Worldwide PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:11 am BST

PDB ID	:	1EF1
Title	:	CRYSTAL STRUCTURE OF THE MOESIN FERM DOMAIN/TAIL DO-MAIN COMPLEX
Authors	:	Pearson, M.A.; Reczek, D.; Bretscher, A.; Karplus, P.A.
Deposited on	:	2000-02-04
Resolution	:	1.90 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 1.90 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.
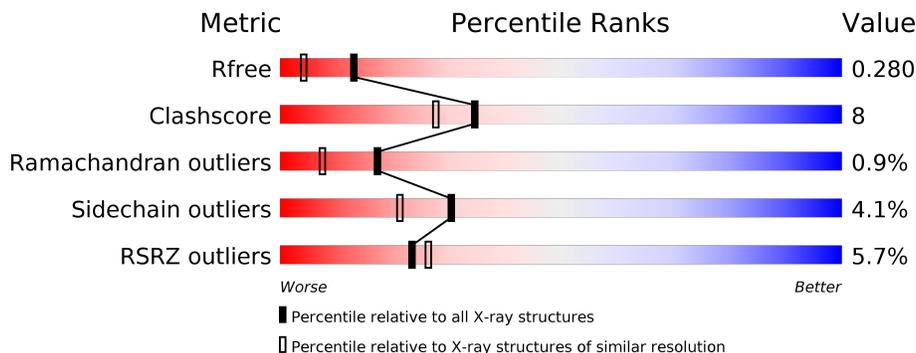
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	294	
1	B	294	
2	C	90	
2	D	90	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6688 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 MOESIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	Se	0	0	0
			2429	1570	415	437	2	5			
1	B	294	Total	C	N	O	S	Se	0	0	0
			2429	1570	415	437	2	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MSE	MET	MODIFIED RESIDUE	UNP P26038
A	182	MSE	MET	MODIFIED RESIDUE	UNP P26038
A	200	MSE	MET	MODIFIED RESIDUE	UNP P26038
A	285	MSE	MET	MODIFIED RESIDUE	UNP P26038
A	292	MSE	MET	MODIFIED RESIDUE	UNP P26038
B	12	MSE	MET	MODIFIED RESIDUE	UNP P26038
B	182	MSE	MET	MODIFIED RESIDUE	UNP P26038
B	200	MSE	MET	MODIFIED RESIDUE	UNP P26038
B	285	MSE	MET	MODIFIED RESIDUE	UNP P26038
B	292	MSE	MET	MODIFIED RESIDUE	UNP P26038

- Molecule 2 is a protein called MOESIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	90	Total	C	N	O	Se	0	0	0
			704	419	136	146	3			
2	D	90	Total	C	N	O	Se	0	0	0
			704	419	136	146	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	543	MSE	MET	MODIFIED RESIDUE	UNP P26038
C	549	MSE	MET	MODIFIED RESIDUE	UNP P26038

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Chain	Residue	Modelled	Actual	Comment	Reference
C	577	MSE	MET	MODIFIED RESIDUE	UNP P26038
D	543	MSE	MET	MODIFIED RESIDUE	UNP P26038
D	549	MSE	MET	MODIFIED RESIDUE	UNP P26038
D	577	MSE	MET	MODIFIED RESIDUE	UNP P26038

