



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:50 PM UTC

PDB ID : 5LEW / pdb_00005lew
Title : DNA polymerase
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Deposited on : 2016-06-30
Resolution : 2.80 Å(reported)

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

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

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

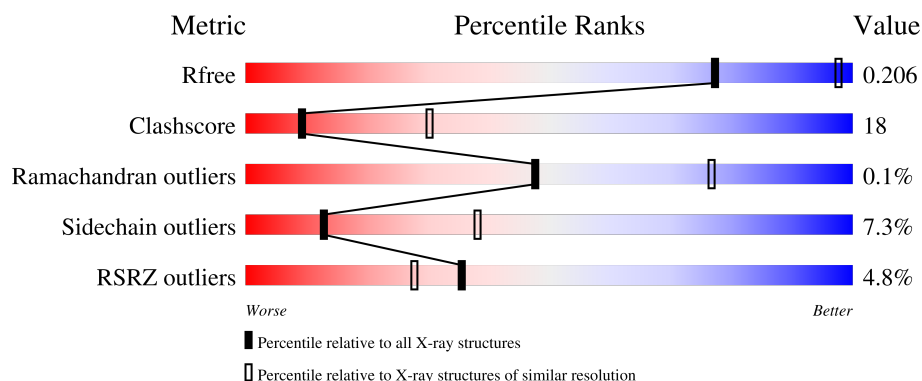
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	A	927	5% 66% 29% ..

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
3	SO4	A	1010	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EPE	A	1013	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7271 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.

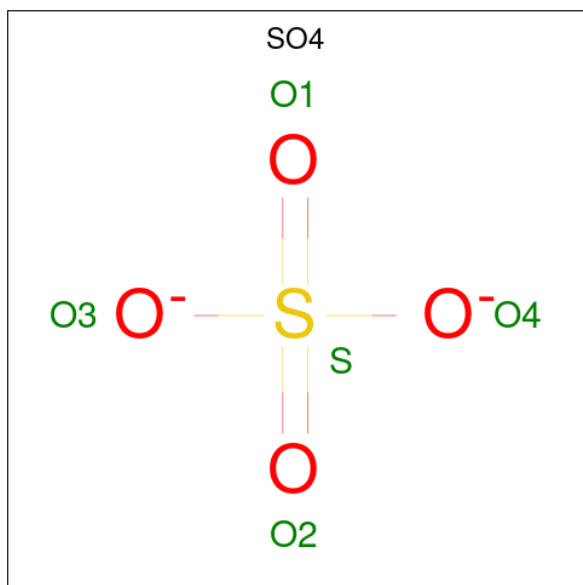
- Molecule 1 is a protein called DNA polymerase III subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	919	Total	C	N	O	S	0	2	0
			7127	4494	1260	1339	34			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



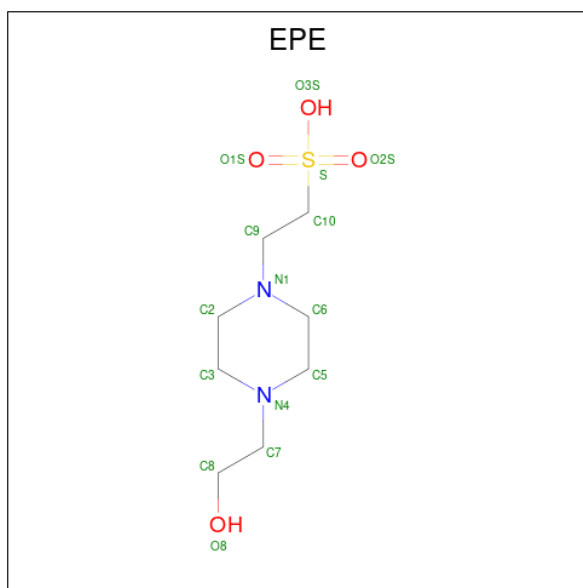
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 15 8 2 4 1	0	0

