Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2023 – 07:46 PM EDT

PDB ID	:	3GEW
Title	:	FaeE-FaeG chaperone-major pilin complex of F4 ad fimbriae
Authors	:	Van Molle, I.; Moonens, K.; Garcia-Pino, A.; Buts, L.; Bouckaert, J.; De Greve, H.
Deposited on	:	2009-02-26
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) 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	:	2.36
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)	:	2.36

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 2.00 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	Percentile Ranks	Value
Rfree		0.257
Clashscore		8
Ramachandran outliers		0.4%
Sidechain outliers		2.0%
RSRZ outliers		2.0%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures
◨ Percentile relative to X-ray structures of similar resolution
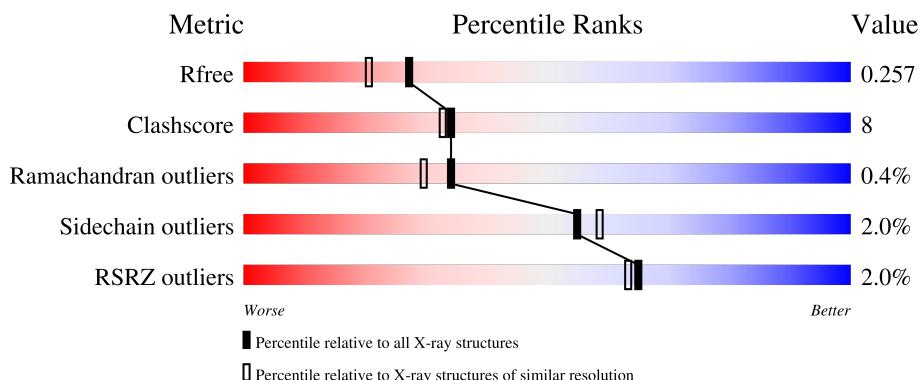
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	B	224	72% 17% 11%
1	C	224	2% / 80% 12% 7%
2	A	253	2% / 72% 12% • 15%
2	D	253	3% / 66% 19% • 14%

WORLDWIDE
wwPDB
PROTEIN DATA BANK
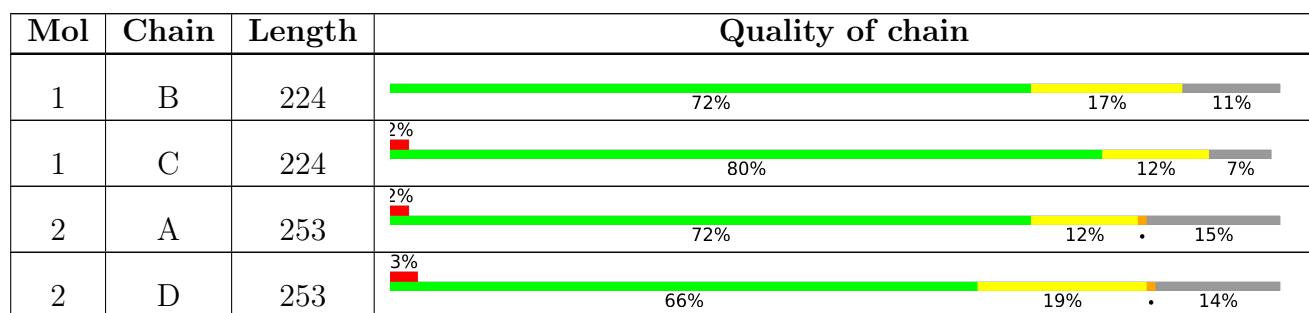
2　Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6440 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 Chaperone protein faeE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	199	Total 1477	C 946	N 247	O 280	S 4	0	0	0
1	C	208	Total 1564	C 995	N 270	O 295	S 4	0	0	0

- Molecule 2 is a protein called K88 fimbrial protein AD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	217	Total 1521	C 964	N 254	O 301	S 2	0	0	0
2	A	215	Total 1507	C 952	N 257	O 296	S 2	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	5	HIS	-	linker	UNP P14191
D	6	HIS	-	linker	UNP P14191
D	7	HIS	-	linker	UNP P14191
D	8	HIS	-	linker	UNP P14191
D	9	HIS	-	linker	UNP P14191
D	10	HIS	-	linker	UNP P14191
D	27	SER	ASN	SEE REMARK 999	UNP P14191
A	5	HIS	-	linker	UNP P14191
A	6	HIS	-	linker	UNP P14191
A	7	HIS	-	linker	UNP P14191
A	8	HIS	-	linker	UNP P14191
A	9	HIS	-	linker	UNP P14191
A	10	HIS	-	linker	UNP P14191
A	27	SER	ASN	SEE REMARK 999	UNP P14191

