



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:46 pm BST

PDB ID : 5BO5  
Title : Structure of a unique ATP synthase subunit NeqB from Nanoarchaeum equitans  
Authors : Mohanty, S.; Jobichen, C.; Chichili, V.P.R.; Sivaraman, J.  
Deposited on : 2015-05-27  
Resolution : 2.81 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.11  
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) : 2.11

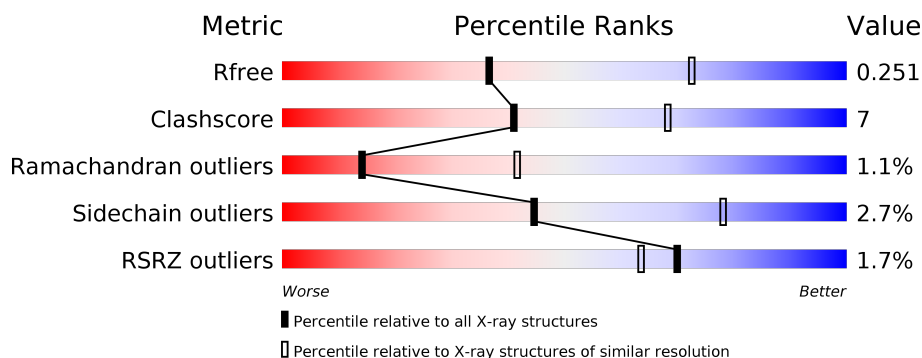
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	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  $\geq 3$ , 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	416	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 78%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>78%</span> <span>16%</span> <span>• 5%</span> </div> </div>
1	B	416	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 78%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>78%</span> <span>16%</span> <span>• 6%</span> </div> </div>
1	C	416	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 17%, green 75%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>2%</span> <span>75%</span> <span>17%</span> <span>• 6%</span> </div> </div>
1	D	416	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 14%, green 75%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>3%</span> <span>75%</span> <span>14%</span> <span>• 10%</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12023 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.

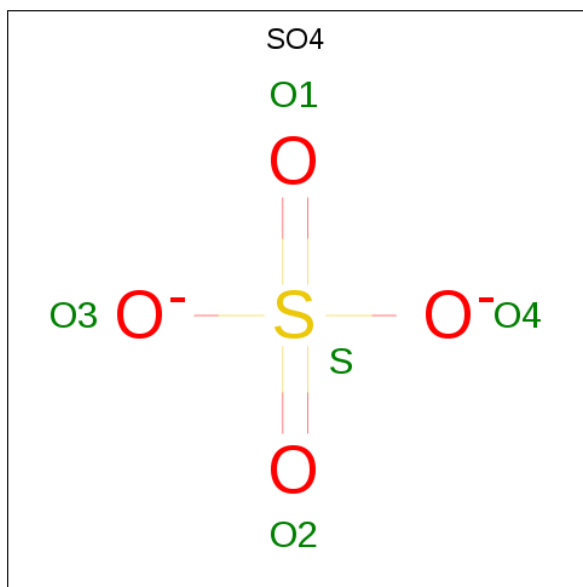
- Molecule 1 is a protein called NEQ263.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3100	2003	497	591	9			
1	B	392	Total	C	N	O	S	0	0	0
			3003	1936	486	573	8			
1	C	392	Total	C	N	O	S	0	0	0
			3017	1946	484	580	7			
1	D	376	Total	C	N	O	S	0	0	0
			2881	1858	467	548	8			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

