Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:09 am BST

PDB ID	:	4RV0
Title	:	Crystal structure of TN complex
Authors	:	Hao, Q.; Jiao, S.; Shi, Z.B.; Zhou, Z.C.
Deposited on	:	2014-11-23
Resolution	:	2.00 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:

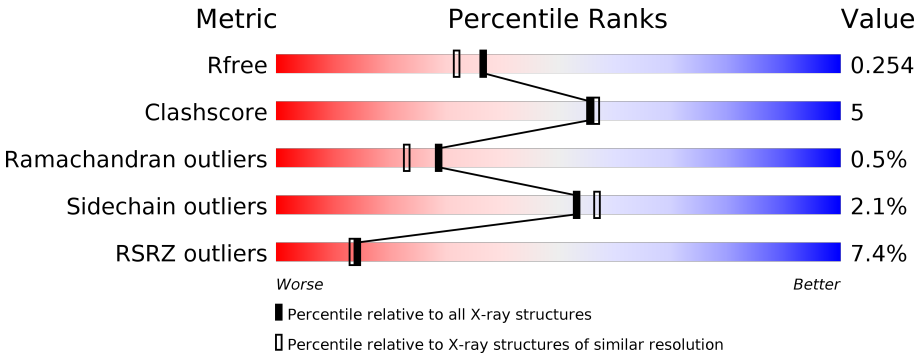
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	171	3% 81% 11% • 7%
1	C	171	% 86% 6% • 7%
1	E	171	3% 81% 12% 7%
1	G	171	4% 88% 9% •
2	B	81	6% 78% 12% • 9%
2	D	81	15% 80% 11% 9%

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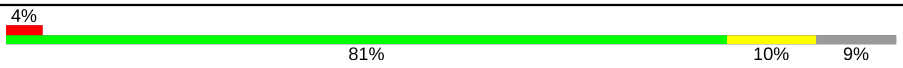
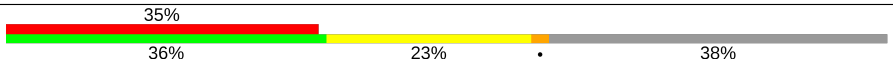
Mol	Chain	Length	Quality of chain
2	F	81	
2	H	81	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8401 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 Transitional endoplasmic reticulum ATPase TER94.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	Se	0	0	0
			1273	806	220	236	6	5			
1	C	159	Total	C	N	O	S	Se	0	1	0
			1284	812	224	237	6	5			
1	E	159	Total	C	N	O	S	Se	0	2	0
			1290	815	222	242	6	5			
1	G	165	Total	C	N	O	S	Se	0	2	0
			1328	839	231	247	6	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLY	-	EXPRESSION TAG	UNP Q7KN62
A	17	ALA	-	EXPRESSION TAG	UNP Q7KN62
A	18	MSE	-	EXPRESSION TAG	UNP Q7KN62
A	19	GLU	-	EXPRESSION TAG	UNP Q7KN62
C	16	GLY	-	EXPRESSION TAG	UNP Q7KN62
C	17	ALA	-	EXPRESSION TAG	UNP Q7KN62
C	18	MSE	-	EXPRESSION TAG	UNP Q7KN62
C	19	GLU	-	EXPRESSION TAG	UNP Q7KN62
E	16	GLY	-	EXPRESSION TAG	UNP Q7KN62
E	17	ALA	-	EXPRESSION TAG	UNP Q7KN62
E	18	MSE	-	EXPRESSION TAG	UNP Q7KN62
E	19	GLU	-	EXPRESSION TAG	UNP Q7KN62
G	16	GLY	-	EXPRESSION TAG	UNP Q7KN62
G	17	ALA	-	EXPRESSION TAG	UNP Q7KN62
G	18	MSE	-	EXPRESSION TAG	UNP Q7KN62
G	19	GLU	-	EXPRESSION TAG	UNP Q7KN62