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
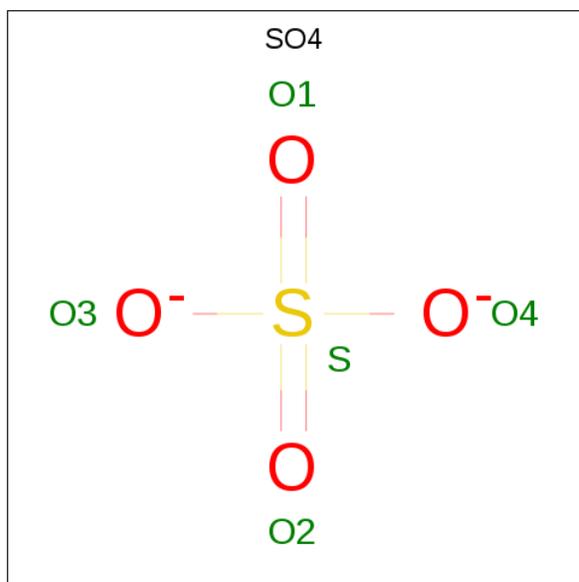
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	145	Total O 145 145	0	0
4	C	59	Total O 59 59	0	0
4	B	145	Total O 145 145	0	0
4	D	63	Total O 63 63	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: MOESIN

Chain A:

- Molecule 1: MOESIN

Chain B:

- Molecule 2: MOESIN

Chain C:

- Molecule 2: MOESIN

Chain D:
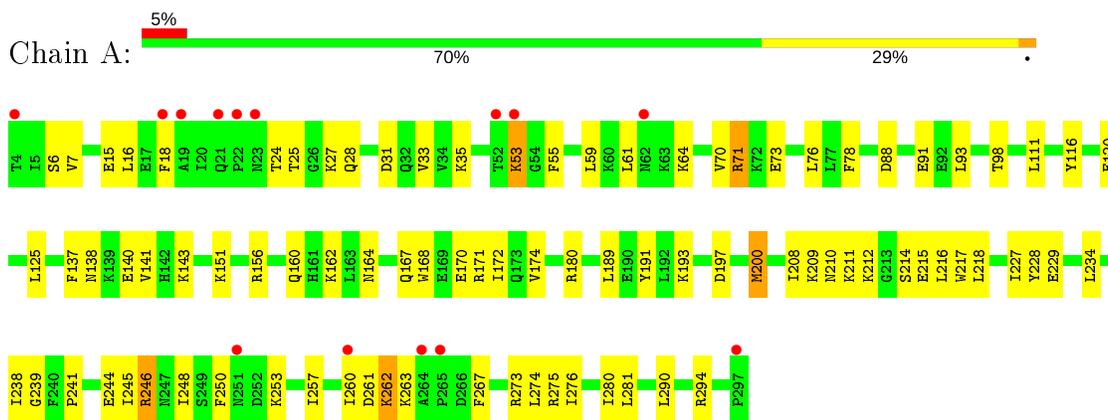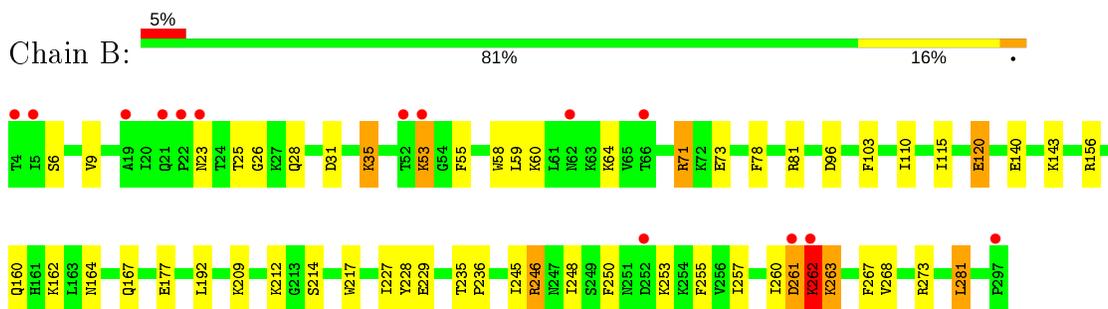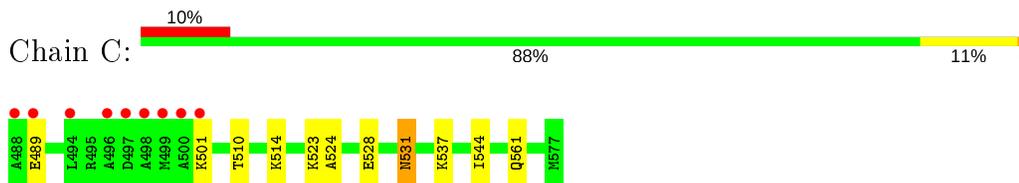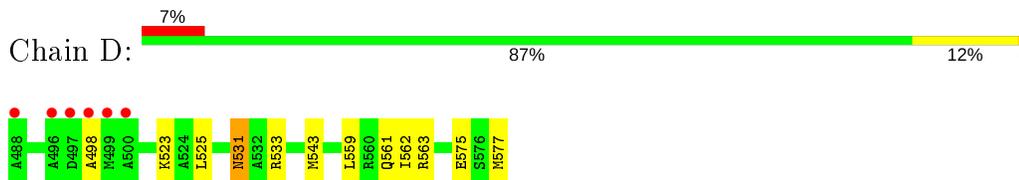
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	54.20Å 153.30Å 112.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 27.57 – 1.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 87.0 (27.57-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 1.79Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.227 , 0.287 0.225 , 0.280	Depositor DCC
R_{free} test set	3923 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.0	EDS
L-test for twinning[2]	$< |L| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6688	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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 46.88 % 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 1.0750e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