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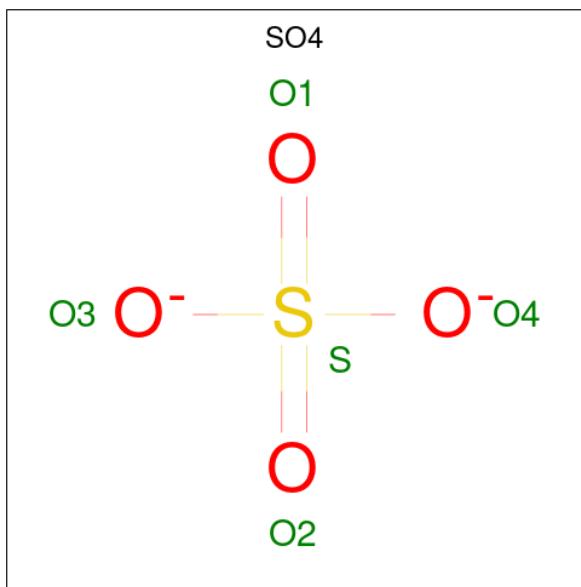
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	76	Total 76	O 76	0	0
5	C	96	Total 96	O 96	0	0
5	D	71	Total 71	O 71	0	0
5	A	56	Total 56	O 56	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Chaperone protein faeE
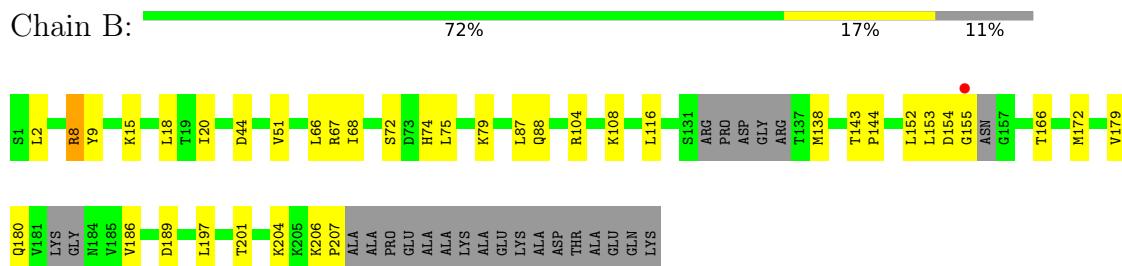
Chain B:

- Molecule 1: Chaperone protein faeE

Chain C:

- Molecule 2: K88 fimbrial protein AD

Chain D:

- Molecule 2: K88 fimbrial protein AD

Chain A:

TRP MET THR GLY HIS HIS HIS HIS HIS R11 K17 G24 S27 VAL L29 N30 D31 L32 T33 N34 G35 G45 R53 T60 P61 VAL THR SER GLY VAL ASP G68 G89 E92 Y97 V115 A131 L138 F139 A140 GLU GLY SER HIS ALA ILE F147

