



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:13 AM UTC

PDB ID : 1NJG / pdb_00001njg
Title : Nucleotide-free form of an Isolated E. coli Clamp Loader Gamma Subunit
Authors : Podobnik, M.; Weitze, T.F.; O'Donnell, M.; Kuriyan, J.
Deposited on : 2002-12-30
Resolution : 2.20 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

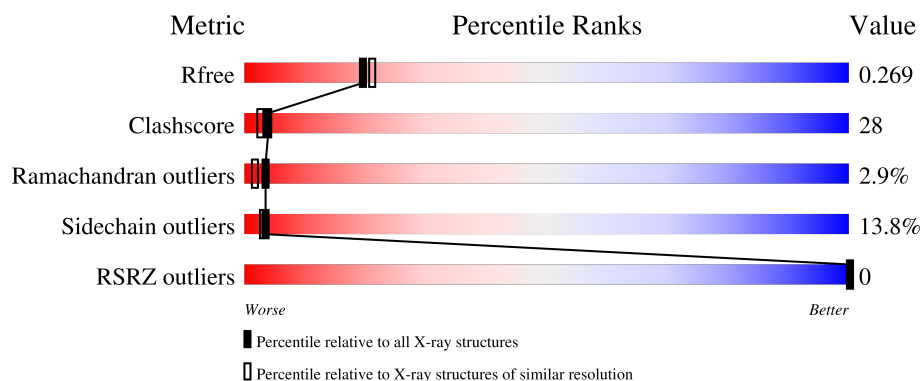
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	250	
1	B	250	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3862 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 gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1862	1164	342	349	7			
1	B	239	Total	C	N	O	S	0	0	0
			1853	1159	340	347	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	cloning artifact	UNP P06710
A	-5	ALA	-	cloning artifact	UNP P06710
A	-4	HIS	-	cloning artifact	UNP P06710
A	-3	MET	-	cloning artifact	UNP P06710
A	-2	GLY	-	cloning artifact	UNP P06710
A	-1	GLY	-	cloning artifact	UNP P06710
A	0	SER	-	cloning artifact	UNP P06710
B	-6	GLY	-	cloning artifact	UNP P06710
B	-5	ALA	-	cloning artifact	UNP P06710
B	-4	HIS	-	cloning artifact	UNP P06710
B	-3	MET	-	cloning artifact	UNP P06710
B	-2	GLY	-	cloning artifact	UNP P06710
B	-1	GLY	-	cloning artifact	UNP P06710
B	0	SER	-	cloning artifact	UNP P06710

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- 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		
3	B	1	Total	O	S	0	0
			5	4	1		

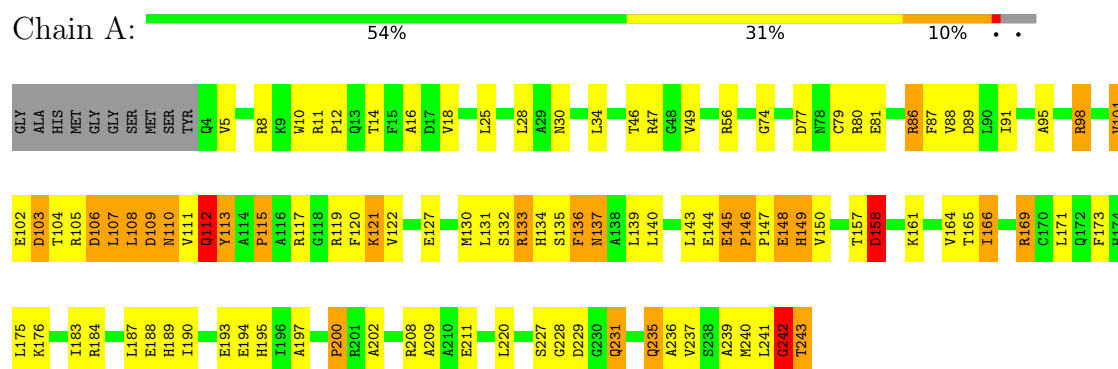
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	64	Total	O	0	0
			64	64		