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	0.79	1/2481 (0.0%)	0.84	1/3341 (0.0%)
1	B	0.76	0/2481	0.85	1/3341 (0.0%)
2	C	0.73	0/704	0.86	0/932
2	D	0.79	0/704	0.84	0/932
All	All	0.77	1/6370 (0.0%)	0.85	2/8546 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	MSE	SE-CE	-9.56	1.39	1.95

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	81	ARG	NE-CZ-NH2	-5.51	117.54	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2429	0	2429	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2429	0	2429	36	0
2	C	704	0	682	5	0
2	D	704	0	682	10	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	145	0	0	1	0
4	B	145	0	0	1	0
4	C	59	0	0	4	0
4	D	63	0	0	2	0
All	All	6688	0	6222	104	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 8.

All (104) 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:246:ARG:HB3	1:A:260:ILE:HG12	1.40	1.03
1:B:246:ARG:HB3	1:B:260:ILE:HG12	1.49	0.92
1:B:246:ARG:HB2	1:B:246:ARG:HH11	1.38	0.88
1:B:263:LYS:HA	1:B:263:LYS:HE3	1.59	0.84
1:B:162:LYS:HD2	4:D:1748:HOH:O	1.82	0.80
1:B:156:ARG:O	1:B:160:GLN:HG3	1.83	0.78
1:A:116:TYR:HB3	1:A:200:MSE:HE3	1.67	0.77
1:B:246:ARG:HB2	1:B:246:ARG:NH1	2.02	0.72
2:C:531:ASN:HB2	4:C:772:HOH:O	1.90	0.71
2:C:524:ALA:O	2:C:528:GLU:HG3	1.93	0.69
1:A:200:MSE:HE2	1:A:234:LEU:HD12	1.75	0.68
1:A:156:ARG:O	1:A:160:GLN:HG3	1.95	0.65
1:A:262:LYS:NZ	1:A:263:LYS:HE2	2.11	0.65
1:A:25:THR:HA	1:A:64:LYS:HA	1.79	0.64
1:A:246:ARG:NH1	1:A:246:ARG:HB2	2.13	0.64
1:A:253:LYS:HZ1	1:A:273:ARG:HH11	1.47	0.62
1:A:164:ASN:OD1	1:A:167:GLN:HG3	1.98	0.62
1:A:273:ARG:NH1	1:A:274:LEU:H	1.98	0.61
2:D:531:ASN:HB2	4:D:1772:HOH:O	2.00	0.61
1:A:246:ARG:HH11	1:A:246:ARG:HB2	1.65	0.61
1:B:164:ASN:OD1	1:B:167:GLN:HG3	2.00	0.61
1:B:25:THR:HA	1:B:64:LYS:HA	1.83	0.61
1:B:31:ASP:O	1:B:35:LYS:HB2	2.01	0.61
1:A:25:THR:OG1	1:A:28:GLN:HG3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:PHE:O	1:B:268:VAL:HG13	2.02	0.59