Y148 G149 G150 T153 E159 S164 T170 E171 S175 L176 S177 V188 N191 N197 V198 PRO GLY SER PHE ASN GLU ASN MET ALA TYR THR ASP GLY S212 V213 N224 T237 THR SER T240 Y253
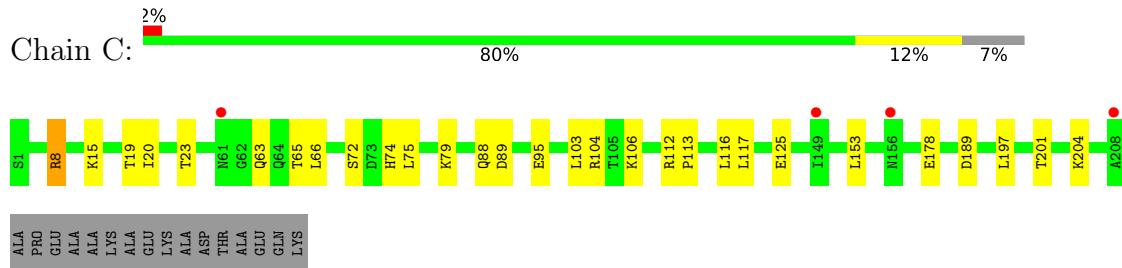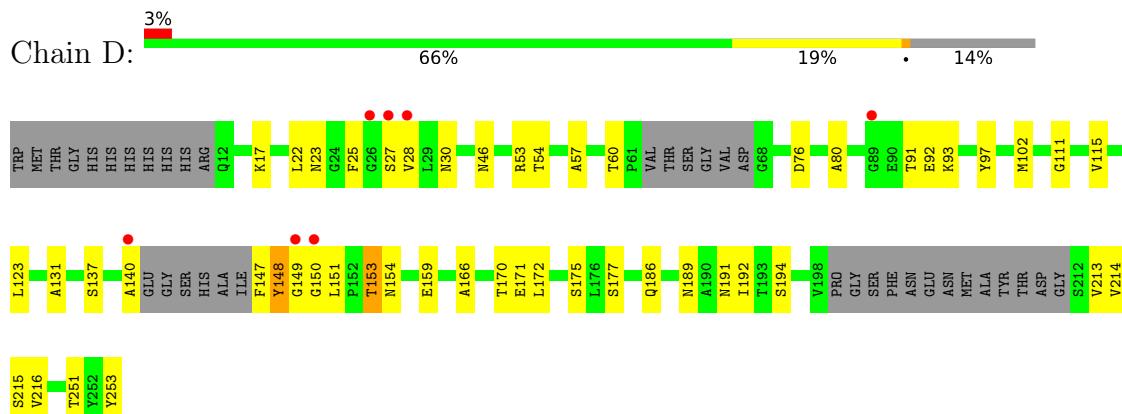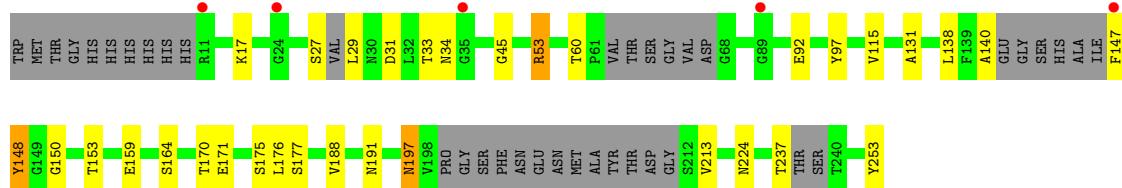
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.58Å 89.76Å 85.83Å 90.00° 113.94° 90.00°	Depositor
Resolution (Å)	17.89 – 2.00 17.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (17.89-2.00) 99.3 (17.89-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.261 0.223 , 0.257	Depositor DCC
R_{free} test set	3481 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 63.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6440	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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 48.29 % 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 8.7869e-05. 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, GOL

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	B	0.44	0/1502	0.63	2/2039 (0.1%)
1	C	0.49	0/1593	0.67	1/2166 (0.0%)
2	A	0.51	0/1529	0.59	1/2072 (0.0%)
2	D	0.54	0/1544	0.62	1/2098 (0.0%)
All	All	0.50	0/6168	0.63	5/8375 (0.1%)

