



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 22, 2024 – 09:22 AM EDT

PDB ID : 9B12
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

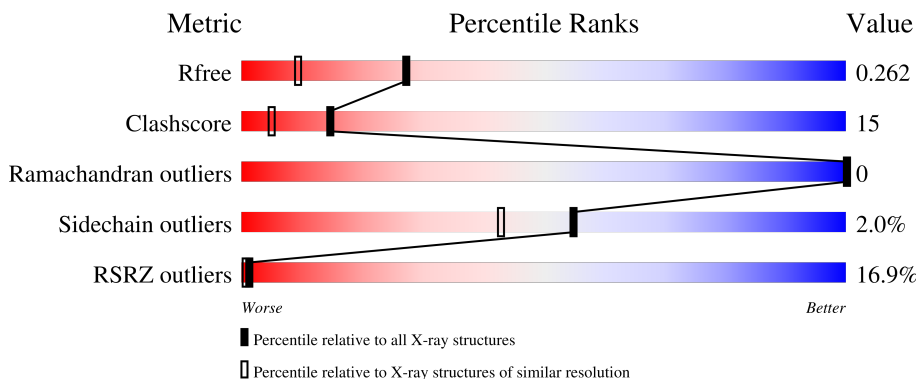
1 Overall quality at a glance

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}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 6% 69% 24% 7%
1	D	96	 3% 65% 27% 8%
1	E	96	 4% 66% 25% 8%
1	F	96	 4% 69% 23% 8%
2	A	152	 33% 74% 24% ..

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

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

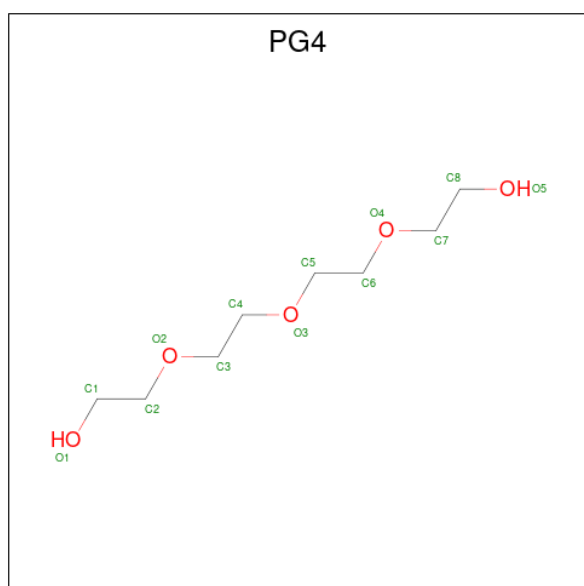
- Molecule 2 is a protein called Ubiquitin.

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

- 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 (three-letter code: PG4) (formula: C₈H₁₈O₅).



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 (three-letter code: PGE) (formula: C₆H₁₄O₄).

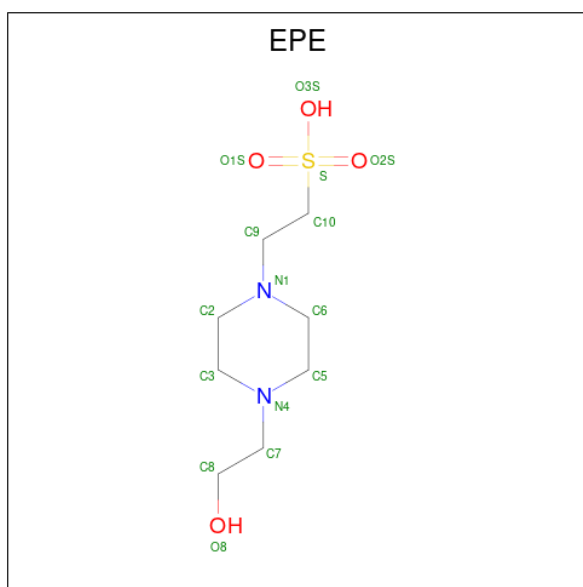


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 8 5 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: 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	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 (three-letter code: 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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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

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.

