wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 01:42 PM EDT

PDB ID	:	3GUA
Title	:	Sulfates bound in the vestibule of AChBP
Authors	:	Hansen, S.B.; Taylor, P.
Deposited on	:	2009-03-28
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

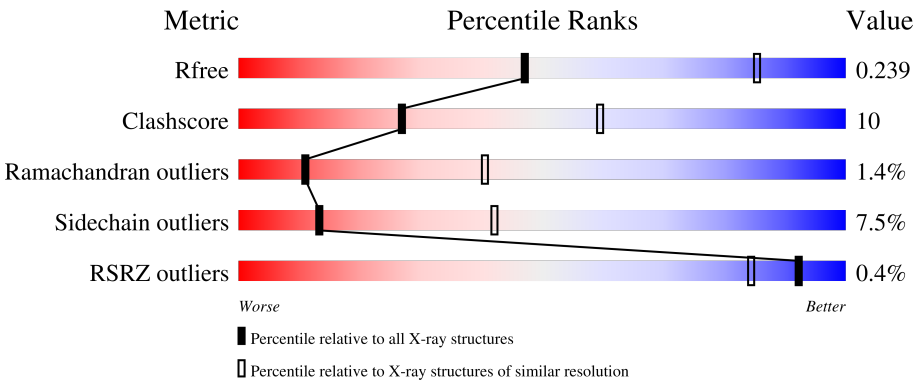
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	A	217	80% 16% • •
1	B	217	82% 13% • •
1	C	217	81% 15% • •
1	D	217	% 85% 9% • •
1	E	217	86% 10% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	217	83% 13%
1	G	217	% 81% 15%
1	H	217	% 82% 12%
1	I	217	86% 10%
1	J	217	82% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17744 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	1736	1094	284	349	9	0	0	0
1	B	216	1726	1088	281	348	9	0	0	0
1	C	217	1737	1094	285	349	9	0	0	0
1	D	217	1737	1094	285	349	9	0	0	0
1	E	217	1737	1094	285	349	9	0	0	0
1	F	217	1736	1094	284	349	9	0	0	0
1	G	216	1726	1088	281	348	9	0	0	0
1	H	217	1737	1094	285	349	9	0	0	0
1	I	217	1737	1094	285	349	9	0	0	0
1	J	217	1737	1094	285	349	9	0	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
A	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
A	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
A	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
A	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
A	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
A	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
A	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
A	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8

Continued on next page...

Continued from previous page...

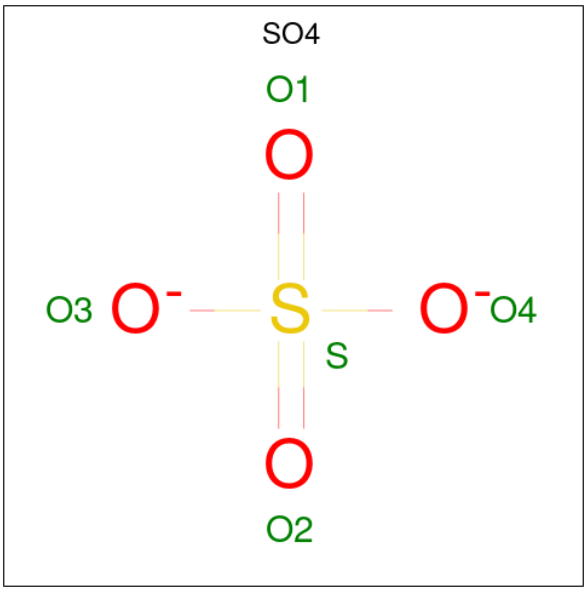
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
B	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
B	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
B	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
B	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
B	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
B	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
B	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
B	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
C	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
C	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
C	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
C	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
C	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
C	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
C	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
C	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
C	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
D	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
D	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
D	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
D	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
D	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
D	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
D	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
D	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
D	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
E	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
E	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
E	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
E	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
E	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
E	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
E	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
E	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
E	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
F	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
F	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
F	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
F	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
F	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
F	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
F	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
F	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
G	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
G	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
G	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
G	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
G	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
G	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
G	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
G	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
G	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
H	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
H	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
H	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
H	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
H	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
H	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
H	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
H	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
H	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
I	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
I	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
I	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
I	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
I	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
I	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
I	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
I	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
I	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8
J	-8	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-7	TYR	-	EXPRESSION TAG	UNP Q8WSF8
J	-6	LYS	-	EXPRESSION TAG	UNP Q8WSF8
J	-5	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-4	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-3	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-2	ASP	-	EXPRESSION TAG	UNP Q8WSF8
J	-1	LYS	-	EXPRESSION TAG	UNP Q8WSF8
J	0	LEU	-	EXPRESSION TAG	UNP Q8WSF8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	G	1	5	4	1	0	0
			Total	O	S		
2	H	1	5	4	1	0	0
			Total	O	S		
2	H	1	5	4	1	0	0
			Total	O	S		
2	I	1	5	4	1	0	0
			Total	O	S		
2	I	1	5	4	1	0	0
			Total	O	S		
2	J	1	5	4	1	0	0
			Total	O	S		
2	J	1	5	4	1	0	0

