



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:17 PM UTC

PDB ID : 9B12 / pdb_00009b12
Title : Structure of Optineurin bound to HOIP NZF1 domain and M1-linked diubiquitin, crystal form 1
Authors : Michel, M.A.; Scutts, S.; Komander, D.
Deposited on : 2024-03-12
Resolution : 1.81 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
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

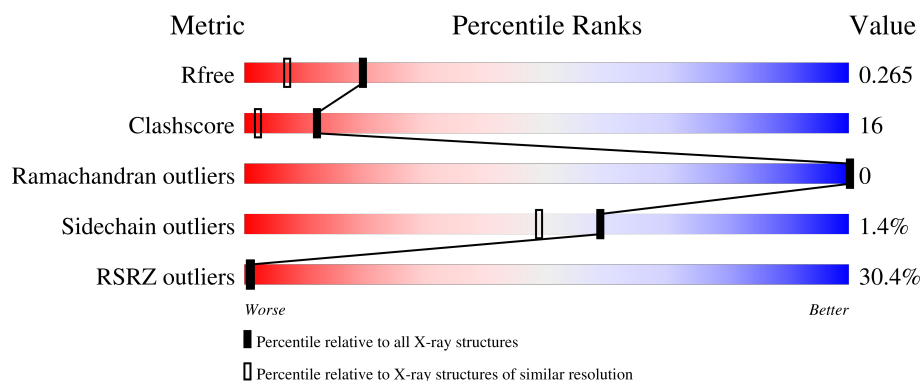
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	C	96	19% 68% 24% 7%
1	D	96	21% 64% 28% 8%
1	E	96	19% 65% 27% 8%
1	F	96	19% 72% 20% 8%
2	A	152	51% 74% 22% ..

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Mol	Chain	Length	Quality of chain
2	B	152	
3	G	30	
3	H	30	
3	I	30	
3	J	30	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CL	B	201	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6106 atoms, of which 17 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 Optineurin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	89	Total	C	N	O	S	0	2	0
			710	441	120	144	5			
1	D	88	Total	C	N	O	S	0	1	0
			690	427	116	142	5			
1	E	88	Total	C	N	O	S	0	2	0
			699	435	117	142	5			
1	F	88	Total	C	N	O	S	0	0	0
			691	430	118	138	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	417	GLY	-	expression tag	UNP Q96CV9
C	418	PRO	-	expression tag	UNP Q96CV9
D	417	GLY	-	expression tag	UNP Q96CV9
D	418	PRO	-	expression tag	UNP Q96CV9
E	417	GLY	-	expression tag	UNP Q96CV9
E	418	PRO	-	expression tag	UNP Q96CV9
F	417	GLY	-	expression tag	UNP Q96CV9
F	418	PRO	-	expression tag	UNP Q96CV9

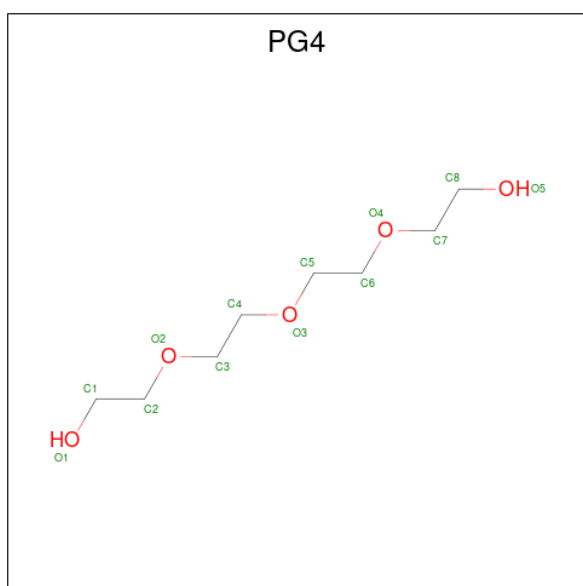
- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	150	Total	C	N	O	S	0	0	0
			1063	670	189	203	1			
2	B	150	Total	C	N	O	S	0	0	0
			1036	647	191	197	1			

- Molecule 3 is a protein called E3 ubiquitin-protein ligase RNF31.

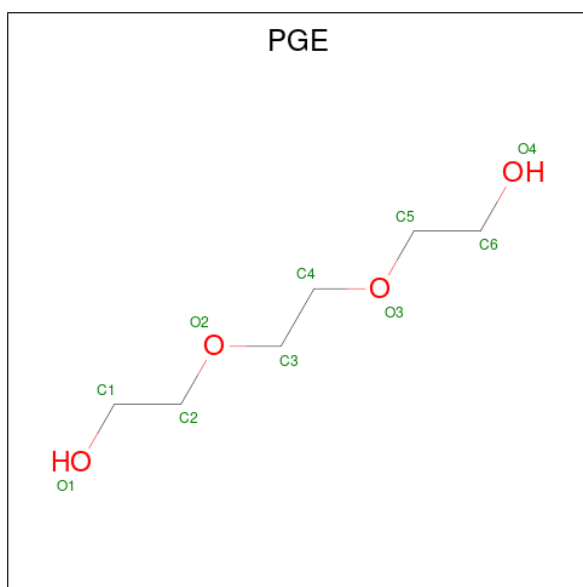
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	29	Total	C	N	O	S	0	0	0
			223	135	44	40	4			
3	H	29	Total	C	N	O	S	0	0	0
			224	135	44	41	4			
3	I	29	Total	C	N	O	S	0	1	0
			231	140	47	40	4			
3	J	29	Total	C	N	O	S	0	2	0
			234	142	47	41	4			

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			13	8	5		
4	J	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).

