GLY:HA2	1.90	0.54
1:B:342:THR:O	1:B:395:ARG:NH2	2.41	0.54
1:I:32:LEU:HB3	1:I:273:VAL:HG12	1.90	0.54
1:I:379:ARG:HH21	1:I:656:GLN:HG3	1.72	0.54
1:L:579:ASN:HB2	1:L:625:VAL:HG21	1.90	0.54
1:I:3:THR:HA	1:I:255:ALA:HB1	1.88	0.54
1:I:150:ARG:NE	1:I:187:GLU:OE2	2.42	0.53
1:L:817:ILE:HG13	1:L:820:ASP:HB2	1.88	0.53
1:L:536:PHE:HB3	1:L:882:PHE:HB3	1.90	0.53
1:E:265:SER:O	1:E:265:SER:OG	2.26	0.53
1:I:150:ARG:NH2	1:I:187:GLU:OE1	2.42	0.53
1:L:334:VAL:HG12	1:L:443:LEU:HD23	1.91	0.53
1:I:201:TRP:HA	1:I:204:TRP:NE1	2.24	0.53
1:L:345:LYS:NZ	1:L:351:ASP:O	2.39	0.53
1:B:659:ILE:HG13	1:B:664:GLY:HA3	1.91	0.52
1:L:571:TYR:CE1	1:L:634:VAL:HB	2.45	0.52
1:L:123:LEU:O	1:L:127:THR:OG1	2.26	0.52
1:L:313:MET:HE2	1:L:316:VAL:HG11	1.91	0.52
1:I:163:LYS:HA	1:I:166:VAL:HG12	1.92	0.52
1:I:584:ALA:HA	1:I:587:ILE:HD12	1.92	0.52
1:B:10:ASP:HB2	1:B:291:ARG:HH21	1.74	0.52
1:I:855:GLU:HA	1:I:858:LEU:HD12	1.92	0.52
1:B:699:LEU:HD12	1:B:779:ALA:HA	1.90	0.52
1:B:281:ILE:HG22	1:B:282:THR:HG23	1.91	0.51
1:E:468:ALA:HA	1:E:505:GLN:HB3	1.91	0.51
1:L:298:ARG:HH12	1:L:427:TYR:HB2	1.75	0.51
1:L:59:LEU:HD22	1:L:127:THR:HG21	1.91	0.51
1:L:286:TYR:HE1	1:L:417:PRO:HG3	1.74	0.51
1:E:490:MET:HE1	1:E:519:ALA:HA	1.91	0.51
1:B:93:LYS:HD3	1:B:94:ALA:N	2.26	0.51
2:A:5:DA:H61	4:D:6:DT:H3	1.58	0.51
1:L:275:PRO:HG2	1:L:324:GLN:HB3	1.93	0.51
1:E:221:ILE:HA	1:E:226:MET:HB3	1.93	0.51
1:I:689:VAL:HB	1:I:692:ALA:HB3	1.92	0.51
1:I:720:ARG:NH1	1:I:721:LYS:O	2.44	0.51
1:L:725:VAL:HG21	1:L:778:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:798:ALA:HB1	1:E:804:ILE:HD13	1.92	0.51
1:L:304:ALA:HA	1:L:307:ARG:HD2	1.92	0.51
1:L:398:LEU:HD11	1:L:439:MET:HE1	1.93	0.51
1:I:342:THR:HG22	1:I:348:PRO:HG3	1.93	0.51
1:L:316:VAL:HG13	1:L:420:MET:HE1	1.93	0.51
1:L:517:GLU:HG3	1:L:532:LEU:HB2	1.93	0.51
1:I:519:ALA:O	1:I:523:HIS:ND1	2.44	0.50
1:I:631:LYS:HE3	1:I:635:MET:HE3	1.93	0.50
1:E:420:MET:HE1	1:E:792:ARG:HD3	1.94	0.50
1:I:89:PHE:HA	1:I:92:VAL:HB	1.93	0.50
1:I:286:TYR:CE1	1:I:417:PRO:HG3	2.46	0.50
1:B:84:ARG:HG3	1:B:219:MET:HB3	1.94	0.50
1:B:347:CYS:HB3	1:B:350:GLU:HB2	1.93	0.50
1:E:160:LYS:HE3	1:E:164:LYS:HZ1	1.77	0.50
1:E:229:LEU:HB2	1:E:242:GLU:HG2	1.93	0.50
1:I:229:LEU:H	1:I:229:LEU:HD23	1.77	0.50
1:B:549:MET:HE3	1:B:842:LEU:HG	1.93	0.50
1:B:791:LEU:HD21	1:B:809:LEU:HD13	1.94	0.50
1:E:472:LYS:NZ	6:E:901:3PO:O2A	2.42	0.50
1:I:549:MET:O	1:I:551:ARG:NH1	2.45	0.50
1:B:110:LYS:HD2	1:B:111:PRO:HD2	1.93	0.50
1:L:462:ILE:O	1:L:466:ASN:N	2.42	0.49
1:I:6:ILE:HD11	1:I:291:ARG:HH11	1.77	0.49
1:I:347:CYS:HB2	1:I:350:GLU:HB2	1.94	0.49
1:I:10:ASP:O	1:I:291:ARG:NH2	2.45	0.49
1:I:536:PHE:HZ	1:I:821:ALA:HB1	1.77	0.49
1:E:696:MET:HG2	1:E:779:ALA:HB1	1.94	0.49
1:L:660:ASP:OD1	1:L:660:ASP:N	2.45	0.49
1:E:688:THR:HG22	1:E:689:VAL:HG13	1.94	0.49
1:L:417:PRO:HG2	1:L:429:VAL:HB	1.95	0.49
1:B:798:ALA:HB1	1:B:804:ILE:HD12	1.93	0.49
1:E:59:LEU:HD12	1:E:60:LYS:HG3	1.93	0.49
1:E:109:ILE:HD11	1:E:149:ALA:HA	1.95	0.49
1:I:537:ASP:HB3	1:I:813:SER:HB2	1.95	0.49
1:L:58:GLN:HG2	1:L:63:GLU:HB2	1.95	0.49
1:I:176:HIS:HD2	1:I:177:VAL:HG13	1.78	0.48
1:I:873:ARG:HD3	1:I:876:LEU:HD12	1.94	0.48
1:B:190:MET:HB3	1:B:195:LEU:HB2	1.95	0.48
1:I:299:THR:HG21	1:I:305:LEU:HG	1.95	0.48
1:L:462:ILE:HG23	1:L:478:ARG:HD3	1.95	0.48
1:L:566:THR:O	1:L:568:GLN:NE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:651:LEU:HA	1:L:655:ILE:HB	1.94	0.48
1:I:623:TYR:HE1	1:I:663:LYS:HB3	1.78	0.48
1:E:155:ARG:O	1:E:160:LYS:HD3	2.13	0.48
1:L:696:MET:O	1:L:700:LYS:HG3	2.13	0.48
1:I:298:ARG:NH2	1:I:419:ASN:OD1	2.46	0.48
1:L:11:PHE:HE2	1:L:48:GLU:HG3	1.79	0.48
1:L:731:ASP:OD2	1:L:792:ARG:NH1	2.47	0.48
1:B:311:VAL:HG21	1:B:734:PRO:HG3	1.96	0.48
1:L:335:LEU:O	1:L:339:ASN:ND2	2.42	0.48