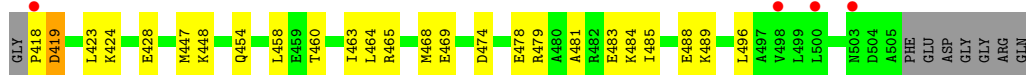
- Molecule 1: Optineurin



- Molecule 1: Optineurin



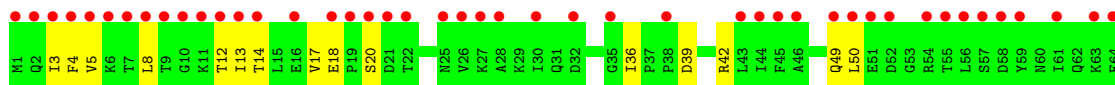
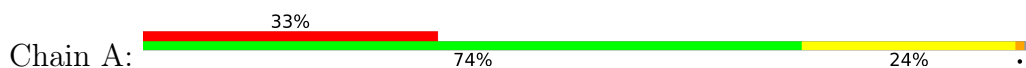
- Molecule 1: Optineurin

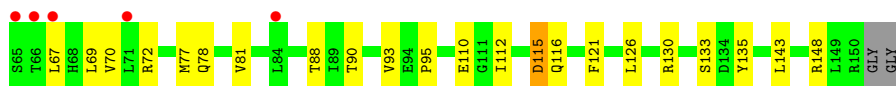


- Molecule 1: Optineurin

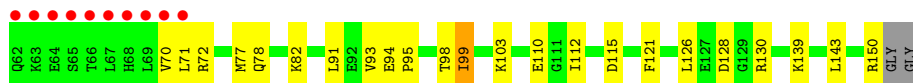
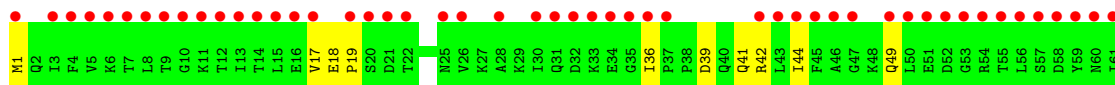
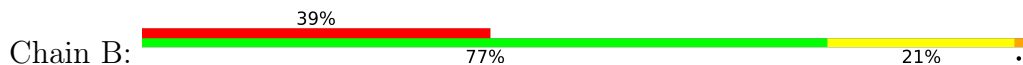


- Molecule 2: Ubiquitin





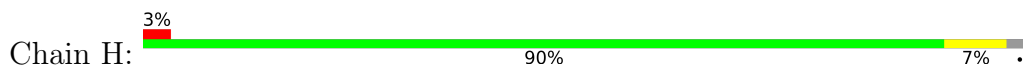
- Molecule 2: Ubiquitin



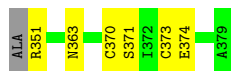
- Molecule 3: E3 ubiquitin-protein ligase RNF31



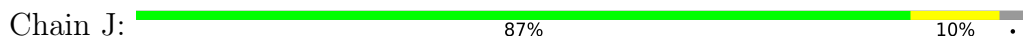
- Molecule 3: E3 ubiquitin-protein ligase RNF31



- 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 – 1.81 189.53 – 1.81	Depositor EDS
% Data completeness (in resolution range)	44.2 (46.15-1.81) 44.2 (189.53-1.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.81Å)	Xtrriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.231 , 0.269 0.229 , 0.262	Depositor DCC
R_{free} test set	2943 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtrriage
Anisotropy	0.086	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PG4, EPE, CL, PGE