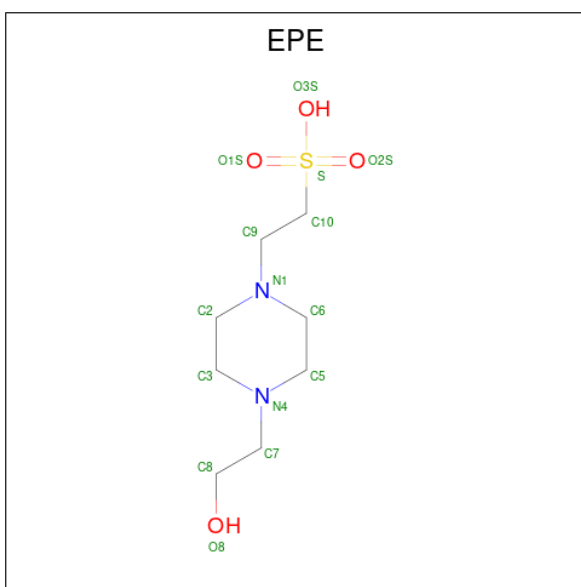


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			8	5	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		
6	J	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	A	1	Total	C	H	N	O	S	0
			32	8	17	2	4	1	
7	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	J	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	1	Total	Zn	0	0
			1	1		
8	H	1	Total	Zn	0	0
			1	1		
8	I	1	Total	Zn	0	0
			1	1		
8	J	1	Total	Zn	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	9	Total	O	0	0
			9	9		

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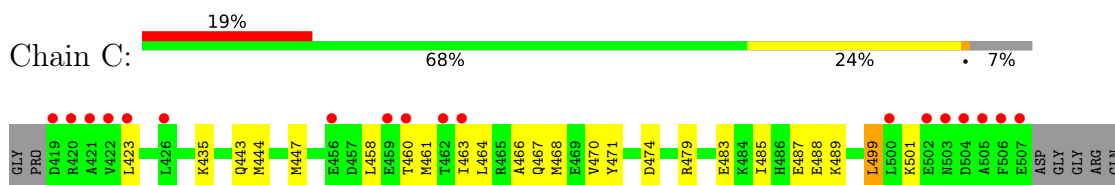
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	18	Total 18	O 18	0	0
9	E	26	Total 26	O 26	0	0
9	F	27	Total 27	O 27	0	0
9	A	19	Total 19	O 19	0	0
9	B	27	Total 27	O 27	0	0
9	G	14	Total 14	O 14	0	0
9	H	10	Total 10	O 10	0	0
9	I	22	Total 22	O 22	0	0
9	J	15	Total 15	O 15	0	0

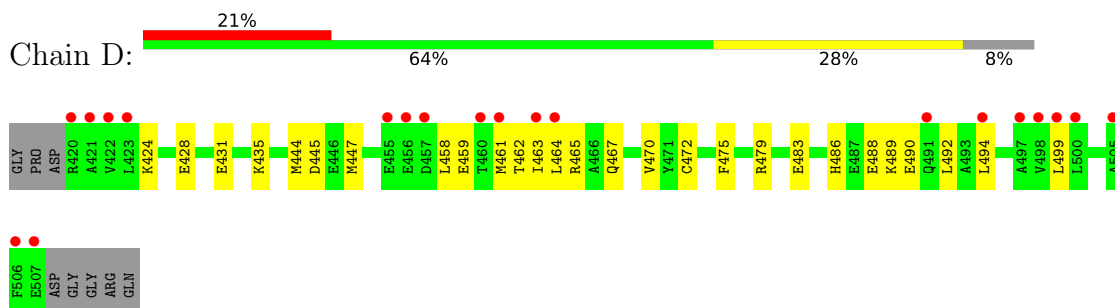
3 Residue-property plots [i](#)

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.

