



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:49 PM UTC

PDB ID : 3GUA / pdb_00003gua
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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

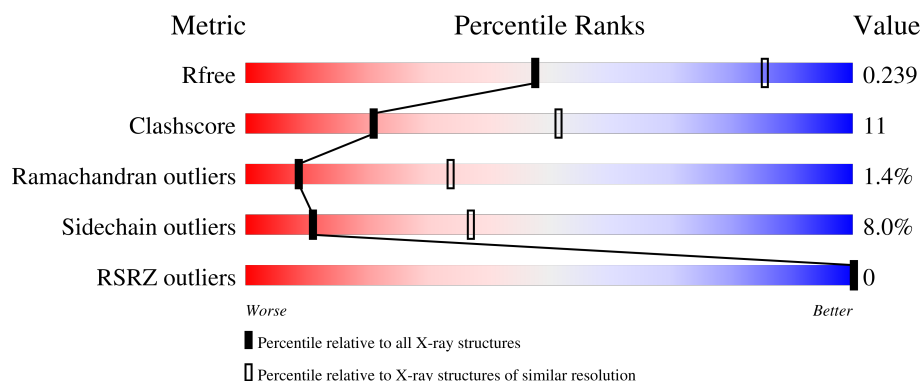
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. 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	217	 79% 17% . .
1	B	217	 82% 14% . .
1	C	217	 81% 14% . .
1	D	217	 83% 11% 5% .
1	E	217	 84% 11% . .

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Mol	Chain	Length	Quality of chain
1	F	217	 82% 14% . .
1	G	217	 78% 17% . .
1	H	217	 80% 13% 5% .
1	I	217	 84% 12% . .
1	J	217	 80% 14% . .

2 Entry composition

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

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

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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

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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 (CCD ID: SO4) (formula: O₄S).



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

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

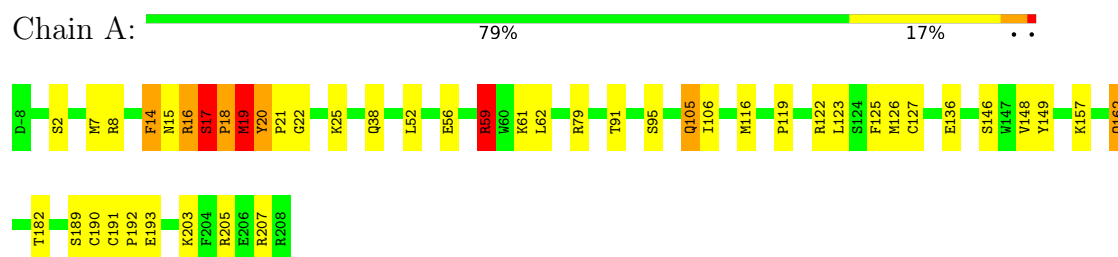
- Molecule 3 is water.

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

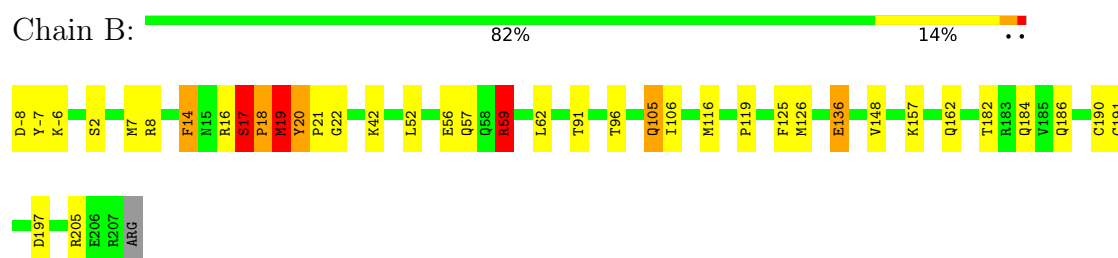
3 Residue-property plots [i](#)

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.

