



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:31 PM UTC

PDB ID : 5OAN / pdb_00005oan
Title : Crystal structure of mutant AChBP in complex with glycine (T53F, Q74R, Y110A, I135S, G162E, S206CCP_KGTG)
Authors : Dawson, A.; Hunter, W.N.; de Souza, J.O.; Trumper, P.
Deposited on : 2017-06-23
Resolution : 2.60 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 : 4-5-2 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

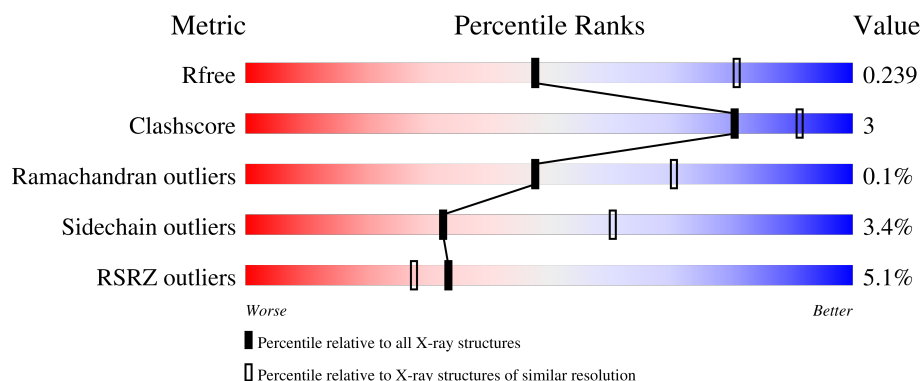
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	249	3% 78% • 17%
1	B	249	4% 78% 7% 15%
1	C	249	6% 79% 5% • 15%
1	D	249	4% 78% 5% • 16%
1	E	249	5% 77% 5% • 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GLY	B	601	-	X	-	-
4	GLY	C	601	-	X	-	-
4	GLY	D	601	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8744 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	206	Total	C	N	O	S	0	2	0
			1660	1049	276	328	7			
1	B	211	Total	C	N	O	S	0	3	0
			1700	1077	283	333	7			
1	C	212	Total	C	N	O	S	0	4	0
			1726	1091	293	334	8			
1	D	208	Total	C	N	O	S	0	4	0
			1693	1075	279	331	8			
1	E	206	Total	C	N	O	S	0	4	0
			1670	1056	277	329	8			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	PHE	THR	engineered mutation	UNP Q8WSF8
A	60	VAL	ALA	engineered mutation	UNP Q8WSF8
A	74	ARG	GLN	engineered mutation	UNP Q8WSF8
A	110	ALA	TYR	engineered mutation	UNP Q8WSF8
A	135	SER	ILE	engineered mutation	UNP Q8WSF8
A	155	VAL	ALA	engineered mutation	UNP Q8WSF8
A	162	GLU	GLY	engineered mutation	UNP Q8WSF8
A	206	LYS	SER	engineered mutation	UNP Q8WSF8
A	207	GLY	CYS	engineered mutation	UNP Q8WSF8
A	208	THR	CYS	engineered mutation	UNP Q8WSF8
A	209	GLY	PRO	engineered mutation	UNP Q8WSF8
A	237	GLU	-	expression tag	UNP Q8WSF8
A	238	ASN	-	expression tag	UNP Q8WSF8
A	239	LEU	-	expression tag	UNP Q8WSF8
A	240	TYR	-	expression tag	UNP Q8WSF8
A	241	PHE	-	expression tag	UNP Q8WSF8
A	242	GLN	-	expression tag	UNP Q8WSF8
A	243	GLY	-	expression tag	UNP Q8WSF8
A	244	HIS	-	expression tag	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	HIS	-	expression tag	UNP Q8WSF8
A	246	HIS	-	expression tag	UNP Q8WSF8
A	247	HIS	-	expression tag	UNP Q8WSF8
A	248	HIS	-	expression tag	UNP Q8WSF8
A	249	HIS	-	expression tag	UNP Q8WSF8
B	53	PHE	THR	engineered mutation	UNP Q8WSF8
B	60	VAL	ALA	engineered mutation	UNP Q8WSF8
B	74	ARG	GLN	engineered mutation	UNP Q8WSF8
B	110	ALA	TYR	engineered mutation	UNP Q8WSF8
B	135	SER	ILE	engineered mutation	UNP Q8WSF8
B	155	VAL	ALA	engineered mutation	UNP Q8WSF8
B	162	GLU	GLY	engineered mutation	UNP Q8WSF8
B	206	LYS	SER	engineered mutation	UNP Q8WSF8
B	207	GLY	CYS	engineered mutation	UNP Q8WSF8
B	208	THR	CYS	engineered mutation	UNP Q8WSF8
B	209	GLY	PRO	engineered mutation	UNP Q8WSF8
B	237	GLU	-	expression tag	UNP Q8WSF8
B	238	ASN	-	expression tag	UNP Q8WSF8
