



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:55 PM UTC

PDB ID : 2DWZ / pdb_00002dwz
Title : Structure of the Oncoprotein Gankyrin in Complex with S6 ATPase of the 26S Proteasome
Authors : Padmanabhan, B.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-08-22
Resolution : 2.40 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

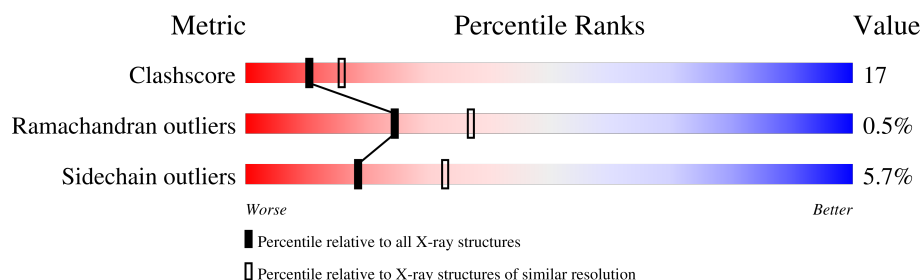
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	231	
1	C	231	
2	B	83	
2	D	83	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4864 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 26S proteasome non-ATPase regulatory subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1719	1072	306	332	9			
1	C	226	Total	C	N	O	S	0	0	0
			1719	1072	306	332	9			

- Molecule 2 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	0	0	0
			589	368	103	114	4			
2	D	73	Total	C	N	O	S	0	0	0
			589	368	103	114	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	336	MET	-	initiating methionine	UNP Q63570
D	336	MET	-	initiating methionine	UNP Q63570

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	38	Total	O	0	0
			38	38		
4	C	78	Total	O	0	0
			78	78		
4	D	14	Total	O	0	0
			14	14		

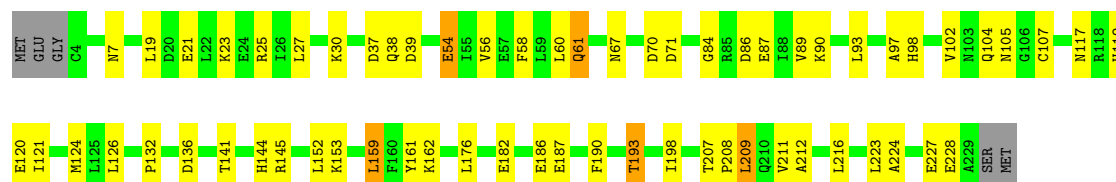
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

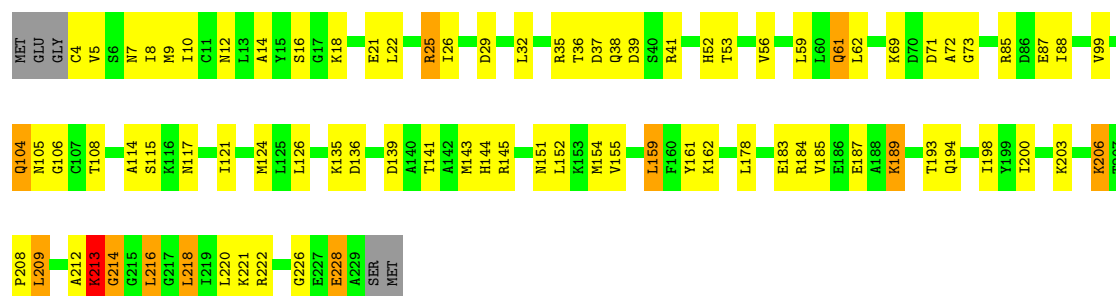
• Molecule 1: 26S proteasome non-ATPase regulatory subunit 10

Chain A: 



• Molecule 1: 26S proteasome non-ATPase regulatory subunit 10

Chain C: 



• Molecule 2: 26S protease regulatory subunit 6B

Chain B: 