- Molecule 3 is water.

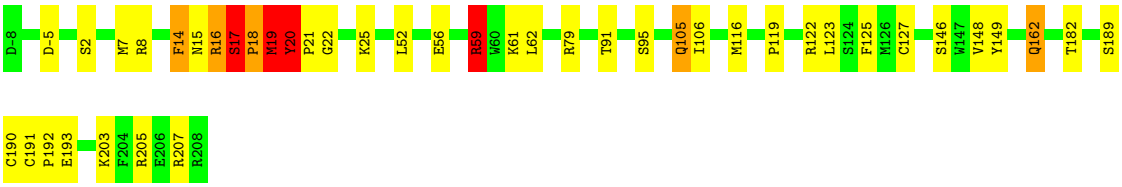
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	H	293	293	293	0	0

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.

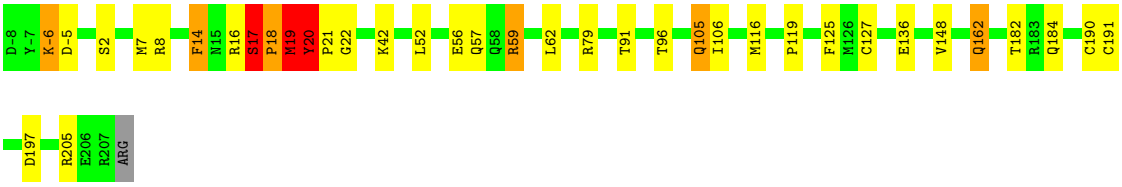
• Molecule 1: Soluble acetylcholine receptor

Chain A:



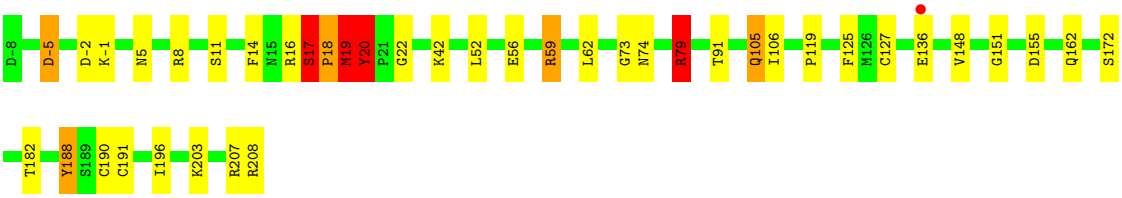
• Molecule 1: Soluble acetylcholine receptor

Chain B:



• Molecule 1: Soluble acetylcholine receptor

Chain C:

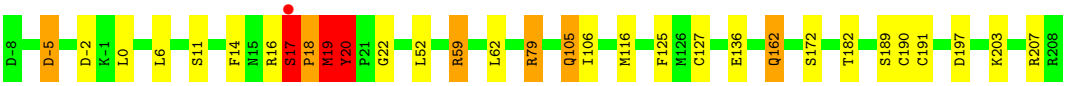


• Molecule 1: Soluble acetylcholine receptor

Chain D:

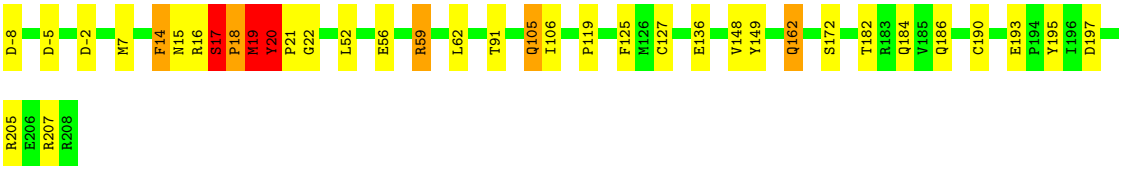
• Molecule 1: Soluble acetylcholine receptor

Chain E:



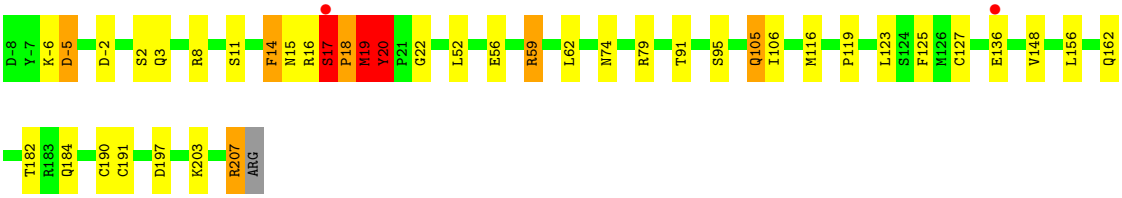
• Molecule 1: Soluble acetylcholine receptor

Chain F:



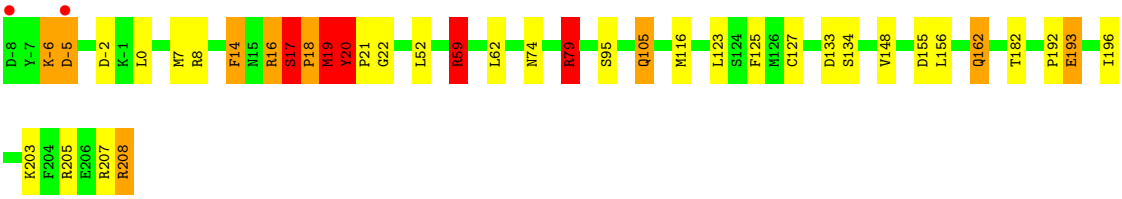
• Molecule 1: Soluble acetylcholine receptor

Chain G:



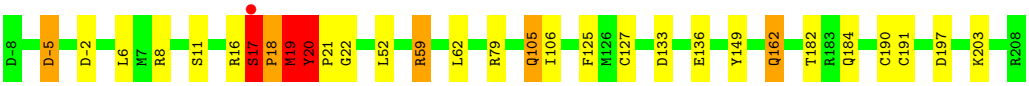
• Molecule 1: Soluble acetylcholine receptor

Chain H:



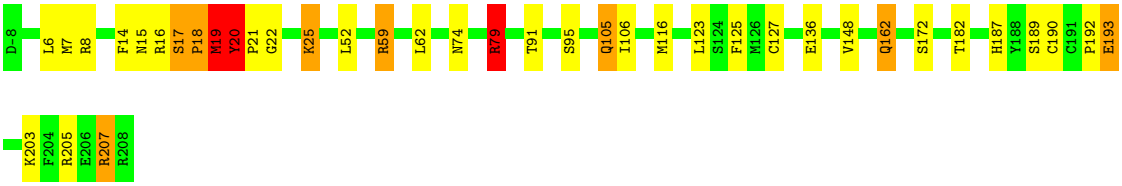
• Molecule 1: Soluble acetylcholine receptor