B	239	LEU	-	expression tag	UNP Q8WSF8
B	240	TYR	-	expression tag	UNP Q8WSF8
B	241	PHE	-	expression tag	UNP Q8WSF8
B	242	GLN	-	expression tag	UNP Q8WSF8
B	243	GLY	-	expression tag	UNP Q8WSF8
B	244	HIS	-	expression tag	UNP Q8WSF8
B	245	HIS	-	expression tag	UNP Q8WSF8
B	246	HIS	-	expression tag	UNP Q8WSF8
B	247	HIS	-	expression tag	UNP Q8WSF8
B	248	HIS	-	expression tag	UNP Q8WSF8
B	249	HIS	-	expression tag	UNP Q8WSF8
C	53	PHE	THR	engineered mutation	UNP Q8WSF8
C	60	VAL	ALA	engineered mutation	UNP Q8WSF8
C	74	ARG	GLN	engineered mutation	UNP Q8WSF8
C	110	ALA	TYR	engineered mutation	UNP Q8WSF8
C	135	SER	ILE	engineered mutation	UNP Q8WSF8
C	155	VAL	ALA	engineered mutation	UNP Q8WSF8
C	162	GLU	GLY	engineered mutation	UNP Q8WSF8
C	206	LYS	SER	engineered mutation	UNP Q8WSF8
C	207	GLY	CYS	engineered mutation	UNP Q8WSF8
C	208	THR	CYS	engineered mutation	UNP Q8WSF8
C	209	GLY	PRO	engineered mutation	UNP Q8WSF8
C	238	GLU	-	expression tag	UNP Q8WSF8
C	239	ASN	-	expression tag	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	240	LEU	-	expression tag	UNP Q8WSF8
C	241	TYR	-	expression tag	UNP Q8WSF8
C	242	PHE	-	expression tag	UNP Q8WSF8
C	243	GLN	-	expression tag	UNP Q8WSF8
C	244	GLY	-	expression tag	UNP Q8WSF8
C	245	HIS	-	expression tag	UNP Q8WSF8
C	246	HIS	-	expression tag	UNP Q8WSF8
C	247	HIS	-	expression tag	UNP Q8WSF8
C	248	HIS	-	expression tag	UNP Q8WSF8
C	249	HIS	-	expression tag	UNP Q8WSF8
C	250	HIS	-	expression tag	UNP Q8WSF8
D	53	PHE	THR	engineered mutation	UNP Q8WSF8
D	60	VAL	ALA	engineered mutation	UNP Q8WSF8
D	74	ARG	GLN	engineered mutation	UNP Q8WSF8
D	110	ALA	TYR	engineered mutation	UNP Q8WSF8
D	135	SER	ILE	engineered mutation	UNP Q8WSF8
D	155	VAL	ALA	engineered mutation	UNP Q8WSF8
D	162	GLU	GLY	engineered mutation	UNP Q8WSF8
D	206	LYS	SER	engineered mutation	UNP Q8WSF8
D	207	GLY	CYS	engineered mutation	UNP Q8WSF8
D	208	THR	CYS	engineered mutation	UNP Q8WSF8
D	209	GLY	PRO	engineered mutation	UNP Q8WSF8
D	237	GLU	-	expression tag	UNP Q8WSF8
D	238	ASN	-	expression tag	UNP Q8WSF8
D	239	LEU	-	expression tag	UNP Q8WSF8
D	240	TYR	-	expression tag	UNP Q8WSF8
D	241	PHE	-	expression tag	UNP Q8WSF8
D	242	GLN	-	expression tag	UNP Q8WSF8
D	243	GLY	-	expression tag	UNP Q8WSF8
D	244	HIS	-	expression tag	UNP Q8WSF8
D	245	HIS	-	expression tag	UNP Q8WSF8
D	246	HIS	-	expression tag	UNP Q8WSF8
D	247	HIS	-	expression tag	UNP Q8WSF8
D	248	HIS	-	expression tag	UNP Q8WSF8
D	249	HIS	-	expression tag	UNP Q8WSF8
E	53	PHE	THR	engineered mutation	UNP Q8WSF8
E	60	VAL	ALA	engineered mutation	UNP Q8WSF8
E	74	ARG	GLN	engineered mutation	UNP Q8WSF8
E	110	ALA	TYR	engineered mutation	UNP Q8WSF8
E	135	SER	ILE	engineered mutation	UNP Q8WSF8
E	155	VAL	ALA	engineered mutation	UNP Q8WSF8
E	162	GLU	GLY	engineered mutation	UNP Q8WSF8

