Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:46 pm BST

PDB ID	:	5ONA
Title	:	Drosophila Bag-of-marbles CBM peptide bound to human CAF40-CNOT1
Authors	:	Raisch, T.; Sgromo, A.; Backhaus, C.; Izaurralde, E.; Weichenrieder, O.
Deposited on	:	2017-08-03
Resolution	:	2.70 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:

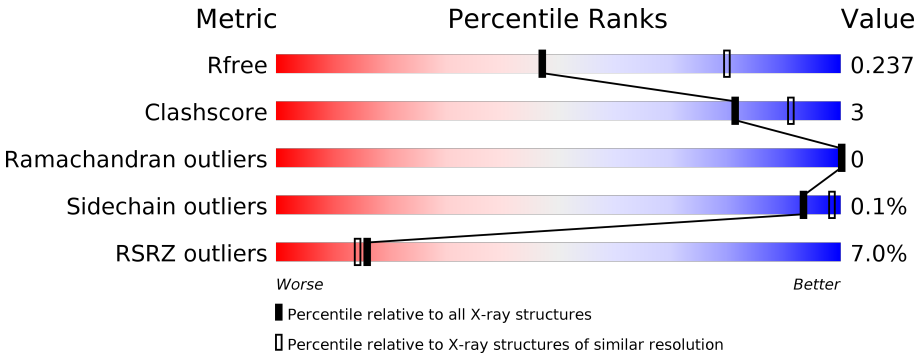
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	244	91% 5%
1	D	244	22% 87% 9%
2	B	273	3% 93% 7%
2	E	273	3% 92% 7%
3	C	24	88% 8%
3	F	24	8% 71% 17% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8481 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 CCR4-NOT transcription complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1866	1163	340	345	18			
1	D	234	Total	C	N	O	S	0	0	0
			1849	1154	335	342	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1345	GLY	-	expression tag	UNP A5YKK6
A	1346	PRO	-	expression tag	UNP A5YKK6
A	1347	HIS	-	expression tag	UNP A5YKK6
A	1348	MET	-	expression tag	UNP A5YKK6
A	1349	LEU	-	expression tag	UNP A5YKK6
A	1350	GLU	-	expression tag	UNP A5YKK6
D	1345	GLY	-	expression tag	UNP A5YKK6
D	1346	PRO	-	expression tag	UNP A5YKK6
D	1347	HIS	-	expression tag	UNP A5YKK6
D	1348	MET	-	expression tag	UNP A5YKK6
D	1349	LEU	-	expression tag	UNP A5YKK6
D	1350	GLU	-	expression tag	UNP A5YKK6

- Molecule 2 is a protein called CCR4-NOT transcription complex subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	273	Total	C	N	O	S	0	0	0
			2182	1398	376	397	11			
2	E	271	Total	C	N	O	S	0	0	0
			2171	1391	374	395	11			

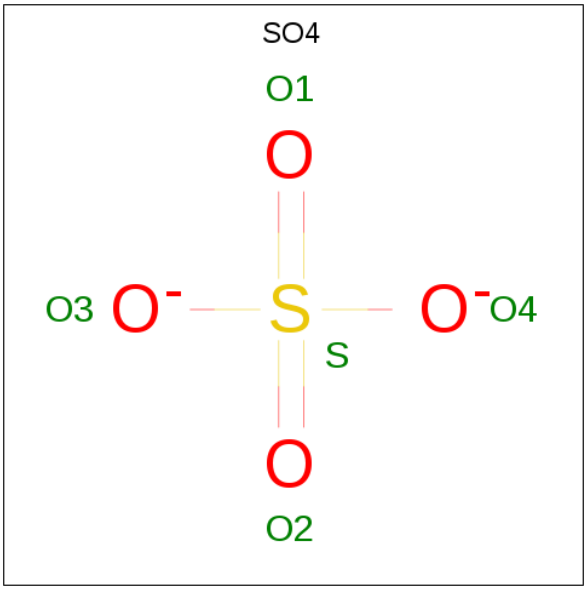
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	GLY	-	expression tag	UNP Q92600
B	14	PRO	-	expression tag	UNP Q92600
B	15	HIS	-	expression tag	UNP Q92600
B	16	MET	-	expression tag	UNP Q92600
B	17	LEU	-	expression tag	UNP Q92600
B	18	GLU	-	expression tag	UNP Q92600
E	13	GLY	-	expression tag	UNP Q92600
E	14	PRO	-	expression tag	UNP Q92600
E	15	HIS	-	expression tag	UNP Q92600
E	16	MET	-	expression tag	UNP Q92600
E	17	LEU	-	expression tag	UNP Q92600
E	18	GLU	-	expression tag	UNP Q92600