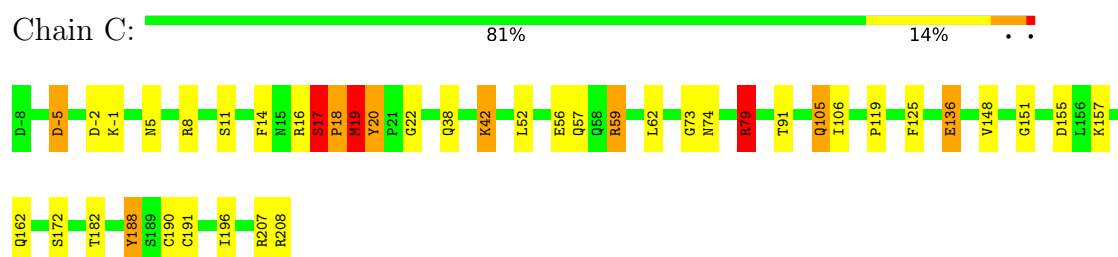
- Molecule 1: Soluble acetylcholine receptor



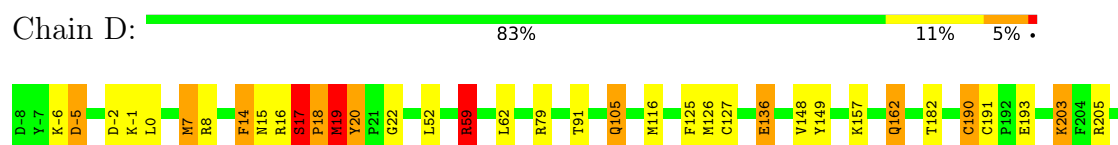
- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor



R208

- Molecule 1: Soluble acetylcholine receptor

Chain E:  84% 11% ..

D-8 D-5 D-2 K-1 L0 L6 M7 S11 F14 R15 R16 P18 P19 Y20 P21 G22 Q38 L52 R59 L62 R79 T80 T91 Q105 I106 M116 F125 M126 C127 E136 K157 Q162 S172 T182 S189 C190 C191 R203

R207
R208

- Molecule 1: Soluble acetylcholine receptor

Chain F:  82% 14% ..

D-8 D-5 D-2 M7 F14 N15 R16 P18 P19 Y20 G22 L52 E56 R59 L62 T91 Q105 I106 P119 F125 M126 E136 V148 Y149 K157 Q162 S172 T182 R183 Q184 Y185 Q186 C190 E193 F194 Y195 I196 D197

V202
R203 F204 E205 R206 R207 R208

- Molecule 1: Soluble acetylcholine receptor

Chain G:  78% 17% ..

D-8 D-5 D-2 S2 Q3 M7 R8 S11 F14 N15 R16 P18 P19 Y20 P21 G22 Q38 K42 L52 E56 Q57 R59 L62 M66 N74 R79 T91 S95 Q105 I106 M116 P119 L123 S124 F125 E136

V148 L156 K157 Q162 T182 R183 Q184 C190 C191 F192 E193 D197 K203 R207 ARG

- Molecule 1: Soluble acetylcholine receptor

Chain H:  80% 13% 5% .

D-8 Y-7 K-6 D-5 D-2 K-1 L0 M7 R8 F14 R15 R16 S17 P18 P19 Y20 P21 G22 L52 R59 L62 N74 R79 T91 S95 Q105 M116 L123 S124 F125 M126 C127 D133 S134 E135 E136 V148 D155 L156 K157 Q162 T182

P192 E193 I196 K203 F204 R205 E206 R207 R208

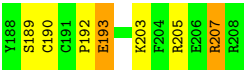
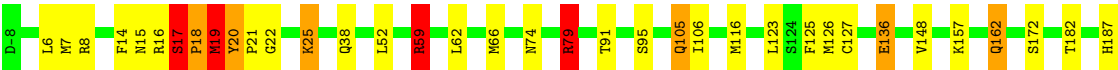
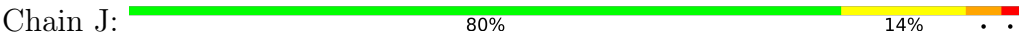
- Molecule 1: Soluble acetylcholine receptor

Chain I:  84% 12% ..

