



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 08:07 PM EST

PDB ID : 4DG4
Title : Human mesotrypsin-S39Y complexed with bovine pancreatic trypsin inhibitor (BPTI)
Authors : Salameh, M.A.; Soares, A.S.; Radisky, E.S.
Deposited on : 2012-01-24
Resolution : 1.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

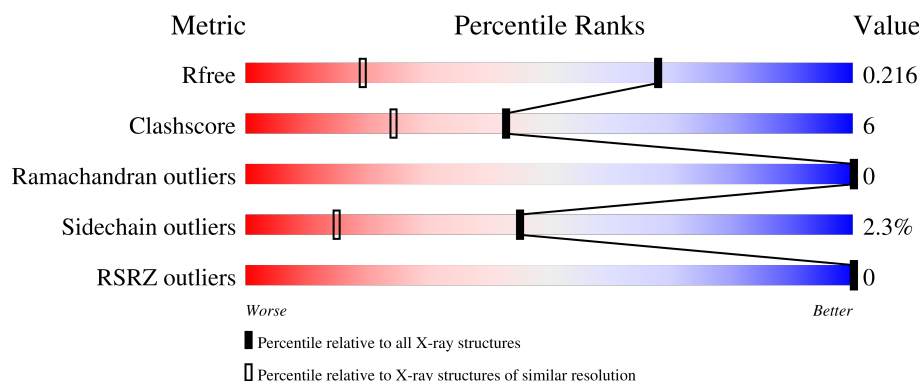
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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.



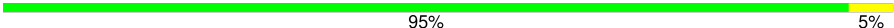


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2247 (1.40-1.40)
Clashscore	180529	2446 (1.40-1.40)
Ramachandran outliers	177936	2398 (1.40-1.40)
Sidechain outliers	177891	2397 (1.40-1.40)
RSRZ outliers	164620	2246 (1.40-1.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	224	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	B	224	<div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	D	224	<div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	G	224	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
2	C	58	<div> <div>84%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	58	 95%5%
2	F	58	 84%16%
2	H	58	 91%9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10168 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 PRSS3 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	4	0
			1733	1095	300	326	12			
1	B	224	Total	C	N	O	S	0	5	0
			1732	1095	296	329	12			
1	D	224	Total	C	N	O	S	0	3	0
			1725	1091	297	325	12			
1	G	224	Total	C	N	O	S	12	1	0
			1711	1079	294	326	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	TYR	SER	engineered mutation	UNP Q8N2U3
A	195	ALA	SER	engineered mutation	UNP Q8N2U3
B	39	TYR	SER	engineered mutation	UNP Q8N2U3
B	195	ALA	SER	engineered mutation	UNP Q8N2U3
D	39	TYR	SER	engineered mutation	UNP Q8N2U3
D	195	ALA	SER	engineered mutation	UNP Q8N2U3
G	39	TYR	SER	engineered mutation	UNP Q8N2U3
G	195	ALA	SER	engineered mutation	UNP Q8N2U3

- Molecule 2 is a protein called Pancreatic trypsin inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	58	Total	C	N	O	S	0	1	0
			459	289	84	79	7			
2	C	58	Total	C	N	O	S	5	0	0
			453	284	84	78	7			
2	F	58	Total	C	N	O	S	0	1	0
			458	288	84	78	8			
2	H	58	Total	C	N	O	S	1	0	0
			454	284	84	79	7			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	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
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
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	265	Total O 266 266	0	1
5	E	87	Total O 87 87	0	0
5	B	265	Total O 265 265	0	0
5	C	82	Total O 84 84	0	2
5	D	247	Total O 248 248	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	62	Total 62	O 62	0	0
5	G	235	Total 237	O 237	0	2
5	H	72	Total 73	O 73	0	1

3 Residue-property plots [i](#)

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: PRSS3 protein

Chain A:  90% 9% .



- Molecule 1: PRSS3 protein

Chain B:  87% 12% .




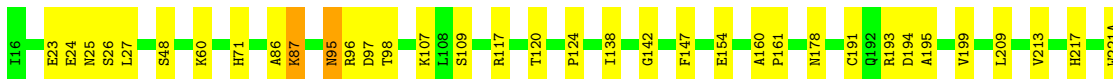
- Molecule 1: PRSS3 protein

Chain D:  90% 8% .



- Molecule 1: PRSS3 protein

Chain G:  83% 16% .




- Molecule 2: Pancreatic trypsin inhibitor

Chain E:  95% 5% .