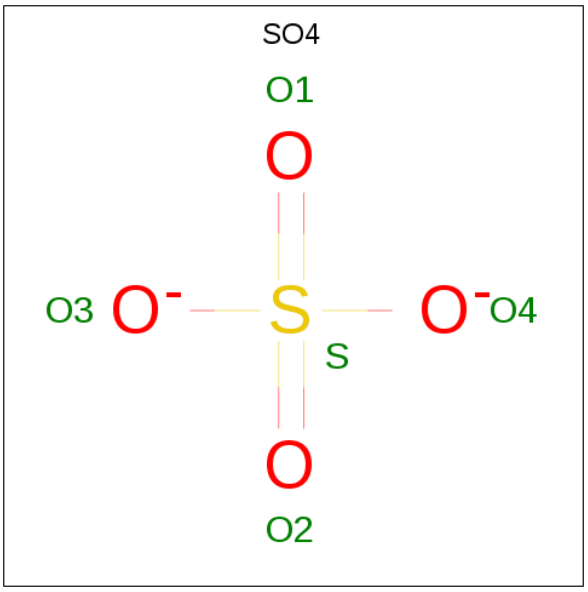
- Molecule 2 is a protein called Nuclear protein localization protein 4 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	74	Total	C	N	O	Se	0	0	0
			582	369	105	107	1			
2	D	74	Total	C	N	O	Se	0	0	0
			582	369	105	107	1			
2	F	74	Total	C	N	O	Se	0	0	0
			586	371	105	109	1			
2	H	50	Total	C	N	O	Se	0	0	0
			395	252	70	72	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	EXPRESSION TAG	UNP Q9VBP9
B	-2	ALA	-	EXPRESSION TAG	UNP Q9VBP9
B	-1	MSE	-	EXPRESSION TAG	UNP Q9VBP9
B	0	GLU	-	EXPRESSION TAG	UNP Q9VBP9
D	-3	GLY	-	EXPRESSION TAG	UNP Q9VBP9
D	-2	ALA	-	EXPRESSION TAG	UNP Q9VBP9
D	-1	MSE	-	EXPRESSION TAG	UNP Q9VBP9
D	0	GLU	-	EXPRESSION TAG	UNP Q9VBP9
F	-3	GLY	-	EXPRESSION TAG	UNP Q9VBP9
F	-2	ALA	-	EXPRESSION TAG	UNP Q9VBP9
F	-1	MSE	-	EXPRESSION TAG	UNP Q9VBP9
F	0	GLU	-	EXPRESSION TAG	UNP Q9VBP9
H	-3	GLY	-	EXPRESSION TAG	UNP Q9VBP9
H	-2	ALA	-	EXPRESSION TAG	UNP Q9VBP9
H	-1	MSE	-	EXPRESSION TAG	UNP Q9VBP9
H	0	GLU	-	EXPRESSION TAG	UNP Q9VBP9

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	217	Total O 217 217	0	0
4	B	82	Total O 82 82	0	0
4	C	193	Total O 193 193	0	0
4	D	38	Total O 38 38	0	0
4	E	221	Total O 221 221	0	0

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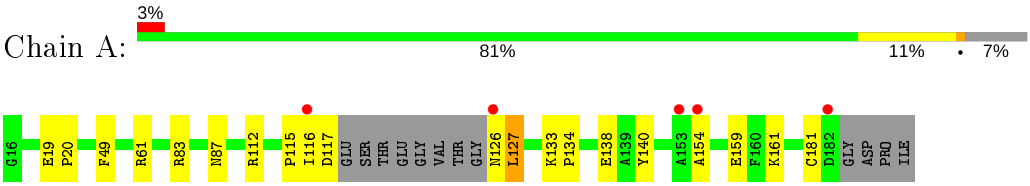
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	89	Total O 89 89	0	0
4	G	175	Total O 175 175	0	0
4	H	31	Total O 31 31	0	0

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.