Continued on next page...

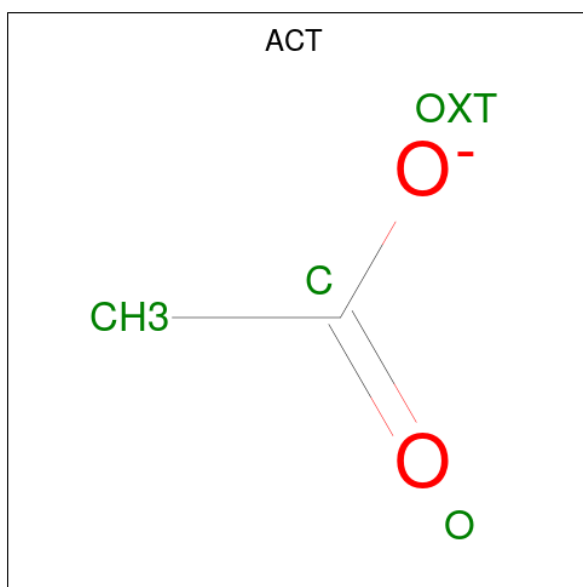
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	206	LYS	SER	engineered mutation	UNP Q8WSF8
E	207	GLY	CYS	engineered mutation	UNP Q8WSF8
E	208	THR	CYS	engineered mutation	UNP Q8WSF8
E	209	GLY	PRO	engineered mutation	UNP Q8WSF8
E	237	GLU	-	expression tag	UNP Q8WSF8
E	238	ASN	-	expression tag	UNP Q8WSF8
E	239	LEU	-	expression tag	UNP Q8WSF8
E	240	TYR	-	expression tag	UNP Q8WSF8
E	241	PHE	-	expression tag	UNP Q8WSF8
E	242	GLN	-	expression tag	UNP Q8WSF8
E	243	GLY	-	expression tag	UNP Q8WSF8
E	244	HIS	-	expression tag	UNP Q8WSF8
E	245	HIS	-	expression tag	UNP Q8WSF8
E	246	HIS	-	expression tag	UNP Q8WSF8
E	247	HIS	-	expression tag	UNP Q8WSF8
E	248	HIS	-	expression tag	UNP Q8WSF8
E	249	HIS	-	expression tag	UNP Q8WSF8