- Molecule 2: Pancreatic trypsin inhibitor

Chain C:  84% 16%



- Molecule 2: Pancreatic trypsin inhibitor

Chain F:  84% 16%



- Molecule 2: Pancreatic trypsin inhibitor

Chain H:  91% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.53Å 109.95Å 81.12Å 90.00° 116.82° 90.00°	Depositor
Resolution (Å)	30.20 – 1.40 30.20 – 1.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.20-1.40) 77.2 (30.20-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 1.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.166 , 0.211 0.179 , 0.216	Depositor DCC
R_{free} test set	2014 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.072 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10168	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 20.16 % 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 9.2330e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CA

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	0.27	0/1786	0.48	0/2429
1	B	0.26	0/1784	0.47	0/2426
1	D	0.25	0/1775	0.47	0/2412
1	G	0.25	0/1754	0.46	0/2385
2	C	0.27	0/464	0.47	0/622
2	E	0.27	0/473	0.44	0/633
2	F	0.26	0/472	0.44	0/632
2	H	0.26	0/465	0.47	0/622
All	All	0.26	0/8973	0.47	0/12161

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	ASN	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	1733	0	1695	17	0
1	B	1732	0	1699	20	0
1	D	1725	0	1687	20	0
1	G	1711	0	1663	24	0
2	C	453	0	438	9	0
2	E	459	0	449	4	0
2	F	458	0	447	12	0
2	H	454	0	438	3	0
3	A	15	0	0	0	0
3	B	5	0	0	1	0
3	C	15	0	0	0	0
3	D	10	0	0	1	0
3	E	10	0	0	0	0
3	F	15	0	0	0	0
3	G	35	0	0	0	0
3	H	15	0	0	0	0
4	A	1	0	0	0	0
5	A	266	0	0	3	0
5	B	265	0	0	3	0
5	C	84	0	0	0	0
5	D	248	0	0	4	0
5	E	87	0	0	0	0
5	F	62	0	0	0	0
5	G	237	0	0	3	0
5	H	73	0	0	0	0
All	All	10168	0	8516	105	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 6.