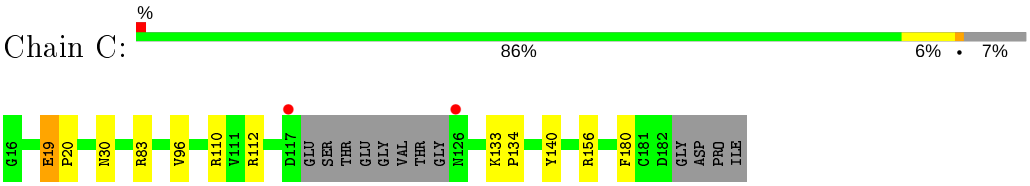
- Molecule 1: Transitional endoplasmic reticulum ATPase TER94

Chain A:



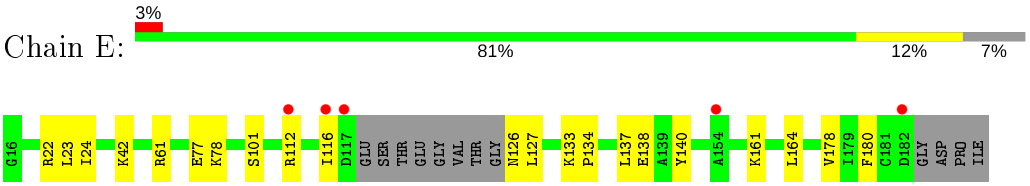
- Molecule 1: Transitional endoplasmic reticulum ATPase TER94

Chain C:



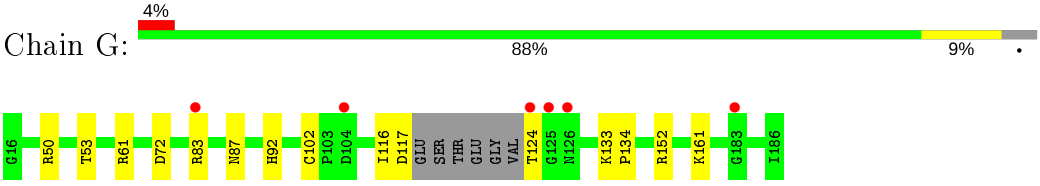
- Molecule 1: Transitional endoplasmic reticulum ATPase TER94

Chain E:



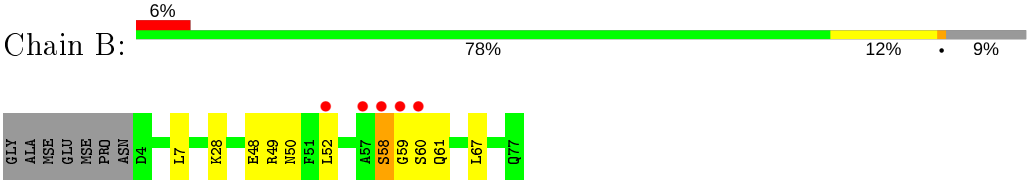
- Molecule 1: Transitional endoplasmic reticulum ATPase TER94

Chain G:



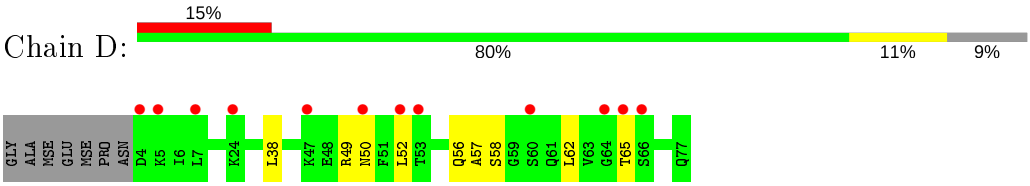
- Molecule 2: Nuclear protein localization protein 4 homolog

Chain B:



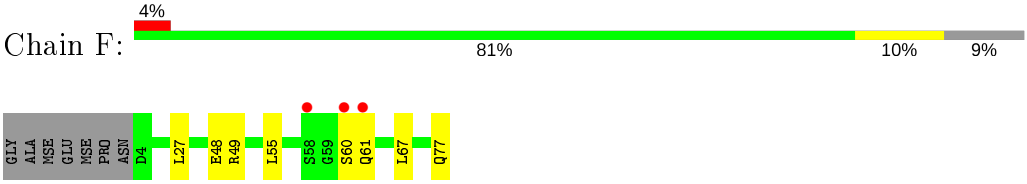
- Molecule 2: Nuclear protein localization protein 4 homolog

Chain D:



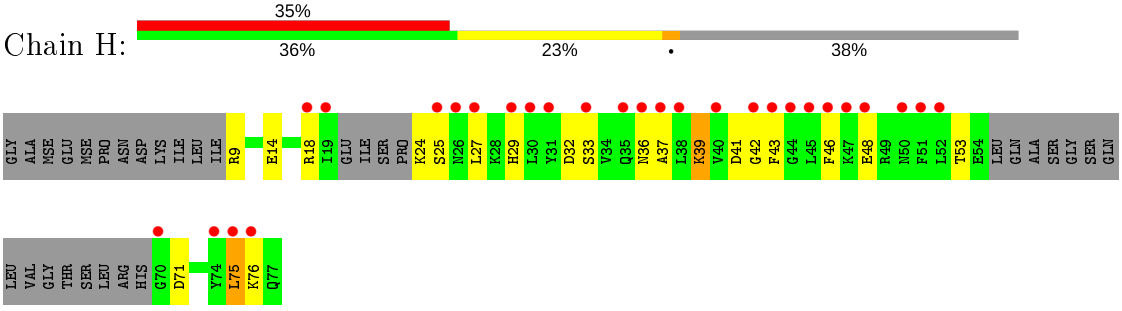
• Molecule 2: Nuclear protein localization protein 4 homolog

Chain F:



• Molecule 2: Nuclear protein localization protein 4 homolog

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.15Å 83.14Å 162.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.38 – 2.00 45.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.38-2.00) 99.7 (45.38-2.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.208 , 0.253 0.209 , 0.254	Depositor DCC
R_{free} test set	3727 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8401	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0592e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.44	0/1289	0.63	0/1736
1	C	0.41	0/1300	0.60	0/1750
1	E	0.42	0/1306	0.63	0/1759
1	G	0.39	0/1345	0.61	0/1812
2	B	0.40	0/588	0.74	1/784 (0.1%)
2	D	0.35	0/588	0.54	0/784
2	F	0.42	0/592	0.64	0/790
2	H	0.32	0/397	0.55	1/525 (0.2%)
All	All	0.41	0/7405	0.62	2/9940 (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
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	61	GLN	N-CA-C	-7.04	92.01	111.00
2	H	75	LEU	CA-CB-CG	5.97	129.03	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	60	SER	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	1273	0	1293	16	1
1	C	1284	0	1305	10	0
1	E	1290	0	1301	17	0
1	G	1328	0	1343	11	0
2	B	582	0	604	9	0
2	D	582	0	604	4	0
2	F	586	0	607	5	0
2	H	395	0	392	9	0
3	A	10	0	0	0	0
3	C	10	0	0	1	0
3	G	15	0	0	2	0
4	A	217	0	0	9	1
4	B	82	0	0	2	1
4	C	193	0	0	3	1
4	D	38	0	0	0	0
4	E	221	0	0	9	3
4	F	89	0	0	1	0
4	G	175	0	0	6	1
4	H	31	0	0	2	0
All	All	8401	0	7449	75	4

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 5.