• Molecule 2: 26S protease regulatory subunit 6B

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.99Å 92.32Å 167.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	88.2 (20.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4864	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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: 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	0.39	0/1746	0.87	0/2362
1	C	0.38	0/1746	0.90	4/2362 (0.2%)
2	B	0.43	0/594	0.95	2/794 (0.3%)
2	D	0.38	0/594	0.80	0/794
All	All	0.39	0/4680	0.89	6/6312 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	THR	N-CA-C	-7.34	101.50	110.31
2	B	366	ARG	CA-C-N	7.29	126.93	119.56
2	B	366	ARG	C-N-CA	7.29	126.93	119.56
1	C	185	VAL	N-CA-C	6.68	117.18	110.23
1	C	104	GLN	N-CA-C	5.24	118.77	112.38
1	C	53	THR	N-CA-C	5.03	116.76	111.28

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	A	1719	0	1716	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1719	0	1716	67	0
2	B	589	0	605	18	0
2	D	589	0	605	24	0
3	A	15	0	18	0	0
4	A	103	0	0	5	0
4	B	38	0	0	0	0
4	C	78	0	0	5	0
4	D	14	0	0	0	0
All	All	4864	0	4660	157	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 (157) 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:C:8:ILE:HG22	1:C:10:ILE:HG22	1.59	0.83
1:C:25:ARG:HH11	1:C:25:ARG:HB2	1.44	0.82
2:D:341:LYS:HE3	2:D:370:ILE:HD11	1.63	0.80
2:D:370:ILE:HD13	2:D:370:ILE:H	1.46	0.80
2:B:369:LYS:HD3	2:B:369:LYS:H	1.48	0.79
1:C:141:THR:H	1:C:144:HIS:CD2	2.04	0.76
1:A:67:ASN:HD21	1:A:98:HIS:H	1.36	0.72
1:C:7:ASN:OD1	1:C:38:GLN:HG2	1.88	0.72
1:A:152:LEU:HD23	1:A:187:GLU:HG2	1.71	0.71
2:B:369:LYS:HD3	2:B:369:LYS:N	2.05	0.71
1:C:121:ILE:HA	1:C:124:MET:HE3	1.73	0.71
2:B:369:LYS:H	2:B:369:LYS:CD	2.05	0.70
1:A:162:LYS:HD2	1:A:162:LYS:N	2.07	0.69
1:A:104:GLN:OE1	2:B:400:GLU:HG3	1.91	0.69
1:A:152:LEU:HD23	1:A:187:GLU:HA	1.73	0.69
1:C:141:THR:H	1:C:144:HIS:HD2	1.41	0.66
1:C:115:SER:HB2	1:C:145:ARG:HD3	1.79	0.65
1:A:224:ALA:O	1:A:228:GLU:HG3	1.95	0.65
1:C:143:MET:HE1	1:C:155:VAL:HA	1.78	0.64
1:C:8:ILE:CG2	1:C:10:ILE:HG22	2.30	0.62
1:C:143:MET:HE1	1:C:155:VAL:HG22	1.82	0.62
1:C:25:ARG:O	1:C:32:LEU:HD12	2.00	0.61
1:C:25:ARG:HH11	1:C:25:ARG:CB	2.14	0.61
2:D:370:ILE:H	2:D:370:ILE:CD1	2.13	0.61
1:A:67:ASN:ND2	1:A:98:HIS:H	1.99	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:LEU:HD23	1:C:194:GLN:HG2	1.85	0.58
2:B:407:ILE:HD12	2:B:407:ILE:N	2.18	0.58
2:D:353:ASN:ND2	2:D:393:ILE:HD13	2.18	0.58
1:A:19:LEU:HD22	1:A:54:GLU:HG2	1.85	0.57
1:A:145:ARG:HH11	1:A:145:ARG:HG3	1.68	0.57
1:C:218:LEU:HD13	1:C:222:ARG:HH12	1.69	0.57
1:C:159:LEU:CD2	1:C:194:GLN:HG2	2.34	0.56
1:C:203:LYS:HE2	4:C:309:HOH:O	2.06	0.56
1:A:223:LEU:O	1:A:227:GLU:HG2	2.06	0.56
2:D:370:ILE:HD13	2:D:370:ILE:N	2.17	0.55