All (105) 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:G:24:GLU:HG2	1:G:117:ARG:NH2	1.94	0.83
1:B:24:GLU:HG2	1:B:117:ARG:NH2	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:52[B]:MET:HA	2:F:52[B]:MET:HE2	1.70	0.73
1:D:24:GLU:HG2	1:D:117:ARG:HH22	1.53	0.73
2:C:1:ARG:HA	2:C:58:ALA:O	1.94	0.67
1:D:71:HIS:HD2	5:D:439:HOH:O	1.78	0.66
1:B:95:ASN:HD22	1:B:97:ASP:H	1.43	0.65
1:A:71:HIS:HD2	5:A:628:HOH:O	1.80	0.64
2:F:1:ARG:N	2:F:2:PRO:CD	2.62	0.63
1:A:24:GLU:HG2	1:A:117:ARG:NH2	2.14	0.62
2:C:1:ARG:N	2:C:2:PRO:CD	2.62	0.62
1:B:125:THR:H	1:B:204:GLN:NE2	1.98	0.62
1:D:217[A]:HIS:HE1	5:D:573:HOH:O	1.82	0.61
1:A:95:ASN:HD22	1:A:97:ASP:H	1.48	0.61
1:D:25:ASN:HB2	1:D:117:ARG:NH2	2.16	0.60
1:B:125:THR:H	1:B:204:GLN:HE21	1.49	0.59
2:F:1:ARG:HA	2:F:58:ALA:HB2	1.83	0.58
2:F:52[B]:MET:HA	2:F:52[B]:MET:CE	2.33	0.58
1:B:95:ASN:ND2	1:B:97:ASP:H	2.02	0.57
2:E:1:ARG:N	2:E:2:PRO:CD	2.68	0.57
2:C:1:ARG:H2	2:C:2:PRO:CD	2.17	0.57
1:G:87:LYS:HD3	1:G:107:LYS:HD3	1.87	0.57
1:B:71:HIS:HD2	5:B:446:HOH:O	1.88	0.57
2:C:1:ARG:N	2:C:2:PRO:HD3	2.19	0.57
1:A:217[B]:HIS:CE1	1:A:221(A):TRP:CZ3	2.95	0.55
1:D:95:ASN:HD22	1:D:97:ASP:H	1.54	0.55
1:D:117:ARG:NH2	5:D:637:HOH:O	2.39	0.54
1:A:217[A]:HIS:HD2	1:A:224[A]:ARG:CZ	2.20	0.54
1:B:142:GLY:HA2	1:B:193:ARG:HB3	1.90	0.53
1:D:95:ASN:ND2	1:D:97:ASP:H	2.06	0.53
1:A:142:GLY:HA2	1:A:193:ARG:HB3	1.91	0.52
2:F:1:ARG:H3	2:F:2:PRO:HD3	1.75	0.52
1:G:71:HIS:HD2	5:G:450:HOH:O	1.93	0.52
1:G:71:HIS:HE1	1:G:154:GLU:OE2	1.93	0.52
2:E:1:ARG:H3	2:E:2:PRO:CD	2.24	0.51
2:E:1:ARG:H3	2:E:2:PRO:HD3	1.76	0.51
1:A:24:GLU:HG2	1:A:117:ARG:HH21	1.77	0.50
1:A:95:ASN:ND2	1:A:97:ASP:H	2.09	0.49
1:G:222:LYS:HE3	1:G:223:ASN:ND2	2.27	0.49
1:G:24:GLU:HG2	1:G:117:ARG:HH21	1.74	0.49
1:B:124:PRO:HA	1:B:204:GLN:HE21	1.78	0.49
2:C:1:ARG:H3	2:C:2:PRO:HD3	1.78	0.49
1:A:87:LYS:HE2	5:A:592:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LYS:CE	3:B:301:SO4:O1	2.61	0.48
1:B:79:ASN:ND2	1:B:117:ARG:HG3	2.28	0.48
1:B:195:ALA:HB2	2:C:15:LYS:C	2.34	0.48
1:D:217[A]:HIS:HD2	5:D:433:HOH:O	1.97	0.48
2:F:1:ARG:N	2:F:2:PRO:HD3	2.28	0.48
1:G:23:GLU:HB2	1:G:26:SER:OG	2.14	0.47
1:A:124:PRO:HG3	1:A:209:LEU:O	2.15	0.47
1:G:60:LYS:HE2	5:G:622:HOH:O	2.14	0.47
1:G:142:GLY:HA2	1:G:193:ARG:HB3	1.96	0.47
1:D:142:GLY:HA2	1:D:193:ARG:HB3	1.97	0.47
2:F:1:ARG:H2	2:F:2:PRO:CD	2.27	0.47
1:G:95:ASN:HD22	1:G:97:ASP:H	1.62	0.47
2:H:49:GLU:H	2:H:49:GLU:CD	2.18	0.47
1:D:79:ASN:CG	1:D:117:ARG:HG3	2.35	0.46
1:B:95:ASN:ND2	1:B:98:THR:H	2.12	0.46
1:B:22:CYS:HB3	1:B:27[A]:LEU:HD23	1.97	0.46
1:D:95:ASN:ND2	1:D:98:THR:H	2.11	0.46
2:F:23:TYR:CE2	2:F:52[B]:MET:HE1	2.51	0.46
1:G:86:ALA:HB2	1:G:109:SER:HA	1.98	0.46
1:G:138:ILE:HG12	1:G:199:VAL:HG22	1.99	0.45