All (75) 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)
3:C:202:SO4:O4	4:C:452:HOH:O	2.04	0.76
1:A:112:ARG:NH1	4:A:418:HOH:O	2.18	0.75
2:B:58:SER:HB3	2:B:59:GLY:CA	2.17	0.73
1:A:181:CYS:HB2	4:A:483:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:SER:HB3	2:B:59:GLY:HA2	1.72	0.70
1:G:50:ARG:O	2:H:9:ARG:NH2	2.21	0.69
2:H:18:ARG:O	4:H:121:HOH:O	2.11	0.69
2:H:41:ASP:O	2:H:43:PHE:N	2.26	0.68
2:D:50:ASN:OD1	2:D:52:LEU:HG	1.95	0.67
3:G:202:SO4:O4	4:G:464:HOH:O	2.13	0.66
1:A:126:ASN:N	4:A:459:HOH:O	2.28	0.66
1:E:126:ASN:N	4:E:291:HOH:O	2.29	0.65
1:G:72:ASP:OD2	4:G:429:HOH:O	2.13	0.65
2:H:36:ASN:O	2:H:39:LYS:NZ	2.30	0.65
2:H:33:SER:O	2:H:37:ALA:N	2.25	0.64
1:C:30:ASN:O	4:C:370:HOH:O	2.15	0.64
1:G:116:ILE:HD11	1:G:161:LYS:HB2	1.84	0.59
1:G:87:ASN:OD1	4:G:456:HOH:O	2.17	0.58
2:F:60:SER:HB2	2:F:61:GLN:HA	1.86	0.57
1:E:24:ILE:HB	1:E:78:LYS:HD3	1.86	0.56
1:G:152:ARG:NH2	3:G:203:SO4:O1	2.38	0.56
1:A:154:ALA:O	1:E:112:ARG:NH1	2.38	0.56
2:B:50:ASN:ND2	4:B:167:HOH:O	2.39	0.55
1:E:77:GLU:OE2	4:E:341:HOH:O	2.19	0.54
1:A:117:ASP:N	4:A:503:HOH:O	2.37	0.53
1:G:92:HIS:NE2	4:G:451:HOH:O	2.33	0.53
2:B:50:ASN:OD1	2:B:52:LEU:HG	2.08	0.53
1:A:140:TYR:CZ	2:B:49:ARG:HD3	2.45	0.52
2:F:55:LEU:HD21	2:F:67:LEU:HD11	1.92	0.51
1:A:154:ALA:N	4:A:399:HOH:O	2.41	0.51
1:E:137:LEU:HG	1:E:138[A]:GLU:HG2	1.93	0.51
1:G:117:ASP:N	4:G:378:HOH:O	2.27	0.50
1:E:116:ILE:HD11	1:E:161:LYS:HB2	1.93	0.49
2:B:58:SER:HB3	2:B:59:GLY:C	2.33	0.49
2:B:67:LEU:O	4:B:155:HOH:O	2.20	0.49
1:E:23:LEU:HD21	1:E:42:LYS:HE3	1.95	0.49
1:E:22:ARG:NH2	4:E:340:HOH:O	2.46	0.49
1:E:61:ARG:NH2	4:E:375:HOH:O	2.45	0.48
2:D:56:GLN:O	2:D:58:SER:N	2.47	0.48
1:E:61:ARG:O	4:E:306:HOH:O	2.20	0.48
4:A:304:HOH:O	1:C:83[B]:ARG:HG3	2.14	0.47
1:E:61:ARG:NH1	4:E:394:HOH:O	2.47	0.47
2:H:46:PHE:HE2	2:H:76:LYS:HB3	1.78	0.47
2:B:28:LYS:H	2:B:58:SER:HB2	1.80	0.46
1:C:156:ARG:NH1	4:C:410:HOH:O	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:LEU:HD22	2:F:55:LEU:HD23	1.98	0.45
1:E:101:SER:HB2	4:E:418:HOH:O	2.16	0.45
2:H:46:PHE:CE2	2:H:76:LYS:HB3	2.51	0.45
1:A:83:ARG:HG2	1:C:83[A]:ARG:NE	2.33	0.44
1:A:116:ILE:HD11	1:A:161:LYS:HB2	2.00	0.44
1:E:133:LYS:HB3	1:E:134:PRO:HD3	1.99	0.44
1:A:49:PHE:CE1	2:B:7:LEU:HD23	2.53	0.44
2:D:62:LEU:HB2	2:D:65:THR:HG23	2.00	0.44
1:G:133:LYS:HB3	1:G:134:PRO:HD3	1.99	0.43
1:A:159:GLU:OE2	4:A:378:HOH:O	2.21	0.43
1:A:133:LYS:HB3	1:A:134:PRO:HD3	2.00	0.43
1:E:112:ARG:NH2	4:E:374:HOH:O	2.52	0.43
2:H:14:GLU:HG2	4:H:111:HOH:O	2.18	0.42
1:G:83[A]:ARG:NH1	1:G:87:ASN:HB2	2.34	0.42
1:C:19:GLU:HA	1:C:20:PRO:HD3	1.91	0.42
1:A:19:GLU:HA	1:A:20:PRO:HD3	1.90	0.41
1:E:180:PHE:HB3	4:E:381:HOH:O	2.19	0.41
1:C:96:VAL:HG21	1:E:178:VAL:HG21	2.02	0.41
1:E:140:TYR:CZ	2:F:49:ARG:HD3	2.55	0.41
1:A:115:PRO:HG3	1:A:127:LEU:HD21	2.01	0.41
1:C:133:LYS:HB3	1:C:134:PRO:HD3	2.01	0.41
2:H:29:HIS:O	2:H:32:ASP:HB2	2.20	0.41
1:C:140:TYR:CZ	2:D:49:ARG:HD3	2.56	0.41
1:C:110:ARG:HD3	1:C:180:PHE:HE2	1.86	0.41
1:G:87:ASN:HB2	4:G:448:HOH:O	2.19	0.41
2:F:77:GLN:HG3	4:F:127:HOH:O	2.21	0.40
1:C:112:ARG:HD2	1:C:112:ARG:HH11	1.74	0.40
1:A:133:LYS:HD3	4:A:344:HOH:O	2.20	0.40
1:G:53:THR:OG1	1:G:102:CYS:O	2.35	0.40
1:A:87:ASN:HB2	4:A:307:HOH:O	2.22	0.40