Chain I:



• Molecule 1: Soluble acetylcholine receptor

Chain J:


D-8
L6
M7
R8
F14
N15
R16
S17
P18
M19
Y20
P21
G22
K25
L52
R59
L62
N74
R79
T91
S95
Q105
I106
M116
L123
S124
F125
M126
C127
E136
V148
Q162
S172
T182
H187
Y188
S189
C190
C191
P192
E193
K203
F204
R205
E206
R207
R208

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	98.43Å 98.43Å 265.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 3.10 49.21 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.21-3.10) 99.9 (49.21-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.95 (at 3.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.212 , 0.250 0.205 , 0.239	Depositor DCC
R_{free} test set	2312 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17744	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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 (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	0.80	2/1778 (0.1%)	1.24	9/2422 (0.4%)
1	B	0.56	1/1768 (0.1%)	0.84	8/2410 (0.3%)
1	C	0.55	1/1779 (0.1%)	1.08	6/2424 (0.2%)
1	D	0.58	3/1779 (0.2%)	0.94	8/2424 (0.3%)
1	E	0.58	2/1779 (0.1%)	1.05	7/2424 (0.3%)
1	F	0.65	2/1778 (0.1%)	0.96	6/2422 (0.2%)
1	G	0.53	1/1768 (0.1%)	0.83	5/2410 (0.2%)
1	H	0.60	3/1779 (0.2%)	1.00	8/2424 (0.3%)
1	I	0.63	1/1779 (0.1%)	0.91	7/2424 (0.3%)
1	J	0.61	2/1779 (0.1%)	1.15	12/2424 (0.5%)
All	All	0.61	18/17766 (0.1%)	1.01	76/24208 (0.3%)

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	2
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	2
All	All	0	14

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	ARG	CZ-NH1	-19.56	1.07	1.33
1	A	205	ARG	CZ-NH2	-16.18	1.12	1.33
1	I	203	LYS	CD-CE	-13.97	1.16	1.51
1	F	205	ARG	CZ-NH1	-12.95	1.16	1.33
1	E	203	LYS	CD-CE	-9.31	1.27	1.51

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	ARG	NE-CZ-NH2	31.25	135.92	120.30
1	F	205	ARG	NE-CZ-NH2	23.98	132.29	120.30
1	C	79	ARG	NE-CZ-NH2	-23.86	108.37	120.30
1	A	205	ARG	NH1-CZ-NH2	-23.70	93.34	119.40
1	C	79	ARG	NE-CZ-NH1	22.12	131.36	120.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	SER	Peptide
1	A	190	CYS	Peptide
1	B	17	SER	Peptide
1	C	17	SER	Peptide
1	D	17	SER	Peptide

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	1736	0	1653	42	0
1	B	1726	0	1642	39	1
1	C	1737	0	1655	38	0
1	D	1737	0	1655	37	0
1	E	1737	0	1655	30	1
1	F	1736	0	1653	39	0
1	G	1726	0	1642	38	0
1	H	1737	0	1655	44	0
1	I	1737	0	1655	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1737	0	1655	41	0
2	A	20	0	0	1	0
2	B	10	0	0	1	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
2	I	10	0	0	0	0
2	J	10	0	0	0	0
3	H	293	0	0	16	2
All	All	17744	0	16520	348	3

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 10.