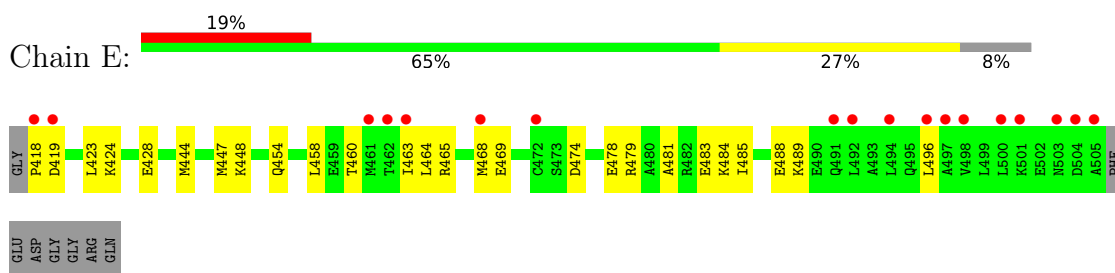
• Molecule 1: Optineurin



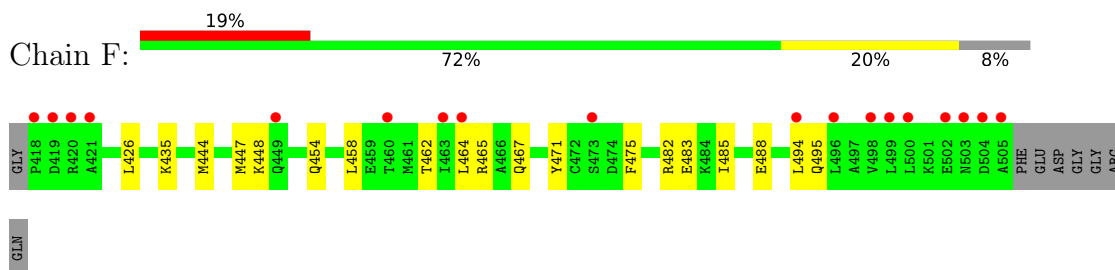
• Molecule 1: Optineurin



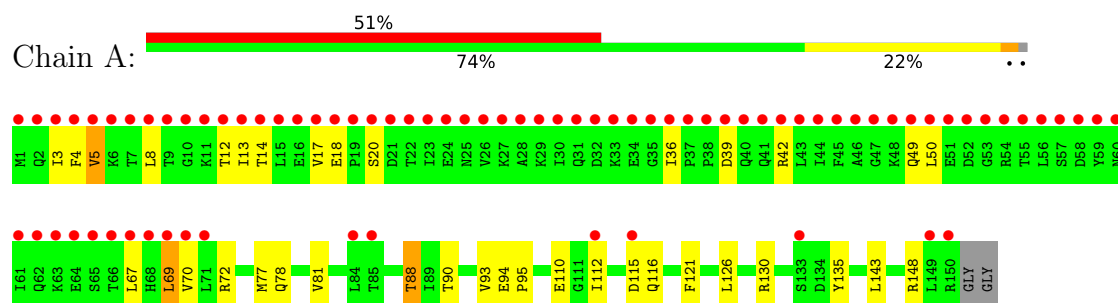
• Molecule 1: Optineurin



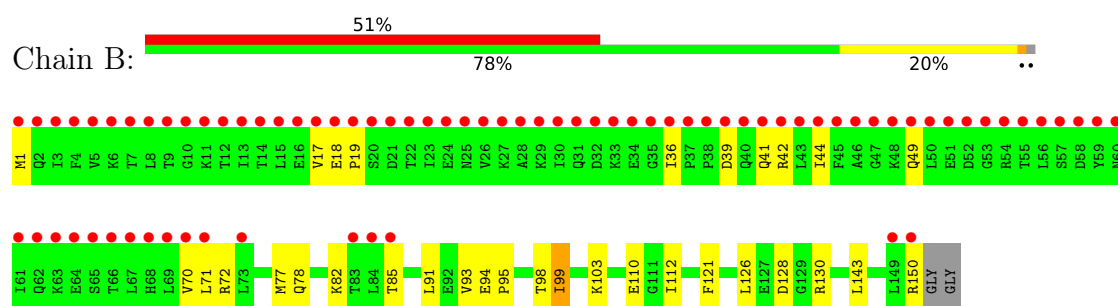
• Molecule 1: Optineurin



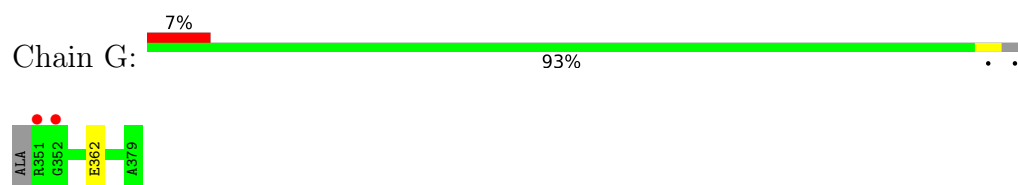
- Molecule 2: Ubiquitin



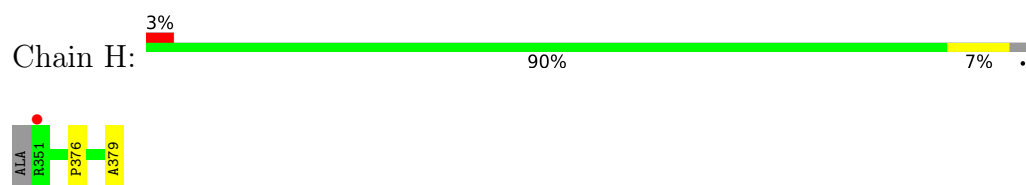
- Molecule 2: Ubiquitin



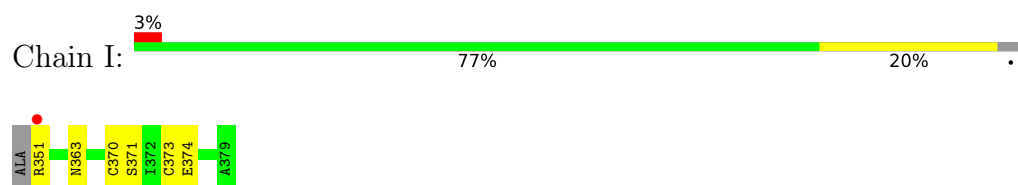
- Molecule 3: E3 ubiquitin-protein ligase RNF31



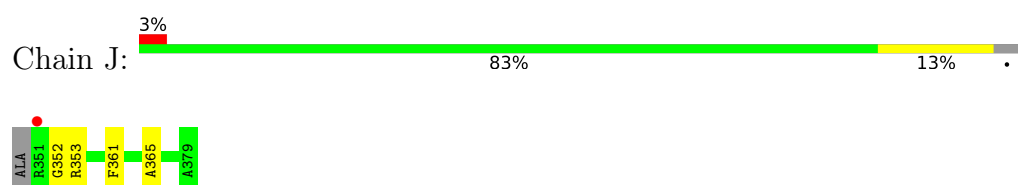
- Molecule 3: E3 ubiquitin-protein ligase RNF31



- Molecule 3: E3 ubiquitin-protein ligase RNF31



- Molecule 3: E3 ubiquitin-protein ligase RNF31



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.41Å 70.19Å 193.94Å 90.00° 102.25° 90.00°	Depositor
Resolution (Å)	46.15 – 1.81 46.15 – 1.81	Depositor EDS
% Data completeness (in resolution range)	44.2 (46.15-1.81) 44.2 (46.15-1.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.231 , 0.269 0.230 , 0.265	Depositor DCC
R_{free} test set	2943 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.0	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	0.93	EDS
Total number of atoms	6106	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.58% 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: PG4, CL, PGE, EPE, ZN

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	C	0.30	0/720	0.50	0/965
1	D	0.28	0/697	0.52	0/935
1	E	0.31	0/709	0.50	0/949
1	F	0.33	0/695	0.53	0/930
2	A	0.29	0/1075	0.50	0/1461
2	B	0.33	0/1048	0.55	0/1425
3	G	0.38	0/226	0.54	0/304
3	H	0.31	0/227	0.52	0/304
3	I	0.41	0/237	0.61	0/318
3	J	0.43	0/243	0.84	0/326
All	All	0.32	0/5877	0.54	0/7917

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

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	C	710	0	695	33	0
1	D	690	0	665	33	0
1	E	699	0	699	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	691	0	692	29	0
2	A	1063	0	992	37	1
2	B	1036	0	917	38	0
3	G	223	0	212	0	1
3	H	224	0	212	1	0
3	I	231	0	224	7	0
3	J	234	0	229	4	0
4	C	13	0	18	4	0
4	J	13	0	18	3	0
5	C	8	0	9	1	0
6	B	1	0	0	2	0
6	F	1	0	0	0	0
6	J	1	0	0	0	0
7	A	15	17	18	4	0
7	F	15	0	18	2	0
7	H	15	0	18	0	0
7	J	15	0	18	2	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
8	I	1	0	0	0	0
8	J	1	0	0	0	0
9	A	19	0	0	0	0
9	B	27	0	0	1	0
9	C	9	0	0	1	0
9	D	18	0	0	1	0
9	E	26	0	0	1	0
9	F	27	0	0	1	0
9	G	14	0	0	0	0
9	H	10	0	0	0	0
9	I	22	0	0	0	0
9	J	15	0	0	0	0
All	All	6089	17	5654	181	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 16.