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	D	1	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	15	LYS	O-C-N	-9.30	107.82	122.70
2	A	17	LYS	CD-CE-NZ	-7.36	94.77	111.70
2	D	148	TYR	N-CA-C	6.27	127.93	111.00
1	B	15	LYS	CA-C-N	5.88	130.14	117.20
1	C	15	LYS	O-C-N	-5.06	114.61	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	154	ASN	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	149	GLY	Peptide
2	D	153	THR	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	B	1477	0	1424	24	0
1	C	1564	0	1541	18	0
2	A	1507	0	1433	25	0
2	D	1521	0	1463	38	0
3	A	5	0	0	0	0
3	B	25	0	0	0	0
3	C	25	0	0	0	0
3	D	5	0	0	0	0
4	A	6	0	8	0	0
4	D	6	0	8	0	0
5	A	56	0	0	0	0
5	B	76	0	0	1	0
5	C	96	0	0	0	0
5	D	71	0	0	0	0
All	All	6440	0	5877	101	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 (101) 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:A:27:SER:C	2:A:29:LEU:N	2.08	1.07
2:D:123:LEU:HD13	2:D:216:VAL:HG22	1.37	1.03
2:A:45:GLY:H	2:A:224:ASN:HD22	1.18	0.87
2:D:147:PHE:O	2:D:148:TYR:CG	2.34	0.81
2:A:53:ARG:HH21	2:A:176:LEU:HD23	1.48	0.78
2:A:138:LEU:HD13	2:A:147:PHE:HE1	1.51	0.76
2:A:138:LEU:HD13	2:A:147:PHE:CE1	2.21	0.75
2:A:140:ALA:HB1	2:A:153:THR:HG22	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:45:GLY:H	2:A:224:ASN:ND2	1.86	0.72
1:C:23:THR:HG22	1:C:63:GLN:HG2	1.71	0.71
2:A:45:GLY:N	2:A:224:ASN:HD22	1.89	0.70
1:C:8:ARG:NH2	2:D:253:TYR:O	2.23	0.69
1:B:166:THR:HG23	1:B:179:VAL:HG11	1.76	0.68
1:B:8:ARG:NH2	2:A:253:TYR:O	2.25	0.67
2:A:147:PHE:CG	2:A:147:PHE:O	2.47	0.66
1:C:88:GLN:NE2	1:C:104:ARG:HE	1.93	0.66
2:D:123:LEU:HD11	2:D:214:VAL:HB	1.78	0.66
1:B:88:GLN:NE2	1:B:104:ARG:HE	1.95	0.65
1:B:72:SER:OG	1:B:74:HIS:HD2	1.81	0.63
2:D:123:LEU:CD1	2:D:216:VAL:HG22	2.24	0.62
1:B:138:MET:HE1	1:B:180:GLN:HG3	1.84	0.60
1:C:178:GLU:O	1:C:178:GLU:HG3	2.02	0.59
2:D:53:ARG:HG3	2:D:54:THR:O	2.02	0.59
2:A:27:SER:O	2:A:29:LEU:N	2.36	0.58
1:C:20:ILE:HD11	1:C:66:LEU:HD12	1.86	0.57
2:D:147:PHE:O	2:D:148:TYR:CD2	2.57	0.57
1:B:108:LYS:HE2	1:B:172:MET:SD	2.45	0.57
1:C:113:PRO:HD2	1:C:116:LEU:HD12	1.86	0.56
1:B:51:VAL:HG22	1:B:68:ILE:HG12	1.88	0.56
1:B:189:ASP:OD2	1:B:197:LEU:HD22	2.06	0.55
2:A:148:TYR:HB3	2:A:150:GLY:H	1.72	0.54
2:A:164:SER:H	2:A:197:ASN:HD21	1.54	0.54
2:D:22:LEU:HD12	2:D:22:LEU:N	2.23	0.54
2:A:170:THR:HB	2:A:175:SER:HB3	1.91	0.53
1:B:166:THR:HG23	1:B:179:VAL:CG1	2.39	0.52
2:D:150:GLY:HA2	2:D:151:LEU:C	2.29	0.52
2:A:92:GLU:HA	2:A:159:GLU:O	2.10	0.52
2:A:131:ALA:HA	2:A:191:ASN:O	2.10	0.52
1:C:201:THR:HB	1:C:204:LYS:HD2	1.92	0.52
2:A:53:ARG:HD3	2:A:176:LEU:HD21	1.92	0.51