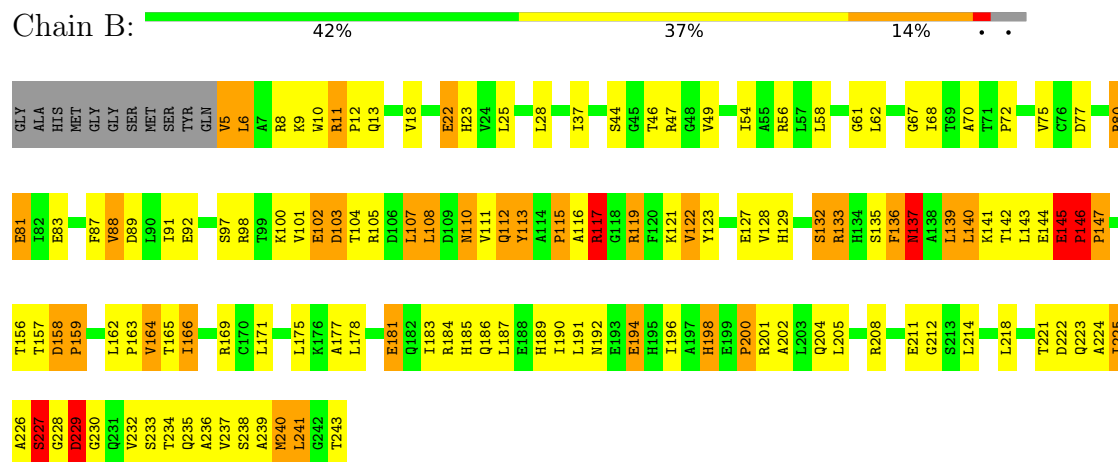
3 Residue-property plots

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 gamma



• Molecule 1: DNA polymerase III subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.34Å 85.47Å 56.93Å 90.00° 93.15° 90.00°	Depositor
Resolution (Å)	56.85 – 2.20 56.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.5 (56.85-2.20) 88.5 (56.85-2.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.73 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.268 0.238 , 0.269	Depositor DCC
R_{free} test set	2108 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3862	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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, 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	0.50	0/1892	1.10	18/2562 (0.7%)
1	B	0.52	0/1883	1.14	19/2550 (0.7%)
All	All	0.51	0/3775	1.12	37/5112 (0.7%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	PRO	N-CA-C	12.25	125.65	110.70
1	A	112	GLN	OE1-CD-NE2	-9.83	112.77	122.60
1	B	194	GLU	N-CA-C	-8.74	102.62	113.28
1	B	113	TYR	N-CA-C	8.49	123.06	112.87
1	B	145	GLU	CA-C-N	8.25	128.88	120.38
1	B	145	GLU	C-N-CA	8.25	128.88	120.38
1	A	145	GLU	CA-C-N	8.13	128.76	120.38
1	A	145	GLU	C-N-CA	8.13	128.76	120.38
1	A	241	LEU	N-CA-C	-7.90	103.53	113.01
1	A	146	PRO	N-CA-C	7.86	120.29	110.70
1	B	198	HIS	N-CA-C	7.23	119.55	108.42
1	A	109	ASP	N-CA-C	-7.21	101.66	112.04
1	A	242	GLY	N-CA-C	7.06	129.90	113.18
1	B	158	ASP	CA-C-N	6.76	127.02	119.32
1	B	158	ASP	C-N-CA	6.76	127.02	119.32
1	B	133	ARG	N-CA-C	-6.74	103.96	111.71
1	A	112	GLN	CG-CD-NE2	6.66	126.40	116.40
1	B	229	ASP	N-CA-C	6.34	119.41	109.96
1	A	171	LEU	N-CA-C	-6.32	99.58	109.25
1	A	158	ASP	CA-C-N	6.21	126.39	119.32
1	A	158	ASP	C-N-CA	6.21	126.39	119.32
1	B	121	LYS	N-CA-C	-6.20	99.90	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	LEU	N-CA-C	-5.90	100.23	109.25
1	A	157	THR	N-CA-C	-5.86	105.78	113.17
1	A	121	LYS	N-CA-C	-5.68	99.98	109.24
1	A	122	VAL	N-CA-C	5.67	116.05	108.11
1	B	122	VAL	N-CA-C	5.63	116.10	107.77
1	A	208	ARG	N-CA-C	-5.58	105.19	111.28
1	B	8	ARG	N-CA-C	-5.44	107.29	114.04
1	B	228	GLY	N-CA-C	-5.36	100.85	111.31
1	B	164	VAL	N-CA-C	-5.24	105.28	110.62
1	A	148	GLU	N-CA-C	5.16	116.91	111.28
1	B	211	GLU	N-CA-C	5.16	118.45	111.17
1	A	166	ILE	N-CA-C	-5.14	107.39	111.81
1	A	115	PRO	CB-CA-C	5.03	119.86	111.56
1	B	137	ASN	N-CA-C	-5.01	107.17	113.28
1	B	225	ILE	N-CA-C	-5.00	104.84	111.09

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	1862	0	1878	94	0
1	B	1853	0	1870	121	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0
4	A	66	0	0	2	0
4	B	64	0	0	2	0
All	All	3862	0	3748	211	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 28.