1:E:151:PHE:CD1	1:E:183:MET:HB3	2.49	0.48
1:I:199:GLU:HB3	1:I:202:SER:HB2	1.95	0.48
1:I:738:GLU:OE2	1:I:740:LYS:NZ	2.39	0.48
1:B:417:PRO:HG2	1:B:429:VAL:HB	1.96	0.48
1:B:427:TYR:HA	1:B:435:GLN:HE22	1.79	0.48
1:E:118:THR:OG1	1:E:119:ILE:N	2.47	0.48
1:E:246:LEU:HD12	1:E:251:ALA:HB2	1.96	0.48
1:I:553:GLU:OE1	1:I:557:ARG:NH2	2.46	0.47
1:L:30:GLU:OE1	1:L:34:ARG:NH1	2.47	0.47
1:B:67:ASN:OD1	1:B:68:ALA:N	2.46	0.47
1:B:794:THR:HA	1:B:831:THR:HG21	1.96	0.47
1:E:541:SER:HA	1:E:544:GLN:HB2	1.97	0.47
1:L:430:SER:OG	1:L:432:PHE:O	2.32	0.47
1:B:141:ILE:O	1:B:145:ILE:HG12	2.15	0.47
1:B:387:LYS:HE2	1:B:387:LYS:HB3	1.80	0.47
1:I:461:LYS:HD2	1:I:479:ILE:HG23	1.95	0.47
1:B:705:LEU:O	1:B:720:ARG:NH2	2.48	0.47
1:E:705:LEU:O	1:E:720:ARG:NH2	2.46	0.47
1:I:826:LYS:O	1:I:830:GLU:HG2	2.15	0.47
1:B:42:GLU:O	1:B:46:MET:HG3	2.13	0.47
1:L:11:PHE:CE1	1:L:44:TYR:HB3	2.50	0.47
1:B:163:LYS:HA	1:B:166:VAL:HG22	1.96	0.47
1:B:386:ARG:NH1	3:C:4:G:OP1	2.47	0.47
1:B:741:LYS:HD2	1:B:770:ASP:HA	1.96	0.47
1:E:5:ASN:OD1	1:E:5:ASN:N	2.43	0.47
1:E:159:ALA:O	1:E:163:LYS:N	2.47	0.47
1:I:804:ILE:HG12	1:I:820:ASP:HB3	1.96	0.47
1:I:826:LYS:HA	1:I:829:ARG:NH1	2.30	0.47
1:L:342:THR:HG21	1:L:402:LEU:HD11	1.97	0.47
1:L:560:ASN:HD21	1:L:567:VAL:HA	1.80	0.47
1:E:117:ILE:O	1:E:121:THR:OG1	2.24	0.47
1:I:740:LYS:HD2	1:I:740:LYS:HA	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:485:ASN:O	1:L:489:ILE:HG13	2.15	0.47
1:B:170:LEU:HD22	1:B:183:MET:HE3	1.97	0.47
1:L:276:LYS:HE2	1:L:287:TRP:HA	1.96	0.47
1:E:42:GLU:O	1:E:46:MET:HG3	2.15	0.47
1:I:557:ARG:H	1:I:557:ARG:HH11	1.63	0.47
1:I:816:THR:HG22	1:I:824:LEU:HD22	1.95	0.47
1:L:44:TYR:HE1	1:L:291:ARG:H	1.62	0.47
1:I:163:LYS:NZ	1:I:167:GLU:HG2	2.30	0.46
1:E:186:VAL:O	1:E:190:MET:HG2	2.16	0.46
1:E:846:TYR:HA	1:E:849:PHE:HE2	1.80	0.46
1:E:226:MET:HE2	1:E:244:ILE:HD11	1.98	0.46
1:I:286:TYR:HE1	1:I:417:PRO:HG3	1.79	0.46
1:I:312:TYR:CZ	1:I:314:PRO:HG3	2.50	0.46
1:I:502:TRP:CG	1:I:512:LEU:HD13	2.51	0.46
1:L:524:HIS:HB2	1:L:528:TYR:HB2	1.97	0.46
1:B:446:LEU:HD13	1:B:806:SER:HB3	1.97	0.46
1:I:589:GLY:HA3	1:I:614:LYS:HB2	1.97	0.46
1:B:692:ALA:O	1:B:696:MET:HG3	2.16	0.46
1:I:490:MET:HE1	1:I:522:GLN:HG3	1.97	0.46
1:L:31:ARG:HA	1:L:34:ARG:HD3	1.97	0.46
1:L:475:PHE:HA	1:L:478:ARG:HD2	1.98	0.46
1:B:551:ARG:NH2	1:B:836:TYR:O	2.48	0.46
1:B:711:LYS:HB3	1:B:718:ILE:HA	1.98	0.46
1:E:231:ARG:HA	1:E:242:GLU:HA	1.97	0.46
1:L:264:ILE:HG22	1:L:291:ARG:CD	2.46	0.46
1:E:231:ARG:HG2	1:E:234:ALA:HB2	1.98	0.45
1:E:329:LYS:HD3	1:E:447:ALA:HA	1.98	0.45
1:B:566:THR:OG1	1:B:567:VAL:N	2.49	0.45
2:A:13:DC:H2'	2:A:14:DG:C8	2.51	0.45
1:E:715:THR:HG23	1:E:717:GLU:H	1.82	0.45
1:E:832:MET:HE2	1:E:832:MET:HB3	1.79	0.45
1:I:577:LYS:HA	1:I:577:LYS:HD3	1.83	0.45
1:L:348:PRO:HD3	1:L:398:LEU:HD21	1.97	0.45
1:I:115:ALA:O	1:I:119:ILE:HG13	2.16	0.45
1:I:298:ARG:HB2	1:I:421:ASP:HA	1.98	0.45
1:L:299:THR:OG1	1:L:301:SER:O	2.30	0.45
1:L:711:LYS:HZ3	1:L:716:GLY:HA2	1.81	0.45
1:I:657:PRO:HA	1:I:660:ASP:HB2	1.98	0.45
1:E:473:VAL:HG13	1:E:477:GLU:HB2	1.97	0.45
2:F:3:DG:H2''	2:F:4:DA:C8	2.51	0.45
1:I:3:THR:HG21	1:I:52:ARG:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:556:GLY:O	1:I:561:LEU:N	2.49	0.45
1:I:816:THR:OG1	1:I:817:ILE:N	2.47	0.45
1:B:36:GLN:NE2	1:B:40:GLU:OE2	2.42	0.45
1:I:462:ILE:HD13	1:I:478:ARG:HD2	1.99	0.45
1:I:613:THR:HA	1:I:616:LEU:HB2	1.99	0.45
1:L:330:ILE:HD13	1:L:409:ALA:HA	1.98	0.45
1:L:471:ASP:O	1:L:478:ARG:NH2	2.50	0.45
1:L:264:ILE:HG13	1:L:292:ARG:HH21	1.81	0.45
1:I:191:LEU:HD23	1:I:191:LEU:HA	1.82	0.45
1:L:577:LYS:HG3	1:L:684:SER:HB3	1.99	0.45
1:B:574:VAL:HG13	1:B:684:SER:HB2	1.99	0.45
1:E:378:LYS:H	1:E:378:LYS:HG2	1.62	0.45
1:I:134:VAL:HG12	1:I:244:ILE:HB	1.98	0.45
1:I:550:LEU:O	1:I:868:GLY:N	2.50	0.45