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

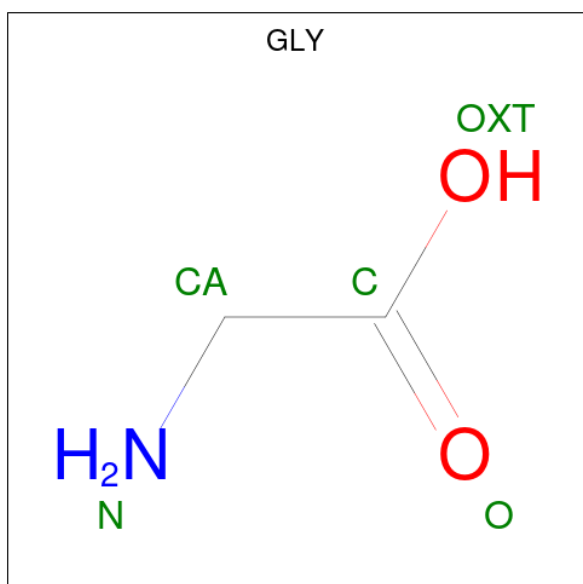
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



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

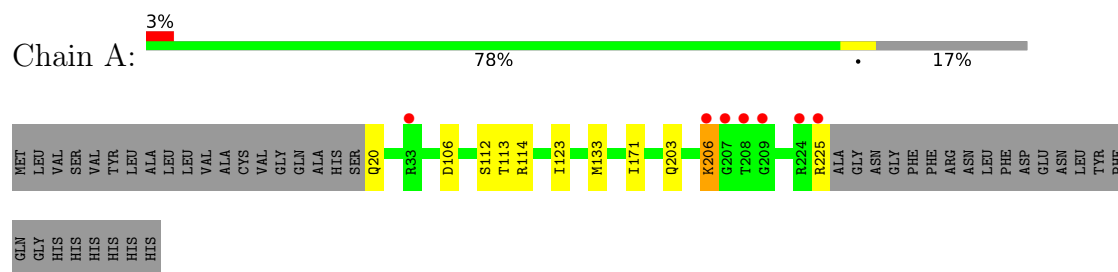
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	44	Total O 44 44	0	0
5	B	55	Total O 55 55	0	0
5	C	66	Total O 66 66	0	0
5	D	43	Total O 43 43	0	0
5	E	42	Total O 42 42	0	0

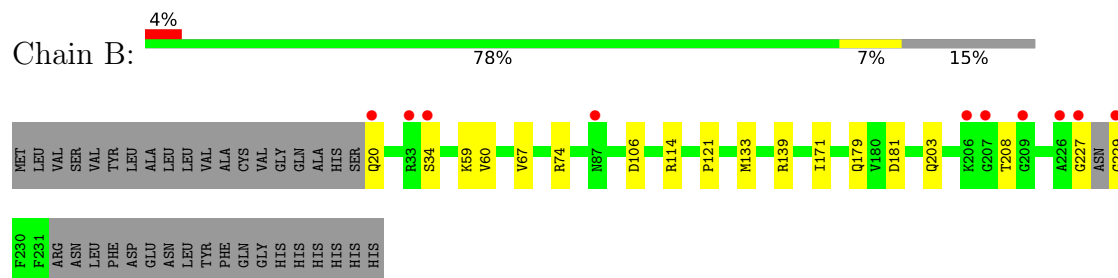
3 Residue-property plots [i](#)

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.

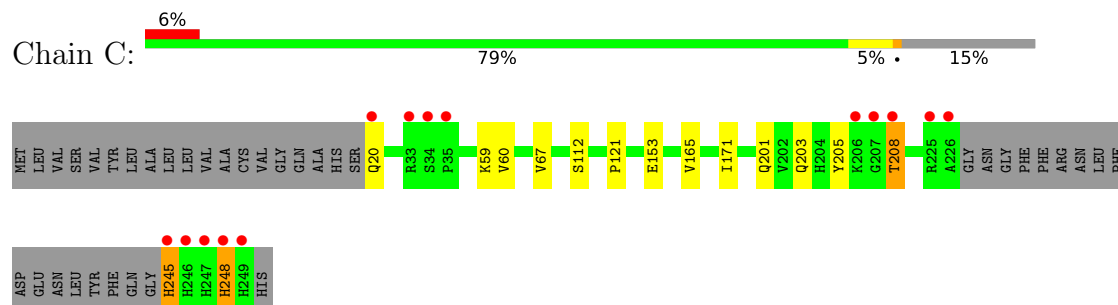
- Molecule 1: Soluble acetylcholine receptor