1:A:217[A]:HIS:CD2	1:A:224[A]:ARG:NH1	2.84	0.45
1:B:213:VAL:HA	1:B:228:TYR:CD2	2.52	0.44
2:C:9:PRO:HD3	2:C:22:PHE:CE1	2.52	0.44
1:G:195:ALA:HB2	2:H:15:LYS:C	2.38	0.44
1:B:217:HIS:HE1	5:B:651:HOH:O	1.99	0.44
2:C:57:GLY:O	2:C:58:ALA:HB2	2.17	0.44
1:D:71:HIS:HE1	1:D:154:GLU:OE2	2.01	0.44
2:F:21:TYR:CE2	2:F:32:THR:HG22	2.53	0.44
1:G:124:PRO:HG3	1:G:209:LEU:O	2.17	0.44
1:D:124:PRO:HG3	1:D:209:LEU:O	2.18	0.43
2:F:23:TYR:HE2	2:F:52[B]:MET:HE1	1.82	0.43
1:B:219:GLY:HA3	1:B:221(A):TRP:CE2	2.52	0.43
1:B:160:ALA:HA	1:B:161:PRO:HD3	1.90	0.43
1:D:87:LYS:HB2	1:D:107:LYS:HB3	2.01	0.43
1:D:95:ASN:HD22	1:D:98:THR:H	1.67	0.43
1:G:26:SER:C	1:G:27:LEU:HD12	2.39	0.42
1:G:213:VAL:HA	1:G:228:TYR:CD2	2.54	0.42
1:D:96:ARG:HH11	1:D:96:ARG:HG3	1.84	0.42
1:A:217[A]:HIS:HB2	1:A:224[A]:ARG:HD2	2.01	0.42
1:G:160:ALA:HA	1:G:161:PRO:HD3	1.88	0.42
1:B:117:ARG:HD2	5:B:477:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:ALA:HB2	2:F:15:LYS:C	2.40	0.42
1:A:213:VAL:HA	1:A:228:TYR:CD2	2.54	0.42
1:B:27[A]:LEU:HD12	1:B:29:TYR:OH	2.20	0.42
1:D:172:TYR:HB3	1:D:175:LYS:HB2	2.01	0.42
2:H:1:ARG:N	2:H:2:PRO:CD	2.83	0.41
1:A:160:ALA:HA	1:A:161:PRO:HD3	1.88	0.41
1:G:178:ASN:HB2	5:G:596:HOH:O	2.21	0.41
1:G:191:CYS:O	1:G:194:ASP:HB2	2.21	0.41
1:D:23:GLU:HG2	3:D:302:SO4:O1	2.20	0.41
1:A:195:ALA:HB2	2:E:15:LYS:C	2.41	0.41
1:G:48:SER:HA	1:G:120:THR:HG21	2.03	0.41
1:A:217[A]:HIS:CD2	1:A:224[A]:ARG:CZ	3.01	0.41
2:F:30:CYS:SG	2:F:52[B]:MET:HE3	2.60	0.41
1:G:95:ASN:ND2	1:G:98:THR:H	2.18	0.41
1:A:223:ASN:HB3	5:A:625:HOH:O	2.21	0.40
1:D:96:ARG:HG3	1:D:96:ARG:NH1	2.36	0.40
1:G:95:ASN:ND2	1:G:97:ASP:H	2.18	0.40
1:B:45:SER:OG	1:B:198:PRO:HB3	2.21	0.40
2:C:49:GLU:H	2:C:49:GLU:CD	2.25	0.40
1:G:71:HIS:CE1	1:G:154:GLU:OE2	2.73	0.40
1:G:217:HIS:CE1	1:G:221(A):TRP:CZ3	3.09	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	226/224 (101%)	221 (98%)	5 (2%)	0	100	100
1	B	227/224 (101%)	220 (97%)	7 (3%)	0	100	100
1	D	225/224 (100%)	218 (97%)	7 (3%)	0	100	100
1	G	223/224 (100%)	217 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
2	E	57/58 (98%)	57 (100%)	0	0	100	100
2	F	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
2	H	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
All	All	1127/1128 (100%)	1099 (98%)	28 (2%)	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	189/185 (102%)	184 (97%)	5 (3%)	41	11
1	B	190/185 (103%)	184 (97%)	6 (3%)	34	7
1	D	188/185 (102%)	183 (97%)	5 (3%)	40	10
1	G	186/185 (100%)	181 (97%)	5 (3%)	40	10
2	C	46/46 (100%)	45 (98%)	1 (2%)	47	16
2	E	47/46 (102%)	47 (100%)	0	100	100
2	F	47/46 (102%)	47 (100%)	0	100	100
2	H	46/46 (100%)	45 (98%)	1 (2%)	47	16
All	All	939/924 (102%)	916 (98%)	23 (2%)	45	13