1:B:550:LEU:HD21	1:B:842:LEU:HD12	1.97	0.44
1:E:118:THR:O	1:E:122:THR:HG23	2.17	0.44
4:D:3:DC:H2''	4:D:4:DG:H5''	1.98	0.44
1:I:651:LEU:HD23	1:I:655:ILE:HD12	2.00	0.44
1:B:412:LYS:HB3	1:B:412:LYS:HE3	1.71	0.44
1:I:639:TYR:HA	1:I:780:PRO:HG3	2.00	0.44
1:I:691:ALA:HA	1:I:694:GLU:HB2	1.99	0.44
1:L:684:SER:O	1:L:688:THR:OG1	2.30	0.44
1:L:705:LEU:HD13	1:L:857:GLN:HB3	2.00	0.44
1:B:722:ARG:HG2	1:B:769:ILE:HB	1.99	0.44
1:I:557:ARG:HH11	1:I:557:ARG:N	2.15	0.44
1:I:734:PRO:HB2	1:I:736:TRP:CZ3	2.53	0.44
1:L:317:TYR:O	1:L:321:ASN:ND2	2.50	0.44
1:B:186:VAL:O	1:B:190:MET:HG3	2.17	0.44
1:E:318:LYS:O	1:E:322:ILE:HG13	2.17	0.44
1:L:545:HIS:HE1	1:L:787:ASP:HA	1.83	0.44
1:I:113:ALA:O	1:I:116:TYR:N	2.49	0.44
1:I:541:SER:HA	1:I:544:GLN:HB2	1.98	0.44
1:L:560:ASN:ND2	1:L:568:GLN:H	2.16	0.44
2:M:13:DC:H2'	2:M:14:DG:C8	2.52	0.44
1:B:110:LYS:HZ1	1:B:112:GLU:HG3	1.82	0.44
1:I:217:ILE:O	1:I:221:ILE:HD12	2.18	0.44
1:B:141:ILE:HD12	1:B:141:ILE:H	1.82	0.44
1:I:557:ARG:HB3	1:I:568:GLN:HE22	1.82	0.44
1:I:879:ASP:OD1	1:I:879:ASP:N	2.51	0.44
1:B:294:LEU:HD21	1:B:429:VAL:HG11	2.00	0.44
1:B:537:ASP:H	1:B:882:PHE:HD2	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:ARG:HH21	1:E:223:SER:HA	1.83	0.44
1:L:537:ASP:OD1	1:L:537:ASP:N	2.50	0.44
1:E:637:LEU:HD13	1:E:685:VAL:HG11	2.00	0.43
1:E:642:LYS:HZ2	1:E:642:LYS:HG3	1.53	0.43
1:I:372:GLU:HB3	1:I:373:ALA:H	1.70	0.43
1:L:832:MET:HE2	1:L:832:MET:HB3	1.90	0.43
1:E:729:THR:HB	1:E:789:SER:HB2	2.00	0.43
1:L:85:ILE:O	1:L:89:PHE:N	2.46	0.43
1:L:40:GLU:HG2	1:L:286:TYR:CD2	2.50	0.43
1:L:394:ARG:O	1:L:398:LEU:HB2	2.19	0.43
1:B:439:MET:HE2	1:B:439:MET:HB3	1.89	0.43
1:I:632:ARG:O	1:I:636:THR:OG1	2.26	0.43
1:B:159:ALA:O	1:B:163:LYS:N	2.39	0.43
1:E:231:ARG:HH11	1:E:242:GLU:HB2	1.83	0.43
1:B:579:ASN:HA	1:B:582:LEU:HB2	2.01	0.43
1:E:30:GLU:OE2	1:E:34:ARG:NH2	2.47	0.43
1:I:186:VAL:HG22	1:I:190:MET:HE3	1.99	0.43
1:L:659:ILE:HD12	1:L:660:ASP:N	2.34	0.43
1:I:826:LYS:O	1:I:829:ARG:HG2	2.18	0.43
1:L:560:ASN:O	1:L:878:SER:OG	2.29	0.43
1:L:804:ILE:HD12	1:L:820:ASP:HB3	2.01	0.43
1:I:48:GLU:HA	1:I:262:ALA:HB1	2.01	0.43
1:I:331:ASN:HB3	1:I:334:VAL:HB	2.01	0.43
1:I:402:LEU:HD21	1:I:439:MET:HE1	2.01	0.43
1:L:824:LEU:O	1:L:828:VAL:HG23	2.19	0.43
1:B:337:VAL:HG21	1:B:512:LEU:HD21	2.00	0.42
1:I:475:PHE:CE2	1:I:879:ASP:HB2	2.54	0.42
1:I:553:GLU:HA	1:I:870:LEU:HG	2.01	0.42
1:L:725:VAL:HG23	1:L:727:TRP:HZ3	1.84	0.42
1:B:131:ASN:HB3	1:B:133:THR:HG22	2.01	0.42
1:I:313:MET:HE2	1:I:316:VAL:HG21	2.01	0.42
1:I:714:LYS:HD3	1:I:714:LYS:HA	1.48	0.42
1:I:808:ALA:HB3	1:I:815:GLY:HA3	2.01	0.42
1:B:389:LYS:O	1:B:393:SER:OG	2.30	0.42
1:I:115:ALA:O	1:I:118:THR:OG1	2.34	0.42
1:I:330:ILE:O	1:I:332:LYS:HD2	2.20	0.42
1:I:727:TRP:HB3	1:I:845:PHE:CD1	2.54	0.42
1:L:332:LYS:H	1:L:332:LYS:HG2	1.55	0.42
1:L:349:VAL:HG21	1:L:508:PRO:HG3	2.01	0.42
1:L:876:LEU:HD12	1:L:876:LEU:H	1.84	0.42
1:B:345:LYS:HB2	1:B:348:PRO:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:LEU:HD23	1:E:78:LEU:HA	1.91	0.42
1:I:138:ALA:HB3	1:I:210:ILE:HG23	2.01	0.42
1:I:536:PHE:CZ	1:I:821:ALA:HB1	2.55	0.42
1:I:728:VAL:HG22	1:I:734:PRO:HB3	2.02	0.42
1:I:731:ASP:CG	1:I:792:ARG:HH21	2.26	0.42
1:L:817:ILE:HD12	1:L:819:ALA:H	1.85	0.42
1:E:122:THR:HG21	1:E:220:LEU:HD22	2.01	0.42
1:I:39:LEU:O	1:I:43:SER:N	2.52	0.42
1:B:272:VAL:HG23	1:B:273:VAL:HG13	2.01	0.42
1:E:269:GLN:HE22	1:E:407:LYS:NZ	2.17	0.42
1:E:700:LYS:HE3	1:E:700:LYS:HB2	1.68	0.42
1:L:345:LYS:HD3	1:L:348:PRO:HA	2.02	0.42
1:L:421:ASP:OD1	1:L:425:ARG:N	2.52	0.42
1:L:264:ILE:HG13	1:L:292:ARG:CZ	2.50	0.42
1:B:833:VAL:HG21	1:B:876:LEU:HG	2.02	0.42
1:I:149:ALA:HB1	1:I:201:TRP:CZ3	2.53	0.42
1:I:532:LEU:HD12	1:I:533:PRO:HD2	2.01	0.42
1:I:725:VAL:HG22	1:I:737:GLN:HB3	2.01	0.42