All (181) 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:E:468:MET:HE1	1:F:464:LEU:HD11	1.44	0.98
2:A:77:MET:HE3	2:A:93:VAL:HG23	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:468:MET:CE	1:F:464:LEU:HD11	1.97	0.94
2:B:99:ILE:HD11	2:B:103:LYS:HE3	1.47	0.93
2:B:99:ILE:CD1	2:B:103:LYS:HE3	1.99	0.93
2:B:77:MET:HE3	2:B:93:VAL:HG23	1.52	0.88
2:B:150:ARG:NH2	6:B:201:CL:CL	2.46	0.86
3:I:363:ASN:HD21	3:I:371:SER:H	1.24	0.81
1:E:448:LYS:HG2	1:F:447:MET:HE1	1.63	0.80
1:E:463:ILE:HD12	1:E:463:ILE:H	1.47	0.80
2:B:36:ILE:HG12	2:B:71:LEU:HD21	1.65	0.79
3:J:353:ARG:HH22	4:J:402:PG4:H42	1.47	0.79
7:J:404:EPE:H62	7:J:404:EPE:H82	1.67	0.76
1:C:464:LEU:HD23	1:D:464:LEU:HD23	1.68	0.75
2:B:99:ILE:HG13	2:B:128:ASP:HA	1.66	0.75
2:A:5:VAL:HG22	2:A:67:LEU:HB2	1.68	0.74
2:A:50:LEU:H	2:A:50:LEU:HD12	1.50	0.74
2:A:42:ARG:O	2:A:70:VAL:HG22	1.88	0.73
2:A:13:ILE:HG13	2:A:14:THR:H	1.53	0.72
1:E:460:THR:HG22	1:E:464:LEU:HD23	1.71	0.71
1:E:424:LYS:O	1:E:428:GLU:HG3	1.91	0.71
1:D:490:GLU:HA	1:D:490:GLU:OE2	1.91	0.69
2:B:18:GLU:HG3	2:B:19:PRO:HD2	1.74	0.69
1:F:448:LYS:HG3	7:F:602:EPE:H102	1.73	0.69
2:A:77:MET:HE1	2:A:95:PRO:N	2.08	0.69
1:D:445:ASP:OD2	9:D:601:HOH:O	2.10	0.68
1:E:460:THR:HA	1:E:463:ILE:HD13	1.74	0.68
2:B:36:ILE:HD12	2:B:36:ILE:O	1.93	0.68
1:E:418:PRO:HG2	1:E:419:ASP:OD1	1.95	0.67
2:A:5:VAL:O	2:A:12:THR:OG1	2.12	0.67
1:C:501:LYS:HZ1	4:C:601:PG4:H12	1.62	0.65
2:B:36:ILE:HG12	2:B:71:LEU:CD2	2.26	0.65
1:E:448:LYS:NZ	9:E:601:HOH:O	2.29	0.65
2:A:115:ASP:O	2:A:148:ARG:HD2	1.96	0.65
1:C:488:GLU:OE1	1:D:489:LYS:HE3	1.96	0.65
1:C:501:LYS:NZ	4:C:601:PG4:H12	2.13	0.64
5:C:602:PGE:O3	2:B:82:LYS:HE2	1.98	0.64
2:A:17:VAL:HG12	2:A:18:GLU:H	1.61	0.63
2:B:94:GLU:HG2	9:B:305:HOH:O	1.98	0.63
2:B:36:ILE:HD11	2:B:41:GLN:CB	2.28	0.62
2:A:130:ARG:HH21	7:A:201:EPE:H102	1.64	0.62
2:B:77:MET:HE1	2:B:95:PRO:N	2.14	0.62
2:A:8:LEU:O	2:A:8:LEU:HD13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:MET:HE2	1:D:467:GLN:HG3	1.82	0.61
2:A:36:ILE:O	2:A:36:ILE:HD12	2.01	0.60
2:B:36:ILE:HD12	2:B:36:ILE:C	2.27	0.59
2:A:116:GLN:O	2:A:148:ARG:HG3	2.02	0.59
3:I:363:ASN:ND2	3:I:371:SER:H	1.98	0.58
1:E:481:ALA:O	1:E:485:ILE:HD12	2.04	0.58
1:E:468:MET:HG3	1:F:471:TYR:CD2	2.38	0.58
1:E:465:ARG:O	1:E:469:GLU:HG3	2.04	0.58
1:E:458:LEU:HD23	1:F:458:LEU:HD23	1.86	0.58
2:B:121:PHE:HB3	2:B:126:LEU:HD21	1.85	0.57
1:C:435:LYS:NZ	9:C:702:HOH:O	2.37	0.57
1:C:464:LEU:HD21	1:D:465:ARG:N	2.19	0.57
2:A:49:GLN:HG2	2:A:49:GLN:O	2.03	0.57
1:E:448:LYS:HG2	1:F:447:MET:CE	2.33	0.56
3:I:351[A]:ARG:CZ	3:I:351[A]:ARG:HB3	2.35	0.56
3:J:353:ARG:NH2	4:J:402:PG4:H42	2.18	0.56
1:E:478:GLU:OE1	1:F:482:ARG:HD3	2.05	0.56
1:E:458:LEU:CD2	1:F:458:LEU:HD23	2.35	0.56
2:A:110:GLU:HB2	2:A:112:ILE:HD12	1.88	0.56
2:A:17:VAL:HG12	2:A:18:GLU:N	2.21	0.55
1:E:460:THR:HG22	1:E:464:LEU:CD2	2.36	0.55
1:F:464:LEU:HD12	1:F:464:LEU:O	2.06	0.55
1:C:499:LEU:HB3	1:D:499:LEU:HD13	1.89	0.55
1:E:474:ASP:HB3	1:F:475:PHE:CE1	2.41	0.55
1:C:461:MET:HE2	1:D:461:MET:HG3	1.89	0.54
2:B:98:THR:HA	2:B:130:ARG:O	2.08	0.54
2:B:1:MET:N	2:B:17:VAL:O	2.27	0.54
1:E:484:LYS:HE3	1:E:488:GLU:OE2	2.07	0.53
1:C:483:GLU:O	1:C:487[A]:GLU:HG3	2.08	0.53
2:A:130:ARG:HE	7:A:201:EPE:H22	1.72	0.53
1:D:479:ARG:O	1:D:483:GLU:HG3	2.08	0.53
1:F:435:LYS:HE3	9:F:719:HOH:O	2.09	0.53
2:A:130:ARG:HG2	2:A:130:ARG:HH11	1.74	0.53
2:B:110:GLU:HB2	2:B:112:ILE:HD12	1.91	0.53
1:C:447:MET:HB2	1:D:447:MET:HE2	1.91	0.53
1:C:464:LEU:HD23	1:D:464:LEU:CD2	2.39	0.53
2:A:130:ARG:NE	7:A:201:EPE:H22	2.25	0.53
1:E:447:MET:HE1	1:F:444:MET:HG2	1.91	0.52
1:E:423:LEU:HD12	1:F:426:LEU:CD1	2.40	0.52
1:E:465:ARG:HA	1:E:468:MET:HE3	1.91	0.52
2:B:39:ASP:O	2:B:72:ARG:NH1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:ARG:HE	2:B:72:ARG:HD2	1.73	0.52
1:E:447:MET:CE	1:F:444:MET:HG2	2.40	0.52
1:E:479:ARG:O	1:E:483:GLU:HG3	2.11	0.51
1:E:496:LEU:HD21	1:F:495:GLN:NE2	2.26	0.51
2:B:77:MET:HE1	2:B:95:PRO:CD	2.41	0.51
1:E:463:ILE:H	1:E:463:ILE:CD1	2.22	0.51
2:B:99:ILE:O	2:B:99:ILE:HD12	2.11	0.51
1:C:489:LYS:HE3	1:D:488:GLU:OE1	2.11	0.51
3:I:370:CYS:O	3:I:374:GLU:HA	2.11	0.51
1:E:423:LEU:HD12	1:F:426:LEU:HD11	1.92	0.50
3:J:361:PHE:HE1	4:J:402:PG4:H71	1.76	0.50
2:B:1:MET:H1	2:B:18:GLU:CD	2.18	0.50
1:D:467:GLN:HA	1:D:470:VAL:HG22	1.94	0.50
1:C:458:LEU:CD2	1:D:458:LEU:HD23	2.42	0.50
1:E:418:PRO:HG2	1:E:419:ASP:H	1.76	0.50
2:A:116:GLN:C	2:A:148:ARG:HG3	2.37	0.50
2:A:5:VAL:CG2	2:A:67:LEU:HD12	2.43	0.49
1:D:467:GLN:O	1:D:470:VAL:HG22	2.13	0.49
1:D:483:GLU:OE2	1:F:483:GLU:OE2	2.31	0.49
1:C:479:ARG:O	1:C:483:GLU:HG3	2.13	0.48
1:E:447:MET:HE3	1:F:447:MET:SD	2.54	0.48
2:A:4:PHE:CB	2:A:12:THR:HG21	2.44	0.48
1:C:447:MET:HB2	1:D:447:MET:CE	2.43	0.48
2:B:36:ILE:CD1	2:B:41:GLN:CB	2.92	0.48
1:D:467:GLN:OE1	2:B:70:VAL:HB	2.14	0.48
1:C:474:ASP:HB3	1:D:475:PHE:CE1	2.49	0.47
1:E:447:MET:HE1	1:F:444:MET:HA	1.96	0.47
3:I:373:CYS:C	3:I:374:GLU:HG2	2.39	0.47
1:D:431:GLU:OE2	1:D:435:LYS:NZ	2.47	0.47
2:A:5:VAL:HG22	2:A:67:LEU:CB	2.43	0.47
1:F:462:THR:O	1:F:465:ARG:HB3	2.15	0.47
1:E:444:MET:HA	1:E:447:MET:HE2	1.97	0.47
1:C:461:MET:HB2	1:C:461:MET:HE3	1.56	0.46
1:D:467:GLN:O	1:D:470:VAL:CG2	2.64	0.46
2:A:130:ARG:HB2	2:A:135:TYR:CE2	2.51	0.46
2:B:77:MET:HE2	2:B:94:GLU:HA	1.97	0.46
1:C:443:GLN:O	1:C:447:MET:HG3	2.16	0.46
1:E:485:ILE:HG21	1:F:485:ILE:HG23	1.97	0.46
1:C:468:MET:HE2	1:D:467:GLN:CG	2.46	0.46
1:E:468:MET:HG3	1:F:471:TYR:CE2	2.52	0.45
2:A:69:LEU:HD13	2:A:70:VAL:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:MET:CE	2:B:94:GLU:HA	2.47	0.45
7:J:404:EPE:H21	7:J:404:EPE:O8	2.17	0.45
2:A:39:ASP:O	2:A:72:ARG:HD3	2.17	0.45
1:C:471:TYR:CD2	1:D:472:CYS:HB2	2.52	0.45
2:A:49:GLN:O	2:A:49:GLN:CG	2.63	0.45
2:B:18:GLU:HG3	2:B:19:PRO:CD	2.44	0.45
2:B:44:ILE:HG12	2:B:49:GLN:CB	2.46	0.45
2:B:150:ARG:CZ	6:B:201:CL:CL	3.02	0.45
2:A:81:VAL:O	2:A:88:THR:HA	2.17	0.44
2:A:130:ARG:HH21	7:A:201:EPE:C10	2.30	0.44
2:A:3:ILE:HD11	2:A:67:LEU:HD21	2.00	0.44
1:E:481:ALA:O	1:E:485:ILE:CD1	2.64	0.44
2:A:18:GLU:O	2:A:20:SER:N	2.51	0.44
1:C:460:THR:O	1:C:463:ILE:CG2	2.65	0.44
1:C:501:LYS:HD2	4:C:601:PG4:H52	1.98	0.44
1:E:454:GLN:HB2	1:F:454:GLN:OE1	2.17	0.44
2:B:78:GLN:HA	2:B:91:LEU:O	2.18	0.44
1:E:463:ILE:HD12	1:E:463:ILE:N	2.25	0.44
3:H:376:PRO:HD2	3:H:379:ALA:HB3	2.00	0.43
1:C:461:MET:HE2	1:D:461:MET:CG	2.49	0.43
1:E:460:THR:HG22	1:E:460:THR:O	2.18	0.43
1:C:466:ALA:O	1:C:470:VAL:HG23	2.19	0.43
1:C:485:ILE:HG21	1:D:486:HIS:HA	2.00	0.43
1:D:424:LYS:O	1:D:428:GLU:HG3	2.19	0.43
2:B:110:GLU:CB	2:B:112:ILE:HD12	2.48	0.43
2:A:18:GLU:OE2	2:A:20:SER:CB	2.67	0.43
2:A:143:LEU:HD12	2:A:143:LEU:N	2.33	0.43
2:A:77:MET:HE1	2:A:94:GLU:C	2.44	0.43
2:B:99:ILE:CG1	2:B:128:ASP:HA	2.44	0.42
1:E:468:MET:HE1	1:F:464:LEU:CD1	2.33	0.42
3:J:352:GLY:C	3:J:365:ALA:HB2	2.45	0.42
1:C:501:LYS:HD3	4:C:601:PG4:H42	2.02	0.42
1:C:467:GLN:HG3	1:F:494:LEU:CD2	2.50	0.42
1:E:464:LEU:HD13	1:E:464:LEU:HA	1.92	0.42
1:C:460:THR:O	1:C:463:ILE:HG23	2.20	0.41
1:E:465:ARG:HA	1:E:468:MET:CE	2.50	0.41
1:E:489:LYS:NZ	1:F:488:GLU:OE1	2.52	0.41
2:B:143:LEU:CD1	2:B:143:LEU:N	2.83	0.41
2:B:143:LEU:N	2:B:143:LEU:HD12	2.35	0.41
2:B:99:ILE:O	2:B:103:LYS:HG3	2.20	0.41
1:C:458:LEU:HD23	1:D:458:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:467:GLN:NE2	1:F:471:TYR:CE1	2.88	0.41
1:F:448:LYS:CG	7:F:602:EPE:H102	2.43	0.41
1:D:494:LEU:HD23	1:D:494:LEU:HA	1.83	0.41
2:A:143:LEU:N	2:A:143:LEU:CD1	2.83	0.41
2:B:99:ILE:HD12	2:B:103:LYS:HE3	1.97	0.41
2:B:77:MET:CE	2:B:95:PRO:HD3	2.51	0.40
1:D:459:GLU:O	1:D:462:THR:OG1	2.34	0.40
1:D:492:LEU:HD23	1:D:492:LEU:HA	1.96	0.40
2:A:121:PHE:HB3	2:A:126:LEU:HD21	2.03	0.40
1:C:444:MET:CG	1:D:444:MET:HG3	2.51	0.40
1:C:471:TYR:CE2	1:D:472:CYS:HB2	2.57	0.40
1:C:464:LEU:HD23	1:D:464:LEU:CG	2.51	0.40
2:A:78:GLN:HB3	2:A:90:THR:CG2	2.51	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)
2:A:148:ARG:NH2	3:G:362:GLU:OE2[2_555]	1.98	0.22