All (211) 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:11:ARG:HH22	1:A:56:ARG:NH1	1.40	1.18
1:A:103:ASP:OD2	1:A:107:LEU:HD11	1.53	1.09
1:B:140:LEU:HD12	1:B:165:THR:HG21	1.43	0.99
1:A:11:ARG:HH22	1:A:56:ARG:HH11	1.16	0.91
1:B:156:THR:HG22	1:B:158:ASP:H	1.34	0.91
1:B:116:ALA:O	1:B:117:ARG:HG2	1.70	0.90
1:A:103:ASP:O	1:A:107:LEU:HG	1.73	0.88
1:A:11:ARG:NH2	1:A:56:ARG:NH1	2.22	0.87
1:B:9:LYS:HE2	1:B:194:GLU:OE2	1.76	0.85
1:B:110:ASN:HD21	1:B:112:GLN:HG2	1.42	0.84
1:B:221:THR:O	1:B:225:ILE:HG12	1.78	0.84
1:A:112:GLN:OE1	1:A:121:LYS:NZ	2.10	0.83
1:B:140:LEU:C	1:B:140:LEU:HD23	2.04	0.83
1:A:98:ARG:HA	1:A:101:VAL:CG1	2.09	0.83
1:A:104:THR:HA	1:A:107:LEU:HD12	1.60	0.82
1:A:131:LEU:HB3	1:A:135:SER:OG	1.79	0.82
1:B:144:GLU:C	1:B:146:PRO:HD3	2.06	0.81
1:A:91:ILE:HD11	1:A:121:LYS:HE3	1.60	0.81
1:A:136:PHE:HE2	1:A:166:ILE:HD12	1.46	0.81
1:B:129:HIS:ND1	1:B:156:THR:HG23	1.96	0.80
1:B:140:LEU:CD1	1:B:165:THR:HG21	2.12	0.80
1:B:28:LEU:HD22	1:B:58:LEU:HD13	1.65	0.78
1:A:137:ASN:HD22	1:A:137:ASN:H	1.33	0.75
1:B:177:ALA:HB1	1:B:212:GLY:HA3	1.67	0.75
1:B:237:VAL:O	1:B:241:LEU:HB2	1.87	0.75
1:A:197:ALA:HB3	1:A:231:GLN:HB3	1.70	0.74
1:B:137:ASN:O	1:B:141:LYS:HB2	1.87	0.73
1:A:47:ARG:HD2	3:A:601:SO4:O2	1.87	0.73
1:B:140:LEU:HD12	1:B:165:THR:CG2	2.16	0.72
1:B:110:ASN:CG	1:B:110:ASN:O	2.33	0.72
1:B:54:ILE:HD12	1:B:175:LEU:HD21	1.69	0.71
1:B:165:THR:O	1:B:169:ARG:HG2	1.89	0.71
1:A:137:ASN:HD22	1:A:137:ASN:N	1.86	0.71
1:A:158:ASP:OD2	1:A:161:LYS:HG3	1.91	0.70
1:B:75:VAL:O	1:B:80:ARG:NH1	2.24	0.70
1:A:11:ARG:NH2	1:A:56:ARG:HH11	1.87	0.70
1:A:30:ASN:O	1:A:34:LEU:HD13	1.91	0.69
1:A:111:VAL:O	1:A:113:TYR:N	2.25	0.69
1:B:67:GLY:HA2	1:B:119:ARG:HH12	1.58	0.68
1:A:133:ARG:O	1:A:137:ASN:ND2	2.27	0.68
1:A:136:PHE:CE2	1:A:166:ILE:HD12	2.26	0.68
1:A:209:ALA:O	1:A:211:GLU:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HD22	1:B:143:LEU:HD11	1.76	0.68
1:B:225:ILE:HG23	1:B:230:GLY:HA2	1.74	0.68
1:A:77:ASP:O	1:A:81:GLU:HG3	1.93	0.67
1:A:149:HIS:N	1:A:149:HIS:CD2	2.62	0.66
1:A:86:ARG:CG	1:A:86:ARG:O	2.43	0.65
1:B:201:ARG:O	1:B:205:LEU:HG	1.96	0.65
1:A:91:ILE:HD11	1:A:121:LYS:CE	2.25	0.65
1:A:109:ASP:O	1:A:111:VAL:N	2.24	0.65
1:A:169:ARG:CG	1:A:169:ARG:HH11	2.10	0.65
1:B:128:VAL:HG13	1:B:162:LEU:HD21	1.78	0.64
1:A:86:ARG:O	1:A:86:ARG:HG2	1.97	0.63