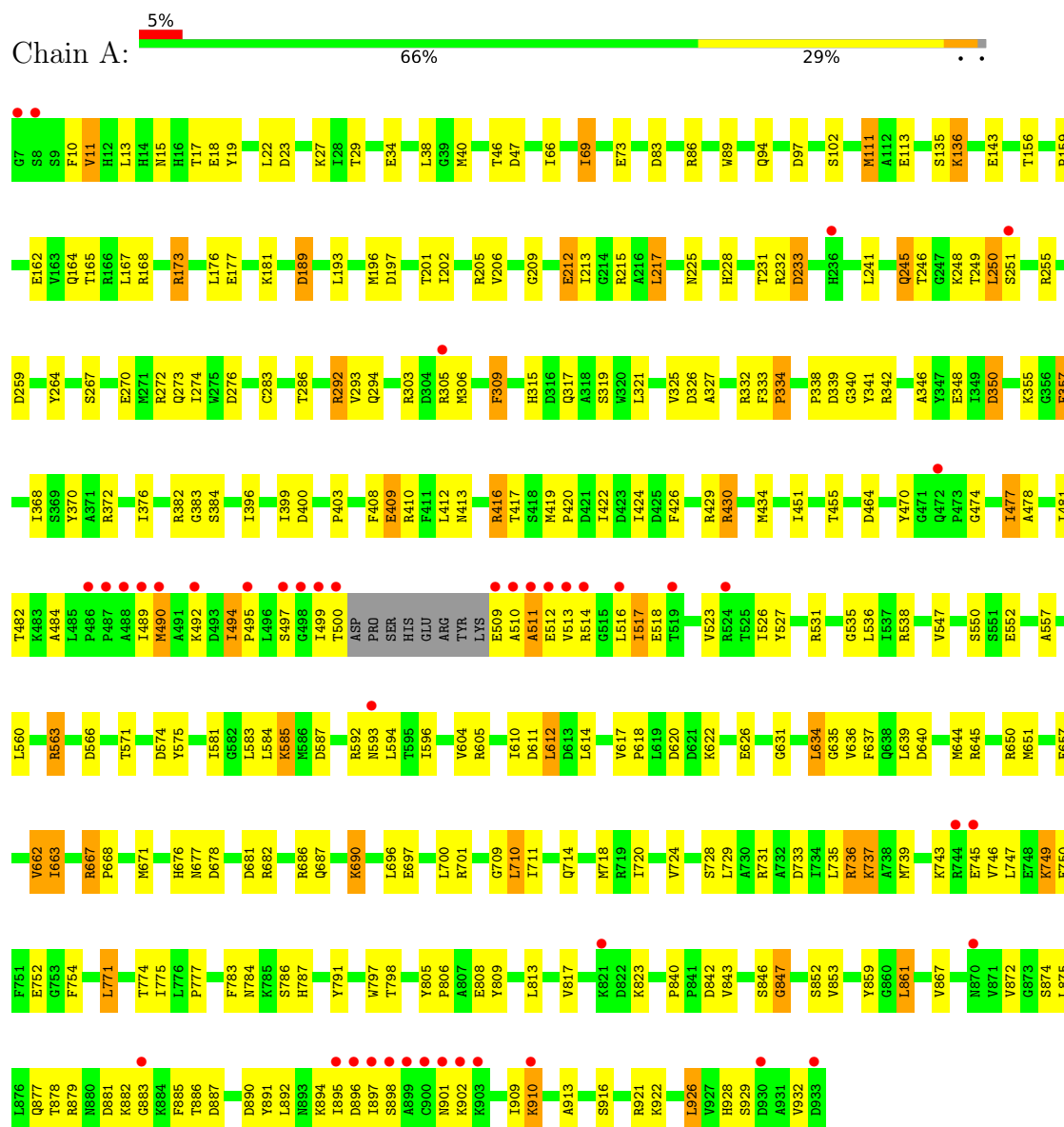
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	81	Total O 81 81	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: DNA polymerase III subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	256.04Å 256.04Å 187.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	143.11 – 2.80 143.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (143.11-2.80) 99.6 (143.11-2.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.196 , 0.231 (Not available) , 0.206	Depositor DCC
R_{free} test set	2925 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.7	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	0.94	EDS
Total number of atoms	7271	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, SO4, EPE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.17	8/7283 (0.1%)	1.36	41/9866 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	PRO	N-CD	16.19	1.70	1.47
1	A	350	ASP	N-CA	-5.79	1.39	1.46
1	A	245	GLN	C-O	-5.66	1.17	1.24
1	A	510	ALA	CA-C	5.62	1.59	1.53
1	A	667[A]	ARG	CA-C	5.41	1.57	1.52
1	A	667[B]	ARG	CA-C	5.41	1.57	1.52
1	A	667[A]	ARG	C-O	5.13	1.28	1.24
1	A	667[B]	ARG	C-O	5.13	1.28	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	910	LYS	CG-CD-CE	7.79	129.22	111.30
1	A	612	LEU	N-CA-C	7.56	121.30	109.96
1	A	910	LYS	CB-CG-CD	7.09	127.60	111.30
1	A	847	GLY	N-CA-C	-6.99	104.40	112.79
1	A	11	VAL	N-CA-C	6.87	118.02	108.12
1	A	417	THR	N-CA-C	-6.58	98.99	109.59
1	A	511	ALA	N-CA-C	6.55	119.58	108.90
1	A	690	LYS	CA-CB-CG	6.33	126.76	114.10
1	A	575	TYR	CA-C-N	-6.32	111.96	118.85
1	A	575	TYR	C-N-CA	-6.32	111.96	118.85
1	A	667[A]	ARG	CA-C-N	-6.07	112.31	119.05
1	A	667[A]	ARG	C-N-CA	-6.07	112.31	119.05
1	A	667[B]	ARG	CA-C-N	-6.07	112.31	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	667[B]	ARG	C-N-CA	-6.07	112.31	119.05
1	A	384	SER	N-CA-C	6.06	118.68	111.71
1	A	196	MET	CA-C-N	-5.99	114.35	122.86
1	A	196	MET	C-N-CA	-5.99	114.35	122.86
1	A	786	SER	CB-CA-C	-5.95	99.62	110.63
1	A	430	ARG	CB-CG-CD	5.80	124.64	111.30
1	A	294	GLN	N-CA-C	5.71	118.23	110.35
1	A	840	PRO	CA-C-N	-5.71	114.05	119.76
1	A	840	PRO	C-N-CA	-5.71	114.05	119.76
1	A	309	PHE	CA-C-N	-5.45	113.97	120.13
1	A	309	PHE	C-N-CA	-5.45	113.97	120.13
1	A	492	LYS	N-CA-C	5.45	119.06	107.67
1	A	197	ASP	N-CA-C	5.45	117.72	108.02
1	A	333	PHE	CA-C-N	-5.26	114.25	119.56
1	A	333	PHE	C-N-CA	-5.26	114.25	119.56
1	A	357	PHE	CA-C-N	-5.24	113.24	119.05
1	A	357	PHE	C-N-CA	-5.24	113.24	119.05
1	A	474	GLY	N-CA-C	-5.21	108.94	114.67
1	A	189	ASP	N-CA-C	5.19	119.25	113.02
1	A	663	ILE	N-CA-C	-5.16	105.51	110.72
1	A	83	ASP	CA-C-N	-5.14	114.43	122.65
1	A	83	ASP	C-N-CA	-5.14	114.43	122.65
1	A	883	GLY	N-CA-C	-5.13	103.62	111.98
1	A	662	VAL	CB-CA-C	-5.12	104.57	112.05
1	A	909	ILE	O-C-N	5.11	126.92	121.91
1	A	69	ILE	CA-C-N	-5.09	116.48	123.14
1	A	69	ILE	C-N-CA	-5.09	116.48	123.14
1	A	470	TYR	N-CA-C	5.07	120.46	113.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7127	0	7037	257	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	0	0	0
3	A	45	0	0	3	0
4	A	15	0	17	10	0
5	A	81	0	0	7	0
All	All	7271	0	7054	258	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 18.