All (4) 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)
4:A:389:HOH:O	4:E:289:HOH:O[4_475]	2.01	0.19
4:B:160:HOH:O	4:E:373:HOH:O[1_455]	2.08	0.12
4:C:452:HOH:O	4:G:443:HOH:O[3_555]	2.13	0.07
1:A:138:GLU:OE2	4:E:354:HOH:O[4_475]	2.14	0.06

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	155/171 (91%)	151 (97%)	4 (3%)	0	100 100
1	C	156/171 (91%)	150 (96%)	6 (4%)	0	100 100
1	E	157/171 (92%)	151 (96%)	6 (4%)	0	100 100
1	G	163/171 (95%)	157 (96%)	6 (4%)	0	100 100
2	B	72/81 (89%)	67 (93%)	4 (6%)	1 (1%)	11 5
2	D	72/81 (89%)	68 (94%)	3 (4%)	1 (1%)	11 5
2	F	72/81 (89%)	71 (99%)	1 (1%)	0	100 100
2	H	44/81 (54%)	40 (91%)	2 (4%)	2 (4%)	2 0
All	All	891/1008 (88%)	855 (96%)	32 (4%)	4 (0%)	29 30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	58	SER
2	H	42	GLY
2	D	57	ALA
2	H	25	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	147/151 (97%)	145 (99%)	2 (1%)	67 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	148/151 (98%)	147 (99%)	1 (1%)	84 88
1	E	149/151 (99%)	147 (99%)	2 (1%)	69 74
1	G	152/151 (101%)	150 (99%)	2 (1%)	69 74
2	B	64/67 (96%)	63 (98%)	1 (2%)	62 67
2	D	64/67 (96%)	63 (98%)	1 (2%)	62 67
2	F	65/67 (97%)	64 (98%)	1 (2%)	65 69
2	H	41/67 (61%)	34 (83%)	7 (17%)	2 1
All	All	830/872 (95%)	813 (98%)	17 (2%)	53 58

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	127	LEU
2	B	48	GLU
1	C	19	GLU
2	D	38	LEU
1	E	127	LEU
1	E	164	LEU
2	F	48	GLU
1	G	61	ARG
1	G	124	THR
2	H	24	LYS
2	H	27	LEU
2	H	39	LYS
2	H	48	GLU
2	H	53	THR
2	H	71	ASP
2	H	75	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	29	HIS

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

7 ligands are 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	SO4	G	203	-	4,4,4	0.15	0	6,6,6	0.49	0
3	SO4	C	201	-	4,4,4	0.27	0	6,6,6	0.48	0
3	SO4	A	201	-	4,4,4	0.15	0	6,6,6	0.30	0
3	SO4	G	202	-	4,4,4	0.18	0	6,6,6	0.29	0
3	SO4	C	202	-	4,4,4	0.19	0	6,6,6	0.27	0
3	SO4	G	201	-	4,4,4	0.20	0	6,6,6	0.34	0
3	SO4	A	202	-	4,4,4	0.13	0	6,6,6	0.16	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	203	SO4	1	0
3	G	202	SO4	1	0
3	C	202	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