- Molecule 3 is a protein called Protein bag-of-marbles.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	22	Total	C	N	O	S	0	0	0
			182	111	31	38	2			
3	F	21	Total	C	N	O	S	0	0	0
			174	107	30	35	2			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

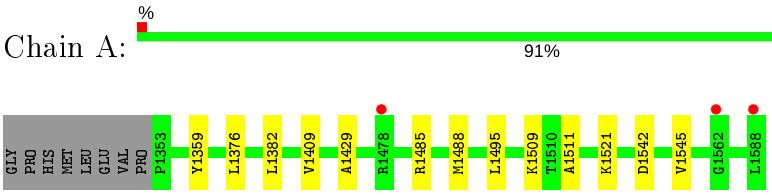
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0

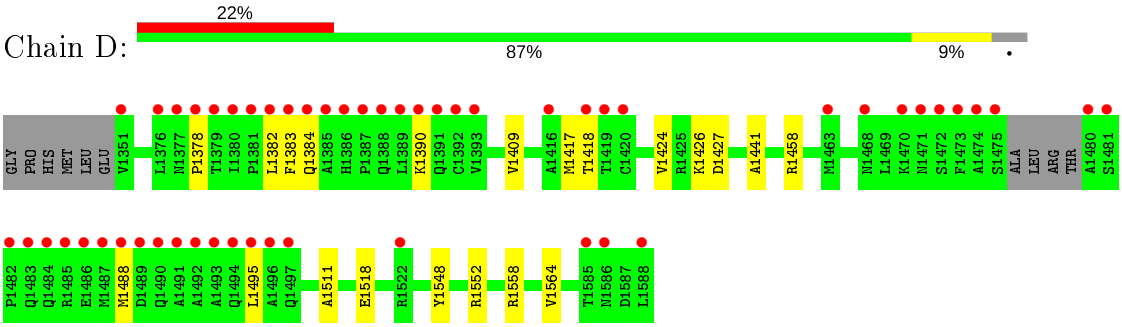
3 Residue-property plots (i)

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.

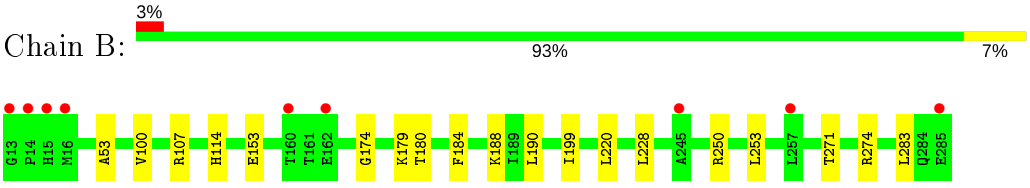
- Molecule 1: CCR4-NOT transcription complex subunit 1



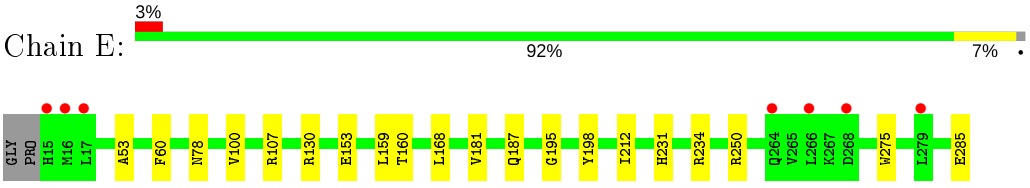
- Molecule 1: CCR4-NOT transcription complex subunit 1