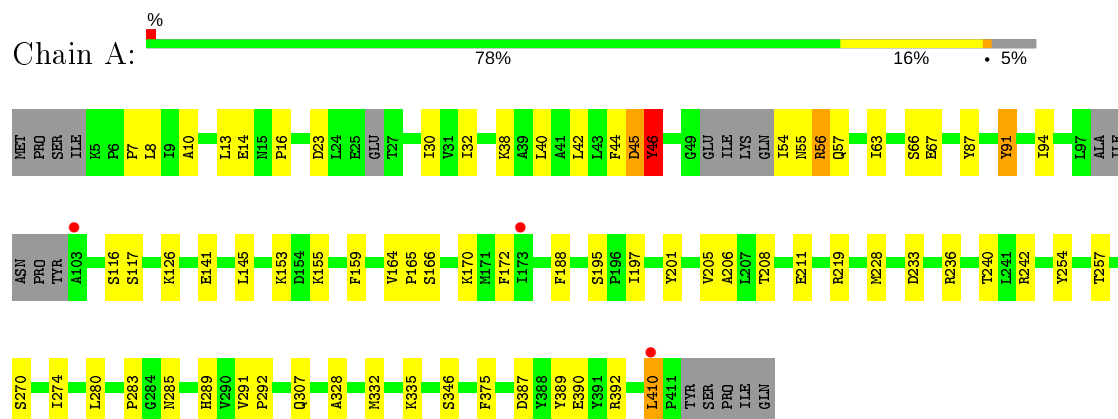


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

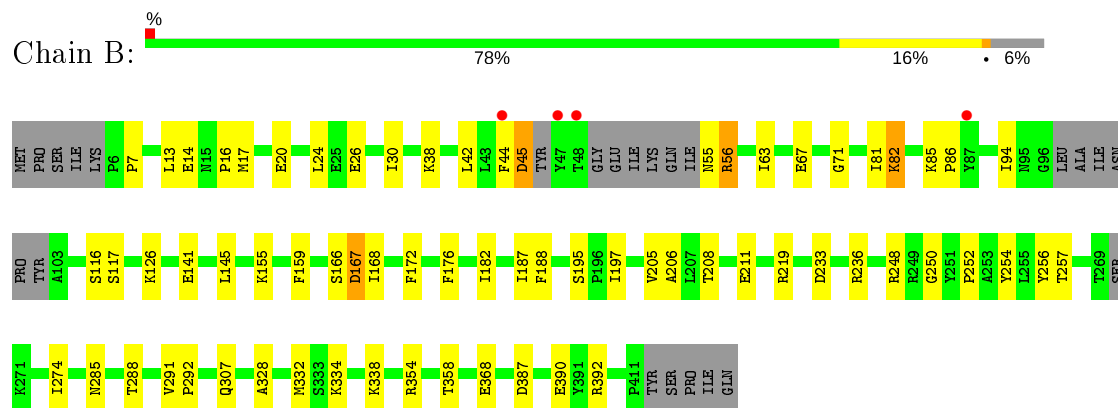
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