1:B:12:PRO:HG3	4:B:528:HOH:O	1.97	0.63
1:B:97:SER:OG	1:B:100:LYS:HG3	1.99	0.63
1:A:164:VAL:HG12	4:A:630:HOH:O	1.99	0.62
1:B:37:ILE:HD11	1:B:68:ILE:HG21	1.81	0.62
1:A:132:SER:O	1:A:134:HIS:N	2.33	0.62
1:B:18:VAL:HB	1:B:25:LEU:HD11	1.82	0.62
1:B:46:THR:O	1:B:49:VAL:HG22	2.01	0.61
1:B:6:LEU:HB2	1:B:222:ASP:OD2	2.01	0.61
1:B:103:ASP:O	1:B:107:LEU:HD23	2.01	0.60
1:A:98:ARG:O	1:A:101:VAL:HG13	2.01	0.60
1:A:98:ARG:HA	1:A:101:VAL:HG12	1.82	0.59
1:A:102:GLU:HA	1:A:105:ARG:HE	1.68	0.59
1:B:13:GLN:HE22	1:B:83:GLU:CD	2.11	0.59
1:B:178:LEU:O	1:B:212:GLY:HA2	2.03	0.58
1:A:133:ARG:HH21	1:B:240:MET:HE3	1.69	0.58
1:B:111:VAL:O	1:B:113:TYR:CD1	2.57	0.58
1:B:61:GLY:HA2	1:B:72:PRO:HG3	1.85	0.57
1:A:137:ASN:N	1:A:137:ASN:ND2	2.53	0.57
1:A:115:PRO:HG3	1:A:121:LYS:N	2.20	0.56
1:A:132:SER:C	1:A:134:HIS:N	2.62	0.56
1:A:119:ARG:HG3	1:A:120:PHE:CD2	2.40	0.56
1:B:140:LEU:C	1:B:140:LEU:CD2	2.76	0.56
1:B:186:GLN:O	1:B:190:ILE:HG13	2.06	0.55
1:B:240:MET:HE2	1:B:241:LEU:HD23	1.87	0.55
1:A:242:GLY:O	1:A:243:THR:OXT	2.24	0.55
1:A:132:SER:C	1:A:134:HIS:H	2.15	0.55
1:B:111:VAL:O	1:B:113:TYR:N	2.39	0.55
1:A:136:PHE:O	1:A:140:LEU:N	2.31	0.55
1:B:202:ALA:HB1	1:B:232:VAL:HG12	1.89	0.55
1:A:46:THR:O	1:A:49:VAL:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:HD3	1:A:121:LYS:HB2	1.89	0.54
1:A:202:ALA:HB1	1:A:237:VAL:HG21	1.89	0.54
1:A:169:ARG:CG	1:A:169:ARG:NH1	2.70	0.54
1:B:202:ALA:HA	1:B:205:LEU:HD12	1.90	0.54
1:A:165:THR:O	1:A:169:ARG:NH1	2.41	0.54
1:B:144:GLU:C	1:B:146:PRO:CD	2.79	0.54
1:A:106:ASP:OD1	1:A:110:ASN:ND2	2.41	0.54
1:B:139:LEU:O	1:B:143:LEU:HG	2.09	0.53
1:B:145:GLU:O	1:B:147:PRO:HD3	2.09	0.53
1:B:229:ASP:O	1:B:229:ASP:OD2	2.27	0.53
1:A:147:PRO:HB2	1:A:150:VAL:HB	1.90	0.53
1:B:11:ARG:NH1	1:B:11:ARG:HG2	2.24	0.53
1:B:191:LEU:CD2	1:B:196:ILE:HD12	2.39	0.52
1:B:233:SER:OG	1:B:236:ALA:HB2	2.09	0.52
1:A:184:ARG:NH2	1:A:188:GLU:OE1	2.42	0.52
1:A:109:ASP:C	1:A:111:VAL:H	2.14	0.52
1:B:87:PHE:O	1:B:88:VAL:C	2.52	0.52
1:A:115:PRO:HG3	1:A:121:LYS:HB2	1.91	0.52
1:B:101:VAL:HG12	1:B:101:VAL:O	2.09	0.52
1:A:112:GLN:OE1	1:A:121:LYS:CE	2.59	0.51
1:B:139:LEU:HD22	1:B:143:LEU:CD1	2.40	0.51
1:B:165:THR:CG2	1:B:166:ILE:N	2.73	0.50
1:B:202:ALA:O	1:B:205:LEU:HB2	2.11	0.50
1:B:6:LEU:HD21	1:B:194:GLU:HG3	1.93	0.50