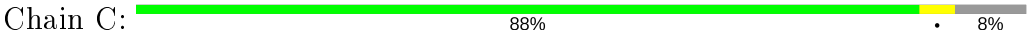
- Molecule 2: CCR4-NOT transcription complex subunit 9

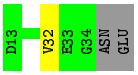


- Molecule 2: CCR4-NOT transcription complex subunit 9



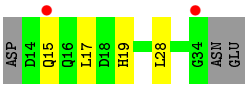
- Molecule 3: Protein bag-of-marbles





• Molecule 3: Protein bag-of-marbles

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.60Å 106.60Å 263.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.41 – 2.70 49.41 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.41-2.70) 99.9 (49.41-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.209 , 0.237 0.209 , 0.237	Depositor DCC
R_{free} test set	2307 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	72.4	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8481	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, CL

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	0.24	0/1900	0.39	0/2567
1	D	0.23	0/1883	0.37	0/2545
2	B	0.24	0/2226	0.38	0/3023
2	E	0.23	0/2214	0.37	0/3006
3	C	0.24	0/184	0.32	0/245
3	F	0.23	0/176	0.31	0/234
All	All	0.24	0/8583	0.37	0/11620

There are no bond length outliers.

There are no bond angle outliers.

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	1866	0	1877	8	0
1	D	1849	0	1855	14	0
2	B	2182	0	2252	11	0
2	E	2171	0	2243	14	0
3	C	182	0	163	2	0
3	F	174	0	159	3	0
4	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	0	1	0
4	D	10	0	0	2	0
4	E	5	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
All	All	8481	0	8549	45	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 3.