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	0.37	0/720	0.54	0/965
1	D	0.35	0/697	0.57	0/935
1	E	0.35	0/709	0.57	0/949
1	F	0.37	0/695	0.60	0/930
2	A	0.32	0/1075	0.59	0/1461
2	B	0.34	0/1048	0.63	0/1425
3	G	0.55	0/226	0.71	0/304
3	H	0.38	0/227	0.67	0/304
3	I	0.54	0/237	0.77	0/318
3	J	0.44	0/243	0.76	0/326
All	All	0.37	0/5877	0.61	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 [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	C	710	0	695	31	0
1	D	690	0	665	32	0
1	E	699	0	699	39	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	38	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	3	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	2	0
9	C	9	0	0	0	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	177	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:ILE:CD1	2:B:103:LYS:HE3	1.99	0.93
2:B:150:ARG:NH2	6:B:201:CL:CL	2.46	0.86
2:B:77:MET:HE1	2:B:95:PRO:HD3	1.58	0.84
1:E:468:MET:HE1	1:F:464:LEU:HD11	1.60	0.83
1:C:501:LYS:HZ1	4:C:601:PG4:H12	1.42	0.83
3:I:363:ASN:HD21	3:I:371:SER:H	1.24	0.81
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
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
2:A:77:MET:HE1	2:A:95:PRO:HD3	1.75	0.67
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:E:448:LYS:HG2	1:F:447:MET:HE1	1.77	0.66
2:B:36:ILE:HG12	2:B:71:LEU:CD2	2.26	0.65
2:B:139:LYS:NZ	9:B:301:HOH:O	2.28	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
1:C:461:MET:HE2	1:D:461:MET:HG3	1.81	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: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)
2:A:77:MET:HE1	2:A:95:PRO:CD	2.31	0.61
2:A:36:ILE:O	2:A:36:ILE:HD12	2.01	0.60
2:B:77:MET:HE1	2:B:95:PRO:CD	2.29	0.59
1:E:448:LYS:HG2	1:F:447:MET:CE	2.33	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
1:C:447:MET:HB2	1:D:447:MET:HE2	1.86	0.57
2:A:49:GLN:HG2	2:A:49:GLN:O	2.03	0.57
2:B:121:PHE:HB3	2:B:126:LEU:HD21	1.85	0.57
1:C:464:LEU:HD21	1:D:465:ARG:N	2.19	0.57
1:E:468:MET:HE2	1:F:464:LEU:HD11	1.83	0.57
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
2:B:36:ILE:HD12	2:B:36:ILE:C	2.27	0.54
1:E:465:ARG:HA	1:E:468:MET:HE3	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:B:77:MET:HE2	2:B:93:VAL:HG23	1.90	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:77:MET:HE2	2:A:93:VAL:HG23	1.91	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: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:423:LEU:HD12	1:F:426:LEU:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ASP:O	2:B:72:ARG:NH1	2.40	0.52
2:B:42:ARG:HE	2:B:72:ARG:HD2	1.73	0.52
2:A:77:MET:CE	2:A:93:VAL:HG23	2.39	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
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
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
1:C:461:MET:HE2	1:D:461:MET:CG	2.42	0.49
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:HE1	1:F:444:MET:HA	1.96	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
1:E:447:MET:HE3	1:F:447:MET:SD	2.54	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
2:B:77:MET:CE	2:B:93:VAL:HG23	2.44	0.47
1:C:474:ASP:HB3	1:D:475:PHE:CE1	2.49	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:C:468:MET:HE2	1:D:467:GLN:HG3	1.97	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
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:E:468:MET:HG3	1:F:471:TYR:CE2	2.52	0.45
1:E:468:MET:HE3	1:E:468:MET:HB3	1.73	0.45
2:A:69:LEU:HD13	2:A:70:VAL:N	2.32	0.45
2:B:77:MET:CE	2:B:94:GLU:HA	2.47	0.45
2:B:1:MET:H1	2:B:18:GLU:CD	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:116:GLN:C	2:A:148:ARG:HG3	2.37	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:C:447:MET:CB	1:D:447:MET:HE2	2.48	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: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
3:I:373:CYS:C	3:I:374:GLU:HG2	2.39	0.43
2:B:99:ILE:CG1	2:B:128:ASP:HA	2.44	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: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
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:F:459:GLU:O	1:F:462:THR:OG1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	73/81 (90%)	72 (99%)	1 (1%)	67	58
1	D	70/81 (86%)	68 (97%)	2 (3%)	42	28
1	E	73/81 (90%)	72 (99%)	1 (1%)	67	58
1	F	71/81 (88%)	69 (97%)	2 (3%)	43	29
2	A	98/136 (72%)	96 (98%)	2 (2%)	55	43
2	B	86/136 (63%)	84 (98%)	2 (2%)	50	37
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%)	23 (92%)	2 (8%)	12	3
All	All	566/688 (82%)	554 (98%)	12 (2%)	55	41

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	423	LEU
1	D	484	LYS
1	D	504	ASP
1	E	419	ASP
1	F	419	ASP
1	F	499	LEU
2	A	115	ASP
2	A	133	SER

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Mol	Chain	Res	Type
2	B	99	ILE
2	B	115	ASP
3	J	351[A]	ARG
3	J	351[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	454	GLN
1	C	495	GLN
1	F	495	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 monosaccharides 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	A	201	-	15,15,15	1.04	1 (6%)	18,20,20	1.33	4 (22%)
7	EPE	H	402	-	15,15,15	0.94	1 (6%)	18,20,20	1.15	2 (11%)
7	EPE	F	602	-	15,15,15	0.88	1 (6%)	18,20,20	0.81	0
7	EPE	J	404	-	15,15,15	0.89	1 (6%)	18,20,20	1.55	4 (22%)
4	PG4	C	601	-	12,12,12	0.30	0	11,11,11	0.22	0
4	PG4	J	402	-	12,12,12	0.25	0	11,11,11	0.28	0
5	PGE	C	602	-	7,7,9	0.31	0	6,6,8	0.49	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	A	201	-	-	8/9/19/19	0/1/1/1
7	EPE	H	402	-	-	4/9/19/19	0/1/1/1
7	EPE	F	602	-	-	4/9/19/19	0/1/1/1
7	EPE	J	404	-	-	2/9/19/19	0/1/1/1
4	PG4	C	601	-	-	1/10/10/10	-
4	PG4	J	402	-	-	7/10/10/10	-
5	PGE	C	602	-	-	2/5/5/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	201	EPE	C10-S	3.06	1.81	1.77
7	H	402	EPE	C10-S	2.87	1.81	1.77
7	J	404	EPE	C10-S	2.65	1.81	1.77
7	F	602	EPE	C10-S	2.57	1.81	1.77