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	C	89/96 (93%)	89 (100%)	0	0	100	100
1	D	87/96 (91%)	86 (99%)	1 (1%)	0	100	100
1	E	88/96 (92%)	88 (100%)	0	0	100	100
1	F	86/96 (90%)	86 (100%)	0	0	100	100
2	A	148/152 (97%)	142 (96%)	6 (4%)	0	100	100
2	B	148/152 (97%)	143 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	27/30 (90%)	27 (100%)	0	0	100	100
3	H	27/30 (90%)	27 (100%)	0	0	100	100
3	I	27/30 (90%)	27 (100%)	0	0	100	100
3	J	28/30 (93%)	28 (100%)	0	0	100	100
All	All	755/808 (93%)	743 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	73/81 (90%)	71 (97%)	2 (3%)	39	22
1	D	70/81 (86%)	69 (99%)	1 (1%)	59	49
1	E	73/81 (90%)	73 (100%)	0	100	100
1	F	71/81 (88%)	71 (100%)	0	100	100
2	A	98/136 (72%)	95 (97%)	3 (3%)	35	17
2	B	86/136 (63%)	84 (98%)	2 (2%)	44	28
3	G	23/23 (100%)	23 (100%)	0	100	100
3	H	23/23 (100%)	23 (100%)	0	100	100
3	I	24/23 (104%)	24 (100%)	0	100	100
3	J	25/23 (109%)	25 (100%)	0	100	100
All	All	566/688 (82%)	558 (99%)	8 (1%)	59	49

