



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 01:58 PM BST

PDB ID : 5LEW
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 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 : 2.13.1
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) : 2.13.1

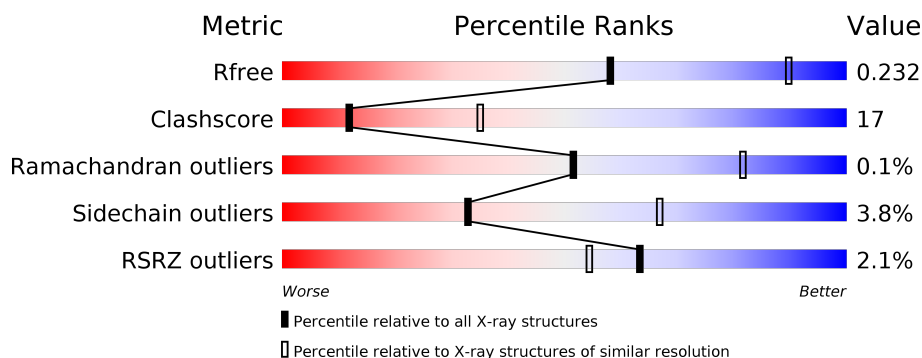
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on 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	<div> <div>2%</div> <div>69%</div> <div>27%</div> <div>• •</div> </div>

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	-
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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



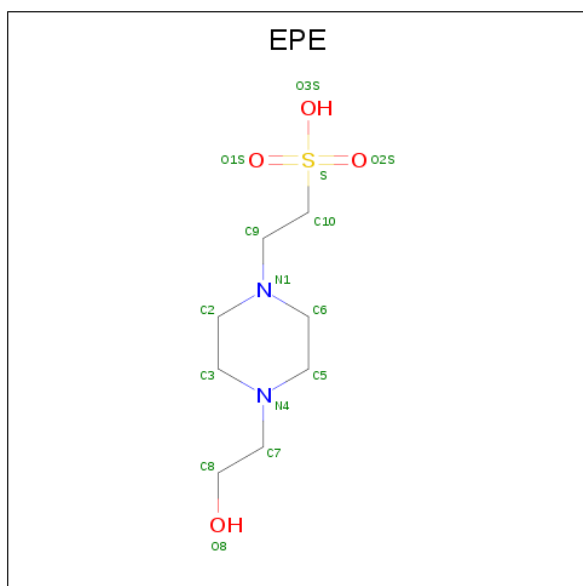
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

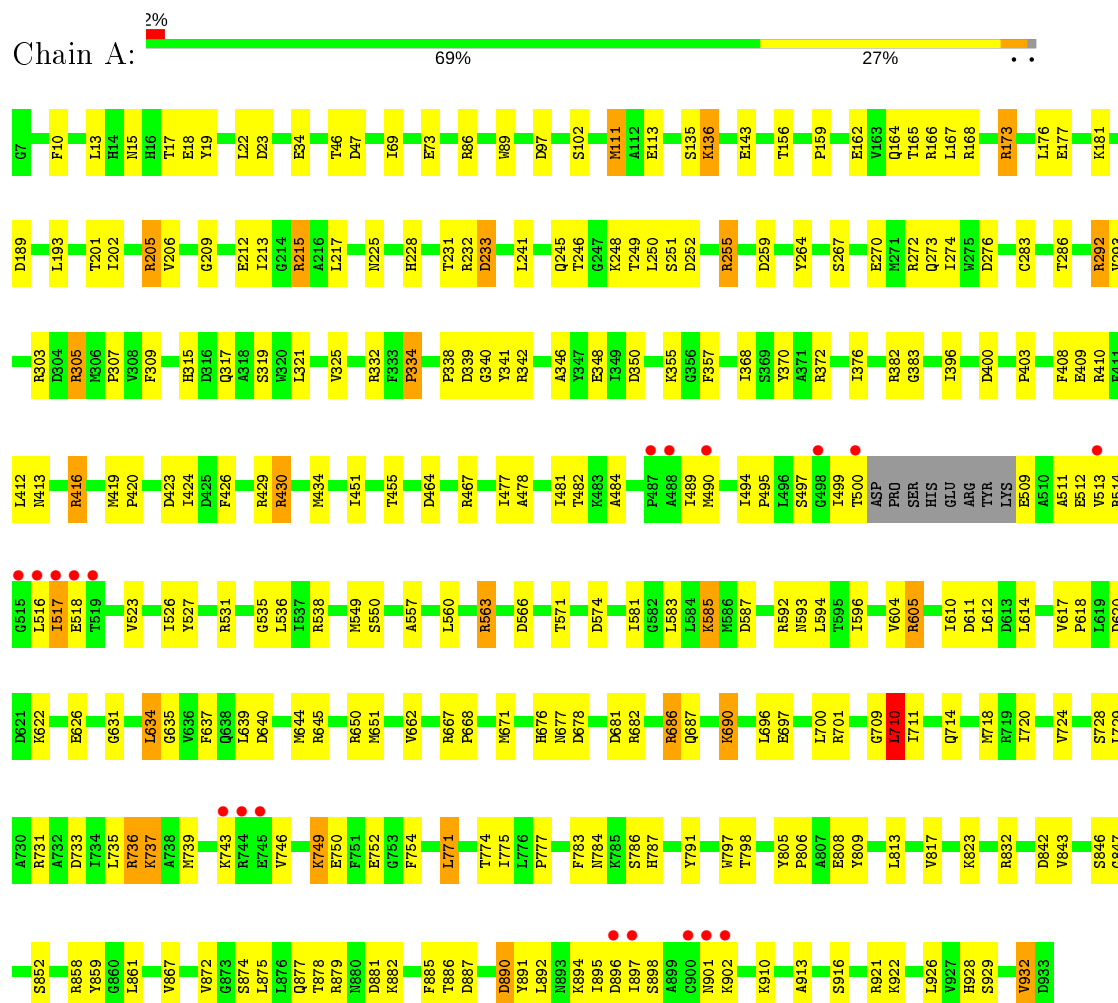
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total	O	0	0
			81	81		