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	201	EPE	C3-C2-N1	2.84	116.46	110.64
7	J	404	EPE	O1S-S-C10	-2.69	103.67	106.92
7	H	402	EPE	C6-N1-C2	2.58	114.63	108.83
7	J	404	EPE	C3-C2-N1	2.43	115.63	110.64
7	J	404	EPE	O2S-S-C10	-2.32	104.12	106.92
7	H	402	EPE	C3-C2-N1	2.30	115.37	110.64
7	A	201	EPE	C7-N4-C5	-2.28	105.41	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	404	EPE	C2-C3-N4	2.14	115.04	110.64
7	A	201	EPE	O1S-S-C10	-2.08	104.41	106.92
7	A	201	EPE	C5-N4-C3	2.05	113.45	108.83

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	F	602	EPE	S-C10-C9-N1
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
7	A	201	EPE	N4-C7-C8-O8
4	J	402	PG4	O3-C5-C6-O4
4	J	402	PG4	O4-C7-C8-O5
4	J	402	PG4	O1-C1-C2-O2
4	J	402	PG4	O2-C3-C4-O3
7	H	402	EPE	C8-C7-N4-C5
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	F	602	EPE	N4-C7-C8-O8
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
4	J	402	PG4	C6-C5-O3-C4
4	J	402	PG4	C5-C6-O4-C7
4	J	402	PG4	C1-C2-O2-C3
5	C	602	PGE	C3-C4-O3-C5
5	C	602	PGE	C4-C3-O2-C2
7	H	402	EPE	C10-C9-N1-C2

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	201	EPE	4	0
7	F	602	EPE	2	0
7	J	404	EPE	2	0
4	C	601	PG4	4	0
4	J	402	PG4	3	0
5	C	602	PGE	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	C	89/96 (92%)	0.24	6 (6%) 17 14	29, 49, 85, 98	0
1	D	88/96 (91%)	0.14	3 (3%) 45 39	31, 52, 74, 105	0
1	E	88/96 (91%)	0.26	4 (4%) 33 27	20, 49, 92, 118	0
1	F	88/96 (91%)	0.19	4 (4%) 33 27	20, 46, 81, 95	0
2	A	150/152 (98%)	2.11	50 (33%) 0 0	31, 65, 174, 226	0
2	B	150/152 (98%)	3.37	60 (40%) 0 0	25, 60, 208, 259	0
3	G	29/30 (96%)	0.14	2 (6%) 16 13	25, 38, 57, 82	0
3	H	29/30 (96%)	0.12	1 (3%) 45 39	27, 37, 63, 94	0
3	I	29/30 (96%)	0.18	0 100 100	20, 27, 44, 48	0
3	J	29/30 (96%)	0.27	0 100 100	21, 27, 48, 53	0
All	All	769/808 (95%)	1.19	130 (16%) 1 1	20, 50, 172, 259	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	13	ILE	26.6
2	B	4	PHE	21.4
2	B	46	ALA	21.0
2	B	12	THR	19.8
2	B	15	LEU	19.5
2	A	3	ILE	19.3
2	B	65	SER	17.8
2	B	50	LEU	17.5
2	B	14	THR	17.4
2	B	9	THR	15.1
2	A	21	ASP	14.7
2	B	10	GLY	14.4
2	A	9	THR	13.5