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	423	LEU
1	C	499	LEU
1	D	463	ILE
2	A	5	VAL

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Mol	Chain	Res	Type
2	A	69	LEU
2	A	88	THR
2	B	85	THR
2	B	99	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	454	GLN
1	C	495	GLN
1	F	486	HIS
1	F	495	GLN
2	A	138	GLN
2	B	40	GLN
3	I	363	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](#)

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 14 ligands modelled in this entry, 7 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
7	EPE	H	402	-	15,15,15	0.95	1 (6%)	19,20,20	1.09	2 (10%)
5	PGE	C	602	-	7,7,9	0.31	0	6,6,8	0.50	0
7	EPE	A	201	-	15,15,15	1.04	1 (6%)	19,20,20	1.23	3 (15%)
7	EPE	J	404	-	15,15,15	0.90	1 (6%)	19,20,20	1.39	3 (15%)
4	PG4	C	601	-	12,12,12	0.31	0	11,11,11	0.22	0
7	EPE	F	602	-	15,15,15	0.89	1 (6%)	19,20,20	0.74	0
4	PG4	J	402	-	12,12,12	0.26	0	11,11,11	0.27	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
7	EPE	H	402	-	-	4/9/19/19	0/1/1/1
5	PGE	C	602	-	-	2/5/5/7	-
7	EPE	A	201	-	-	8/9/19/19	0/1/1/1
7	EPE	J	404	-	-	2/9/19/19	0/1/1/1
4	PG4	C	601	-	-	1/10/10/10	-
7	EPE	F	602	-	-	4/9/19/19	0/1/1/1
4	PG4	J	402	-	-	7/10/10/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	201	EPE	C10-S	3.05	1.81	1.77
7	H	402	EPE	C10-S	2.85	1.81	1.77
7	J	404	EPE	C10-S	2.63	1.81	1.77
7	F	602	EPE	C10-S	2.55	1.81	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	201	EPE	C3-C2-N1	2.88	116.46	110.65
7	H	402	EPE	C6-N1-C2	2.69	114.63	108.84
7	J	404	EPE	C3-C2-N1	2.47	115.63	110.65
7	H	402	EPE	C3-C2-N1	2.34	115.37	110.65
7	A	201	EPE	C7-N4-C5	-2.19	105.41	111.24
7	J	404	EPE	C2-C3-N4	2.18	115.04	110.65
7	A	201	EPE	C5-N4-C3	2.14	113.45	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	404	EPE	O1S-S-C10	-2.02	103.67	106.73