All (258) 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:A:334:PRO:N	1:A:334:PRO:CD	1.70	1.33
1:A:890:ASP:OD2	1:A:894:LYS:NZ	1.61	1.32
1:A:497:SER:O	1:A:500:THR:HG22	1.00	1.17
1:A:890:ASP:CG	1:A:894:LYS:NZ	2.01	1.17
1:A:497:SER:O	1:A:500:THR:CG2	1.92	1.16
1:A:711:ILE:H	4:A:1013:EPE:H22	0.98	1.08
1:A:890:ASP:CG	1:A:894:LYS:HZ2	1.58	1.03
1:A:902:LYS:HG3	1:A:928:HIS:CE1	1.96	0.99
1:A:622:LYS:NZ	1:A:626:GLU:OE1	1.95	0.99
1:A:710:LEU:HD12	4:A:1013:EPE:H101	1.43	0.97
1:A:711:ILE:N	4:A:1013:EPE:H22	1.81	0.95
1:A:383:GLY:HA2	1:A:787[B]:HIS:CE1	2.04	0.93
1:A:650:ARG:NH1	1:A:677:ASN:OD1	2.03	0.92
1:A:481:ILE:HD11	1:A:523:VAL:HG22	1.49	0.91
1:A:464:ASP:OD2	1:A:538:ARG:NH1	2.03	0.90
1:A:497:SER:C	1:A:500:THR:HG22	1.98	0.88
1:A:592:ARG:HG2	5:A:1168:HOH:O	1.75	0.86
1:A:512:GLU:HG3	1:A:513:VAL:N	1.90	0.86
1:A:711:ILE:H	4:A:1013:EPE:C2	1.88	0.84
1:A:902:LYS:HD2	1:A:932:VAL:HG11	1.59	0.83
1:A:733:ASP:OD1	1:A:736:ARG:NH1	2.12	0.82
1:A:922:LYS:O	1:A:926:LEU:HD13	1.80	0.82
1:A:929:SER:O	1:A:932:VAL:HG22	1.82	0.80
1:A:484:ALA:HB1	1:A:513:VAL:HB	1.64	0.79
1:A:682:ARG:NH1	1:A:710:LEU:HD13	1.98	0.78
1:A:413:ASN:HB3	1:A:416:ARG:HG3	1.66	0.77
1:A:896:ASP:OD1	1:A:901:ASN:ND2	2.18	0.77
1:A:631:GLY:O	1:A:645:ARG:HG2	1.85	0.76
1:A:639:LEU:HD22	1:A:644:MET:CE	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:THR:O	1:A:205:ARG:HG3	1.85	0.76
1:A:678:ASP:OD1	1:A:687:GLN:NE2	2.13	0.75
1:A:267:SER:OG	1:A:270:GLU:HG3	1.86	0.74
1:A:376:ILE:HD12	1:A:434:MET:HE3	1.70	0.74
1:A:651:MET:HE1	1:A:662:VAL:HG12	1.69	0.73
1:A:305:ARG:NH1	1:A:557:ALA:HB1	2.03	0.73
1:A:38:LEU:HD13	1:A:40:MET:HE3	1.71	0.73
1:A:874:SER:O	1:A:878:THR:HG23	1.89	0.72
1:A:173:ARG:HH11	1:A:177:GLU:CD	1.98	0.72
1:A:231:THR:HG22	1:A:232:ARG:N	2.03	0.72
1:A:17:THR:HG22	1:A:19:TYR:H	1.54	0.71
1:A:255:ARG:HG2	1:A:255:ARG:HH21	1.55	0.71
1:A:681:ASP:OD1	1:A:686:ARG:NH1	2.24	0.70
1:A:787[A]:HIS:NE2	1:A:791:TYR:CE2	2.60	0.70
1:A:527:TYR:CZ	1:A:531:ARG:HD2	2.27	0.70
1:A:306:MET:HE2	1:A:584:LEU:HD13	1.74	0.69
1:A:17:THR:HG22	1:A:18:GLU:N	2.07	0.69
1:A:897:ILE:H	1:A:897:ILE:HD12	1.58	0.69
1:A:419:MET:HE3	1:A:420:PRO:HD2	1.73	0.69
1:A:787[A]:HIS:NE2	1:A:791:TYR:CZ	2.60	0.69
1:A:512:GLU:HG3	1:A:513:VAL:H	1.58	0.68
1:A:355:LYS:HD2	1:A:412:LEU:HD22	1.74	0.68
1:A:902:LYS:CD	1:A:932:VAL:HG11	2.22	0.68
1:A:710:LEU:CD1	4:A:1013:EPE:H101	2.20	0.68
1:A:376:ILE:CD1	1:A:434:MET:HE3	2.24	0.67
1:A:13:LEU:HB3	1:A:111:MET:CE	2.24	0.67
1:A:159:PRO:O	1:A:168:ARG:NH2	2.27	0.67
1:A:737:LYS:NZ	5:A:1101:HOH:O	2.14	0.67
1:A:13:LEU:HB3	1:A:111:MET:HE2	1.78	0.66
1:A:305:ARG:NH1	1:A:581:ILE:HD12	2.10	0.66
1:A:309:PHE:O	1:A:317:GLN:NE2	2.29	0.66
1:A:668:PRO:HD2	5:A:1132:HOH:O	1.96	0.66
1:A:709:GLY:O	4:A:1013:EPE:H102	1.97	0.65
1:A:231:THR:HG22	1:A:232:ARG:H	1.62	0.65
1:A:574:ASP:HB2	5:A:1158:HOH:O	1.95	0.65
1:A:46:THR:O	1:A:46:THR:HG22	1.97	0.64