The worst 5 of 348 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:59:ARG:NH2	3:H:346:HOH:O	1.68	1.22
1:H:20:TYR:HE2	1:H:62:LEU:HD22	1.08	1.18
1:D:20:TYR:HE2	1:D:62:LEU:HD22	1.09	1.17
1:F:20:TYR:HE2	1:F:62:LEU:HD22	1.11	1.16
1:E:20:TYR:HE2	1:E:62:LEU:HD22	1.09	1.14

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:285:HOH:O	3:H:451:HOH:O[3_555]	1.59	0.61
3:H:285:HOH:O	3:H:450:HOH:O[3_555]	2.00	0.20
1:B:57:GLN:OE1	1:E:189:SER:O[4_554]	2.02	0.18

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	215/217 (99%)	207 (96%)	5 (2%)	3 (1%)	11	40
1	B	214/217 (99%)	206 (96%)	5 (2%)	3 (1%)	11	40
1	C	215/217 (99%)	208 (97%)	4 (2%)	3 (1%)	11	40
1	D	215/217 (99%)	208 (97%)	4 (2%)	3 (1%)	11	40
1	E	215/217 (99%)	208 (97%)	4 (2%)	3 (1%)	11	40
1	F	215/217 (99%)	206 (96%)	6 (3%)	3 (1%)	11	40
1	G	214/217 (99%)	206 (96%)	5 (2%)	3 (1%)	11	40
1	H	215/217 (99%)	207 (96%)	5 (2%)	3 (1%)	11	40
1	I	215/217 (99%)	207 (96%)	5 (2%)	3 (1%)	11	40
1	J	215/217 (99%)	207 (96%)	5 (2%)	3 (1%)	11	40
All	All	2148/2170 (99%)	2070 (96%)	48 (2%)	30 (1%)	11	40

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PRO
1	B	18	PRO
1	C	18	PRO
1	D	18	PRO
1	E	18	PRO

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	198/198 (100%)	181 (91%)	17 (9%)	10	37
1	B	197/198 (100%)	183 (93%)	14 (7%)	14	44
1	C	198/198 (100%)	183 (92%)	15 (8%)	13	41
1	D	198/198 (100%)	182 (92%)	16 (8%)	11	39
1	E	198/198 (100%)	185 (93%)	13 (7%)	16	47
1	F	198/198 (100%)	185 (93%)	13 (7%)	16	47
1	G	197/198 (100%)	183 (93%)	14 (7%)	14	44
1	H	198/198 (100%)	180 (91%)	18 (9%)	9	33
1	I	198/198 (100%)	187 (94%)	11 (6%)	21	52
1	J	198/198 (100%)	181 (91%)	17 (9%)	10	37
All	All	1978/1980 (100%)	1830 (92%)	148 (8%)	13	42

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	162	GLN
1	J	182	THR
1	H	208	ARG
1	I	182	THR
1	D	0	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	162	GLN
1	J	15	ASN
1	H	184	GLN
1	I	162	GLN
1	J	105	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