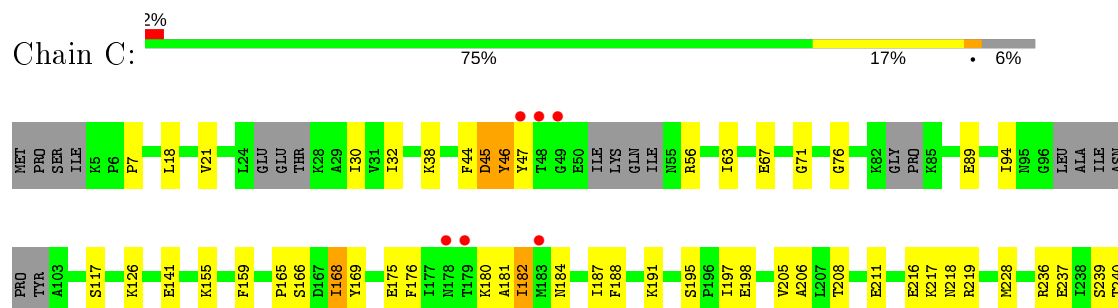
#### • Molecule 1: NEQ263

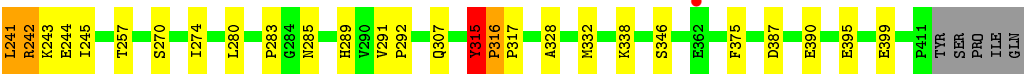


#### • Molecule 1: NEQ263

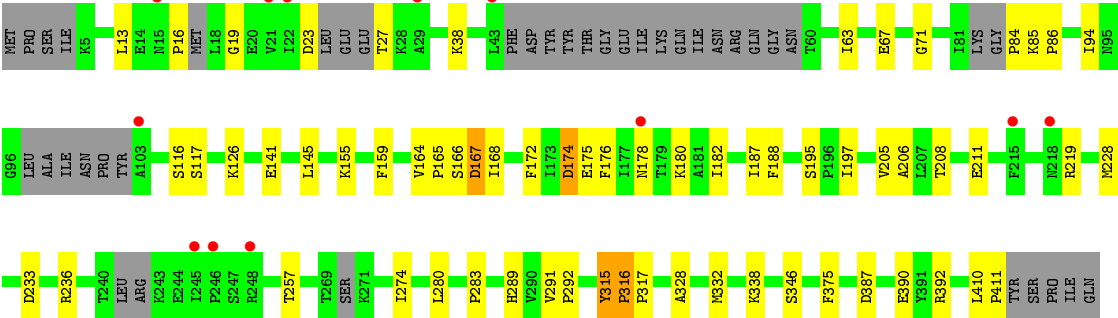
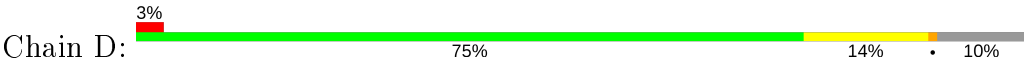


#### • Molecule 1: NEQ263





● Molecule 1: NEQ263



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.23Å 155.23Å 177.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 2.81 29.91 – 2.81	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.78-2.81) 95.3 (29.91-2.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.216 , 0.257 0.211 , 0.251	Depositor DCC
$R_{free}$ test set	1999 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.1	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12023	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, 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	0.53	5/3160 (0.2%)	0.65	0/4281
1	B	0.42	0/3061	0.63	4/4142 (0.1%)
1	C	0.50	4/3074 (0.1%)	0.62	1/4163 (0.0%)
1	D	0.42	0/2931	0.58	1/3960 (0.0%)
All	All	0.47	9/12226 (0.1%)	0.62	6/16546 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	TYR	CE2-CZ	-8.03	1.28	1.38
1	A	46	TYR	CG-CD2	-7.92	1.28	1.39
1	A	46	TYR	CE2-CZ	-7.85	1.28	1.38
1	A	46	TYR	CE1-CZ	-7.29	1.29	1.38
1	A	46	TYR	CG-CD1	-7.03	1.30	1.39
1	C	46	TYR	CE1-CZ	-6.67	1.29	1.38
1	C	46	TYR	CG-CD2	-6.47	1.30	1.39
1	A	91	TYR	CD1-CE1	-5.97	1.30	1.39
1	C	46	TYR	CG-CD1	-5.63	1.31	1.39

All (6) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	ILE	C-N-CA	-8.48	100.51	121.70
1	B	81	ILE	CA-C-N	7.18	133.00	117.20
1	B	81	ILE	O-C-N	-7.17	111.23	122.70
1	D	315	TYR	C-N-CD	-6.68	105.90	120.60
1	C	315	TYR	C-N-CD	-6.51	106.28	120.60
1	B	82	LYS	CB-CA-C	5.65	121.70	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	410	LEU	Peptide
1	C	315	TYR	Peptide
1	D	315	TYR	Peptide

## 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	3100	0	3132	53	1
1	B	3003	0	2999	40	1
1	C	3017	0	3020	56	1
1	D	2881	0	2899	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
All	All	12023	0	12050	171	2

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 7.