1:A:144:GLU:HG2	1:A:169:ARG:HH21	1.75	0.50
1:A:165:THR:O	1:A:169:ARG:HG3	2.10	0.50
1:A:127:GLU:OE1	1:A:127:GLU:HA	2.10	0.50
1:B:205:LEU:HB2	1:B:237:VAL:HG11	1.94	0.50
1:B:143:LEU:O	1:B:146:PRO:HD3	2.11	0.50
1:A:87:PHE:CE2	1:A:89:ASP:HB2	2.47	0.49
1:B:164:VAL:CG1	1:B:165:THR:N	2.73	0.49
1:A:109:ASP:OD2	1:B:47:ARG:NH1	2.45	0.49
1:B:110:ASN:ND2	1:B:112:GLN:HG2	2.19	0.49
1:B:140:LEU:HA	1:B:143:LEU:HD12	1.95	0.49
1:A:10:TRP:CE2	1:A:190:ILE:HG23	2.47	0.49
1:A:183:ILE:O	1:A:187:LEU:HG	2.13	0.49
1:A:139:LEU:O	1:A:143:LEU:HD13	2.12	0.48
1:B:91:ILE:HD12	1:B:123:TYR:CZ	2.48	0.48
1:A:189:HIS:O	1:A:193:GLU:HG2	2.12	0.48
1:B:11:ARG:HG2	1:B:11:ARG:HH11	1.77	0.48
1:B:132:SER:HB3	1:B:135:SER:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ASP:N	1:B:159:PRO:CD	2.76	0.48
1:A:103:ASP:OD2	1:A:107:LEU:CD1	2.42	0.48
1:B:140:LEU:HD23	1:B:141:LYS:N	2.28	0.48
1:B:136:PHE:HE2	1:B:166:ILE:HD12	1.77	0.48
1:B:185:HIS:ND1	1:B:185:HIS:C	2.71	0.48
1:B:191:LEU:HD23	1:B:196:ILE:HD12	1.96	0.48
1:A:109:ASP:C	1:A:111:VAL:N	2.71	0.47
1:B:70:ALA:C	1:B:72:PRO:HD3	2.39	0.47
1:B:145:GLU:N	1:B:146:PRO:HD3	2.28	0.47
1:B:44:SER:HB3	1:B:159:PRO:HG3	1.96	0.47
1:B:158:ASP:N	1:B:159:PRO:HD3	2.28	0.47
1:B:181:GLU:HB3	4:B:519:HOH:O	2.13	0.47
1:A:74:GLY:HA2	1:A:79:CYS:HB3	1.97	0.47
1:B:136:PHE:CE2	1:B:166:ILE:HD12	2.49	0.47
1:B:243:THR:HG22	1:B:243:THR:OXT	2.15	0.47
1:A:12:PRO:HG3	4:A:651:HOH:O	2.14	0.47
1:B:22:GLU:HG3	1:B:23:HIS:N	2.27	0.47
1:B:237:VAL:O	1:B:241:LEU:CB	2.62	0.47
1:B:46:THR:HG22	1:B:47:ARG:N	2.29	0.46
1:A:18:VAL:HB	1:A:25:LEU:HD11	1.96	0.46
1:A:169:ARG:HH11	1:A:169:ARG:HG2	1.78	0.46
1:A:140:LEU:HD23	1:A:166:ILE:HG13	1.96	0.46
1:A:145:GLU:O	1:B:98:ARG:NH2	2.48	0.46
1:B:5:VAL:O	1:B:6:LEU:C	2.59	0.46
1:B:44:SER:HB2	1:B:159:PRO:HG2	1.98	0.46
1:B:227:SER:HB2	1:B:240:MET:HB3	1.98	0.46
1:B:10:TRP:CE2	1:B:190:ILE:HG23	2.51	0.46
1:A:81:GLU:OE1	1:A:117:ARG:NH1	2.50	0.45
1:A:235:GLN:HG2	1:A:236:ALA:N	2.31	0.45
1:B:136:PHE:HZ	1:B:162:LEU:CD2	2.29	0.45
1:B:165:THR:HG23	1:B:166:ILE:N	2.32	0.45
1:B:183:ILE:O	1:B:187:LEU:HG	2.16	0.45
1:B:5:VAL:O	1:B:5:VAL:HG22	2.16	0.45
1:B:233:SER:O	1:B:234:THR:C	2.59	0.45
1:A:139:LEU:HD23	1:A:143:LEU:HD13	1.98	0.45
1:B:223:GLN:O	1:B:226:ALA:HB3	2.16	0.45
1:A:28:LEU:HD21	1:A:173:PHE:CE2	2.52	0.44
1:B:77:ASP:O	1:B:81:GLU:HB2	2.18	0.44