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 49.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (143.11-2.80) 99.6 (49.09-2.80)	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 0.198 , 0.232	Depositor DCC
R_{free} test set	2925 reflections (5.08%)	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 , 54.0	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	0.94	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EPE, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	2/7283 (0.0%)	1.06	24/9866 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	PRO	N-CD	16.12	1.70	1.47
1	A	890	ASP	CB-CG	-5.00	1.41	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	A	215	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	173	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	A	710	LEU	CA-CB-CG	6.51	130.27	115.30
1	A	690	LYS	CD-CE-NZ	6.33	126.26	111.70
1	A	910	LYS	CB-CG-CD	6.15	127.60	111.60
1	A	292	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	690	LYS	CA-CB-CG	6.07	126.76	113.40
1	A	430	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	255	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	A	910	LYS	CG-CD-CE	5.77	129.22	111.90
1	A	467	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	832	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	205	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	423	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	786	SER	CB-CA-C	-5.51	99.62	110.10
1	A	858	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	605	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	832	ARG	NE-CZ-NH2	-5.31	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	932	VAL	CG1-CB-CG2	5.20	119.22	110.90
1	A	252	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	305	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	430	ARG	CB-CG-CD	5.01	124.64	111.60
1	A	686	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	246	0
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	247	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 17.

All (247) 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:CD	1:A:334:PRO:N	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:497:SER:O	1:A:500:THR:CG2	1.92	1.16
1:A:890:ASP:CG	1:A:894:LYS:NZ	2.01	1.13
1:A:711:ILE:H	4:A:1013:EPE:H22	0.98	1.08
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:890:ASP:CG	1:A:894:LYS:HZ2	1.58	0.99
1:A:710:LEU:HD12	4:A:1013:EPE:H101	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:497:SER:C	1:A:500:THR:HG22	1.98	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
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:305:ARG:NH1	1:A:557:ALA:HB1	2.03	0.73
1:A:13:LEU:HB3	1:A:111:MET:HE2	1.72	0.72
1:A:890:ASP:OD1	1:A:894:LYS:NZ	2.14	0.72
1:A:874:SER:O	1:A:878:THR:HG23	1.89	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: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: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:173:ARG:HH11	1:A:177:GLU:CD	1.98	0.67
1:A:13:LEU:HB3	1:A:111:MET:CE	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HG22	1:A:46:THR:O	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:348:GLU:HG2	1:A:408:PHE:CD1	2.35	0.61
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: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: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: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:592:ARG:N	3:A:1005:SO4:O4	2.37	0.57
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:563:ARG:NH1	1:A:566:ASP:OD2	2.39	0.55
1:A:89:TRP:HH2	1:A:162:GLU:HG3	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:376:ILE:CD1	1:A:434:MET:HE3	2.37	0.55
1:A:728:SER:HB3	1:A:731:ARG:H	1.71	0.55
1:A:651:MET:CE	1:A:662:VAL:HG12	2.36	0.54