1:A:190:PHE:O	1:A:193:THR:HB	2.07	0.55
1:A:38:GLN:OE1	2:B:389:GLU:HG2	2.06	0.54
4:A:2321:HOH:O	1:C:189:LYS:HE2	2.05	0.54
1:C:143:MET:CE	1:C:155:VAL:HG22	2.37	0.54
2:D:389:GLU:CD	2:D:391:ARG:HH21	2.15	0.54
1:C:145:ARG:HH11	1:C:145:ARG:HG3	1.73	0.54
2:B:385:LEU:HD13	2:B:401:LYS:HD2	1.89	0.54
1:C:105:ASN:O	1:C:136:ASP:HB2	2.08	0.54
2:D:354:LEU:HD12	2:D:354:LEU:N	2.23	0.54
1:C:87:GLU:CD	1:C:87:GLU:H	2.16	0.54
1:A:21:GLU:OE2	1:A:25:ARG:NH1	2.41	0.53
1:C:14:ALA:O	1:C:52:HIS:HD2	1.91	0.53
2:B:384:MET:HA	2:B:384:MET:HE2	1.90	0.53
1:C:85:ARG:NH2	2:D:356:GLU:HG3	2.24	0.52
1:A:105:ASN:HB2	4:A:2268:HOH:O	2.09	0.52
1:C:39:ASP:HA	1:C:71:ASP:OD2	2.10	0.52
2:D:407:ILE:O	2:D:408:LYS:HB2	2.10	0.52
1:C:206:LYS:HE3	1:C:206:LYS:HA	1.92	0.51
1:C:214:GLY:C	1:C:216:LEU:H	2.18	0.51
1:A:27:LEU:HA	1:A:30:LYS:HE3	1.91	0.51
1:C:35:ARG:NE	4:C:264:HOH:O	2.43	0.51
1:C:56:VAL:HG11	1:C:88:ILE:HG23	1.91	0.51
2:D:403:TYR:O	2:D:407:ILE:HG12	2.11	0.51
2:B:366:ARG:NH2	2:B:400:GLU:OE2	2.43	0.50
1:A:119:HIS:H	1:A:119:HIS:HD1	1.58	0.50
1:C:143:MET:HE3	1:C:143:MET:HA	1.93	0.50
1:A:87:GLU:HB2	4:A:2252:HOH:O	2.10	0.50
1:A:161:TYR:C	1:A:162:LYS:HD2	2.37	0.50
1:C:99:VAL:HG22	4:C:251:HOH:O	2.11	0.50
1:C:29:ASP:HB3	1:C:32:LEU:HD12	1.94	0.49
1:C:69:LYS:HB3	1:C:73:GLY:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:HH21	2:B:362:ASP:HA	1.77	0.49
1:A:198:ILE:HB	1:A:209:LEU:HD13	1.94	0.49
1:C:212:ALA:HB1	1:C:216:LEU:HB3	1.94	0.49
1:A:102:VAL:HA	1:A:107:CYS:O	2.12	0.49
1:C:184:ARG:HB3	1:C:187:GLU:OE1	2.12	0.49
2:D:374:ASP:O	2:D:378:ILE:HG13	2.13	0.49
1:A:186:GLU:HG2	4:A:2283:HOH:O	2.13	0.49
1:C:226:GLY:C	1:C:228:GLU:H	2.20	0.49
1:C:72:ALA:O	1:C:104:GLN:HG2	2.13	0.48
1:A:89:VAL:O	1:A:93:LEU:HG	2.12	0.48
2:D:370:ILE:HG21	2:D:407:ILE:CD1	2.43	0.48
2:B:407:ILE:HG22	2:B:407:ILE:O	2.12	0.48
1:C:218:LEU:CD1	1:C:222:ARG:HH12	2.26	0.48
1:A:56:VAL:O	1:A:60:LEU:HG	2.14	0.48
1:A:152:LEU:CD2	1:A:187:GLU:HA	2.42	0.48
1:C:9:MET:HG3	4:C:279:HOH:O	2.14	0.48
2:D:388:ARG:HH11	2:D:388:ARG:HG2	1.79	0.48
1:A:141:THR:OG1	1:A:144:HIS:HD2	1.96	0.47
1:C:213:LYS:HA	1:C:213:LYS:NZ	2.29	0.47
2:B:391:ARG:HG2	2:B:393:ILE:O	2.13	0.47
1:A:98:HIS:HA	4:A:2339:HOH:O	2.14	0.47
1:A:39:ASP:HA	1:A:71:ASP:OD2	2.15	0.46
2:D:370:ILE:CG2	2:D:407:ILE:HD12	2.45	0.46
1:A:27:LEU:HA	1:A:30:LYS:CE	2.46	0.46
1:A:39:ASP:O	1:A:70:ASP:HB2	2.15	0.46
1:A:120:GLU:H	1:A:120:GLU:CD	2.22	0.46
1:C:216:LEU:HD22	1:C:220:LEU:HG	1.96	0.46
2:D:348:ILE:HD13	2:D:376:ASN:HA	1.98	0.46
1:C:114:ALA:HA	1:C:154:MET:HE3	1.98	0.46
1:C:16:SER:CB	1:C:18:LYS:HE2	2.46	0.46
1:C:228:GLU:HB2	4:C:274:HOH:O	2.16	0.45
2:D:355:SER:OG	2:D:358:VAL:HG23	2.15	0.45
1:A:207:THR:O	1:A:211:VAL:HG23	2.17	0.45
1:A:227:GLU:OE2	1:C:189:LYS:NZ	2.49	0.45
2:D:370:ILE:HG21	2:D:407:ILE:HD12	1.99	0.45