1:A:175:LEU:N	1:A:175:LEU:HD22	2.33	0.44
1:A:169:ARG:NH1	1:A:169:ARG:HG3	2.32	0.44
1:A:240:MET:C	1:A:242:GLY:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:THR:O	1:B:147:PRO:HD2	2.17	0.44
1:B:127:GLU:OE2	1:B:127:GLU:HA	2.17	0.44
1:A:235:GLN:O	1:A:239:ALA:HB2	2.17	0.44
1:A:135:SER:O	1:A:139:LEU:HB2	2.18	0.43
1:A:220:LEU:HD22	1:A:240:MET:HE1	2.00	0.43
1:B:44:SER:HB2	1:B:159:PRO:CG	2.48	0.43
1:B:98:ARG:C	1:B:100:LYS:H	2.25	0.43
1:B:108:LEU:HD12	1:B:108:LEU:HA	1.78	0.43
1:B:189:HIS:ND1	1:B:189:HIS:C	2.76	0.43
1:B:61:GLY:CA	1:B:72:PRO:HG3	2.48	0.43
1:B:192:ASN:OD1	1:B:198:HIS:HE1	2.02	0.43
1:B:235:GLN:O	1:B:239:ALA:CB	2.66	0.43
1:A:14:THR:HG23	1:A:16:ALA:HB3	2.01	0.43
1:B:214:LEU:O	1:B:218:LEU:HD12	2.19	0.43
1:A:95:ALA:HB2	1:A:131:LEU:CD2	2.48	0.42
1:A:240:MET:C	1:A:242:GLY:H	2.23	0.42
1:A:133:ARG:HH21	1:B:240:MET:CE	2.32	0.42
1:B:200:PRO:O	1:B:201:ARG:C	2.62	0.42
1:B:202:ALA:CB	1:B:232:VAL:HG12	2.49	0.42
1:B:226:ALA:O	1:B:227:SER:C	2.63	0.42
1:A:140:LEU:CD2	1:A:166:ILE:HG13	2.50	0.42
1:B:140:LEU:HD23	1:B:140:LEU:O	2.18	0.42
1:A:91:ILE:HD12	1:A:91:ILE:H	1.85	0.42
1:A:136:PHE:CE2	1:A:166:ILE:CD1	3.00	0.42
1:A:228:GLY:HA3	1:A:236:ALA:HB2	2.02	0.42
1:A:146:PRO:HA	1:A:147:PRO:HD3	1.91	0.41
1:B:102:GLU:C	1:B:104:THR:N	2.77	0.41
1:A:127:GLU:HB3	1:A:130:MET:HE3	2.02	0.41
1:A:194:GLU:O	1:A:195:HIS:HB2	2.20	0.41
1:B:224:ALA:HA	1:B:240:MET:SD	2.60	0.41
1:A:112:GLN:OE1	1:A:121:LYS:HE2	2.21	0.41
1:B:89:ASP:OD2	1:B:117:ARG:HB2	2.20	0.41
1:B:98:ARG:C	1:B:100:LYS:N	2.78	0.41
1:B:9:LYS:HE2	1:B:194:GLU:CD	2.43	0.41
1:B:56:ARG:NH2	1:B:92:GLU:CD	2.78	0.41
1:B:62:LEU:O	1:B:119:ARG:NE	2.52	0.41
1:A:108:LEU:HD13	1:A:108:LEU:HA	1.78	0.41
1:B:156:THR:HG22	1:B:157:THR:N	2.36	0.41
1:B:181:GLU:OE1	1:B:184:ARG:NH1	2.54	0.41
1:B:189:HIS:C	1:B:189:HIS:HD1	2.29	0.41
1:B:102:GLU:O	1:B:103:ASP:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLN:OE1	1:B:208:ARG:NH1	2.55	0.40
1:B:54:ILE:HD12	1:B:175:LEU:CD2	2.45	0.40
1:B:233:SER:O	1:B:236:ALA:HB3	2.21	0.40
1:B:91:ILE:N	1:B:122:VAL:O	2.50	0.40
1:A:98:ARG:C	1:A:101:VAL:HG13	2.47	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	238/250 (95%)	219 (92%)	12 (5%)	7 (3%)	3	2
1	B	237/250 (95%)	212 (90%)	18 (8%)	7 (3%)	3	1
All	All	475/500 (95%)	431 (91%)	30 (6%)	14 (3%)	3	2