1:B:53:LYS:HB2	1:B:55:PHE:CD1	2.37	0.59
1:A:241:PRO:HG2	1:A:244:GLU:HG3	1.84	0.59
1:A:59:LEU:HD13	1:A:78:PHE:CE2	2.39	0.58
1:A:59:LEU:HD13	1:A:78:PHE:HE2	1.68	0.58
1:B:53:LYS:HB2	1:B:55:PHE:HD1	1.69	0.57
1:A:290:LEU:O	1:A:294:ARG:HG3	2.05	0.57
1:A:189:LEU:O	1:A:193:LYS:HG3	2.05	0.56
1:A:262:LYS:HZ2	1:A:263:LYS:HE2	1.69	0.56
1:A:200:MSE:HE2	1:A:234:LEU:CD1	2.36	0.56
1:B:212:LYS:HE2	2:D:575:GLU:O	2.06	0.56
1:A:168:TRP:O	1:A:172:ILE:HG12	2.07	0.55
1:A:93:LEU:HD22	1:A:98:THR:HG22	1.89	0.55
1:A:71:ARG:O	1:A:73:GLU:HG2	2.08	0.54
2:C:510:THR:O	2:C:514:LYS:HG2	2.08	0.54
1:A:162:LYS:HD2	4:C:748:HOH:O	2.08	0.53
1:A:245:ILE:HD12	1:A:257:ILE:CG2	2.38	0.53
1:B:160:GLN:OE1	2:D:533:ARG:NH2	2.42	0.53
1:A:116:TYR:CB	1:A:200:MSE:HE3	2.37	0.53
1:B:248:ILE:HG22	1:B:257:ILE:HG12	1.90	0.52
1:A:246:ARG:HB3	1:A:260:ILE:CG1	2.27	0.52
1:A:171:ARG:HG2	4:C:613:HOH:O	2.09	0.51
1:A:31:ASP:O	1:A:35:LYS:HB2	2.11	0.51
1:B:59:LEU:HD13	1:B:78:PHE:CE2	2.46	0.51
1:B:59:LEU:HD13	1:B:78:PHE:HE2	1.75	0.51
1:A:7:VAL:HG22	1:A:76:LEU:HB2	1.93	0.50
1:B:140:GLU:O	1:B:143:LYS:HE2	2.11	0.50
1:A:209:LYS:HA	1:A:214:SER:O	2.11	0.50
1:A:137:PHE:O	1:A:180:ARG:NH2	2.43	0.50
1:B:209:LYS:HA	1:B:214:SER:O	2.11	0.49
1:A:210:ASN:ND2	1:A:214:SER:HB2	2.26	0.49
2:C:537:LYS:HE3	4:C:788:HOH:O	2.11	0.49
1:A:53:LYS:HB2	1:A:55:PHE:HD1	1.78	0.48
1:B:103:PHE:HA	1:B:192:LEU:HD21	1.94	0.48
1:A:138:ASN:ND2	1:A:141:VAL:HG23	2.29	0.48
1:A:210:ASN:OD1	1:A:212:LYS:HG3	2.14	0.48
1:B:120:GLU:CD	1:B:120:GLU:H	2.16	0.47
1:A:120:GLU:H	1:A:120:GLU:CD	2.17	0.47
1:A:250:PHE:HE1	1:A:274:LEU:HD11	1.79	0.47
1:B:217:TRP:HB2	1:B:228:TYR:HB2	1.96	0.47
1:B:58:TRP:O	1:B:60:LYS:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:HA	1:A:28:GLN:OE1	2.15	0.47
1:A:125:LEU:HB3	1:A:191:TYR:CE1	2.50	0.46
1:A:170:GLU:O	1:A:174:VAL:HG23	2.15	0.46
1:B:253:LYS:HE3	1:B:273:ARG:HA	1.97	0.46