All (45) 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)
2:B:107:ARG:NH1	2:B:153:GLU:OE2	2.27	0.67
1:D:1382:LEU:HD22	1:D:1488:MET:HA	1.83	0.60
2:E:181:VAL:HG21	3:F:28:LEU:HD13	1.85	0.59
2:E:187:GLN:OE1	2:E:231:HIS:ND1	2.36	0.59
2:B:250:ARG:NH2	4:B:303:SO4:O4	2.37	0.58
2:B:184:PHE:HB2	3:C:32:VAL:HG13	1.86	0.58
2:B:174:GLY:O	2:B:179:LYS:NZ	2.32	0.56
2:E:250:ARG:NH1	2:E:285:GLU:OE2	2.39	0.55
2:B:180:THR:HG22	3:C:32:VAL:HG11	1.88	0.55
1:D:1409:VAL:HG22	1:D:1511:ALA:HB2	1.90	0.54
1:A:1542:ASP:HB3	1:A:1545:VAL:HB	1.91	0.52
1:D:1418:THR:OG1	4:D:1602:SO4:O3	2.27	0.51
2:B:220:LEU:HD21	2:B:228:LEU:HD23	1.92	0.51
1:D:1378:PRO:O	1:D:1384:GLN:NE2	2.45	0.50
2:E:130:ARG:HG2	3:F:17:LEU:HD21	1.94	0.48
1:D:1426:LYS:NZ	1:D:1427:ASP:OD1	2.43	0.48
2:E:53:ALA:HB1	2:E:100:VAL:HA	1.95	0.48
1:A:1359:TYR:CZ	1:A:1509:LYS:HG3	2.49	0.48
1:A:1409:VAL:HG22	1:A:1511:ALA:HB2	1.96	0.47
1:D:1417:MET:HE3	1:D:1518:GLU:HB3	1.96	0.47
1:D:1424:VAL:HG11	1:D:1441:ALA:HB2	1.97	0.47
2:E:168:LEU:HB3	2:E:212:ILE:HG13	1.96	0.47
1:D:1458:ARG:NH1	2:E:78:ASN:O	2.48	0.46
2:B:271:THR:HG22	2:B:274:ARG:HH12	1.80	0.46
3:F:15:GLN:O	3:F:19:HIS:ND1	2.49	0.46
1:A:1521:LYS:HE3	2:E:160:THR:OG1	2.16	0.45
1:D:1383:PHE:HZ	1:D:1495:LEU:HD11	1.82	0.45
2:E:107:ARG:NH1	2:E:153:GLU:OE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:ALA:HB1	2:B:100:VAL:HA	1.99	0.44
1:A:1376:LEU:HD12	1:A:1495:LEU:HD21	1.99	0.44
2:E:234:ARG:HD3	2:E:275:TRP:CE3	2.53	0.43
2:E:159:LEU:HD11	2:E:195:GLY:HA2	2.00	0.43
1:D:1383:PHE:HB3	1:D:1390:LYS:HE2	2.00	0.43
1:A:1429:ALA:HB3	1:A:1545:VAL:HG11	2.00	0.43
1:A:1485:ARG:HA	1:A:1488:MET:HE2	2.02	0.42
2:E:234:ARG:HD3	2:E:275:TRP:CD2	2.54	0.42
1:D:1548:TYR:CE2	1:D:1552:ARG:HD3	2.55	0.42
1:D:1558:ARG:NH2	4:D:1601:SO4:O2	2.32	0.41
1:D:1564:VAL:HG21	2:E:60:PHE:CZ	2.55	0.41
2:B:188:LYS:HA	2:B:188:LYS:HD2	1.86	0.41
1:D:1424:VAL:HG21	1:D:1441:ALA:HA	2.02	0.41
2:E:159:LEU:HD22	2:E:198:TYR:CD2	2.56	0.41
2:B:190:LEU:HD21	2:B:199:ILE:HD12	2.03	0.40
1:A:1382:LEU:HD22	1:A:1488:MET:HA	2.02	0.40
2:B:253:LEU:HD22	2:B:283:LEU:HD12	2.03	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	234/244 (96%)	231 (99%)	3 (1%)	0	100	100
1	D	230/244 (94%)	228 (99%)	2 (1%)	0	100	100
2	B	271/273 (99%)	268 (99%)	3 (1%)	0	100	100
2	E	269/273 (98%)	266 (99%)	3 (1%)	0	100	100
3	C	20/24 (83%)	19 (95%)	1 (5%)	0	100	100
3	F	19/24 (79%)	19 (100%)	0	0	100	100
All	All	1043/1082 (96%)	1031 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	203/210 (97%)	203 (100%)	0	100 100
1	D	202/210 (96%)	202 (100%)	0	100 100
2	B	246/246 (100%)	245 (100%)	1 (0%)	91 97
2	E	245/246 (100%)	245 (100%)	0	100 100
3	C	20/22 (91%)	20 (100%)	0	100 100
3	F	19/22 (86%)	19 (100%)	0	100 100
All	All	935/956 (98%)	934 (100%)	1 (0%)	93 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	114	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