1:A:509:GLU:HB2	1:A:514:ARG:HH22	1.61	0.63
1:A:484:ALA:CB	1:A:513:VAL:HB	2.29	0.63
1:A:97:ASP:OD1	1:A:168:ARG:HD2	1.98	0.62
1:A:370:TYR:CD2	1:A:434:MET:HE1	2.33	0.62
1:A:348:GLU:HG2	1:A:408:PHE:CD1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:LEU:CD2	1:A:644:MET:CE	2.79	0.61
1:A:891:TYR:O	1:A:895:ILE:HG23	2.00	0.61
1:A:877:GLN:NE2	1:A:881:ASP:OD2	2.31	0.61
1:A:886:THR:HG22	1:A:887:ASP:OD2	2.00	0.61
1:A:902:LYS:CG	1:A:928:HIS:CE1	2.80	0.61
1:A:892:LEU:HA	1:A:895:ILE:HG12	1.83	0.61
1:A:17:THR:CG2	1:A:18:GLU:N	2.64	0.60
1:A:305:ARG:NH1	1:A:557:ALA:CB	2.65	0.60
1:A:676:HIS:CE1	1:A:677:ASN:HD22	2.20	0.60
1:A:306:MET:HE1	1:A:419:MET:HE1	1.84	0.59
1:A:89:TRP:CH2	1:A:162:GLU:HG3	2.38	0.59
1:A:17:THR:HG21	1:A:19:TYR:HD1	1.68	0.59
1:A:842:ASP:OD1	1:A:916:SER:HB2	2.03	0.59
1:A:340:GLY:N	3:A:1010:SO4:O4	2.25	0.58
1:A:902:LYS:HG3	1:A:928:HIS:NE2	2.19	0.58
1:A:517:ILE:HG22	1:A:523:VAL:HG12	1.85	0.58
1:A:604:VAL:HG22	1:A:808:GLU:HG2	1.85	0.58
1:A:563:ARG:HH11	1:A:566:ASP:CG	2.11	0.58
1:A:17:THR:CG2	1:A:19:TYR:HD1	2.17	0.57
1:A:368:ILE:HD12	1:A:396:ILE:HA	1.86	0.57
1:A:718:MET:HE2	1:A:733:ASP:HA	1.86	0.57
1:A:735:LEU:HD13	1:A:750:GLU:CG	2.34	0.57
1:A:511:ALA:HB1	1:A:513:VAL:HG12	1.85	0.57
1:A:651:MET:HE1	1:A:662:VAL:CG1	2.33	0.57
1:A:592:ARG:N	3:A:1005:SO4:O4	2.37	0.57
1:A:563:ARG:NH1	1:A:566:ASP:CG	2.64	0.56
1:A:370:TYR:HD2	1:A:434:MET:HE1	1.71	0.56
1:A:270:GLU:O	1:A:274:ILE:HG13	2.05	0.56
1:A:383:GLY:CA	1:A:787[B]:HIS:CE1	2.86	0.56
1:A:563:ARG:NH1	1:A:566:ASP:OD1	2.33	0.55
1:A:89:TRP:HH2	1:A:162:GLU:HG3	1.71	0.55
1:A:563:ARG:NH1	1:A:566:ASP:OD2	2.39	0.55
1:A:926:LEU:N	1:A:926:LEU:HD12	2.22	0.55
1:A:168:ARG:HD3	1:A:202:ILE:HG13	1.87	0.55
1:A:511:ALA:HB1	1:A:513:VAL:CG1	2.37	0.55
1:A:735:LEU:HD13	1:A:750:GLU:HG2	1.89	0.55
1:A:355:LYS:HD3	5:A:1155:HOH:O	2.06	0.55
1:A:728:SER:HB3	1:A:731:ARG:H	1.71	0.55
1:A:38:LEU:CD1	1:A:40:MET:HE3	2.35	0.55
1:A:15:ASN:H	1:A:46:THR:HB	1.72	0.54
1:A:413:ASN:HB3	1:A:416:ARG:CG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:HG22	1:A:248:LYS:HG3	1.89	0.54
1:A:902:LYS:HE3	1:A:932:VAL:HG21	1.89	0.54
1:A:348:GLU:HG2	1:A:408:PHE:CE1	2.43	0.54
1:A:867:VAL:HG12	1:A:872:VAL:CG2	2.37	0.54
1:A:383:GLY:HA2	1:A:787[B]:HIS:ND1	2.20	0.54
1:A:481:ILE:CD1	1:A:523:VAL:HG22	2.30	0.54
1:A:651:MET:CE	1:A:662:VAL:HG12	2.36	0.54
1:A:164:GLN:HG2	1:A:206:VAL:HG11	1.89	0.53
1:A:478:ALA:O	1:A:482:THR:HG23	2.09	0.53
1:A:477:ILE:O	1:A:481:ILE:HG12	2.08	0.53
1:A:509:GLU:CG	1:A:514:ARG:HH22	2.22	0.53
1:A:682:ARG:NH1	1:A:710:LEU:CD1	2.71	0.53
1:A:817:VAL:HG13	1:A:823:LYS:HB2	1.89	0.53
1:A:517:ILE:HG22	1:A:523:VAL:CG1	2.38	0.53
1:A:926:LEU:N	1:A:926:LEU:CD1	2.71	0.53
1:A:926:LEU:CD1	1:A:926:LEU:H	2.21	0.53
1:A:23:ASP:OD1	1:A:228:HIS:CD2	2.62	0.53
1:A:513:VAL:O	1:A:516:LEU:N	2.42	0.53
1:A:513:VAL:O	1:A:514:ARG:C	2.48	0.53
1:A:409:GLU:HG3	1:A:729:LEU:HB3	1.90	0.52