1:B:67:ARG:NH1	5:B:616:HOH:O	2.43	0.51
2:A:33:THR:OG1	2:A:34:ASN:ND2	2.42	0.51
2:A:53:ARG:NH2	2:A:176:LEU:HD23	2.22	0.51
2:D:123:LEU:HD12	2:D:215:SER:O	2.12	0.50
2:D:91:THR:O	2:D:93:LYS:HG2	2.12	0.50
2:D:92:GLU:HA	2:D:159:GLU:O	2.12	0.50
1:C:89:ASP:OD2	1:C:103:LEU:HB3	2.12	0.49
2:D:148:TYR:HB3	2:D:150:GLY:H	1.76	0.49
2:D:150:GLY:HA2	2:D:151:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:53:ARG:HH21	2:A:176:LEU:CD2	2.21	0.49
1:B:9:TYR:HB3	1:B:18:LEU:HD21	1.95	0.49
1:B:88:GLN:HE22	1:B:104:ARG:HE	1.57	0.49
2:A:164:SER:N	2:A:197:ASN:HD21	2.10	0.49
2:D:148:TYR:HB2	2:D:151:LEU:HD22	1.95	0.48
2:D:102:MET:HG2	2:D:111:GLY:C	2.34	0.48
1:C:112:ARG:HG2	1:C:117:LEU:HD23	1.96	0.47
1:B:155:GLY:HA2	1:B:186:VAL:HG21	1.96	0.47
1:C:19:THR:HG23	1:C:65:THR:HG23	1.96	0.47
2:D:57:ALA:HB1	2:D:213:VAL:HG13	1.97	0.47
1:B:2:LEU:HB3	1:B:87:LEU:HD21	1.96	0.47
1:B:79:LYS:HA	1:B:116:LEU:HD11	1.98	0.46
1:B:75:LEU:HD12	1:B:75:LEU:N	2.31	0.46
2:D:170:THR:HB	2:D:175:SER:HB3	1.98	0.46
1:C:95:GLU:H	2:D:23:ASN:ND2	2.14	0.45
2:A:188:VAL:HG11	2:A:213:VAL:HG21	1.99	0.45
2:D:25:PHE:O	2:D:28:VAL:HG12	2.17	0.45
2:D:186:GLN:HG3	2:D:192:ILE:O	2.16	0.45
2:D:46:ASN:ND2	2:D:172:LEU:HD11	2.32	0.45
1:B:138:MET:CE	1:B:180:GLN:HG3	2.45	0.44
2:D:140:ALA:CB	2:D:153:THR:HA	2.47	0.44
2:D:148:TYR:HD1	2:D:151:LEU:HD22	1.82	0.44
2:D:28:VAL:C	2:D:30:ASN:H	2.19	0.44
1:B:72:SER:OG	1:B:74:HIS:CD2	2.66	0.44
1:C:189:ASP:OD2	1:C:197:LEU:HD22	2.18	0.44
2:D:171:GLU:HB2	2:D:177:SER:HA	1.99	0.43
1:B:143:THR:HB	1:B:144:PRO:HD2	2.00	0.43
2:D:189:ASN:HB3	2:D:191:ASN:OD1	2.19	0.43
1:B:201:THR:HB	1:B:204:LYS:HD2	2.01	0.42
1:B:206:LYS:HA	1:B:207:PRO:HD3	1.79	0.42
2:D:159:GLU:H	2:D:159:GLU:CD	2.22	0.42
1:B:154:ASP:OD1	1:B:154:ASP:C	2.57	0.42
1:C:75:LEU:HD12	1:C:75:LEU:N	2.35	0.42
2:A:171:GLU:HB2	2:A:177:SER:HA	2.01	0.42
1:C:79:LYS:HA	1:C:116:LEU:HD11	2.01	0.41
2:D:151:LEU:CD1	2:D:151:LEU:N	2.82	0.41
2:A:53:ARG:HD3	2:A:176:LEU:CD2	2.50	0.41
2:D:97:TYR:HA	2:D:115:VAL:O	2.21	0.41
1:B:20:ILE:HD11	1:B:66:LEU:HD12	2.02	0.41
1:C:106:LYS:HE3	2:D:251:THR:OG1	2.20	0.41
1:C:125:GLU:HG2	1:C:201:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:SER:OG	1:C:74:HIS:HD2	2.04	0.41
2:D:131:ALA:HA	2:D:191:ASN:O	2.21	0.41
2:D:137:SER:HB2	2:D:166:ALA:HB2	2.01	0.41
2:D:151:LEU:N	2:D:151:LEU:HD12	2.36	0.41
1:B:152:LEU:O	1:B:153:LEU:HD12	2.21	0.41
1:C:88:GLN:NE2	1:C:104:ARG:HH21	2.19	0.41
2:D:150:GLY:HA2	2:D:151:LEU:HB2	2.03	0.41
2:D:76:ASP:OD2	2:D:80:ALA:HB3	2.21	0.40
2:D:22:LEU:N	2:D:22:LEU:CD1	2.85	0.40
2:D:150:GLY:HA2	2:D:151:LEU:CB	2.50	0.40
2:A:97:TYR:HA	2:A:115:VAL:O	2.22	0.40