2:D:341:LYS:HE2	2:D:364:VAL:HA	1.99	0.45
1:C:4:CYS:HB2	1:C:12:ASN:OD1	2.16	0.45
1:C:143:MET:HE1	1:C:155:VAL:HG13	1.98	0.45
1:A:126:LEU:HD13	1:A:161:TYR:CD2	2.52	0.45
1:C:21:GLU:HG2	1:C:25:ARG:HH22	1.82	0.45
1:C:200:ILE:O	1:C:208:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LEU:HD13	1:C:222:ARG:NH1	2.30	0.45
1:A:141:THR:H	1:A:144:HIS:CD2	2.35	0.45
1:C:106:GLY:O	1:C:136:ASP:HA	2.17	0.45
1:A:67:ASN:HD21	1:A:98:HIS:N	2.11	0.44
1:A:212:ALA:HB1	1:A:216:LEU:HB3	1.99	0.44
1:A:67:ASN:HD21	1:A:97:ALA:HA	1.83	0.44
1:C:25:ARG:HB2	1:C:25:ARG:NH1	2.22	0.44
1:A:104:GLN:CD	2:B:400:GLU:HG3	2.42	0.44
2:D:341:LYS:CE	2:D:370:ILE:HD11	2.41	0.44
1:A:152:LEU:CD2	1:A:187:GLU:HG2	2.45	0.43
1:A:176:LEU:HG	1:A:208:PRO:HB3	2.00	0.43
1:A:152:LEU:C	1:A:152:LEU:HD13	2.43	0.43
1:A:21:GLU:HG2	1:A:25:ARG:HH11	1.83	0.43
1:C:5:VAL:O	2:D:391:ARG:HD3	2.19	0.43
1:C:21:GLU:HG2	1:C:25:ARG:HH12	1.84	0.43
1:C:135:LYS:HB3	1:C:139:ASP:HA	2.00	0.43
1:A:182:GLU:HA	2:B:339:ARG:HD2	2.00	0.43
2:B:407:ILE:N	2:B:407:ILE:CD1	2.81	0.43
1:C:218:LEU:O	1:C:218:LEU:HD22	2.19	0.43
2:D:401:LYS:O	2:D:401:LYS:HD3	2.19	0.43
1:A:58:PHE:O	1:A:61:GLN:HG3	2.19	0.42
1:C:16:SER:HB3	1:C:18:LYS:HE2	2.00	0.42
1:C:56:VAL:HG21	1:C:88:ILE:HD13	2.01	0.42
2:D:402:ALA:O	2:D:406:VAL:HG23	2.18	0.42
2:D:345:PHE:HB3	2:D:360:LEU:HD13	2.01	0.42
1:A:7:ASN:OD1	1:A:37:ASP:HB2	2.19	0.42
1:C:198:ILE:HB	1:C:209:LEU:HD13	2.01	0.42
1:A:159:LEU:HD12	1:A:159:LEU:HA	1.90	0.42
1:A:117:ASN:ND2	1:A:119:HIS:HE1	2.17	0.42
1:C:32:LEU:HD23	1:C:35:ARG:HD2	2.01	0.42
1:A:132:PRO:HG3	1:A:161:TYR:O	2.20	0.42
2:B:384:MET:HA	2:B:384:MET:CE	2.49	0.42
1:C:36:THR:HA	1:C:41:ARG:O	2.19	0.42
1:A:21:GLU:HG2	1:A:25:ARG:NH1	2.35	0.42
1:A:54:GLU:OE1	1:A:54:GLU:HA	2.20	0.42
1:C:126:LEU:HD13	1:C:161:TYR:CD2	2.55	0.42
1:A:86:ASP:HB3	1:A:124:MET:HE1	2.02	0.42
1:C:61:GLN:OE1	1:C:61:GLN:C	2.63	0.42
1:A:86:ASP:OD1	1:A:121:ILE:HG13	2.20	0.41
1:C:59:LEU:O	1:C:62:LEU:HB3	2.20	0.41
1:A:84:GLY:HA2	1:A:121:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASP:OD1	1:A:136:ASP:C	2.62	0.41
2:B:368:ASP:HB2	2:B:403:TYR:OH	2.20	0.41
1:C:117:ASN:ND2	1:C:151:ASN:OD1	2.53	0.41
1:C:7:ASN:OD1	1:C:37:ASP:HB2	2.20	0.41
1:C:22:LEU:CD2	1:C:26:ILE:HD12	2.51	0.41
2:D:384:MET:O	2:D:387:VAL:HB	2.21	0.41
2:B:384:MET:HE2	2:B:384:MET:CA	2.51	0.41
1:C:183:GLU:HB2	1:C:213:LYS:HG3	2.03	0.41
1:A:23:LYS:O	1:A:27:LEU:HG	2.21	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	224/231 (97%)	214 (96%)	10 (4%)	0	100	100
1	C	224/231 (97%)	210 (94%)	12 (5%)	2 (1%)	14	22
2	B	71/83 (86%)	69 (97%)	2 (3%)	0	100	100
2	D	71/83 (86%)	66 (93%)	4 (6%)	1 (1%)	9	13
All	All	590/628 (94%)	559 (95%)	28 (5%)	3 (0%)	24	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	213	LYS
1	C	214	GLY
2	D	338	ARG