1:L:278:TRP:CD2	1:L:296:LEU:HD23	2.55	0.42
1:E:8:LYS:HE2	1:E:8:LYS:HB2	1.74	0.41
1:E:54:MET:O	1:E:58:GLN:HG3	2.19	0.41
1:I:248:PRO:O	1:I:252:GLU:HG2	2.20	0.41
1:L:67:ASN:OD1	1:L:68:ALA:N	2.54	0.41
1:L:549:MET:HB3	1:L:842:LEU:HD11	2.02	0.41
1:L:566:THR:OG1	1:L:567:VAL:N	2.53	0.41
1:B:550:LEU:HB2	1:B:691:ALA:HB1	2.02	0.41
1:B:718:ILE:H	1:B:718:ILE:HG13	1.71	0.41
1:E:117:ILE:HG23	1:E:751:PHE:CE2	2.55	0.41
1:E:308:TYR:OH	1:E:734:PRO:O	2.35	0.41
1:B:163:LYS:O	1:B:167:GLU:N	2.53	0.41
1:B:574:VAL:HG21	1:B:685:VAL:HG22	2.01	0.41
1:I:267:MET:HG2	1:I:431:MET:HE1	2.02	0.41
1:L:801:LYS:HD2	1:L:801:LYS:HA	1.90	0.41
1:B:829:ARG:NH2	1:B:882:PHE:H	2.19	0.41
1:I:138:ALA:HA	1:I:141:ILE:HD12	2.03	0.41
1:E:183:MET:HA	1:E:183:MET:HE2	2.02	0.41
1:L:666:MET:SD	1:L:666:MET:N	2.90	0.41
1:E:6:ILE:HD12	1:E:6:ILE:HA	1.92	0.41
1:E:278:TRP:CD2	1:E:296:LEU:HD23	2.55	0.41
1:I:272:VAL:HA	1:I:414:ILE:HG22	2.02	0.41
1:L:118:THR:O	1:L:122:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:THR:HG22	1:B:137:VAL:HG13	2.03	0.41
1:E:37:LEU:HD12	1:E:288:ALA:HB2	2.03	0.41
1:I:466:ASN:OD1	1:I:478:ARG:NH1	2.53	0.41
1:B:180:LYS:HA	1:B:750:MET:HE1	2.03	0.41
1:B:396:ILE:HD12	1:B:397:SER:N	2.35	0.41
1:B:432:PHE:HE2	1:B:444:LEU:HD21	1.86	0.41
1:E:248:PRO:HA	1:E:251:ALA:HB3	2.03	0.41
1:I:57:ARG:HH12	2:J:17:DG:H5''	1.85	0.41
1:L:457:TYR:CD1	1:L:521:VAL:HG11	2.56	0.41
1:I:142:GLY:O	1:I:146:GLU:HB2	2.20	0.41
1:I:303:LYS:HD3	1:I:303:LYS:N	2.36	0.41
1:I:713:LYS:H	1:I:713:LYS:HG2	1.62	0.41
1:I:842:LEU:HD23	1:I:842:LEU:HA	1.84	0.41
1:I:861:MET:HA	1:I:862:PRO:HD3	1.96	0.41
1:L:13:ASP:OD1	1:L:13:ASP:N	2.53	0.41
1:L:51:PHE:CD1	1:L:262:ALA:HB2	2.55	0.41
1:L:281:ILE:HD12	1:L:282:THR:OG1	2.21	0.41
1:L:392:LYS:O	1:L:396:ILE:HG13	2.21	0.41
1:L:826:LYS:HA	1:L:826:LYS:HD3	1.89	0.41
1:B:100:PRO:HB2	1:B:215:ARG:NH1	2.36	0.41
1:E:113:ALA:O	1:E:117:ILE:HD12	2.21	0.41
1:E:119:ILE:H	1:E:119:ILE:HG13	1.67	0.41
1:E:281:ILE:HG21	1:E:309:GLU:HA	2.02	0.41
1:I:176:HIS:CD2	1:I:177:VAL:HG13	2.53	0.41
1:I:397:SER:O	1:I:401:MET:HG2	2.21	0.41
1:B:772:HIS:CD2	2:A:8:DG:H4'	2.56	0.40
1:E:53:LYS:HB3	1:E:53:LYS:HE3	1.70	0.40
1:E:412:LYS:H	1:E:412:LYS:HG2	1.65	0.40
1:L:316:VAL:HG21	1:L:733:PHE:HB2	2.02	0.40
1:B:226:MET:HG2	1:B:227:VAL:HG13	2.04	0.40
1:B:274:PRO:HA	1:B:275:PRO:HD3	1.93	0.40
1:L:418:TYR:HD2	1:L:426:VAL:HG12	1.86	0.40
1:L:677:MET:HA	1:L:680:LEU:HD12	2.03	0.40
1:L:710:VAL:HG23	1:L:719:LEU:HB2	2.04	0.40
1:B:153:ARG:HG3	1:B:157:LEU:HD21	2.04	0.40
1:B:810:ILE:HB	1:B:813:SER:HB3	2.03	0.40
1:E:281:ILE:HD12	1:E:305:LEU:HG	2.03	0.40
1:E:572:GLY:O	1:E:576:LYS:HG2	2.22	0.40
1:I:494:LYS:HD2	1:I:494:LYS:HA	1.88	0.40
1:I:647:ARG:HE	1:I:647:ARG:HB3	1.70	0.40
1:B:102:ALA:O	1:B:106:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:LYS:O	1:B:484:GLU:HG3	2.21	0.40
1:E:11:PHE:HE2	1:E:48:GLU:HB2	1.86	0.40
1:E:199:GLU:HB2	1:E:201:TRP:CE3	2.55	0.40
1:I:281:ILE:H	1:I:281:ILE:HG13	1.72	0.40
1:E:135:GLN:H	1:E:135:GLN:HG2	1.65	0.40
1:E:853:LEU:HD12	1:E:853:LEU:HA	1.88	0.40
1:I:204:TRP:N	1:I:204:TRP:CD1	2.88	0.40
1:I:307:ARG:HD3	1:I:736:TRP:CE2	2.56	0.40
1:L:264:ILE:HD13	1:L:264:ILE:HG21	1.91	0.40
1:L:681:ILE:O	1:L:685:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

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	B	850/883 (96%)	824 (97%)	24 (3%)	2 (0%)	43	72
1	E	831/883 (94%)	813 (98%)	18 (2%)	0	100	100
1	I	823/883 (93%)	800 (97%)	23 (3%)	0	100	100
1	L	726/883 (82%)	711 (98%)	15 (2%)	0	100	100
All	All	3230/3532 (91%)	3148 (98%)	80 (2%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	811	HIS
1	B	227	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	695/729 (95%)	663 (95%)	32 (5%)	24	57
1	E	688/729 (94%)	670 (97%)	18 (3%)	40	73