1:A:735:LEU:CD1	1:A:750:GLU:HG2	2.38	0.52
1:A:400:ASP:CG	1:A:403:PRO:HD2	2.35	0.52
1:A:410:ARG:NH2	1:A:714:GLN:OE1	2.38	0.52
1:A:455:THR:HG23	1:A:535:GLY:HA2	1.92	0.52
1:A:233:ASP:OD1	1:A:233:ASP:N	2.43	0.52
1:A:255:ARG:HG2	1:A:255:ARG:NH2	2.23	0.52
1:A:455:THR:CG2	1:A:535:GLY:HA2	2.40	0.52
1:A:513:VAL:HG13	1:A:514:ARG:N	2.25	0.52
1:A:784:ASN:ND2	1:A:787[B]:HIS:CE1	2.78	0.52
1:A:231:THR:CG2	1:A:232:ARG:H	2.24	0.51
1:A:231:THR:CG2	1:A:232:ARG:N	2.70	0.51
1:A:635:GLY:HA3	1:A:813:LEU:HD21	1.91	0.51
1:A:593:ASN:OD1	1:A:594:LEU:N	2.44	0.51
1:A:610:ILE:HG22	1:A:611:ASP:N	2.26	0.50
1:A:667[A]:ARG:HD2	1:A:783:PHE:CE1	2.46	0.50
1:A:639:LEU:CD2	1:A:644:MET:HE2	2.42	0.50
1:A:173:ARG:NH1	1:A:177:GLU:OE1	2.45	0.50
1:A:209:GLY:O	1:A:213:ILE:HG13	2.12	0.49
1:A:509:GLU:HG3	1:A:514:ARG:HH22	1.76	0.49
1:A:700:LEU:HD22	1:A:720:ILE:HG12	1.94	0.49
1:A:321:LEU:O	1:A:325:VAL:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLU:CB	1:A:514:ARG:HH22	2.26	0.49
1:A:697:GLU:OE1	1:A:701:ARG:NH1	2.45	0.49
1:A:46:THR:HG22	1:A:73:GLU:HB2	1.94	0.49
1:A:272:ARG:HD3	1:A:276:ASP:OD2	2.12	0.49
1:A:429:ARG:C	1:A:430:ARG:HG2	2.38	0.49
1:A:787[A]:HIS:CE1	1:A:791:TYR:CZ	3.00	0.49
1:A:156:THR:HG21	1:A:193:LEU:HD12	1.95	0.49
1:A:817:VAL:CG1	1:A:823:LYS:HB2	2.43	0.49
1:A:890:ASP:OD1	1:A:894:LYS:NZ	2.14	0.49
1:A:173:ARG:NH1	1:A:177:GLU:CD	2.69	0.49
1:A:808:GLU:HA	1:A:852:SER:OG	2.13	0.48
1:A:113:GLU:OE2	1:A:292:ARG:HD2	2.13	0.48
1:A:671:MET:HE3	1:A:676:HIS:CD2	2.48	0.48
1:A:805:TYR:N	1:A:806:PRO:HD3	2.29	0.48
1:A:867:VAL:HG12	1:A:872:VAL:HG23	1.94	0.48
1:A:451:ILE:HB	1:A:571:THR:O	2.12	0.48
1:A:639:LEU:HD23	1:A:644:MET:HE2	1.96	0.48
1:A:877:GLN:NE2	1:A:881:ASP:CG	2.72	0.48
1:A:527:TYR:CE1	1:A:531:ARG:HD2	2.49	0.47
1:A:232:ARG:HG3	1:A:264:TYR:CE1	2.49	0.47
1:A:550:SER:HB2	1:A:583:LEU:HD22	1.95	0.47
1:A:618:PRO:HB2	1:A:620:ASP:OD1	2.14	0.47
1:A:843:VAL:HG23	1:A:913:ALA:HB1	1.95	0.47
1:A:494:ILE:O	1:A:495:PRO:C	2.58	0.47
1:A:355:LYS:CD	1:A:412:LEU:HD22	2.44	0.47
1:A:490:MET:O	1:A:490:MET:HG3	2.14	0.46
1:A:342:ARG:HB2	3:A:1010:SO4:O3	2.14	0.46
1:A:22:LEU:HB3	1:A:245:GLN:HB2	1.98	0.46
1:A:346:ALA:O	1:A:350:ASP:HB2	2.16	0.46
1:A:212:GLU:HG3	1:A:215:ARG:NH2	2.31	0.46
1:A:315:HIS:ND1	1:A:319:SER:HB3	2.31	0.46
1:A:614:LEU:HD13	1:A:797:TRP:CD2	2.51	0.46
1:A:735:LEU:HG	1:A:739:MET:HE2	1.99	0.45
1:A:651:MET:O	1:A:651:MET:HG2	2.16	0.45
1:A:743:LYS:HG2	1:A:746:VAL:HB	1.97	0.45
1:A:650:ARG:CZ	1:A:677:ASN:OD1	2.62	0.45
1:A:754:PHE:HZ	1:A:771:LEU:HD13	1.82	0.45
1:A:634:LEU:HB2	5:A:1126:HOH:O	2.16	0.45
1:A:424:ILE:CD1	1:A:426:PHE:HE2	2.30	0.45
1:A:874:SER:O	1:A:877:GLN:HB3	2.17	0.45
1:A:710:LEU:HA	4:A:1013:EPE:C10	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:THR:CG2	1:A:73:GLU:HB2	2.47	0.45
1:A:846:SER:O	1:A:879:ARG:NH2	2.49	0.44
1:A:842:ASP:OD1	1:A:916:SER:CB	2.64	0.44