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	180/184 (98%)	173 (96%)	7 (4%)	28	48
1	C	180/184 (98%)	165 (92%)	15 (8%)	10	17
2	B	66/76 (87%)	62 (94%)	4 (6%)	17	30
2	D	66/76 (87%)	64 (97%)	2 (3%)	36	58
All	All	492/520 (95%)	464 (94%)	28 (6%)	18	33

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

Mol	Chain	Res	Type
1	A	54	GLU
1	A	61	GLN
1	A	90	LYS
1	A	153	LYS
1	A	159	LEU
1	A	193	THR
1	A	209	LEU
2	B	340	GLN
2	B	369	LYS
2	B	384	MET
2	B	408	LYS
1	C	25	ARG
1	C	61	GLN
1	C	152	LEU
1	C	159	LEU
1	C	162	LYS
1	C	178	LEU
1	C	189	LYS
1	C	193	THR
1	C	206	LYS
1	C	209	LEU
1	C	213	LYS
1	C	216	LEU
1	C	218	LEU

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Mol	Chain	Res	Type
1	C	221	LYS
1	C	228	GLU
2	D	370	ILE
2	D	401	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	67	ASN
1	A	98	HIS
1	A	105	ASN
1	A	119	HIS
1	A	144	HIS
1	A	194	GLN
2	B	340	GLN
2	B	376	ASN
1	C	38	GLN
1	C	52	HIS
1	C	104	GLN
1	C	117	ASN
1	C	137	HIS
1	C	144	HIS
2	D	353	ASN
2	D	380	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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	EPE	A	2241	-	15,15,15	1.27	1 (6%)	19,20,20	1.29	2 (10%)

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
3	EPE	A	2241	-	-	1/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2241	EPE	C10-S	3.43	1.82	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2241	EPE	O1S-S-C10	3.56	112.11	106.73
3	A	2241	EPE	O3S-S-O1S	-2.30	105.65	111.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2241	EPE	N4-C7-C8-O8

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.