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	242	GLY
1	B	88	VAL
1	B	112	GLN
1	B	115	PRO
1	B	117	ARG
1	B	227	SER
1	A	110	ASN
1	A	112	GLN
1	A	113	TYR
1	A	133	ARG
1	B	6	LEU
1	B	102	GLU

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Mol	Chain	Res	Type
1	A	200	PRO

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	200/206 (97%)	177 (88%)	23 (12%)	5	5
1	B	199/206 (97%)	167 (84%)	32 (16%)	2	2
All	All	399/412 (97%)	344 (86%)	55 (14%)	3	3

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	8	ARG
1	A	80	ARG
1	A	86	ARG
1	A	88	VAL
1	A	98	ARG
1	A	101	VAL
1	A	103	ASP
1	A	106	ASP
1	A	107	LEU
1	A	108	LEU
1	A	136	PHE
1	A	137	ASN
1	A	148	GLU
1	A	149	HIS
1	A	158	ASP
1	A	169	ARG
1	A	176	LYS
1	A	200	PRO
1	A	229	ASP
1	A	231	GLN
1	A	235	GLN

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Mol	Chain	Res	Type
1	A	243	THR
1	B	5	VAL
1	B	11	ARG
1	B	22	GLU
1	B	80	ARG
1	B	81	GLU
1	B	103	ASP
1	B	105	ARG
1	B	107	LEU
1	B	108	LEU
1	B	110	ASN
1	B	115	PRO
1	B	117	ARG
1	B	119	ARG
1	B	132	SER
1	B	133	ARG
1	B	136	PHE
1	B	137	ASN
1	B	139	LEU
1	B	140	LEU
1	B	145	GLU
1	B	146	PRO
1	B	147	PRO
1	B	159	PRO
1	B	163	PRO
1	B	166	ILE
1	B	181	GLU
1	B	200	PRO
1	B	227	SER
1	B	229	ASP
1	B	238	SER
1	B	240	MET
1	B	241	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	63	ASN
1	A	137	ASN
1	A	149	HIS
1	A	195	HIS

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Mol	Chain	Res	Type
1	A	198	HIS
1	A	223	GLN
1	B	13	GLN
1	B	110	ASN
1	B	112	GLN
1	B	134	HIS
1	B	137	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	501	-	4,4,4	0.31	0	6,6,6	0.24	0
3	SO4	B	502	-	4,4,4	0.48	0	6,6,6	0.15	0
3	SO4	A	601	-	4,4,4	0.47	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	SO4	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	A	240/250 (96%)	-1.23	0 100 100	22, 42, 74, 88	0
1	B	239/250 (95%)	-1.20	0 100 100	21, 47, 78, 84	0
All	All	479/500 (95%)	-1.21	0 100 100	21, 44, 77, 88	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	601	5/5	0.97	0.04	80,80,81,81	0
2	ZN	B	402	1/1	1.00	0.01	25,25,25,25	0
3	SO4	A	501	5/5	1.00	0.02	19,23,25,26	0
2	ZN	A	401	1/1	1.00	0.01	26,26,26,26	0
3	SO4	B	502	5/5	1.00	0.02	23,24,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.