1:A:176:LEU:HD11	1:A:217:LEU:HD13	1.98	0.44
1:A:135:SER:OG	1:A:136:LYS:N	2.51	0.44
1:A:676:HIS:CG	1:A:677:ASN:N	2.85	0.44
1:A:847:GLY:O	1:A:861:LEU:HB2	2.18	0.44
1:A:593:ASN:ND2	1:A:637:PHE:CE1	2.85	0.44
1:A:464:ASP:CG	1:A:538:ARG:HH12	2.21	0.44
1:A:690:LYS:HB2	4:A:1013:EPE:O3S	2.18	0.44
1:A:305:ARG:HH12	1:A:557:ALA:HB1	1.83	0.43
1:A:735:LEU:HD13	1:A:750:GLU:HG3	1.99	0.43
1:A:481:ILE:HD12	1:A:523:VAL:HG13	2.00	0.43
1:A:499:ILE:CG2	1:A:514:ARG:HB2	2.48	0.43
1:A:13:LEU:HB3	1:A:111:MET:HE1	1.99	0.43
1:A:181:LYS:HB3	1:A:181:LYS:HE2	1.85	0.43
1:A:250:LEU:HD12	1:A:250:LEU:HA	1.89	0.43
1:A:637:PHE:H	1:A:798:THR:HG21	1.83	0.43
1:A:225:ASN:ND2	1:A:264:TYR:O	2.52	0.42
1:A:273:GLN:O	1:A:273:GLN:HG2	2.19	0.42
1:A:843:VAL:HG12	1:A:885:PHE:HD2	1.83	0.42
1:A:604:VAL:CG2	1:A:808:GLU:HG2	2.49	0.42
1:A:97:ASP:O	1:A:165:THR:HG23	2.19	0.42
1:A:241:LEU:HD22	1:A:536:LEU:HD13	2.00	0.42
1:A:774:THR:O	1:A:777:PRO:HD2	2.19	0.42
1:A:798:THR:HG23	1:A:809:TYR:OH	2.19	0.42
1:A:509:GLU:HG3	1:A:514:ARG:NH2	2.33	0.42
1:A:749:LYS:O	1:A:752:GLU:HB2	2.19	0.42
1:A:477:ILE:HG12	1:A:526:ILE:HD12	2.02	0.42
1:A:34:GLU:HA	1:A:34:GLU:OE1	2.20	0.42
1:A:639:LEU:HD22	1:A:644:MET:HE3	1.97	0.42
1:A:382:ARG:CZ	1:A:791:TYR:HE1	2.32	0.42
1:A:843:VAL:CG1	1:A:885:PHE:CD2	3.02	0.42
1:A:272:ARG:NH1	1:A:283:CYS:HB2	2.35	0.42
1:A:338:PRO:HG2	1:A:341:TYR:CE1	2.54	0.42
1:A:513:VAL:O	1:A:516:LEU:HB3	2.20	0.42
1:A:696:LEU:HD23	1:A:696:LEU:HA	1.89	0.42
1:A:348:GLU:HG2	1:A:408:PHE:CG	2.55	0.41
1:A:605:ARG:HA	1:A:610:ILE:O	2.20	0.41
1:A:617:VAL:HG13	1:A:618:PRO:HD2	2.01	0.41
4:A:1013:EPE:H61	4:A:1013:EPE:O2S	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:THR:HG22	1:A:251:SER:N	2.35	0.41
1:A:326:ASP:O	1:A:327:ALA:C	2.63	0.41
1:A:10:PHE:CE2	1:A:286:THR:HG21	2.56	0.41
1:A:69:ILE:HD12	1:A:293:VAL:HG21	2.02	0.41
1:A:592:ARG:O	1:A:596:ILE:HG13	2.20	0.41
1:A:585:LYS:HE3	1:A:587:ASP:OD1	2.21	0.41
1:A:775:ILE:HD13	1:A:775:ILE:HG21	1.88	0.41
1:A:514:ARG:O	1:A:518:GLU:HG3	2.21	0.41
1:A:17:THR:CG2	1:A:18:GLU:H	2.33	0.41
1:A:509:GLU:CG	1:A:514:ARG:NH2	2.83	0.41
1:A:513:VAL:HG13	1:A:514:ARG:H	1.86	0.41
1:A:593:ASN:OD1	1:A:593:ASN:C	2.64	0.41
1:A:813:LEU:HD12	1:A:813:LEU:HA	1.83	0.41
1:A:17:THR:HB	1:A:47:ASP:OD2	2.20	0.41
1:A:885:PHE:CD1	1:A:891:TYR:HA	2.56	0.41
1:A:372:ARG:NH2	5:A:1110:HOH:O	2.54	0.40
1:A:167:LEU:CD1	1:A:206:VAL:HG13	2.51	0.40
1:A:489:ILE:O	1:A:489:ILE:HD12	2.21	0.40
1:A:711:ILE:HG13	4:A:1013:EPE:H21	2.02	0.40
1:A:735:LEU:CG	1:A:739:MET:HE2	2.52	0.40
1:A:86:ARG:HH11	1:A:102:SER:HB3	1.86	0.40
1:A:383:GLY:CA	1:A:787[B]:HIS:ND1	2.84	0.40
1:A:745:GLU:H	1:A:745:GLU:CD	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	917/927 (99%)	852 (93%)	64 (7%)	1 (0%)	48 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	PHE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	739/745 (99%)	685 (93%)	54 (7%)	13	38