All (171) 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:335:LYS:HB2	1:D:178:ASN:HD21	1.13	1.07
1:C:7:PRO:HB3	1:C:46:TYR:HE2	1.21	1.02
1:A:389:TYR:HB3	1:C:217:LYS:HD3	1.46	0.97
1:A:46:TYR:CD2	1:A:254:TYR:HB3	2.04	0.93
1:C:7:PRO:HB3	1:C:46:TYR:CE2	2.05	0.90
1:A:46:TYR:HD2	1:A:254:TYR:HB3	1.41	0.84
1:A:390:GLU:HA	1:C:67:GLU:OE1	1.78	0.83
1:C:169:TYR:CE2	1:C:191:LYS:HG2	2.16	0.80
1:A:54:ILE:O	1:A:55:ASN:ND2	2.17	0.77
1:B:248:ARG:HA	1:C:236:ARG:NH2	2.00	0.77
1:C:67:GLU:OE2	1:C:219:ARG:NH2	2.19	0.76
1:C:240:THR:HA	1:C:245:ILE:HD12	1.67	0.75
1:B:67:GLU:OE2	1:B:219:ARG:NH2	2.20	0.75
1:A:14:GLU:O	1:A:56:ARG:NH2	2.20	0.74
1:A:67:GLU:OE2	1:A:219:ARG:NH2	2.21	0.74
1:A:335:LYS:CB	1:D:178:ASN:HD21	1.98	0.73
1:D:67:GLU:OE2	1:D:219:ARG:NH2	2.22	0.72
1:A:389:TYR:HB3	1:C:217:LYS:CD	2.20	0.71
1:A:335:LYS:HB2	1:D:178:ASN:ND2	1.97	0.69
1:C:241:LEU:O	1:C:244:GLU:N	2.19	0.68
1:A:23:ASP:HB3	1:A:57:GLN:HG2	1.75	0.67
1:B:167:ASP:N	1:B:167:ASP:OD1	2.28	0.66
1:A:389:TYR:O	1:C:217:LYS:NZ	2.28	0.66
1:B:17:MET:N	1:B:20:GLU:OE2	2.29	0.64
1:C:63:ILE:HD13	1:C:205:VAL:HG13	1.82	0.62
1:D:63:ILE:HD13	1:D:205:VAL:HG13	1.84	0.60
1:C:180:LYS:HA	1:C:182:ILE:HG22	1.84	0.59
1:C:47:TYR:CE1	1:C:241:LEU:HD12	2.37	0.59
1:A:45:ASP:OD1	1:A:45:ASP:N	2.35	0.59
1:C:141:GLU:HG2	1:C:168:ILE:HG21	1.83	0.59
1:A:389:TYR:CE2	1:C:218:ASN:ND2	2.71	0.59
1:D:233:ASP:OD1	1:D:236:ARG:NH2	2.36	0.58
1:C:45:ASP:N	1:C:45:ASP:OD1	2.35	0.58
1:B:288:THR:HG21	1:C:243:LYS:H	1.69	0.58
1:D:174:ASP:C	1:D:176:PHE:H	2.07	0.58
1:D:141:GLU:HG2	1:D:168:ILE:HD12	1.88	0.56
1:C:239:SER:O	1:C:245:ILE:HD12	2.05	0.56
1:D:174:ASP:O	1:D:176:PHE:N	2.38	0.56
1:C:188:PHE:CE2	1:C:205:VAL:HG12	2.41	0.55
1:B:233:ASP:OD1	1:B:236:ARG:NH2	2.38	0.55
1:B:45:ASP:OD1	1:B:45:ASP:N	2.39	0.55
1:D:126:LYS:HD3	1:D:155:LYS:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:PHE:O	1:D:176:PHE:HB3	2.06	0.54