D-8 D-5 D-2 L6 M7 S11 R16 S17 P18 P19 Y20 P21 G22 Q38 L52 R59 L62 R79 T80 T91 Q105 I106 F125 M126 C127 D133 E136 Y149 K157 Q162 T182 R183 Q184 C190 C191 D197 K203



● Molecule 1: Soluble acetylcholine receptor



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.33 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	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.*

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 [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	0.85	2/1778 (0.1%)	1.13	10/2422 (0.4%)
1	B	0.65	1/1768 (0.1%)	0.94	5/2410 (0.2%)
1	C	0.64	1/1779 (0.1%)	1.03	8/2424 (0.3%)
1	D	0.68	2/1779 (0.1%)	1.01	8/2424 (0.3%)
1	E	0.67	1/1779 (0.1%)	1.00	8/2424 (0.3%)
1	F	0.73	2/1778 (0.1%)	1.02	7/2422 (0.3%)
1	G	0.61	0/1768	0.95	7/2410 (0.3%)
1	H	0.69	2/1779 (0.1%)	1.00	9/2424 (0.4%)
1	I	0.69	1/1779 (0.1%)	1.00	9/2424 (0.4%)
1	J	0.68	2/1779 (0.1%)	1.09	13/2424 (0.5%)
All	All	0.69	14/17766 (0.1%)	1.02	84/24208 (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 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	ARG	CZ-NH1	-17.95	1.07	1.32
1	A	205	ARG	CZ-NH2	-16.49	1.12	1.33
1	I	203	LYS	CD-CE	-12.04	1.16	1.52
1	F	205	ARG	CZ-NH1	-11.81	1.16	1.32
1	F	205	ARG	CZ-NH2	-9.44	1.21	1.33

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ARG	NH1-CZ-NH2	-19.97	93.34	119.30
1	A	205	ARG	NE-CZ-NH2	18.58	135.92	119.20
1	F	205	ARG	NE-CZ-NH2	14.55	132.29	119.20
1	F	17	SER	CA-C-N	12.77	135.80	119.84
1	F	17	SER	C-N-CA	12.77	135.80	119.84

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	45	0
1	B	1726	0	1642	41	1
1	C	1737	0	1655	39	0
1	D	1737	0	1655	42	0
1	E	1737	0	1655	32	1
1	F	1736	0	1653	42	0
1	G	1726	0	1642	43	0
1	H	1737	0	1655	48	0
1	I	1737	0	1655	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1737	0	1655	46	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	373	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 11.

The worst 5 of 373 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

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	A	215/217 (99%)	207 (96%)	5 (2%)	3 (1%)	9	34
1	B	214/217 (99%)	206 (96%)	5 (2%)	3 (1%)	9	34
1	C	215/217 (99%)	208 (97%)	4 (2%)	3 (1%)	9	34
1	D	215/217 (99%)	208 (97%)	4 (2%)	3 (1%)	9	34
1	E	215/217 (99%)	208 (97%)	4 (2%)	3 (1%)	9	34
1	F	215/217 (99%)	206 (96%)	6 (3%)	3 (1%)	9	34
1	G	214/217 (99%)	206 (96%)	5 (2%)	3 (1%)	9	34
1	H	215/217 (99%)	207 (96%)	5 (2%)	3 (1%)	9	34
1	I	215/217 (99%)	207 (96%)	5 (2%)	3 (1%)	9	34
1	J	215/217 (99%)	207 (96%)	5 (2%)	3 (1%)	9	34
All	All	2148/2170 (99%)	2070 (96%)	48 (2%)	30 (1%)	9	34

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

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	34
1	B	197/198 (100%)	185 (94%)	12 (6%)	17	46
1	C	198/198 (100%)	182 (92%)	16 (8%)	11	36
1	D	198/198 (100%)	181 (91%)	17 (9%)	10	34
1	E	198/198 (100%)	182 (92%)	16 (8%)	11	36
1	F	198/198 (100%)	184 (93%)	14 (7%)	13	41
1	G	197/198 (100%)	182 (92%)	15 (8%)	12	39
1	H	198/198 (100%)	178 (90%)	20 (10%)	7	28
1	I	198/198 (100%)	185 (93%)	13 (7%)	15	43
1	J	198/198 (100%)	180 (91%)	18 (9%)	9	32
All	All	1978/1980 (100%)	1820 (92%)	158 (8%)	11	37

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	59	ARG
1	J	19	MET
1	H	127	CYS
1	I	19	MET
1	J	136	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	58	GLN
1	J	121	GLN
1	G	105	GLN
1	J	105	GLN
1	I	121	GLN

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 [i](#)