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	27	LYS
1	A	29	THR
1	A	66	ILE
1	A	94	GLN
1	A	111	MET
1	A	136	LYS
1	A	143	GLU
1	A	173	ARG
1	A	189	ASP
1	A	212	GLU
1	A	217	LEU
1	A	233	ASP
1	A	250	LEU
1	A	259	ASP
1	A	292	ARG
1	A	303	ARG
1	A	332	ARG
1	A	339	ASP
1	A	399	ILE
1	A	409	GLU
1	A	416	ARG
1	A	422	ILE
1	A	477	ILE
1	A	490	MET
1	A	494	ILE

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Mol	Chain	Res	Type
1	A	517	ILE
1	A	547	VAL
1	A	552	GLU
1	A	560	LEU
1	A	563	ARG
1	A	585	LYS
1	A	612	LEU
1	A	634	LEU
1	A	636	VAL
1	A	640	ASP
1	A	657	GLU
1	A	663	ILE
1	A	710	LEU
1	A	724	VAL
1	A	736	ARG
1	A	737	LYS
1	A	747	LEU
1	A	749	LYS
1	A	771	LEU
1	A	853	VAL
1	A	859	TYR
1	A	861	LEU
1	A	875	LEU
1	A	882	LYS
1	A	898	SER
1	A	910	LYS
1	A	921	ARG
1	A	926	LEU