1	I	674/729 (92%)	646 (96%)	28 (4%)	26	60
1	L	530/729 (73%)	502 (95%)	28 (5%)	20	52
All	All	2587/2916 (89%)	2481 (96%)	106 (4%)	27	61

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	THR
1	B	6	ILE
1	B	75	THR
1	B	109	ILE
1	B	114	VAL
1	B	121	THR
1	B	133	THR
1	B	137	VAL
1	B	157	LEU
1	B	160	LYS
1	B	195	LEU
1	B	236	VAL
1	B	254	ILE
1	B	265	SER
1	B	310	ASP
1	B	375	THR
1	B	398	LEU
1	B	402	LEU
1	B	527	SER
1	B	559	VAL
1	B	564	SER
1	B	594	VAL
1	B	606	SER
1	B	627	ARG

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Mol	Chain	Res	Type
1	B	628	SER
1	B	687	VAL
1	B	701	SER
1	B	718	ILE
1	B	728	VAL
1	B	776	SER
1	B	783	VAL
1	B	795	VAL
1	E	8	LYS
1	E	22	ASN
1	E	121	THR
1	E	229	LEU
1	E	242	GLU
1	E	265	SER
1	E	388	ASP
1	E	473	VAL
1	E	626	THR
1	E	628	SER
1	E	690	VAL
1	E	721	LYS
1	E	735	VAL
1	E	783	VAL
1	E	805	GLU
1	E	811	HIS
1	E	812	ASP
1	E	851	ASP
1	I	3	THR
1	I	121	THR
1	I	161	HIS
1	I	168	GLU
1	I	180	LYS
1	I	220	LEU
1	I	223	SER
1	I	230	HIS
1	I	243	THR
1	I	291	ARG
1	I	397	SER
1	I	430	SER
1	I	438	ASP
1	I	452	ILE
1	I	472	LYS
1	I	492	CYS

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Mol	Chain	Res	Type
1	I	495	SER
1	I	507	SER
1	I	546	PHE
1	I	557	ARG
1	I	632	ARG
1	I	643	GLU
1	I	654	THR
1	I	689	VAL
1	I	711	LYS
1	I	776	SER
1	I	778	ILE
1	I	848	GLN
1	L	3	THR
1	L	21	PHE
1	L	23	THR
1	L	27	HIS
1	L	78	LEU
1	L	127	THR
1	L	133	THR
1	L	273	VAL
1	L	337	VAL
1	L	349	VAL
1	L	438	ASP
1	L	460	LEU
1	L	471	ASP
1	L	527	SER
1	L	528	TYR
1	L	537	ASP
1	L	540	CYS
1	L	566	THR
1	L	567	VAL
1	L	570	ILE
1	L	576	LYS
1	L	680	LEU
1	L	684	SER
1	L	690	VAL
1	L	710	VAL
1	L	783	VAL
1	L	841	VAL
1	L	855	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	233	ASN
1	B	269	GLN
1	B	321	ASN
1	B	404	GLN
1	B	463	HIS
1	B	499	ASN
1	B	529	ASN
1	B	811	HIS
1	B	823	ASN
1	B	857	GLN
1	E	27	HIS
1	E	67	ASN
1	E	86	ASN
1	E	232	GLN
1	E	300	HIS
1	E	404	GLN
1	E	410	ASN
1	E	437	ASN
1	E	529	ASN
1	E	544	GLN
1	E	601	ASN
1	I	5	ASN
1	I	131	ASN
1	I	176	HIS
1	I	488	ASN
1	I	524	HIS
1	I	544	GLN
1	I	823	ASN
1	L	41	HIS
1	L	486	HIS
1	L	545	HIS
1	L	560	ASN
1	L	786	GLN
1	L	857	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	6/12 (50%)	0	0
3	G	6/12 (50%)	0	0
3	K	6/12 (50%)	0	0
3	N	6/12 (50%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	24/48 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\# Z > 2$
5	GOL	I	901	-	5,5,5	0.94	0	5,5,5	1.04	0
6	3PO	B	902	7	10,12,12	2.41	2 (20%)	17,20,20	0.83	0
5	GOL	B	901	-	5,5,5	0.96	0	5,5,5	1.07	0
6	3PO	L	901	7	10,12,12	2.47	2 (20%)	17,20,20	0.80	0
6	3PO	I	902	7	10,12,12	2.50	2 (20%)	17,20,20	0.83	0
5	GOL	C	101	-	5,5,5	0.95	0	5,5,5	1.07	0
6	3PO	E	901	7	10,12,12	2.45	2 (20%)	17,20,20	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	I	901	-	-	3/4/4/4	-
6	3PO	B	902	7	-	1/12/12/12	-
5	GOL	B	901	-	-	0/4/4/4	-
6	3PO	L	901	7	-	3/12/12/12	-
6	3PO	I	902	7	-	2/12/12/12	-
5	GOL	C	101	-	-	2/4/4/4	-
6	3PO	E	901	7	-	0/12/12/12	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	901	3PO	PB-O3B	5.45	1.65	1.59
6	I	902	3PO	PB-O3A	5.41	1.65	1.59
6	I	902	3PO	PB-O3B	5.40	1.65	1.59
6	E	901	3PO	PB-O3B	5.29	1.65	1.59
6	E	901	3PO	PB-O3A	5.28	1.65	1.59
6	B	902	3PO	PB-O3A	5.21	1.65	1.59
6	B	902	3PO	PB-O3B	5.19	1.65	1.59
6	L	901	3PO	PB-O3A	5.16	1.65	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

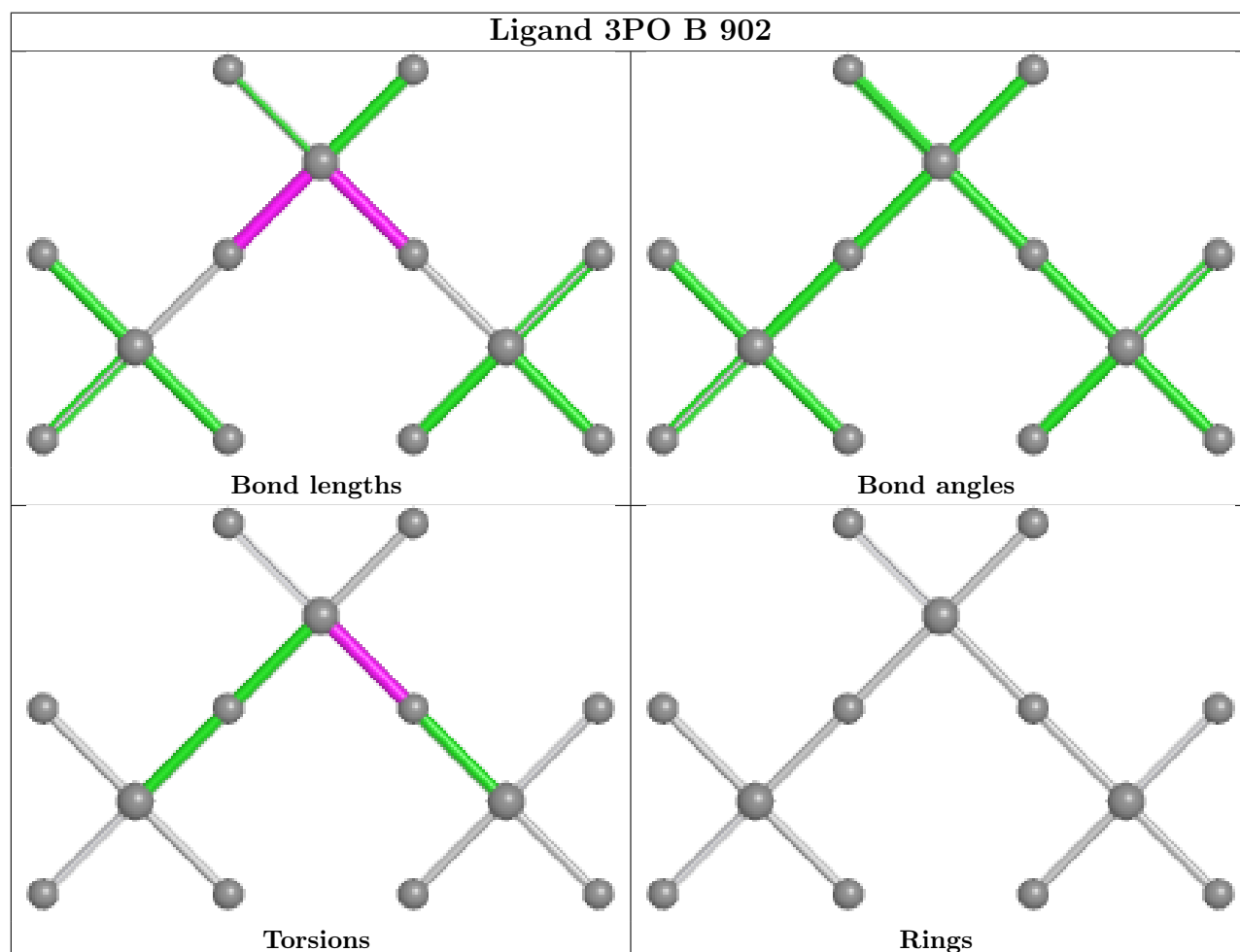
Mol	Chain	Res	Type	Atoms
6	L	901	3PO	PB-O3B-PG-O2G
6	L	901	3PO	PB-O3B-PG-O3G
5	C	101	GOL	O1-C1-C2-C3
5	I	901	GOL	O1-C1-C2-C3
5	C	101	GOL	O1-C1-C2-O2
5	I	901	GOL	O1-C1-C2-O2
5	I	901	GOL	C1-C2-C3-O3
6	I	902	3PO	PA-O3A-PB-O1B
6	B	902	3PO	PG-O3B-PB-O1B
6	I	902	3PO	PA-O3A-PB-O2B
6	L	901	3PO	PA-O3A-PB-O2B

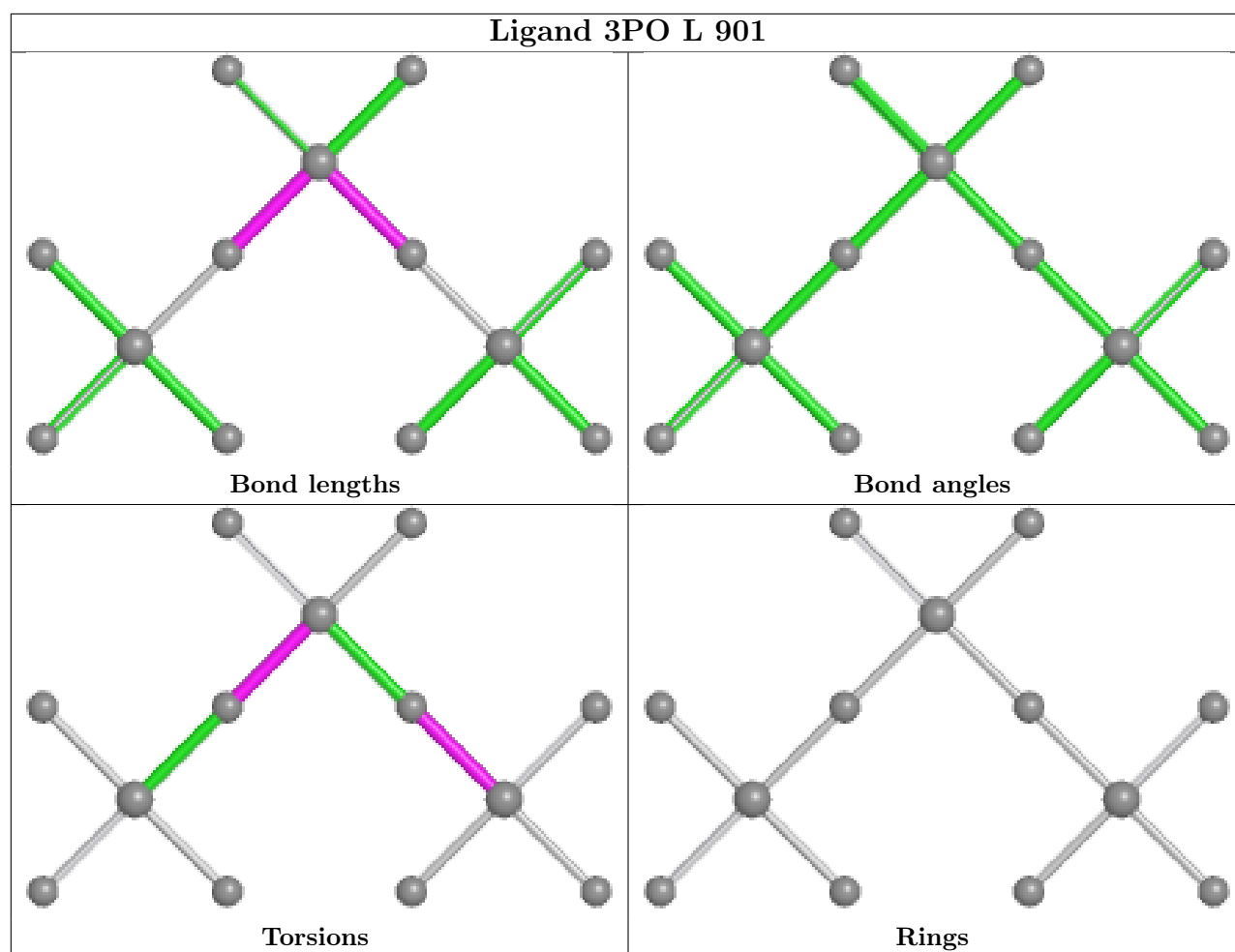
There are no ring outliers.