1:A:8:LEU:HD11	1:A:32:ILE:HD11	1.89	0.54
1:A:233:ASP:OD1	1:A:236:ARG:NH2	2.41	0.54
1:A:188:PHE:CE2	1:A:205:VAL:HG12	2.44	0.53
1:C:283:PRO:HG2	1:C:289:HIS:CD2	2.43	0.53
1:D:188:PHE:CE2	1:D:205:VAL:HG12	2.44	0.53
1:C:126:LYS:HD3	1:C:155:LYS:HE2	1.89	0.53
1:B:126:LYS:HD3	1:B:155:LYS:HE2	1.89	0.53
1:A:389:TYR:O	1:C:217:LYS:HD2	2.08	0.52
1:B:188:PHE:CE2	1:B:205:VAL:HG12	2.45	0.52
1:C:169:TYR:CZ	1:C:191:LYS:HE2	2.44	0.52
1:C:32:ILE:HG22	1:C:241:LEU:HD11	1.92	0.51
1:A:126:LYS:HD3	1:A:155:LYS:HE2	1.91	0.51
1:D:168:ILE:HG22	1:D:172:PHE:CE2	2.46	0.51
1:D:283:PRO:HG2	1:D:289:HIS:CD2	2.45	0.51
1:D:167:ASP:OD1	1:D:167:ASP:N	2.38	0.51
1:B:63:ILE:HD13	1:B:205:VAL:HG13	1.92	0.51
1:A:283:PRO:HG2	1:A:289:HIS:CD2	2.46	0.51
1:C:176:PHE:O	1:C:182:ILE:HB	2.11	0.51
1:D:410:LEU:HD23	1:D:411:PRO:HD2	1.93	0.50
1:C:395:GLU:O	1:C:399:GLU:HG3	2.12	0.50
1:D:13:LEU:HB3	1:D:16:PRO:HB3	1.93	0.50
1:C:47:TYR:HE1	1:C:241:LEU:HD12	1.75	0.50
1:A:236:ARG:O	1:A:240:THR:OG1	2.26	0.50
1:C:195:SER:OG	1:C:197:ILE:HG22	2.12	0.49
1:B:30:ILE:HD11	1:B:44:PHE:CE1	2.48	0.49
1:C:328:ALA:O	1:C:332:MET:HG3	2.12	0.49
1:A:63:ILE:HD13	1:A:205:VAL:HG13	1.95	0.49
1:B:17:MET:O	1:B:20:GLU:HG2	2.13	0.49
1:D:94:ILE:HA	1:D:208:THR:OG1	2.13	0.49
1:A:46:TYR:CD1	1:A:46:TYR:N	2.81	0.48
1:B:248:ARG:HA	1:C:236:ARG:HH21	1.76	0.48
1:D:328:ALA:O	1:D:332:MET:HG3	2.13	0.48
1:A:387:ASP:HB3	1:A:390:GLU:HB2	1.95	0.48
1:B:94:ILE:HA	1:B:208:THR:OG1	2.12	0.48
1:B:55:ASN:O	1:B:56:ARG:HB2	2.12	0.48
1:C:181:ALA:O	1:C:184:ASN:N	2.36	0.48
1:A:328:ALA:O	1:A:332:MET:HG3	2.14	0.48
1:A:13:LEU:O	1:A:16:PRO:HD3	2.14	0.48
1:A:170:LYS:HD3	1:A:170:LYS:HA	1.70	0.47
1:C:94:ILE:HA	1:C:208:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASN:ND2	1:A:307:GLN:OE1	2.48	0.47
1:A:116:SER:OG	1:A:392:ARG:HD2	2.15	0.47
1:B:387:ASP:HB3	1:B:390:GLU:HB2	1.96	0.47