21 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	$\#\|Z\| > 2$
2	SO4	F	303	-	4,4,4	0.30	0	6,6,6	0.30	0
2	SO4	D	301	-	4,4,4	0.31	0	6,6,6	0.18	0
2	SO4	E	302	-	4,4,4	0.24	0	6,6,6	0.40	0
2	SO4	A	304	-	4,4,4	0.41	0	6,6,6	0.28	0
2	SO4	B	301	-	4,4,4	0.30	0	6,6,6	0.43	0
2	SO4	B	304	-	4,4,4	0.20	0	6,6,6	0.21	0
2	SO4	H	302	-	4,4,4	0.24	0	6,6,6	0.38	0
2	SO4	J	301	-	4,4,4	0.25	0	6,6,6	0.19	0
2	SO4	J	302	-	4,4,4	0.21	0	6,6,6	0.28	0
2	SO4	C	301	-	4,4,4	0.29	0	6,6,6	0.51	0
2	SO4	I	302	-	4,4,4	0.30	0	6,6,6	0.27	0
2	SO4	E	301	-	4,4,4	0.26	0	6,6,6	0.32	0
2	SO4	A	301	-	4,4,4	0.20	0	6,6,6	0.19	0
2	SO4	D	302	-	4,4,4	0.27	0	6,6,6	0.45	0
2	SO4	A	303	-	4,4,4	0.34	0	6,6,6	0.38	0
2	SO4	F	301	-	4,4,4	0.29	0	6,6,6	0.30	0
2	SO4	A	302	-	4,4,4	0.28	0	6,6,6	0.29	0
2	SO4	H	301	-	4,4,4	0.27	0	6,6,6	0.12	0
2	SO4	C	303	-	4,4,4	0.32	0	6,6,6	0.24	0
2	SO4	G	301	-	4,4,4	0.36	0	6,6,6	0.31	0
2	SO4	I	301	-	4,4,4	0.23	0	6,6,6	0.27	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
2	A	304	SO4	1	0
2	B	301	SO4	1	0
2	C	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	217/217 (100%)	-0.16	0	100	100	42, 50, 60, 66	0
1	B	216/217 (99%)	-0.15	0	100	100	42, 50, 59, 63	0
1	C	217/217 (100%)	-0.07	1 (0%)	91	81	42, 50, 59, 64	0
1	D	217/217 (100%)	-0.14	2 (0%)	84	69	41, 50, 59, 64	0
1	E	217/217 (100%)	-0.11	1 (0%)	91	81	42, 50, 59, 65	0
1	F	217/217 (100%)	-0.10	0	100	100	42, 50, 59, 64	0
1	G	216/217 (99%)	-0.09	2 (0%)	84	69	42, 50, 58, 63	0
1	H	217/217 (100%)	-0.15	2 (0%)	84	69	41, 50, 59, 65	0
1	I	217/217 (100%)	-0.09	1 (0%)	91	81	42, 51, 58, 64	0
1	J	217/217 (100%)	-0.17	0	100	100	42, 50, 60, 63	0
All	All	2168/2170 (99%)	-0.12	9 (0%)	92	84	41, 50, 59, 66	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-8	ASP	3.6
1	H	-5	ASP	2.6
1	H	-8	ASP	2.5
1	D	-5	ASP	2.5
1	G	17	SER	2.2

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(Å^2)	Q<0.9
2	SO4	H	301	5/5	0.83	0.17	88,88,89,89	0
2	SO4	G	301	5/5	0.94	0.20	64,65,65,66	0
2	SO4	H	302	5/5	0.94	0.15	60,60,61,61	0
2	SO4	C	303	5/5	0.95	0.16	88,89,89,89	0
2	SO4	F	301	5/5	0.95	0.23	56,56,57,58	0
2	SO4	F	303	5/5	0.95	0.13	72,74,74,75	0
2	SO4	J	302	5/5	0.95	0.17	62,62,62,63	0
2	SO4	A	302	5/5	0.96	0.20	65,67,68,68	0
2	SO4	E	302	5/5	0.96	0.29	60,60,61,62	0
2	SO4	A	304	5/5	0.96	0.12	81,81,82,82	0
2	SO4	J	301	5/5	0.96	0.17	64,65,65,65	0
2	SO4	C	301	5/5	0.96	0.25	64,64,64,65	0
2	SO4	A	301	5/5	0.97	0.15	66,67,67,67	0
2	SO4	D	301	5/5	0.97	0.10	84,84,85,85	0
2	SO4	D	302	5/5	0.97	0.14	64,64,65,65	0
2	SO4	E	301	5/5	0.97	0.15	71,73,73,73	0
2	SO4	I	301	5/5	0.97	0.15	79,80,80,80	0
2	SO4	I	302	5/5	0.97	0.32	59,59,60,61	0
2	SO4	B	301	5/5	0.97	0.23	54,54,55,55	0
2	SO4	A	303	5/5	0.97	0.13	66,67,68,68	0
2	SO4	B	304	5/5	0.98	0.07	74,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.