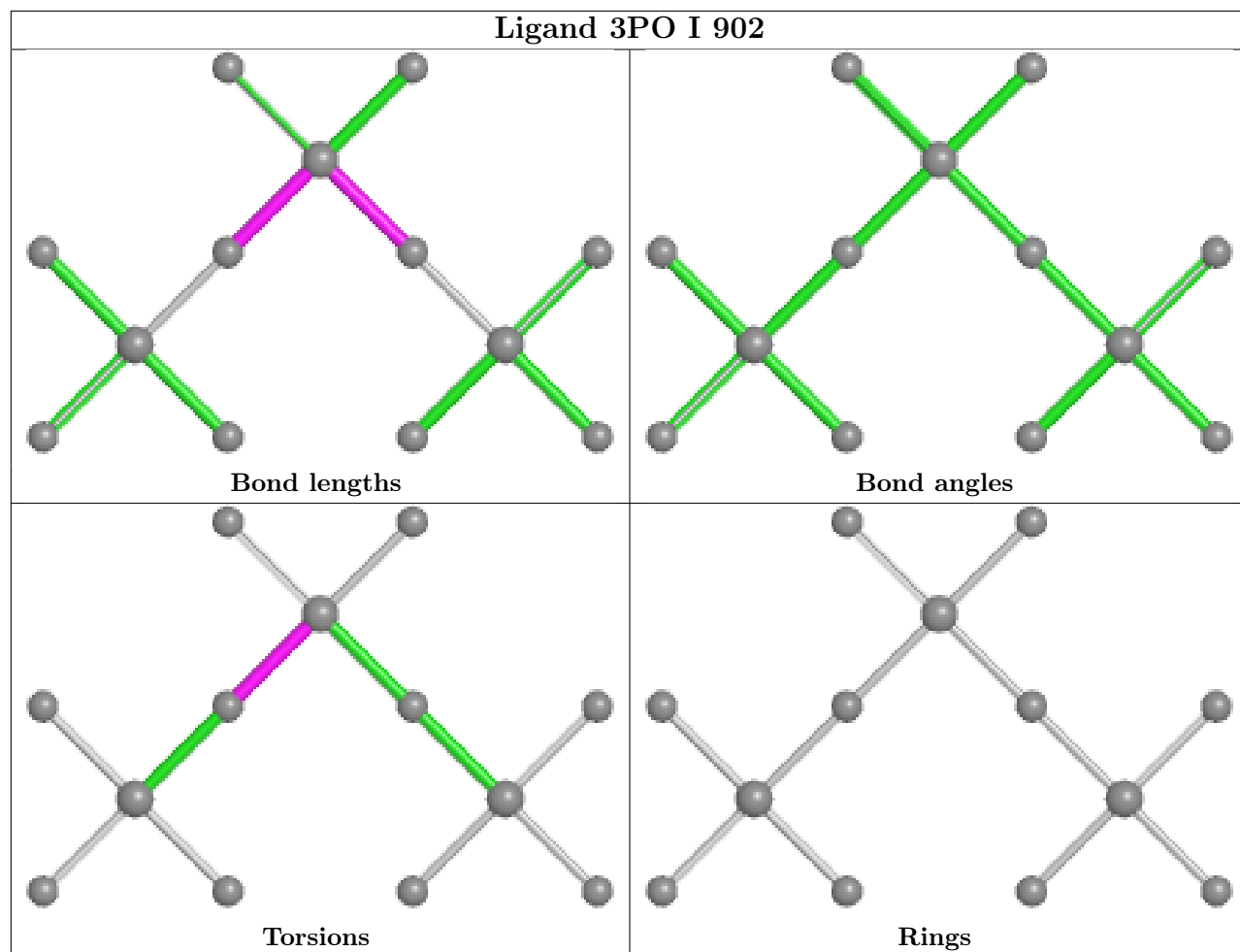
1 monomer is involved in 2 short contacts:

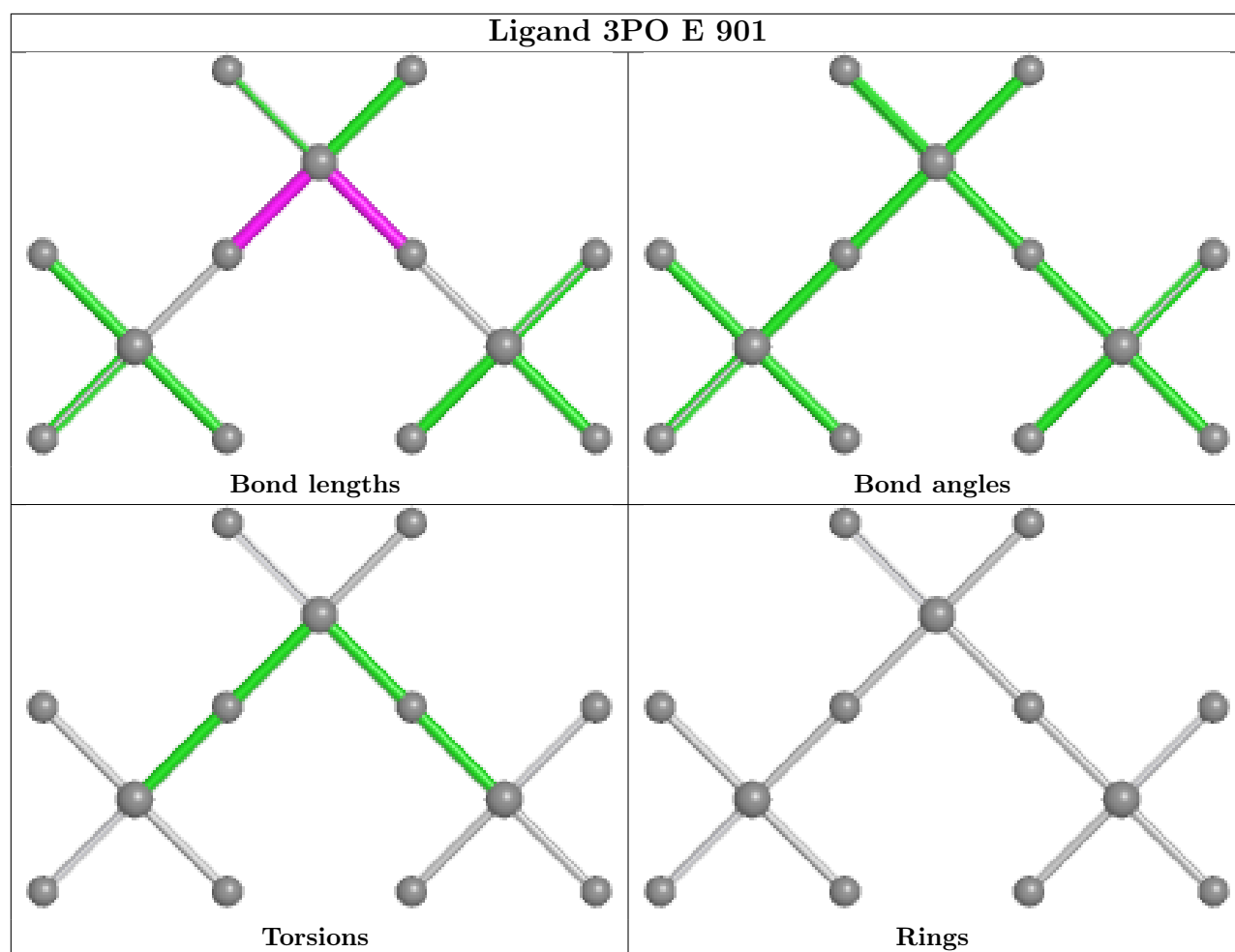
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	901	3PO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	B	856/883 (96%)	0.32	36 (4%)	40	32	39, 81, 191, 296	0
1	E	841/883 (95%)	0.30	24 (2%)	53	45	46, 81, 202, 308	0
1	I	833/883 (94%)	0.68	59 (7%)	22	17	86, 153, 225, 304	0
1	L	741/883 (83%)	0.50	38 (5%)	33	26	84, 128, 189, 245	0
2	A	16/18 (88%)	-0.00	0	100	100	68, 109, 266, 271	0
2	F	16/18 (88%)	0.30	0	100	100	63, 119, 255, 275	0
2	J	11/18 (61%)	-0.06	0	100	100	105, 111, 194, 228	0
2	M	13/18 (72%)	0.09	0	100	100	104, 127, 200, 238	0
3	C	8/12 (66%)	-0.51	0	100	100	63, 80, 96, 113	0
3	G	8/12 (66%)	-0.21	0	100	100	65, 90, 148, 176	0
3	K	8/12 (66%)	-0.12	0	100	100	119, 121, 163, 193	0
3	N	8/12 (66%)	-0.03	0	100	100	110, 137, 190, 191	0
4	D	8/9 (88%)	0.50	0	100	100	205, 222, 229, 271	0
4	H	8/9 (88%)	0.85	1 (12%)	8	7	189, 207, 227, 255	0
4	O	5/9 (55%)	0.18	0	100	100	200, 215, 229, 246	0
All	All	3380/3679 (91%)	0.44	158 (4%)	36	28	39, 121, 209, 308	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	883	ALA	8.7
1	I	558	ALA	5.8
1	L	816	THR	4.9
1	L	122	THR	4.4
1	E	883	ALA	4.4
1	I	541	SER	4.3
1	L	613	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	L	809	LEU	4.2
1	I	570	ILE	4.1
1	E	4	ILE	3.9
1	B	883	ALA	3.9
1	I	122	THR	3.9
1	B	74	ILE	3.8
1	I	791	LEU	3.8
1	B	2	ASN	3.8
1	I	670	PRO	3.8
1	L	535	ALA	3.8
1	I	691	ALA	3.6
1	I	550	LEU	3.6
1	I	629	VAL	3.6
1	B	195	LEU	3.6
1	I	782	PHE	3.6
1	L	682	TRP	3.5
1	L	428	ALA	3.5
1	B	85	ILE	3.5
1	I	64	VAL	3.4
1	L	883	ALA	3.4
1	E	14	ILE	3.4
1	B	752	LEU	3.4
1	I	573	ILE	3.4
1	E	137	VAL	3.4
1	I	459	TRP	3.4
1	I	677	MET	3.3
1	B	78	LEU	3.3
1	B	244	ILE	3.2
1	I	671	ASN	3.2