1:C:387:ASP:HB3	1:C:390:GLU:HB2	1.96	0.47
1:A:94:ILE:HA	1:A:208:THR:OG1	2.15	0.47
1:D:195:SER:OG	1:D:197:ILE:HG22	2.14	0.47
1:B:13:LEU:HB3	1:B:16:PRO:HB3	1.96	0.47
1:B:328:ALA:O	1:B:332:MET:HG3	2.15	0.47
1:C:291:VAL:HB	1:C:292:PRO:HD3	1.97	0.47
1:A:30:ILE:HD11	1:A:44:PHE:CE1	2.50	0.46
1:A:7:PRO:O	1:A:42:LEU:HD12	2.15	0.46
1:D:23:ASP:OD1	1:D:27:THR:N	2.48	0.46
1:A:188:PHE:CE2	1:A:206:ALA:HA	2.50	0.46
1:A:389:TYR:CB	1:C:217:LYS:HA	2.46	0.46
1:D:387:ASP:HB3	1:D:390:GLU:HB2	1.98	0.46
1:A:145:LEU:HD21	1:A:172:PHE:HD1	1.81	0.46
1:D:211:GLU:HA	1:D:274:ILE:HD11	1.98	0.46
1:B:211:GLU:HA	1:B:274:ILE:HD11	1.98	0.46
1:C:169:TYR:HE2	1:C:191:LYS:HG2	1.77	0.46
1:C:21:VAL:HG13	1:C:44:PHE:HZ	1.79	0.46
1:B:195:SER:OG	1:B:197:ILE:HG22	2.16	0.46
1:A:346:SER:HB2	1:A:375:PHE:CE2	2.51	0.46
1:C:71:GLY:HA2	1:C:182:ILE:O	2.16	0.45
1:A:211:GLU:HA	1:A:274:ILE:HD11	1.98	0.45
1:D:187:ILE:C	1:D:188:PHE:HD1	2.20	0.45
1:A:46:TYR:CD2	1:A:254:TYR:CB	2.88	0.45
1:A:228:MET:HB2	1:A:280:LEU:HB3	1.99	0.45
1:B:338:LYS:HA	1:B:338:LYS:HD3	1.79	0.45
1:A:153:LYS:HD3	1:C:89:GLU:O	2.17	0.44
1:A:195:SER:OG	1:A:197:ILE:HG22	2.17	0.44
1:D:291:VAL:HB	1:D:292:PRO:HD3	1.99	0.44
1:B:176:PHE:CG	1:B:187:ILE:HD11	2.52	0.44
1:B:188:PHE:CE2	1:B:206:ALA:HA	2.53	0.44
1:C:187:ILE:C	1:C:188:PHE:HD1	2.21	0.44
1:C:30:ILE:HD11	1:C:44:PHE:CE1	2.53	0.44
1:D:316:PRO:HA	1:D:317:PRO:HD2	1.90	0.44
1:C:76:GLY:HA3	1:C:198:GLU:HG2	1.99	0.44
1:D:338:LYS:HA	1:D:338:LYS:HD3	1.72	0.44
1:A:46:TYR:HD1	1:A:46:TYR:N	2.16	0.44
1:B:71:GLY:HA2	1:B:182:ILE:O	2.18	0.43
1:B:285:ASN:ND2	1:B:307:GLN:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:HIS:O	1:A:292:PRO:HD2	2.18	0.43
1:C:211:GLU:HA	1:C:274:ILE:HD11	2.00	0.43
1:D:116:SER:OG	1:D:392:ARG:HD2	2.18	0.43
1:B:116:SER:OG	1:B:392:ARG:HD2	2.19	0.43
1:B:14:GLU:O	1:B:56:ARG:NH2	2.34	0.43
1:A:389:TYR:CD1	1:C:216:GLU:O	2.71	0.42