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	A	95	ASN
1	A	147	PHE
1	A	217[A]	HIS
1	A	217[B]	HIS
1	B	25	ASN

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Mol	Chain	Res	Type
1	B	62	ARG
1	B	95	ASN
1	B	96	ARG
1	B	147	PHE
1	B	217	HIS
2	C	29	LEU
1	D	87	LYS
1	D	95	ASN
1	D	147	PHE
1	D	217[A]	HIS
1	D	217[B]	HIS
1	G	25	ASN
1	G	87	LYS
1	G	95	ASN
1	G	96	ARG
1	G	147	PHE
2	H	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	50	GLN
1	A	71	HIS
1	A	95	ASN
1	A	202	ASN
1	B	25	ASN
1	B	30	GLN
1	B	50	GLN
1	B	71	HIS
1	B	79	ASN
1	B	95	ASN
1	B	178	ASN
1	B	204	GLN
1	B	217	HIS
1	D	25	ASN
1	D	30	GLN
1	D	50	GLN
1	D	71	HIS
1	D	95	ASN
1	D	178	ASN
1	D	202	ASN

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Mol	Chain	Res	Type
1	G	30	GLN
1	G	50	GLN
1	G	71	HIS
1	G	95	ASN
1	G	202	ASN
1	G	217	HIS
1	G	223	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	C	101	-	4,4,4	0.24	0	6,6,6	0.18	0
3	SO4	E	101	-	4,4,4	0.24	0	6,6,6	0.20	0
3	SO4	F	102	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	D	302	-	4,4,4	0.26	0	6,6,6	0.07	0
3	SO4	B	301	-	4,4,4	0.21	0	6,6,6	0.08	0
3	SO4	G	305	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	G	302	-	4,4,4	0.23	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	D	301	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	G	301	-	4,4,4	0.26	0	6,6,6	0.12	0
3	SO4	F	101	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	G	307	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	E	102	-	4,4,4	0.22	0	6,6,6	0.19	0
3	SO4	H	103	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	G	304	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	A	301	-	4,4,4	0.23	0	6,6,6	0.21	0
3	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	H	102	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	A	302	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	G	303	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	C	103	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	H	101	-	4,4,4	0.26	0	6,6,6	0.12	0
3	SO4	F	103	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	G	306	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	C	102	-	4,4,4	0.23	0	6,6,6	0.08	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	SO4	1	0
3	B	301	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 [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(Å ²)	Q<0.9
1	A	224/224 (100%)	-1.51	0 100 100	8, 12, 16, 24	136 (60%)
1	B	224/224 (100%)	-1.47	0 100 100	7, 13, 17, 25	158 (70%)
1	D	224/224 (100%)	-1.46	0 100 100	6, 13, 19, 24	150 (66%)
1	G	224/224 (100%)	-1.43	0 100 100	6, 14, 21, 28	176 (78%)
2	C	58/58 (100%)	-1.38	0 100 100	9, 12, 21, 30	44 (75%)
2	E	58/58 (100%)	-1.48	0 100 100	6, 12, 17, 18	40 (68%)
2	F	58/58 (100%)	-1.25	0 100 100	9, 14, 36, 45	47 (81%)
2	H	58/58 (100%)	-1.41	0 100 100	10, 13, 19, 23	49 (84%)
All	All	1128/1128 (100%)	-1.45	0 100 100	6, 13, 20, 45	800 (70%)

There are no RSRZ outliers to report.

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 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(\AA^2)	Q<0.9
3	SO4	A	302	5/5	0.95	0.11	72,72,72,72	0
3	SO4	A	303	5/5	0.95	0.16	114,114,114,114	0
3	SO4	G	307	5/5	0.95	0.12	100,101,101,101	0
3	SO4	D	301	5/5	0.97	0.07	66,66,66,66	3
3	SO4	F	103	5/5	0.97	0.10	70,70,70,70	2
3	SO4	C	103	5/5	0.97	0.09	77,77,77,78	0
3	SO4	D	302	5/5	0.98	0.07	80,80,80,80	0
3	SO4	G	302	5/5	0.98	0.07	75,75,75,75	3
3	SO4	G	303	5/5	0.98	0.06	62,62,62,62	3
3	SO4	G	305	5/5	0.98	0.05	68,68,68,68	3
3	SO4	F	102	5/5	0.98	0.06	55,55,55,56	0
3	SO4	A	301	5/5	0.99	0.03	27,27,27,27	2
3	SO4	G	301	5/5	0.99	0.03	40,40,40,40	3
3	SO4	E	102	5/5	0.99	0.04	40,41,41,41	2
3	SO4	B	301	5/5	1.00	0.02	25,25,25,25	5
3	SO4	C	101	5/5	1.00	0.03	21,21,21,22	5
3	SO4	F	101	5/5	1.00	0.02	24,24,24,24	5
3	SO4	G	304	5/5	1.00	0.03	23,23,23,23	3
3	SO4	C	102	5/5	1.00	0.01	20,20,20,20	4
3	SO4	G	306	5/5	1.00	0.02	38,38,38,38	4
3	SO4	E	101	5/5	1.00	0.01	17,17,17,18	4
3	SO4	H	101	5/5	1.00	0.02	19,19,19,19	4
3	SO4	H	102	5/5	1.00	0.02	20,20,20,21	5
3	SO4	H	103	5/5	1.00	0.02	33,33,33,33	3
4	CA	A	304	1/1	1.00	0.04	23,23,23,23	1

6.5 Other polymers

There are no such residues in this entry.