There are no symmetry-related clashes.

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	B	191/224 (85%)	185 (97%)	5 (3%)	1 (0%)	29	23
1	C	206/224 (92%)	200 (97%)	6 (3%)	0	100	100
2	A	203/253 (80%)	197 (97%)	5 (2%)	1 (0%)	29	23
2	D	209/253 (83%)	199 (95%)	9 (4%)	1 (0%)	29	23
All	All	809/954 (85%)	781 (96%)	25 (3%)	3 (0%)	34	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	154	ASN
1	B	44	ASP
2	A	31	ASP

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	B	148/189 (78%)	147 (99%)	1 (1%)	84	88
1	C	161/189 (85%)	159 (99%)	2 (1%)	71	76
2	A	143/196 (73%)	138 (96%)	5 (4%)	36	35
2	D	146/196 (74%)	142 (97%)	4 (3%)	44	46
All	All	598/770 (78%)	586 (98%)	12 (2%)	55	58

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	ARG
1	C	8	ARG
1	C	153	LEU
2	D	17	LYS
2	D	27	SER
2	D	60	THR
2	D	194	SER
2	A	53	ARG
2	A	60	THR
2	A	148	TYR
2	A	197	ASN
2	A	237	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	74	HIS
1	B	88	GLN
1	C	74	HIS
1	C	88	GLN
1	C	168	GLN
2	D	23	ASN
2	D	34	ASN

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Mol	Chain	Res	Type
2	D	184	GLN
2	A	23	ASN
2	A	34	ASN
2	A	71	HIS
2	A	189	ASN
2	A	197	ASN
2	A	224	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 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	C	228	-	4,4,4	0.18	0	6,6,6	0.09	0
3	SO4	C	225	-	4,4,4	0.15	0	6,6,6	0.26	0
3	SO4	D	254	-	4,4,4	0.12	0	6,6,6	0.13	0
4	GOL	A	255	-	5,5,5	0.33	0	5,5,5	0.46	0
3	SO4	C	226	-	4,4,4	0.17	0	6,6,6	0.23	0
3	SO4	B	227	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	B	225	-	4,4,4	0.14	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	SO4	C	229	-	4,4,4	0.13	0	6,6,6	0.13	0
3	SO4	B	229	-	4,4,4	0.14	0	6,6,6	0.07	0
4	GOL	D	255	-	5,5,5	0.41	0	5,5,5	0.60	0
3	SO4	B	228	-	4,4,4	0.19	0	6,6,6	0.16	0
3	SO4	B	226	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	C	227	-	4,4,4	0.12	0	6,6,6	0.09	0
3	SO4	A	254	-	4,4,4	0.15	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	255	-	-	0/4/4/4	-
4	GOL	A	255	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	255	GOL	C1-C2-C3-O3
4	A	255	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	B	199/224 (88%)	-0.20	1 (0%) 91	90	19, 33, 63, 76	0
1	C	208/224 (92%)	-0.34	4 (1%) 66	65	15, 28, 44, 56	0
2	A	215/253 (84%)	-0.19	5 (2%) 60	59	20, 33, 57, 79	0
2	D	217/253 (85%)	-0.11	7 (3%) 47	46	17, 32, 54, 65	0
All	All	839/954 (87%)	-0.21	17 (2%) 65	63	15, 32, 55, 79	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	27	SER	6.7
2	D	28	VAL	6.0
2	A	147	PHE	3.1
2	D	140	ALA	3.1
1	C	156	ASN	3.0
1	C	208	ALA	2.9
2	D	26	GLY	2.5
2	A	11	ARG	2.4
2	A	35	GLY	2.4
2	A	24	GLY	2.4
1	C	149	ILE	2.3
2	D	150	GLY	2.2
1	C	61	ASN	2.1
2	A	89	GLY	2.1
2	D	149	GLY	2.1
1	B	155	GLY	2.1
2	D	89	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

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6.3 Carbohydrates (i)

There are no monosaccharides 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	B	227	5/5	0.85	0.26	87,89,89,90	0
3	SO4	B	229	5/5	0.86	0.31	108,108,108,109	0
3	SO4	C	229	5/5	0.88	0.17	91,91,92,93	0
3	SO4	C	228	5/5	0.89	0.18	82,82,82,82	0
3	SO4	D	254	5/5	0.91	0.17	98,98,98,98	0
3	SO4	A	254	5/5	0.92	0.15	94,95,95,95	0
4	GOL	D	255	6/6	0.94	0.11	29,35,38,42	0
3	SO4	C	226	5/5	0.95	0.14	57,57,60,60	0
4	GOL	A	255	6/6	0.95	0.12	35,41,41,43	0
3	SO4	B	226	5/5	0.97	0.13	60,61,61,61	0
3	SO4	C	225	5/5	0.98	0.09	42,44,46,48	0
3	SO4	B	228	5/5	0.98	0.09	40,43,44,47	0
3	SO4	C	227	5/5	0.98	0.12	48,49,50,52	0
3	SO4	B	225	5/5	0.99	0.10	45,45,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.