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
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:481:ILE:CD1	1:A:523:VAL:HG22	2.30	0.54
1:A:383:GLY:HA2	1:A:787[B]:HIS:ND1	2.20	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:H	1:A:926:LEU:CD1	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: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:410:ARG:NH2	1:A:714:GLN:OE1	2.38	0.52
1:A:563:ARG:HH11	1:A:566:ASP:CG	2.11	0.52
1:A:455:THR:HG23	1:A:535:GLY:HA2	1.92	0.52
1:A:233:ASP:N	1:A:233:ASP:OD1	2.43	0.52
1:A:255:ARG:HG2	1:A:255:ARG:NH2	2.23	0.52
1:A:513:VAL:HG13	1:A:514:ARG:N	2.25	0.52
1:A:455:THR:CG2	1:A:535:GLY:HA2	2.40	0.52
1:A:784:ASN:ND2	1:A:787[B]:HIS:CE1	2.78	0.52
1:A:718:MET:HE2	1:A:733:ASP:HA	1.91	0.51
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:563:ARG:NH1	1:A:566:ASP:CG	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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: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:513:VAL:O	1:A:514:ARG:C	2.48	0.48
1:A:527:TYR:CE1	1:A:531:ARG:HD2	2.49	0.47
1:A:400:ASP:CG	1:A:403:PRO:HD2	2.35	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: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:370:TYR:CE2	1:A:434:MET:HE2	2.51	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:651:MET:HG2	1:A:651:MET:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:MET:HE3	1:A:420:PRO:HD2	1.99	0.45
1:A:639:LEU:CD2	1:A:644:MET:HE2	2.46	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
1:A:46:THR:CG2	1:A:73:GLU:HB2	2.47	0.45
1:A:429:ARG:C	1:A:430:ARG:HG2	2.38	0.44
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:173:ARG:NH1	1:A:177:GLU:CD	2.69	0.44
1:A:135:SER:OG	1:A:136:LYS:N	2.51	0.44
1:A:639:LEU:HD23	1:A:644:MET:HE2	1.98	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:651:MET:HE3	1:A:662:VAL:HG12	1.99	0.44
1:A:690:LYS:HB2	4:A:1013:EPE:O3S	2.18	0.44
1:A:376:ILE:HD12	1:A:434:MET:CE	2.48	0.43
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:877:GLN:NE2	1:A:881:ASP:CG	2.72	0.43
1:A:181:LYS:HE2	1:A:181:LYS:HB3	1.85	0.43
1:A:250:LEU:HA	1:A:250:LEU:HD12	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:HG2	1:A:273:GLN:O	2.19	0.42
1:A:843:VAL:HG12	1:A:885:PHE:HD2	1.83	0.42
1:A:376:ILE:HD12	1:A:434:MET:HE3	2.01	0.42
1:A:494:ILE:O	1:A:495:PRO:C	2.58	0.42
1:A:604:VAL:CG2	1:A:808:GLU:HG2	2.49	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:97:ASP:O	1:A:165:THR:HG23	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:382:ARG:CZ	1:A:791:TYR:HE1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:696:LEU:HD23	1.89	0.42
1:A:348:GLU:HG2	1:A:408:PHE:CG	2.55	0.41
4:A:1013:EPE:H61	4:A:1013:EPE:O2S	2.21	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
1:A:249:THR:HG22	1:A:251:SER:N	2.35	0.41
1:A:10:PHE:CE2	1:A:286:THR:HG21	2.56	0.41
1:A:592:ARG:O	1:A:596:ILE:HG13	2.20	0.41
1:A:69:ILE:HD12	1:A:293:VAL:HG21	2.02	0.41
1:A:585:LYS:HE3	1:A:587:ASP:OD1	2.21	0.41
1:A:775:ILE:HG21	1:A:775:ILE:HD13	1.88	0.41
1:A:514:ARG:O	1:A:518:GLU:HG3	2.21	0.41
1:A:307:PRO:HG2	1:A:549:MET:HE2	2.03	0.41
1:A:651:MET:HE1	1:A:662:VAL:HG12	2.03	0.41
1:A:509:GLU:CG	1:A:514:ARG:NH2	2.83	0.41
1:A:813:LEU:HD12	1:A:813:LEU:HA	1.83	0.41
1:A:17:THR:CG2	1:A:18:GLU:H	2.33	0.41
1:A:513:VAL:HG13	1:A:514:ARG:H	1.86	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:711:ILE:HG13	4:A:1013:EPE:H21	2.02	0.40
1:A:167:LEU:CD1	1:A:206:VAL:HG13	2.51	0.40
1:A:489:ILE:HD12	1:A:489:ILE:O	2.21	0.40
1:A:735:LEU:HG	1:A:739:MET:HE2	2.03	0.40
1:A:383:GLY:CA	1:A:787[B]:HIS:ND1	2.84	0.40
1:A:86:ARG:HH11	1:A:102:SER:HB3	1.86	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%)	51 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	739/745 (99%)	711 (96%)	28 (4%)	33 67