4	SO4	A	1601	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	B	303	2	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	304	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	1603	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	1604	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	1602	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	D	1601	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	E	301	-	4,4,4	0.15	0	6,6,6	0.08	0
4	SO4	A	1602	-	4,4,4	0.15	0	6,6,6	0.06	0
4	SO4	B	302	-	4,4,4	0.13	0	6,6,6	0.05	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
4	B	303	SO4	1	0
4	D	1602	SO4	1	0
4	D	1601	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	236/244 (96%)	0.17	3 (1%) 77 78	52, 77, 123, 171	0
1	D	234/244 (95%)	1.19	53 (22%) 0 0	75, 108, 206, 239	0
2	B	273/273 (100%)	0.20	9 (3%) 46 46	53, 75, 112, 193	0
2	E	271/273 (99%)	0.40	7 (2%) 56 57	78, 98, 144, 186	0
3	C	22/24 (91%)	0.11	0 100 100	67, 80, 118, 142	0
3	F	21/24 (87%)	0.71	2 (9%) 8 6	104, 117, 146, 179	0
All	All	1057/1082 (97%)	0.47	74 (7%) 16 14	52, 88, 166, 239	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1385	ALA	8.7
1	D	1488	MET	7.1
1	D	1483	GLN	6.9
1	D	1393	VAL	6.8
3	F	34	GLY	6.7
1	D	1482	PRO	6.4
1	D	1490	GLN	6.3
1	D	1383	PHE	6.2
1	D	1389	LEU	5.8
1	D	1473	PHE	5.7
1	D	1487	MET	5.5
1	D	1376	LEU	5.3
1	D	1377	ASN	5.0
1	D	1495	LEU	5.0
1	D	1493	ALA	5.0
1	D	1486	GLU	4.8
1	D	1492	ALA	4.7
2	E	15	HIS	4.5
1	D	1381	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	1588	LEU	4.5
1	D	1471	ASN	4.5
1	D	1472	SER	4.4
2	E	17	LEU	4.4
1	D	1382	LEU	4.4
1	D	1475	SER	4.3
1	D	1474	ALA	4.3
1	D	1378	PRO	4.3
1	D	1391	GLN	4.2
1	D	1379	THR	4.2
1	D	1380	ILE	4.2
1	D	1386	HIS	4.1
1	D	1390	LYS	4.0
1	D	1484	GLN	3.9
1	A	1562	GLY	3.8
2	E	16	MET	3.7
1	D	1491	ALA	3.7
2	B	16	MET	3.7
1	D	1481	SER	3.6
2	B	14	PRO	3.6
2	B	15	HIS	3.3
1	D	1489	ASP	3.3
1	D	1463	MET	3.1
1	D	1496	ALA	3.1
1	A	1478	ARG	3.1
2	E	264	GLN	3.1
1	D	1468	ASN	3.1
1	D	1384	GLN	3.0
2	B	285	GLU	3.0
1	D	1387	PRO	2.9
1	D	1485	ARG	2.9
2	B	245	ALA	2.8
1	D	1418	THR	2.7
2	E	279	LEU	2.7
1	A	1588	LEU	2.6
2	B	160	THR	2.6
1	D	1586	ASN	2.5
1	D	1497	GLN	2.5
2	B	257	LEU	2.5
1	D	1388	GLN	2.5
1	D	1416	ALA	2.5
1	D	1392	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	268	ASP	2.5
3	F	15	GLN	2.4
1	D	1480	ALA	2.4
1	D	1585	THR	2.3
1	D	1522	ARG	2.3
1	D	1419	THR	2.3
1	D	1470	LYS	2.3
2	B	13	GLY	2.3
1	D	1420	CYS	2.2
1	D	1351	VAL	2.2
2	E	266	LEU	2.1
2	B	162	GLU	2.1
1	D	1494	GLN	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
5	CL	C	101	1/1	0.74	0.16	102,102,102,102	0
4	SO4	A	1603	5/5	0.81	0.78	175,175,176,176	0
4	SO4	A	1604	5/5	0.81	0.21	184,185,186,186	0
4	SO4	B	303	5/5	0.82	0.28	122,128,132,133	0
4	SO4	D	1602	5/5	0.83	0.54	160,162,163,164	0
4	SO4	B	304	5/5	0.83	0.27	173,173,174,175	0
5	CL	A	1605	1/1	0.84	0.14	114,114,114,114	0
4	SO4	A	1602	5/5	0.87	0.62	146,147,148,150	0
4	SO4	A	1601	5/5	0.89	0.17	138,138,143,143	5
4	SO4	B	301	5/5	0.91	0.31	131,132,132,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	E	301	5/5	0.95	0.13	100,102,108,118	0
4	SO4	D	1601	5/5	0.96	0.15	164,167,168,168	5
4	SO4	B	302	5/5	0.96	0.12	131,133,134,135	0

6.5 Other polymers (i)

There are no such residues in this entry.