There are no oligosaccharides 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	J	302	-	4,4,4	0.21	0	6,6,6	0.28	0
2	SO4	A	302	-	4,4,4	0.28	0	6,6,6	0.29	0
2	SO4	E	301	-	4,4,4	0.26	0	6,6,6	0.32	0
2	SO4	H	301	-	4,4,4	0.27	0	6,6,6	0.12	0
2	SO4	H	302	-	4,4,4	0.24	0	6,6,6	0.38	0
2	SO4	A	303	-	4,4,4	0.34	0	6,6,6	0.38	0
2	SO4	B	304	-	4,4,4	0.20	0	6,6,6	0.21	0
2	SO4	F	303	-	4,4,4	0.30	0	6,6,6	0.30	0
2	SO4	D	302	-	4,4,4	0.27	0	6,6,6	0.45	0
2	SO4	I	302	-	4,4,4	0.30	0	6,6,6	0.27	0
2	SO4	F	301	-	4,4,4	0.29	0	6,6,6	0.30	0
2	SO4	G	301	-	4,4,4	0.36	0	6,6,6	0.31	0
2	SO4	C	301	-	4,4,4	0.29	0	6,6,6	0.51	0
2	SO4	I	301	-	4,4,4	0.23	0	6,6,6	0.27	0
2	SO4	C	303	-	4,4,4	0.32	0	6,6,6	0.24	0
2	SO4	A	301	-	4,4,4	0.20	0	6,6,6	0.19	0
2	SO4	D	301	-	4,4,4	0.31	0	6,6,6	0.18	0
2	SO4	J	301	-	4,4,4	0.25	0	6,6,6	0.19	0
2	SO4	B	301	-	4,4,4	0.30	0	6,6,6	0.43	0
2	SO4	A	304	-	4,4,4	0.41	0	6,6,6	0.28	0
2	SO4	E	302	-	4,4,4	0.24	0	6,6,6	0.40	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	C	301	SO4	1	0
2	B	301	SO4	1	0
2	A	304	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%)	-1.62	0 100 100	42, 50, 60, 66	0
1	B	216/217 (99%)	-1.60	0 100 100	42, 50, 59, 63	0
1	C	217/217 (100%)	-1.54	0 100 100	42, 50, 59, 64	0
1	D	217/217 (100%)	-1.59	0 100 100	41, 50, 59, 64	0
1	E	217/217 (100%)	-1.57	0 100 100	42, 50, 59, 65	0
1	F	217/217 (100%)	-1.58	0 100 100	42, 50, 59, 64	0
1	G	216/217 (99%)	-1.53	0 100 100	42, 50, 58, 63	0
1	H	217/217 (100%)	-1.59	0 100 100	41, 50, 59, 65	0
1	I	217/217 (100%)	-1.56	0 100 100	42, 51, 58, 64	0
1	J	217/217 (100%)	-1.59	0 100 100	42, 50, 60, 63	0
All	All	2168/2170 (99%)	-1.58	0 100 100	41, 50, 59, 66	0

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 oligosaccharides 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	0.97	0.04	88,88,89,89	0
2	SO4	A	304	5/5	0.98	0.07	81,81,82,82	0
2	SO4	F	301	5/5	0.98	0.05	56,56,57,58	0
2	SO4	A	301	5/5	0.98	0.05	66,67,67,67	0
2	SO4	B	301	5/5	0.99	0.05	54,54,55,55	0
2	SO4	B	304	5/5	0.99	0.03	74,75,75,75	0
2	SO4	C	301	5/5	0.99	0.07	64,64,64,65	0
2	SO4	C	303	5/5	0.99	0.04	88,89,89,89	0
2	SO4	D	301	5/5	0.99	0.03	84,84,85,85	0
2	SO4	D	302	5/5	0.99	0.05	64,64,65,65	0
2	SO4	E	301	5/5	0.99	0.03	71,73,73,73	0
2	SO4	E	302	5/5	0.99	0.07	60,60,61,62	0
2	SO4	A	303	5/5	0.99	0.07	66,67,68,68	0
2	SO4	F	303	5/5	0.99	0.03	72,74,74,75	0
2	SO4	G	301	5/5	0.99	0.05	64,65,65,66	0
2	SO4	A	302	5/5	0.99	0.05	65,67,68,68	0
2	SO4	H	302	5/5	0.99	0.03	60,60,61,61	0
2	SO4	I	301	5/5	0.99	0.04	79,80,80,80	0
2	SO4	I	302	5/5	0.99	0.09	59,59,60,61	0
2	SO4	J	301	5/5	0.99	0.05	64,65,65,65	0
2	SO4	J	302	5/5	0.99	0.04	62,62,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.