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^{th} 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	154/171 (90%)	0.11	5 (3%) 47 46	2, 9, 23, 40	0
1	C	154/171 (90%)	0.06	2 (1%) 77 76	3, 11, 24, 42	0
1	E	154/171 (90%)	0.21	5 (3%) 47 46	5, 11, 24, 41	0
1	G	160/171 (93%)	0.34	6 (3%) 40 39	5, 13, 27, 39	0
2	B	73/81 (90%)	0.59	5 (6%) 17 16	6, 20, 35, 45	0
2	D	73/81 (90%)	1.02	12 (16%) 1 1	13, 29, 40, 43	0
2	F	73/81 (90%)	0.29	3 (4%) 37 36	6, 15, 29, 40	0
2	H	49/81 (60%)	2.49	28 (57%) 0 0	21, 40, 57, 62	0
All	All	890/1008 (88%)	0.42	66 (7%) 14 13	2, 13, 39, 62	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	27	LEU	11.1
2	B	60	SER	8.2
2	B	59	GLY	5.6
2	D	53	THR	5.4
2	F	58	SER	5.1
2	H	29	HIS	4.8
2	H	30	LEU	4.8
2	F	61	GLN	4.5
2	H	26	ASN	4.3
2	H	43	PHE	4.1
2	D	60	SER	4.0
2	D	4	ASP	4.0
2	H	19	ILE	3.9
2	H	76	LYS	3.9
1	E	182	ASP	3.9
2	D	66	SER	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	58	SER	3.8
1	A	153	ALA	3.7
2	F	60	SER	3.5
2	H	25	SER	3.4
2	H	31	TYR	3.4
2	H	75	LEU	3.4
1	G	183	GLY	3.3
2	H	42	GLY	3.3
2	D	52	LEU	3.3
2	H	40	VAL	3.3
2	H	38	LEU	3.3
2	H	36	ASN	3.2
2	H	51	PHE	3.2
2	B	52	LEU	3.2
2	H	74	TYR	3.0
2	H	70	GLY	3.0
2	H	33	SER	3.0
1	A	116	ILE	2.8
1	C	126	ASN	2.8
1	G	104	ASP	2.8
1	A	182	ASP	2.7
2	D	65	THR	2.7
2	H	35	GLN	2.7
2	H	44	GLY	2.7
2	H	37	ALA	2.7
1	G	125	GLY	2.6
2	D	24	LYS	2.6
2	H	45	LEU	2.6
1	G	83[A]	ARG	2.6
2	H	50	ASN	2.6
1	C	117	ASP	2.5
2	D	47	LYS	2.5
1	A	126	ASN	2.5
1	E	117	ASP	2.4
2	H	52	LEU	2.4
2	D	7	LEU	2.3
2	B	57	ALA	2.3
2	H	18	ARG	2.3
2	H	47	LYS	2.3
2	H	48	GLU	2.3
1	G	124	THR	2.3
1	G	126	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	154	ALA	2.2
1	E	154	ALA	2.2
2	D	64	GLY	2.1
2	D	5	LYS	2.1
1	E	116	ILE	2.0
2	D	50	ASN	2.0
1	E	112	ARG	2.0
2	H	46	PHE	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^{th} 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	G	202	5/5	0.93	0.17	29,30,35,38	0
3	SO4	C	202	5/5	0.96	0.15	22,24,29,31	0
3	SO4	G	203	5/5	0.98	0.12	12,12,16,18	0
3	SO4	C	201	5/5	0.98	0.10	6,9,11,11	0
3	SO4	A	201	5/5	0.99	0.12	7,9,11,16	0
3	SO4	G	201	5/5	0.99	0.08	13,15,17,23	0
3	SO4	A	202	5/5	0.99	0.08	17,18,21,22	0

6.5 Other polymers (i)

There are no such residues in this entry.