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Mol	Chain	Res	Type	RSRZ
2	A	32	ASP	13.4
2	A	12	THR	12.6
2	A	1	MET	12.4
2	B	56	LEU	11.7
2	B	61	ILE	11.3
2	B	7	THR	11.2
2	A	20	SER	11.1
2	A	50	LEU	11.1
2	B	32	ASP	10.7
2	B	66	THR	10.4
2	B	35	GLY	10.4
2	B	57	SER	10.2
2	B	5	VAL	10.2
2	B	43	LEU	9.8
2	A	19	PRO	9.5
2	B	8	LEU	9.4
2	B	34	GLU	9.0
2	A	65	SER	8.5
2	B	19	PRO	8.3
2	B	45	PHE	8.2
2	B	64	GLU	8.2
2	A	10	GLY	8.1
2	B	21	ASP	7.9
2	B	3	ILE	7.8
2	A	13	ILE	7.7
2	A	14	THR	7.6
2	A	52	ASP	7.5
2	B	6	LYS	7.3
2	A	56	LEU	7.0
2	A	22	THR	6.9
2	B	16	GLU	6.9
2	B	67	LEU	6.8
2	A	61	ILE	6.5
2	A	57	SER	6.4
2	A	46	ALA	6.4
2	B	63	LYS	6.2
2	B	62	GLN	6.2
2	B	54	ARG	6.2
2	A	5	VAL	6.1
2	B	59	TYR	6.1
2	A	55	THR	6.1
2	B	31	GLN	5.9

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Mol	Chain	Res	Type	RSRZ
2	A	4	PHE	5.9
2	B	26	VAL	5.9
2	A	6	LYS	5.8
2	A	59	TYR	5.7
2	A	54	ARG	5.5
1	E	418	PRO	5.2
2	A	11	LYS	5.0
2	A	27	LYS	5.0
2	B	53	GLY	5.0
2	B	17	VAL	5.0
2	B	51	GLU	4.9
2	B	37	PRO	4.7
2	A	44	ILE	4.7
2	B	36	ILE	4.6
2	A	18	GLU	4.6
2	B	33	LYS	4.5
2	B	42	ARG	4.4
2	B	30	ILE	4.3
2	B	11	LYS	4.2
2	A	66	THR	4.2
2	B	20	SER	4.1
1	F	418	PRO	4.0
2	B	28	ALA	4.0
2	B	69	LEU	3.9
2	B	55	THR	3.8
2	B	22	THR	3.7
2	B	60	ASN	3.7
2	A	16	GLU	3.7
2	B	58	ASP	3.7
2	B	68	HIS	3.6
2	B	1	MET	3.5
2	A	67	LEU	3.5
2	B	25	ASN	3.4
1	D	420	ARG	3.4
2	B	70	VAL	3.4
2	B	52	ASP	3.3
2	A	25	ASN	3.2
1	F	494	LEU	3.2
2	A	63	LYS	3.2
2	B	47	GLY	3.2
1	E	500	LEU	3.1
1	C	505	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	38	PRO	2.9
2	B	44	ILE	2.9
1	C	421	ALA	2.8
2	A	49	GLN	2.8
2	A	64	GLU	2.7
2	B	49	GLN	2.7
2	B	71	LEU	2.7
2	A	7	THR	2.7
2	A	45	PHE	2.7
1	C	504	ASP	2.6
2	A	2	GLN	2.6
1	D	421	ALA	2.5
2	A	28	ALA	2.5
1	C	506	PHE	2.5
2	A	43	LEU	2.5
1	F	504	ASP	2.4
1	E	498	VAL	2.4
2	A	26	VAL	2.4
3	G	351	ARG	2.4
2	A	51	GLU	2.4
2	A	8	LEU	2.3
2	A	84	LEU	2.3
1	D	463	ILE	2.3
2	A	30	ILE	2.3
1	C	500	LEU	2.3
2	A	71	LEU	2.3
2	A	58	ASP	2.2
3	G	352	GLY	2.2
3	H	351	ARG	2.1
1	F	498	VAL	2.1
1	E	503	ASN	2.1
2	A	35	GLY	2.1
1	C	463	ILE	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.66	0.27	64,77,117,127	0
7	EPE	A	201	15/15	0.75	0.28	68,92,113,115	0
7	EPE	J	404	15/15	0.81	0.33	45,71,88,103	0
7	EPE	F	602	15/15	0.85	0.26	45,67,110,113	0
4	PG4	J	402	13/13	0.86	0.15	38,43,57,58	0
4	PG4	C	601	13/13	0.90	0.15	47,60,65,70	0
5	PGE	C	602	8/10	0.90	0.11	52,59,65,70	0
6	CL	B	201	1/1	0.92	0.09	62,62,62,62	0
6	CL	J	403	1/1	0.92	0.14	54,54,54,54	0
6	CL	F	601	1/1	0.96	0.08	69,69,69,69	0
8	ZN	G	401	1/1	0.99	0.17	35,35,35,35	0
8	ZN	H	401	1/1	0.99	0.17	30,30,30,30	0
8	ZN	I	401	1/1	0.99	0.17	27,27,27,27	0
8	ZN	J	401	1/1	1.00	0.18	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.