1:B:261:ASP:CG	1:B:262:LYS:H	2.20	0.46
4:B:1771:HOH:O	2:D:533:ARG:HG2	2.16	0.46
2:D:559:LEU:O	2:D:563:ARG:HG3	2.16	0.46
1:B:9:VAL:HG22	1:B:78:PHE:HB2	1.98	0.45
1:A:290:LEU:HD22	4:A:696:HOH:O	2.16	0.45
1:B:25:THR:OG1	1:B:28:GLN:HG3	2.15	0.45
1:A:208:ILE:HD13	1:A:218:LEU:HB2	1.97	0.45
1:B:26:GLY:HA2	1:B:59:LEU:HD21	1.97	0.45
1:A:111:LEU:HB3	1:A:151:LYS:HD3	1.97	0.44
1:A:140:GLU:O	1:A:143:LYS:HE2	2.16	0.44
1:B:235:THR:HA	1:B:236:PRO:HD2	1.79	0.44
1:A:245:ILE:HD12	1:A:257:ILE:HG21	1.98	0.44
1:A:15:GLU:O	1:A:16:LEU:HD23	2.18	0.44
1:A:263:LYS:HA	1:A:263:LYS:HD3	1.49	0.44
2:D:559:LEU:HA	2:D:559:LEU:HD12	1.79	0.43
2:C:544:ILE:HA	2:D:543:MSE:HE1	2.00	0.43
1:A:211:LYS:HB2	1:A:211:LYS:HE2	1.87	0.43
1:A:276:ILE:O	1:A:280:ILE:HG13	2.19	0.43
1:A:238:ILE:HG22	1:A:239:GLY:N	2.35	0.42
1:B:212:LYS:HE3	2:D:577:MSE:OXT	2.19	0.42
1:A:273:ARG:NH2	1:A:275:ARG:HB2	2.35	0.42
1:A:217:TRP:HB2	1:A:228:TYR:HB2	2.00	0.42
1:A:27:LYS:HB2	1:A:61:LEU:HB3	2.01	0.42
1:A:257:ILE:HD12	1:A:267:PHE:CD1	2.55	0.41
1:A:18:PHE:HE2	1:A:33:VAL:HG22	1.85	0.41
1:A:88:ASP:HB3	1:A:91:GLU:HG2	2.02	0.41
1:A:215:GLU:O	1:A:216:LEU:HD23	2.20	0.41
1:B:227:ILE:HD11	1:B:267:PHE:HZ	1.85	0.41
1:B:236:PRO:HG2	2:D:562:ILE:HD13	2.02	0.41
1:B:250:PHE:CE2	1:B:281:LEU:HD13	2.55	0.41
1:B:71:ARG:O	1:B:73:GLU:HG2	2.21	0.41
1:B:245:ILE:HD12	1:B:257:ILE:CG2	2.51	0.41
2:D:525:LEU:HD23	2:D:525:LEU:HA	1.88	0.41
1:B:110:ILE:HG13	1:B:115:ILE:HD12	2.02	0.40
1:A:227:ILE:HD11	1:A:267:PHE:HZ	1.85	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	292/294 (99%)	284 (97%)	6 (2%)	2 (1%)	22	12
1	B	292/294 (99%)	282 (97%)	7 (2%)	3 (1%)	15	6
2	C	88/90 (98%)	84 (96%)	3 (3%)	1 (1%)	14	5
2	D	88/90 (98%)	84 (96%)	3 (3%)	1 (1%)	14	5
All	All	760/768 (99%)	734 (97%)	19 (2%)	7 (1%)	17	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	ASP
1	A	262	LYS
1	B	261	ASP
1	B	71	ARG
1	B	262	LYS
2	C	501	LYS
2	D	498	ALA