1	B	158	GLU	3.1
1	B	89	PHE	3.1
1	I	814	PHE	3.1
1	I	665	LEU	3.1
1	L	123	LEU	3.1
1	I	543	ILE	3.0
1	B	217	ILE	3.0
1	I	605	ILE	3.0
1	I	811	HIS	2.9
1	I	548	ALA	2.9
1	L	65	ALA	2.9
1	I	882	PHE	2.8
1	I	845	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	123	LEU	2.8
1	B	118	THR	2.8
1	B	137	VAL	2.7
1	B	4	ILE	2.7
1	E	165	ASN	2.7
1	E	6	ILE	2.7
1	I	688	THR	2.7
1	B	216	CYS	2.7
1	I	246	LEU	2.7
1	L	804	ILE	2.6
1	I	640	GLY	2.6
1	I	638	ALA	2.6
1	I	696	MET	2.6
1	E	278	TRP	2.6
1	E	20	PRO	2.6
1	E	752	LEU	2.6
1	B	168	GLU	2.6
1	L	634	VAL	2.6
1	I	204	TRP	2.6
1	I	547	SER	2.5
1	I	620	TRP	2.5
1	L	418	TYR	2.5
1	L	746	ARG	2.5
1	E	100	PRO	2.5
1	B	247	ALA	2.5
1	I	631	LYS	2.5
1	I	426	VAL	2.5
1	I	609	VAL	2.5
1	I	571	TYR	2.5
1	E	169	GLN	2.5
1	I	669	GLN	2.5
1	B	402	LEU	2.4
1	L	398	LEU	2.4
1	I	676	TYR	2.4
1	L	587	ILE	2.4
1	L	685	VAL	2.4
1	B	241	SER	2.4
1	B	243	THR	2.4
1	B	374	LEU	2.4
1	I	594	VAL	2.4
1	E	7	ALA	2.4
1	L	435	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	3	THR	2.4
1	L	835	THR	2.4
1	B	157	LEU	2.4
1	B	248	PRO	2.4
1	I	129	ALA	2.4
1	L	267	MET	2.4
1	I	103	PHE	2.3
1	I	881	ALA	2.3
1	E	195	LEU	2.3
1	L	243	THR	2.3
1	I	552	ASP	2.3
1	E	162	PHE	2.3
1	L	807	PHE	2.3
1	E	255	ALA	2.3
1	L	377	TRP	2.3
1	B	220	LEU	2.3
1	I	561	LEU	2.3
1	I	784	HIS	2.3
1	B	132	THR	2.3
1	L	574	VAL	2.3
1	I	825	PHE	2.2
1	I	747	LEU	2.2
1	I	787	ASP	2.2
4	H	2	DT	2.2
1	E	234	ALA	2.2
1	B	196	LEU	2.2
1	I	592	ASN	2.2
1	L	14	ILE	2.2
1	B	133	THR	2.2
1	E	814	PHE	2.2
1	I	569	ASP	2.2
1	B	226	MET	2.2
1	B	261	LEU	2.2
1	L	688	THR	2.2
1	B	246	LEU	2.2
1	E	322	ILE	2.1
1	L	667	PHE	2.1
1	I	810	ILE	2.1
1	L	817	ILE	2.1
1	E	751	PHE	2.1
1	I	536	PHE	2.1
1	L	327	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	543	ILE	2.1
1	B	1	MET	2.1
1	E	196	LEU	2.1
1	I	16	LEU	2.1
1	I	65	ALA	2.1