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	602	EPE	C10-C9-N1-C6
7	A	201	EPE	C10-C9-N1-C2
7	H	402	EPE	S-C10-C9-N1
7	J	404	EPE	C10-C9-N1-C2
7	J	404	EPE	C10-C9-N1-C6
4	J	402	PG4	O3-C5-C6-O4
7	A	201	EPE	N4-C7-C8-O8
4	J	402	PG4	O4-C7-C8-O5
4	J	402	PG4	O2-C3-C4-O3
7	H	402	EPE	C8-C7-N4-C5
4	J	402	PG4	O1-C1-C2-O2
4	C	601	PG4	O3-C5-C6-O4
7	H	402	EPE	C8-C7-N4-C3
7	F	602	EPE	C10-C9-N1-C2
7	A	201	EPE	C10-C9-N1-C6
7	A	201	EPE	C9-C10-S-O3S
7	A	201	EPE	C8-C7-N4-C3
7	A	201	EPE	C8-C7-N4-C5
7	A	201	EPE	C9-C10-S-O1S
7	A	201	EPE	C9-C10-S-O2S
7	F	602	EPE	N4-C7-C8-O8
7	F	602	EPE	S-C10-C9-N1
4	J	402	PG4	C6-C5-O3-C4
4	J	402	PG4	C5-C6-O4-C7
4	J	402	PG4	C1-C2-O2-C3
7	H	402	EPE	C10-C9-N1-C2
5	C	602	PGE	C3-C4-O3-C5
5	C	602	PGE	C4-C3-O2-C2

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	602	PGE	1	0
7	A	201	EPE	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	404	EPE	2	0
4	C	601	PG4	4	0
7	F	602	EPE	2	0
4	J	402	PG4	3	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, 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(Å²)	Q<0.9	
1	C	89/96 (92%)	1.14	18 (20%)	3	3	27, 49, 85, 98	2 (2%)
1	D	88/96 (91%)	1.18	20 (22%)	2	2	29, 52, 74, 105	1 (1%)
1	E	88/96 (91%)	1.07	18 (20%)	2	3	17, 49, 92, 118	2 (2%)
1	F	88/96 (91%)	0.95	18 (20%)	2	3	20, 46, 81, 95	0
2	A	150/152 (98%)	3.80	78 (52%)	0	0	31, 65, 174, 226	0
2	B	150/152 (98%)	3.70	77 (51%)	0	0	25, 60, 208, 259	0
3	G	29/30 (96%)	0.45	2 (6%)	23	26	25, 38, 57, 82	0
3	H	29/30 (96%)	0.34	1 (3%)	48	55	27, 37, 63, 94	0
3	I	29/30 (96%)	-0.05	1 (3%)	48	55	20, 27, 43, 45	1 (3%)
3	J	29/30 (96%)	0.04	1 (3%)	48	55	19, 26, 40, 48	2 (6%)
All	All	769/808 (95%)	1.99	234 (30%)	1	1	17, 49, 172, 259	8 (1%)

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	3	ILE	16.2
2	B	4	PHE	15.1
2	A	50	LEU	14.1
2	A	61	ILE	13.9
2	A	19	PRO	13.8
2	A	21	ASP	12.4
2	B	66	THR	11.9
2	B	46	ALA	11.8
2	B	15	LEU	11.1
2	B	61	ILE	11.1
2	A	32	ASP	11.1
2	B	65	SER	10.9
2	A	65	SER	10.8

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Mol	Chain	Res	Type	RSRZ
2	B	67	LEU	10.7
2	A	20	SER	10.5
2	A	13	ILE	10.4
2	B	50	LEU	10.4
2	B	14	THR	10.1
2	B	6	LYS	10.0
2	A	14	THR	10.0
2	B	45	PHE	9.9
2	B	19	PRO	9.9
2	B	13	ILE	9.8
2	B	8	LEU	9.8
2	A	52	ASP	9.8
2	A	1	MET	9.7
2	B	56	LEU	9.7
2	A	17	VAL	9.6
2	A	9	THR	9.6
2	B	69	LEU	9.3
2	A	8	LEU	9.2
2	B	64	GLU	9.2
2	B	3	ILE	9.1
2	A	4	PHE	8.8
2	A	55	THR	8.8
2	B	5	VAL	8.8
2	B	2	GLN	8.8
1	E	505	ALA	8.7
2	B	7	THR	8.5
2	B	43	LEU	8.5
2	A	16	GLU	8.4
2	A	5	VAL	8.2
2	A	26	VAL	8.1
2	A	12	THR	8.1
2	B	12	THR	8.1
2	A	66	THR	8.1
2	B	62	GLN	8.0
2	A	27	LYS	8.0
2	A	51	GLU	7.9
2	A	15	LEU	7.9
2	A	59	TYR	7.9
2	A	6	LYS	7.8
2	A	25	ASN	7.7
2	A	22	THR	7.7
2	A	64	GLU	7.6