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	261/260 (100%)	253 (97%)	8 (3%)	40	32
1	B	261/260 (100%)	249 (95%)	12 (5%)	27	17
2	C	71/73 (97%)	67 (94%)	4 (6%)	21	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	71/73 (97%)	68 (96%)	3 (4%)	30	20
All	All	664/666 (100%)	637 (96%)	27 (4%)	30	21

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	53	LYS
1	A	70	VAL
1	A	71	ARG
1	A	229	GLU
1	A	246	ARG
1	A	248	ILE
1	A	281	LEU
2	C	489	GLU
2	C	523	LYS
2	C	531	ASN
2	C	561	GLN
1	B	6	SER
1	B	23	ASN
1	B	35	LYS
1	B	53	LYS
1	B	96	ASP
1	B	120	GLU
1	B	177	GLU
1	B	229	GLU
1	B	246	ARG
1	B	262	LYS
1	B	263	LYS
1	B	281	LEU
2	D	523	LYS
2	D	531	ASN
2	D	561	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	230	GLN
2	C	519	GLN
1	B	23	ASN

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Mol	Chain	Res	Type
1	B	112	ASN
1	B	230	GLN
2	D	519	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	A	2001	-	4,4,4	0.97	0	6,6,6	0.55	0
3	SO4	B	3001	-	4,4,4	0.63	0	6,6,6	1.24	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	3001	SO4	O4-S-O2	2.25	121.05	109.31

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 (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(Å²)	Q<0.9
1	A	289/294 (98%)	0.38	14 (4%)	30	33	15, 31, 62, 84	0
1	B	289/294 (98%)	0.20	14 (4%)	30	33	13, 26, 56, 79	0
2	C	87/90 (96%)	0.44	9 (10%)	6	7	13, 35, 78, 99	0
2	D	87/90 (96%)	0.23	6 (6%)	16	19	13, 26, 60, 80	0
All	All	752/768 (97%)	0.30	43 (5%)	23	26	13, 30, 62, 99	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	498	ALA	8.9
2	C	497	ASP	6.8
2	D	496	ALA	6.5
2	D	497	ASP	5.4
2	C	496	ALA	5.1
1	A	19	ALA	4.4
1	B	19	ALA	4.3
1	B	23	ASN	4.0
1	A	260	ILE	3.8
1	A	4	THR	3.8
2	D	498	ALA	3.7
1	B	21	GLN	3.7
1	B	261	ASP	3.6
1	A	21	GLN	3.5
2	C	488	ALA	3.5
2	C	499	MET	3.4
1	B	53	LYS	3.3
1	A	264	ALA	3.3
1	A	52	THR	3.2
2	D	500	ALA	3.1
2	C	500	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	499	MET	3.1
1	B	22	PRO	3.1
1	B	5	ILE	3.0
2	D	488	ALA	3.0
1	B	252	ASP	2.9
2	C	494	LEU	2.8
1	A	23	ASN	2.8
1	B	52	THR	2.7
1	B	4	THR	2.7
1	B	62	ASN	2.7
1	A	18	PHE	2.5
1	A	22	PRO	2.5
1	A	297	PRO	2.5
1	B	262	LYS	2.3
2	C	501	LYS	2.3
1	A	265	PRO	2.3
1	B	66	THR	2.2
2	C	489	GLU	2.2
1	B	297	PRO	2.1
1	A	62	ASN	2.0
1	A	251	ASN	2.0
1	A	53	LYS	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, 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	2001	5/5	0.98	0.07	26,31,32,34	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	SO4	B	3001	5/5	0.99	0.08	35,37,40,41	5

6.5 Other polymers (i)

There are no such residues in this entry.