1	I	695	ALA	2.1
1	L	266	PRO	2.1
1	B	601	ASN	2.1
1	E	753	GLY	2.1
1	L	646	PHE	2.1
1	E	377	TRP	2.1
1	B	607	GLU	2.1
1	L	265	SER	2.0
1	L	536	PHE	2.0
1	B	224	THR	2.0
1	L	19	ILE	2.0
1	L	116	TYR	2.0
1	B	297	VAL	2.0
1	I	625	VAL	2.0
1	I	686	SER	2.0
1	L	841	VAL	2.0
1	I	730	PRO	2.0
1	E	755	PHE	2.0
1	B	221	ILE	2.0
1	E	376	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

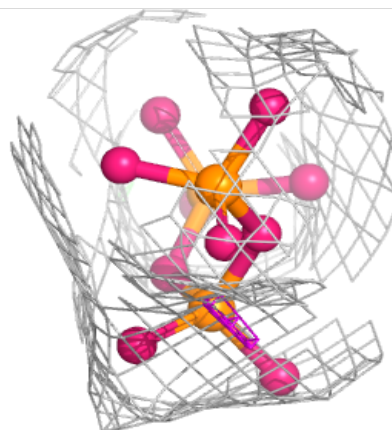
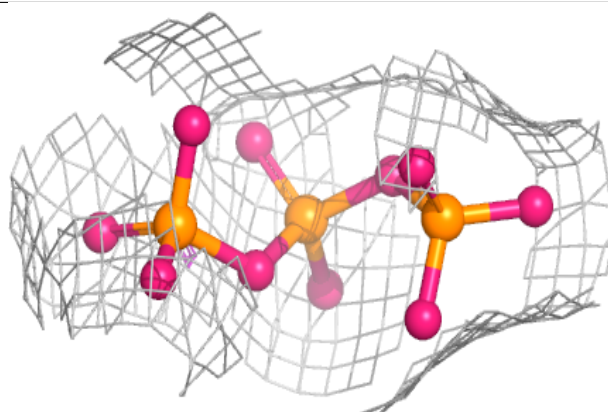
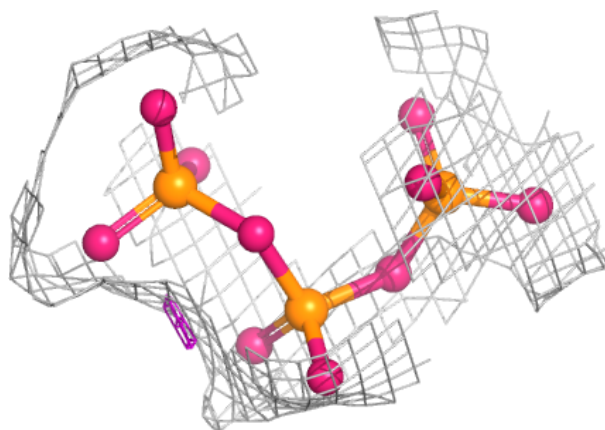
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	I	901	6/6	0.54	0.19	135,140,144,150	0
6	3PO	I	902	13/13	0.60	0.09	148,166,176,176	0
5	GOL	C	101	6/6	0.72	0.14	77,88,95,101	0
6	3PO	L	901	13/13	0.73	0.08	141,154,163,168	0
6	3PO	B	902	13/13	0.79	0.10	72,103,111,126	0
7	MG	L	902	1/1	0.81	0.13	124,124,124,124	0
6	3PO	E	901	13/13	0.83	0.07	77,108,138,139	0
7	MG	I	903	1/1	0.88	0.09	125,125,125,125	0
7	MG	E	902	1/1	0.90	0.06	74,74,74,74	0
5	GOL	B	901	6/6	0.92	0.10	69,70,90,90	0
7	MG	B	903	1/1	0.93	0.15	66,66,66,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

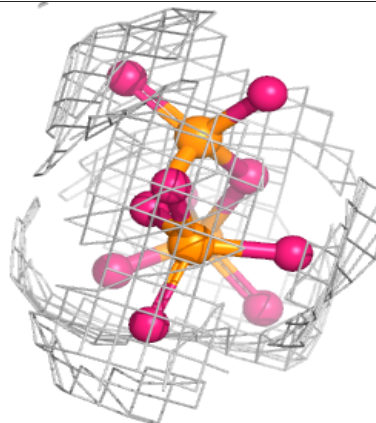
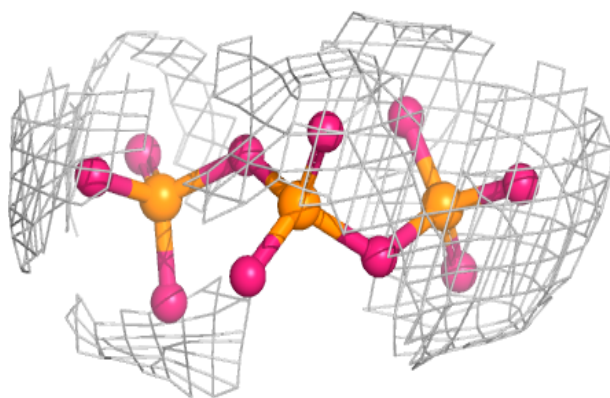
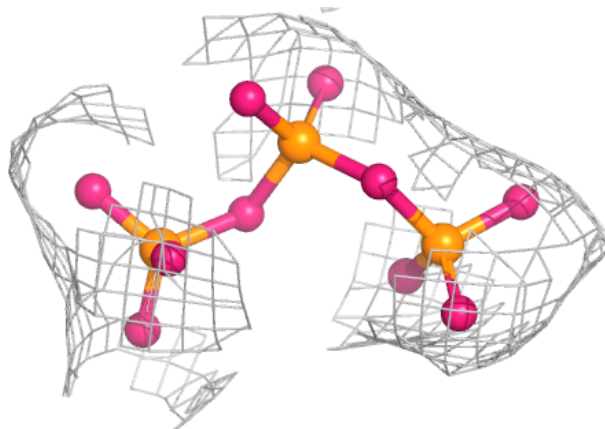
Electron density around 3PO I 902:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



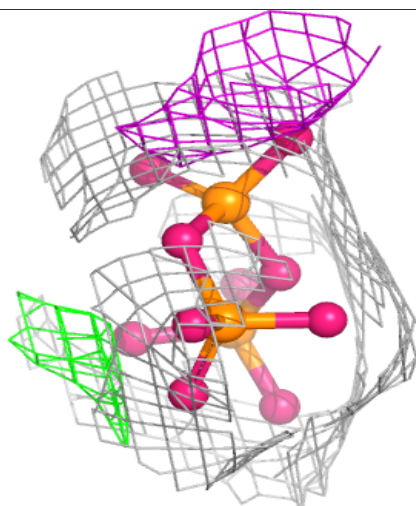
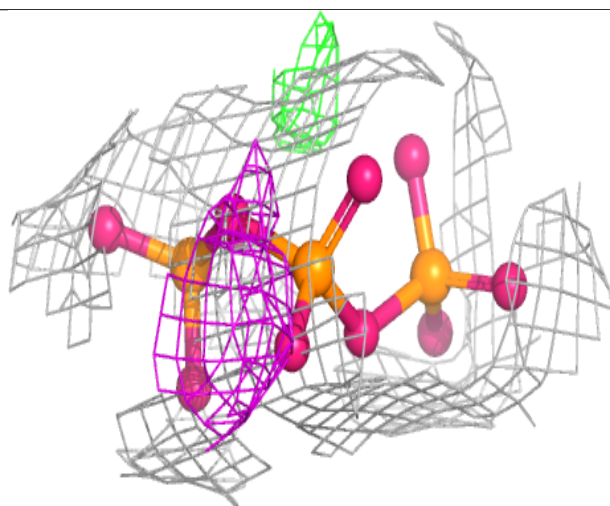
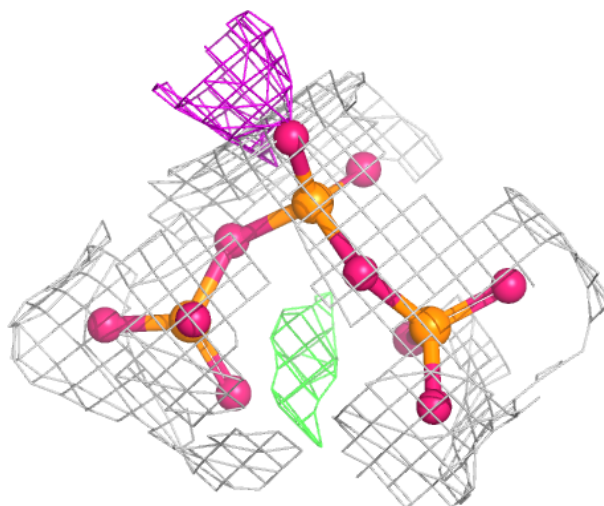
Electron density around 3PO L 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



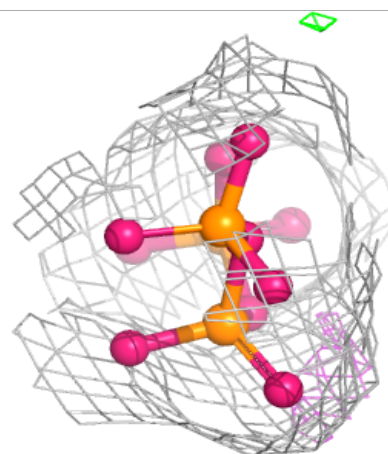
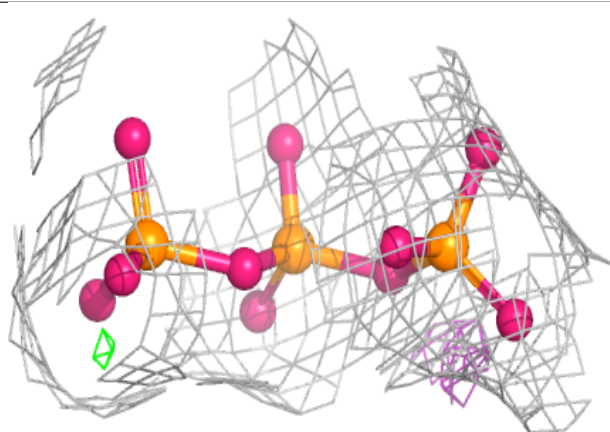
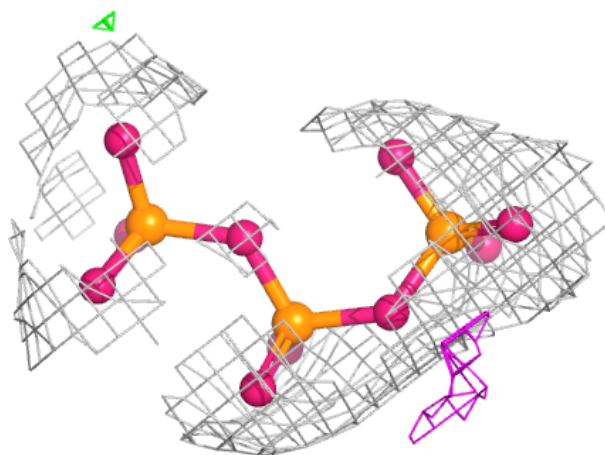
Electron density around 3PO B 902:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 3PO E 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.