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

Mol	Chain	Res	Type
1	A	127	HIS
1	A	148	HIS
1	A	245	GLN
1	A	469	HIS
1	A	674	ASN
1	A	684	ASN
1	A	685	ASN
1	A	849	ASN
1	A	928	HIS

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 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\# Z > 2$
3	SO4	A	1005	-	4,4,4	0.51	0	6,6,6	0.59	0
3	SO4	A	1012	-	4,4,4	0.61	0	6,6,6	0.47	0
3	SO4	A	1007	-	4,4,4	0.72	0	6,6,6	1.30	1 (16%)
3	SO4	A	1008	-	4,4,4	0.59	0	6,6,6	0.35	0
3	SO4	A	1011	-	4,4,4	0.59	0	6,6,6	0.19	0
4	EPE	A	1013	-	15,15,15	2.35	1 (6%)	19,20,20	2.79	9 (47%)
3	SO4	A	1006	-	4,4,4	0.52	0	6,6,6	0.31	0
3	SO4	A	1004	-	4,4,4	0.68	0	6,6,6	0.74	0
3	SO4	A	1009	-	4,4,4	0.57	0	6,6,6	1.18	1 (16%)
3	SO4	A	1010	-	4,4,4	0.56	0	6,6,6	1.11	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
4	EPE	A	1013	-	-	6/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1013	EPE	C10-S	-7.93	1.66	1.77

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1013	EPE	O1S-S-C10	-6.15	97.43	106.73
4	A	1013	EPE	O2S-S-C10	6.14	116.01	106.73
4	A	1013	EPE	C2-C3-N4	-4.33	101.91	110.65
4	A	1013	EPE	C6-C5-N4	-3.59	103.41	110.65
4	A	1013	EPE	O3S-S-C10	3.29	112.45	106.00
4	A	1013	EPE	C7-N4-C5	2.63	118.25	111.24
3	A	1007	SO4	O4-S-O3	2.47	122.17	108.54
4	A	1013	EPE	C3-C2-N1	2.37	115.43	110.65
4	A	1013	EPE	C6-N1-C2	2.35	113.89	108.84
3	A	1009	SO4	O4-S-O1	-2.34	97.35	109.56
4	A	1013	EPE	C7-N4-C3	2.33	117.46	111.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1013	EPE	S-C10-C9-N1
4	A	1013	EPE	C9-C10-S-O3S
4	A	1013	EPE	C9-C10-S-O1S
4	A	1013	EPE	C10-C9-N1-C2
4	A	1013	EPE	C9-C10-S-O2S
4	A	1013	EPE	C10-C9-N1-C6

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1005	SO4	1	0
4	A	1013	EPE	10	0
3	A	1010	SO4	2	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(Å ²)	Q<0.9
1	A	919/927 (99%)	-0.27	44 (4%) 35 28	19, 44, 90, 161	2 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	897	ILE	7.5
1	A	902	LYS	6.7
1	A	498	GLY	6.6
1	A	896	ASP	6.1
1	A	899	ALA	5.9
1	A	510	ALA	5.5
1	A	500	THR	5.5
1	A	895	ILE	4.9
1	A	499	ILE	4.5
1	A	511	ALA	4.4
1	A	513	VAL	4.2
1	A	489	ILE	4.2
1	A	490	MET	4.2
1	A	488	ALA	4.0
1	A	900	CYS	4.0
1	A	933	ASP	3.9
1	A	492	LYS	3.8
1	A	497	SER	3.8
1	A	7	GLY	3.7
1	A	472	GLN	3.5
1	A	8	SER	3.4
1	A	487	PRO	3.3
1	A	910	LYS	3.2
1	A	744	ARG	3.0
1	A	593	ASN	2.9
1	A	495	PRO	2.9
1	A	516	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	745	GLU	2.9
1	A	898	SER	2.8
1	A	903	LYS	2.7
1	A	930	ASP	2.7
1	A	901	ASN	2.5
1	A	486	PRO	2.4
1	A	870	ASN	2.4
1	A	305	ARG	2.3
1	A	883	GLY	2.3
1	A	236	HIS	2.2
1	A	519	THR	2.2
1	A	251	SER	2.2
1	A	514	ARG	2.2
1	A	512	GLU	2.2
1	A	509	GLU	2.1
1	A	821	LYS	2.1
1	A	524	ARG	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($\text{\AA}^2$)	Q<0.9
3	SO4	A	1011	5/5	0.83	0.20	106,123,129,151	0
3	SO4	A	1010	5/5	0.85	0.12	84,88,90,94	0
3	SO4	A	1012	5/5	0.85	0.21	105,131,136,149	0
4	EPE	A	1013	15/15	0.85	0.25	69,89,113,116	0
3	SO4	A	1009	5/5	0.90	0.15	71,77,100,102	0
3	SO4	A	1008	5/5	0.92	0.20	101,104,114,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1005	5/5	0.93	0.17	69,75,83,106	0
3	SO4	A	1007	5/5	0.93	0.22	51,63,88,97	0
3	SO4	A	1006	5/5	0.95	0.14	95,95,101,106	0
3	SO4	A	1004	5/5	0.95	0.11	53,58,68,70	0
2	ZN	A	1002	1/1	1.00	0.01	25,25,25,25	0
2	ZN	A	1003	1/1	1.00	0.01	29,29,29,29	0
2	ZN	A	1001	1/1	1.00	0.01	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.