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	MET
1	A	136	LYS
1	A	143	GLU
1	A	189	ASP
1	A	233	ASP
1	A	259	ASP
1	A	303	ARG
1	A	332	ARG
1	A	339	ASP
1	A	416	ARG
1	A	517	ILE
1	A	560	LEU
1	A	563	ARG
1	A	585	LYS
1	A	612	LEU
1	A	634	LEU
1	A	640	ASP
1	A	710	LEU

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Mol	Chain	Res	Type
1	A	724	VAL
1	A	736	ARG
1	A	737	LYS
1	A	749	LYS
1	A	771	LEU
1	A	859	TYR
1	A	875	LEU
1	A	882	LYS
1	A	898	SER
1	A	921	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	GLN
1	A	317	GLN
1	A	469	HIS
1	A	928	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1012	-	4,4,4	0.53	0	6,6,6	0.47	0
3	SO4	A	1008	-	4,4,4	0.50	0	6,6,6	0.32	0
3	SO4	A	1005	-	4,4,4	0.41	0	6,6,6	0.57	0
3	SO4	A	1011	-	4,4,4	0.50	0	6,6,6	0.26	0
3	SO4	A	1004	-	4,4,4	0.61	0	6,6,6	0.75	0
3	SO4	A	1010	-	4,4,4	0.47	0	6,6,6	1.28	1 (16%)
4	EPE	A	1013	-	15,15,15	2.30	1 (6%)	18,20,20	3.30	9 (50%)
3	SO4	A	1007	-	4,4,4	0.67	0	6,6,6	1.49	1 (16%)
3	SO4	A	1009	-	4,4,4	0.49	0	6,6,6	1.22	1 (16%)
3	SO4	A	1006	-	4,4,4	0.43	0	6,6,6	0.40	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	-7.76	1.66	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1013	EPE	O1S-S-C10	-7.88	97.43	106.92
4	A	1013	EPE	O2S-S-C10	7.55	116.01	106.92
4	A	1013	EPE	C2-C3-N4	-4.25	101.91	110.64
4	A	1013	EPE	O3S-S-C10	4.13	112.45	105.77
4	A	1013	EPE	C6-C5-N4	-3.52	103.41	110.64
3	A	1007	SO4	O4-S-O3	3.07	122.17	109.06
4	A	1013	EPE	C7-N4-C5	2.74	118.25	111.23
4	A	1013	EPE	C7-N4-C3	2.43	117.46	111.23
4	A	1013	EPE	C3-C2-N1	2.33	115.43	110.64
3	A	1009	SO4	O4-S-O1	-2.29	97.35	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1013	EPE	C6-N1-C2	2.25	113.89	108.83
3	A	1010	SO4	O4-S-O3	-2.05	100.33	109.06

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
3	A	1010	SO4	2	0
4	A	1013	EPE	10	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%)	-0.19	19 (2%) 63 54	21, 44, 90, 161	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	902	LYS	5.7
1	A	897	ILE	4.1
1	A	900	CYS	3.9
1	A	490	MET	3.8
1	A	498	GLY	3.5
1	A	516	LEU	3.3
1	A	500	THR	3.1
1	A	901	ASN	2.7
1	A	487	PRO	2.7
1	A	743	LYS	2.6
1	A	488	ALA	2.6
1	A	513	VAL	2.5
1	A	517	ILE	2.5
1	A	896	ASP	2.4
1	A	518	GLU	2.4
1	A	515	GLY	2.4
1	A	744	ARG	2.3
1	A	745	GLU	2.2
1	A	519	THR	2.1

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

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

6.3 Carbohydrates [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(\AA^2)	Q<0.9
3	SO4	A	1011	5/5	0.81	0.28	106,123,129,151	0
3	SO4	A	1012	5/5	0.83	0.31	105,131,136,149	0
4	EPE	A	1013	15/15	0.86	0.35	69,89,113,116	0
3	SO4	A	1007	5/5	0.86	0.26	51,63,88,97	0
3	SO4	A	1009	5/5	0.92	0.24	71,77,100,102	0
3	SO4	A	1010	5/5	0.94	0.16	84,88,90,94	0
3	SO4	A	1005	5/5	0.94	0.16	69,75,83,106	0
3	SO4	A	1006	5/5	0.94	0.13	95,95,101,106	0
3	SO4	A	1008	5/5	0.95	0.23	101,104,114,118	0
3	SO4	A	1004	5/5	0.96	0.22	53,58,68,70	0
2	ZN	A	1001	1/1	1.00	0.16	28,28,28,28	0
2	ZN	A	1003	1/1	1.00	0.17	29,29,29,29	0
2	ZN	A	1002	1/1	1.00	0.16	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.