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Mol	Chain	Res	Type	RSRZ
2	B	34	GLU	7.6
2	B	36	ILE	7.6
2	A	18	GLU	7.5
2	A	63	LYS	7.5
2	A	43	LEU	7.5
2	A	56	LEU	7.4
2	A	67	LEU	7.4
2	B	17	VAL	7.3
2	B	49	GLN	7.3
2	B	16	GLU	7.3
2	A	10	GLY	7.2
2	B	57	SER	7.1
2	B	35	GLY	7.1
2	A	54	ARG	7.1
2	B	51	GLU	7.0
2	B	30	ILE	7.0
2	A	46	ALA	7.0
2	A	36	ILE	6.9
2	B	22	THR	6.8
1	F	418	PRO	6.7
2	B	32	ASP	6.7
2	B	31	GLN	6.6
2	B	20	SER	6.6
2	A	2	GLN	6.6
2	A	53	GLY	6.6
2	B	54	ARG	6.6
2	A	57	SER	6.6
2	B	26	VAL	6.5
2	B	9	THR	6.5
2	B	11	LYS	6.5
2	B	55	THR	6.5
1	E	418	PRO	6.4
2	B	59	TYR	6.4
2	A	7	THR	6.3
2	A	62	GLN	6.3
2	A	11	LYS	6.2
2	B	52	ASP	6.0
2	B	10	GLY	6.0
2	B	21	ASP	5.9
2	B	42	ARG	5.8
2	A	44	ILE	5.8
2	B	27	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
2	B	1	MET	5.7
2	B	37	PRO	5.7
2	B	29	LYS	5.5
2	A	38	PRO	5.4
2	B	68	HIS	5.4
2	B	33	LYS	5.4
2	B	18	GLU	5.3
2	A	45	PHE	5.3
2	A	35	GLY	5.2
1	C	506	PHE	5.2
2	B	23	ILE	5.2
2	B	60	ASN	5.2
3	J	351[A]	ARG	5.1
2	A	58	ASP	5.1
2	B	63	LYS	5.1
2	A	23	ILE	5.0
2	B	44	ILE	5.0
1	C	505	ALA	5.0
2	B	38	PRO	5.0
1	F	505	ALA	4.9
2	B	28	ALA	4.9
2	A	29	LYS	4.8
2	A	34	GLU	4.8
3	G	351	ARG	4.8
1	E	500	LEU	4.8
2	B	47	GLY	4.8
2	B	53	GLY	4.7
2	B	58	ASP	4.7
2	A	30	ILE	4.7
2	A	71	LEU	4.7
1	D	420	ARG	4.6
1	E	504	ASP	4.6
2	A	60	ASN	4.6
2	B	71	LEU	4.6
2	A	28	ALA	4.5
2	A	49	GLN	4.5
1	E	503	ASN	4.5
3	I	351[A]	ARG	4.4
2	B	70	VAL	4.4
1	C	423	LEU	4.3
1	C	422	VAL	4.3
2	A	33	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	48	LYS	4.2
1	D	421	ALA	4.1
2	A	24	GLU	4.1
2	A	84	LEU	4.0
1	D	463	ILE	4.0
3	H	351	ARG	3.8
2	B	24	GLU	3.7
2	A	47	GLY	3.7
2	A	68	HIS	3.7
1	C	504	ASP	3.7
2	B	25	ASN	3.7
2	B	150	ARG	3.7
1	F	421	ALA	3.6
1	F	463	ILE	3.6
2	B	85	THR	3.6
1	C	419	ASP	3.6
1	F	419	ASP	3.6
1	D	506	PHE	3.6
2	B	149	LEU	3.6
2	A	69	LEU	3.5
1	E	461	MET	3.5
2	B	84	LEU	3.5
2	A	48	LYS	3.5
2	A	150	ARG	3.4
3	G	352	GLY	3.4
1	C	507	GLU	3.4
2	A	70	VAL	3.3
2	B	40	GLN	3.3
1	E	501	LYS	3.3
2	A	31	GLN	3.3
1	F	494	LEU	3.3
1	F	498	VAL	3.2
1	D	456	GLU	3.2
1	E	419	ASP	3.1
1	E	472	CYS	3.1
2	A	133	SER	3.1
1	C	462	THR	3.1
1	C	421	ALA	3.1
1	D	423	LEU	3.0
1	C	502	GLU	3.0
1	F	499	LEU	3.0
1	D	464	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	A	149	LEU	2.9
1	F	504	ASP	2.9
1	D	422	VAL	2.9
1	E	497	ALA	2.9
2	B	41	GLN	2.9
1	E	494	LEU	2.9
1	C	463	ILE	2.8
1	F	420	ARG	2.7
1	F	464	LEU	2.7
1	D	455	GLU	2.6
1	F	503	ASN	2.6
1	E	498	VAL	2.6
1	C	460	THR	2.6
2	A	39	ASP	2.6
2	A	85	THR	2.6
2	A	42	ARG	2.5
1	E	468	MET	2.5
1	C	503	ASN	2.5
1	C	456	GLU	2.5
2	A	40	GLN	2.5
1	D	500	LEU	2.4
1	E	496	LEU	2.4
1	D	498	VAL	2.4
1	D	499	LEU	2.4
1	D	505	ALA	2.4
1	D	507	GLU	2.4
1	C	500	LEU	2.4
1	D	461	MET	2.4
1	D	491[A]	GLN	2.3
1	D	494	LEU	2.3
1	E	462	THR	2.3
2	B	39	ASP	2.3
1	C	459	GLU	2.2
1	E	463	ILE	2.2
1	F	473	SER	2.2
2	A	115	ASP	2.2
1	C	420	ARG	2.2
1	F	449	GLN	2.2
1	F	500	LEU	2.2
2	A	41	GLN	2.2
1	D	457	ASP	2.2
1	D	497	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	112	ILE	2.1
1	D	460	THR	2.1
2	B	83	THR	2.1
1	C	426	LEU	2.1
1	E	492	LEU	2.1
1	F	460	THR	2.1
2	A	37	PRO	2.1
2	B	73	LEU	2.1
1	F	496	LEU	2.0
1	F	502	GLU	2.0
1	E	491	GLN	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 oligosaccharides 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, 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(Å ²)	Q<0.9
7	EPE	H	402	15/15	0.71	0.24	64,77,117,127	0
7	EPE	A	201	15/15	0.74	0.22	68,92,113,115	0
7	EPE	F	602	15/15	0.75	0.20	45,67,110,113	0
7	EPE	J	404	15/15	0.75	0.23	45,71,88,103	0
4	PG4	C	601	13/13	0.86	0.16	47,60,65,70	0
4	PG4	J	402	13/13	0.87	0.16	38,43,57,58	0
5	PGE	C	602	8/10	0.90	0.15	52,59,65,70	0
6	CL	B	201	1/1	0.90	0.13	62,62,62,62	0
6	CL	F	601	1/1	0.91	0.12	69,69,69,69	0
6	CL	J	403	1/1	0.92	0.12	54,54,54,54	0
8	ZN	G	401	1/1	0.99	0.03	35,35,35,35	0
8	ZN	H	401	1/1	0.99	0.02	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	ZN	I	401	1/1	0.99	0.02	27,27,27,27	0
8	ZN	J	401	1/1	0.99	0.02	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.