1:C:289:HIS:O	1:C:292:PRO:HD2	2.19	0.42
1:B:85:LYS:HA	1:B:86:PRO:HD3	1.90	0.42
1:D:188:PHE:N	1:D:188:PHE:CD1	2.87	0.42
1:A:8:LEU:HA	1:A:8:LEU:HD12	1.90	0.42
1:D:346:SER:HB2	1:D:375:PHE:CE2	2.54	0.42
1:B:250:GLY:HA3	1:C:237:GLU:CD	2.39	0.42
1:C:165:PRO:HD2	1:C:168:ILE:HG13	2.00	0.42
1:C:188:PHE:CE2	1:C:206:ALA:HA	2.55	0.42
1:A:141:GLU:CD	1:A:141:GLU:H	2.23	0.42
1:D:228:MET:HB2	1:D:280:LEU:HB3	2.01	0.42
1:B:168:ILE:HG22	1:B:172:PHE:CE2	2.55	0.41
1:C:188:PHE:N	1:C:188:PHE:CD1	2.88	0.41
1:B:188:PHE:N	1:B:188:PHE:CD1	2.89	0.41
1:D:188:PHE:CE2	1:D:206:ALA:HA	2.55	0.41
1:C:242:ARG:HB2	1:C:244:GLU:OE2	2.21	0.41
1:D:164:VAL:HA	1:D:165:PRO:HD3	1.89	0.41
1:D:145:LEU:HD21	1:D:172:PHE:HD1	1.85	0.41
1:A:66:SER:HB2	1:A:87:TYR:O	2.20	0.41
1:B:334:LYS:HD2	1:B:334:LYS:HA	1.73	0.41
1:A:188:PHE:CD2	1:A:206:ALA:HA	2.55	0.41
1:B:354:ARG:O	1:B:358:THR:HG23	2.21	0.41
1:B:55:ASN:HB3	1:B:56:ARG:H	1.67	0.41
1:C:228:MET:HB2	1:C:280:LEU:HB3	2.03	0.41
1:D:176:PHE:HD2	1:D:187:ILE:HD11	1.86	0.41
1:D:84:PRO:O	1:D:86:PRO:N	2.54	0.41
1:A:10:ALA:HB1	1:A:201:TYR:CZ	2.56	0.41
1:B:7:PRO:O	1:B:42:LEU:HD12	2.21	0.41
1:B:291:VAL:HB	1:B:292:PRO:HD3	2.01	0.41
1:D:71:GLY:HA2	1:D:182:ILE:O	2.21	0.41
1:B:13:LEU:O	1:B:16:PRO:HD3	2.20	0.40
1:C:285:ASN:ND2	1:C:307:GLN:OE1	2.54	0.40
1:A:164:VAL:HA	1:A:165:PRO:HD3	1.88	0.40
1:A:8:LEU:HG	1:A:40:LEU:HD22	2.02	0.40
1:B:141:GLU:CD	1:B:141:GLU:H	2.24	0.40
1:C:316:PRO:HA	1:C:317:PRO:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:VAL:HB	1:A:292:PRO:HD3	2.02	0.40
1:B:145:LEU:HD21	1:B:172:PHE:HD1	1.86	0.40
1:B:252:PRO:HB3	1:B:254:TYR:CE2	2.56	0.40
1:C:315:TYR:CG	1:C:316:PRO:N	2.89	0.40
1:C:346:SER:HB2	1:C:375:PHE:CE2	2.56	0.40
1:D:174:ASP:C	1:D:176:PHE:N	2.74	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:TYR:OH	1:C:399:GLU:OE1[1_655]	1.51	0.69
1:B:256:TYR:OH	1:B:368:GLU:OE2[4_455]	2.11	0.09

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	389/416 (94%)	371 (95%)	16 (4%)	2 (0%)	29	61
1	B	382/416 (92%)	365 (96%)	14 (4%)	3 (1%)	19	49
1	C	382/416 (92%)	362 (95%)	14 (4%)	6 (2%)	9	31
1	D	360/416 (86%)	335 (93%)	20 (6%)	5 (1%)	11	34
All	All	1513/1664 (91%)	1433 (95%)	64 (4%)	16 (1%)	14	41

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	LEU
1	B	26	GLU
1	C	56	ARG

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Mol	Chain	Res	Type
1	C	175	GLU
1	C	242	ARG
1	D	85	LYS
1	D	175	GLU
1	A	56	ARG
1	C	182	ILE
1	C	241	LEU
1	C	316	PRO
1	D	316	PRO
1	B	56	ARG
1	D	174	ASP
1	A	410	LEU
1	D	19	GLY

### 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	334/360 (93%)	325 (97%)	9 (3%)	44	78
1	B	318/360 (88%)	310 (98%)	8 (2%)	47	80
1	C	322/360 (89%)	312 (97%)	10 (3%)	40	74
1	D	307/360 (85%)	300 (98%)	7 (2%)	50	82
All	All	1281/1440 (89%)	1247 (97%)	34 (3%)	44	78

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	45	ASP
1	A	46	TYR
1	A	117	SER
1	A	159	PHE
1	A	166	SER
1	A	242	ARG
1	A	257	THR

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Mol	Chain	Res	Type
1	A	270	SER
1	B	38	LYS
1	B	45	ASP
1	B	82	LYS
1	B	117	SER
1	B	159	PHE
1	B	166	SER
1	B	167	ASP
1	B	257	THR
1	C	18	LEU
1	C	38	LYS
1	C	45	ASP
1	C	117	SER
1	C	159	PHE
1	C	166	SER
1	C	168	ILE
1	C	257	THR
1	C	270	SER
1	C	338	LYS
1	D	38	LYS
1	D	117	SER
1	D	159	PHE
1	D	166	SER
1	D	167	ASP
1	D	180	LYS
1	D	257	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	218	ASN
1	D	178	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	D	501	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	A	502	-	4,4,4	0.24	0	6,6,6	0.14	0
3	SO4	C	501	-	4,4,4	0.29	0	6,6,6	0.33	0
3	SO4	B	502	-	4,4,4	0.18	0	6,6,6	0.27	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.

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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	397/416 (95%)	-0.13	3 (0%) 86 81	31, 47, 75, 97	0
1	B	392/416 (94%)	-0.25	4 (1%) 82 77	31, 49, 80, 99	0
1	C	392/416 (94%)	0.01	7 (1%) 68 61	33, 50, 83, 108	0
1	D	376/416 (90%)	-0.06	12 (3%) 47 37	34, 51, 88, 122	0
All	All	1557/1664 (93%)	-0.11	26 (1%) 70 63	31, 49, 81, 122	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	179	THR	6.1
1	D	21	VAL	4.3
1	B	47	TYR	4.3
1	B	44	PHE	3.8
1	C	48	THR	3.8
1	D	178	ASN	3.6
1	C	47	TYR	3.3
1	D	103	ALA	3.2
1	D	246	PRO	3.1
1	C	49	GLY	2.9
1	B	87	TYR	2.9
1	D	245	ILE	2.7
1	D	43	LEU	2.6
1	C	178	ASN	2.6
1	B	48	THR	2.5
1	C	362	GLU	2.4
1	C	183	MET	2.3
1	D	22	ILE	2.3
1	D	15	ASN	2.2
1	D	218	ASN	2.2
1	D	29	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	215	PHE	2.1
1	D	248	ARG	2.1
1	A	173	ILE	2.1
1	A	410	LEU	2.1
1	A	103	ALA	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 carbohydrates 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, 95<sup>th</sup> 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	C	501	5/5	0.90	0.16	39,46,51,108	0
2	MG	A	501	1/1	0.91	0.20	66,66,66,66	0
3	SO4	D	501	5/5	0.92	0.13	57,63,73,105	0
3	SO4	B	502	5/5	0.96	0.10	35,50,70,102	0
3	SO4	A	502	5/5	0.97	0.09	46,57,76,89	0
2	MG	B	501	1/1	0.97	0.23	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.