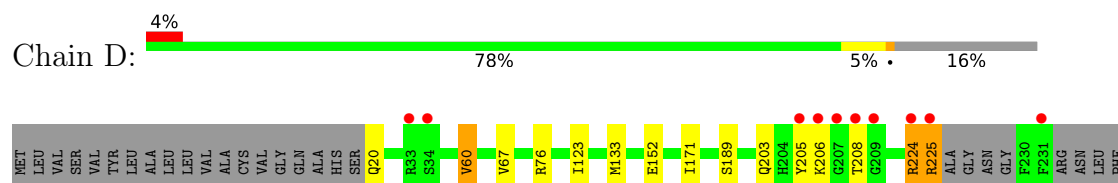
- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor

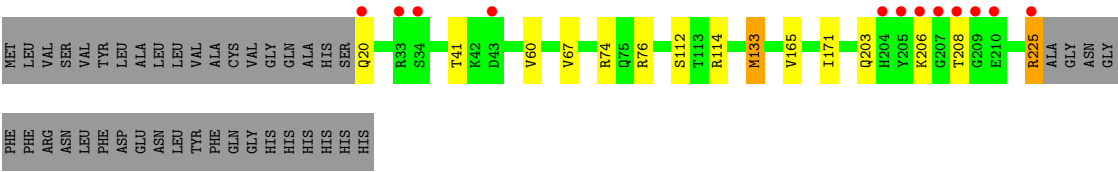
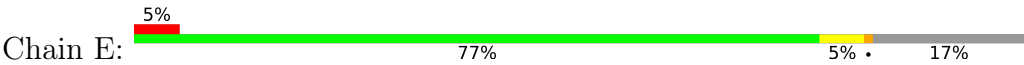


- Molecule 1: Soluble acetylcholine receptor



ASP
GLU
ASN
LEU
TYR
PHE
GLN
GLY
HIS
HIS
HIS
HIS
HIS

● Molecule 1: Soluble acetylcholine receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	89.92Å 100.27Å 165.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.90 – 2.60 32.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.90-2.60) 99.9 (32.90-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.202 , 0.235 0.206 , 0.239	Depositor DCC
R_{free} test set	2381 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8744	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: ACT, CL

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	0.66	0/1705	0.77	0/2320
1	B	0.68	0/1751	0.83	2/2381 (0.1%)
1	C	0.69	1/1782 (0.1%)	0.79	0/2423
1	D	0.65	0/1746	0.77	0/2374
1	E	0.66	0/1722	0.79	2/2344 (0.1%)
All	All	0.67	1/8706 (0.0%)	0.79	4/11842 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	248	HIS	N-CA	5.05	1.52	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	THR	CA-C-O	-7.05	113.60	121.00
1	E	208	THR	CA-C-O	-6.14	114.55	121.00
1	E	208	THR	N-CA-C	5.25	116.69	110.97
1	B	208	THR	N-CA-C	5.12	116.55	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1660	0	1600	9	0
1	B	1700	0	1639	11	1
1	C	1726	0	1659	8	1
1	D	1693	0	1635	10	0
1	E	1670	0	1616	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	4	0	3	1	0
3	B	4	0	3	0	0
3	C	4	0	3	1	0
3	D	4	0	3	0	0
3	E	4	0	3	1	0
4	B	5	0	2	0	0
4	C	5	0	2	0	0
4	D	5	0	2	0	0
4	E	5	0	2	0	0
5	A	44	0	0	0	0
5	B	55	0	0	0	0
5	C	66	0	0	0	1
5	D	43	0	0	0	0
5	E	42	0	0	2	0
All	All	8744	0	8172	43	2

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 3.

All (43) 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:B:114[B]:ARG:HH11	1:B:114[B]:ARG:HG3	1.15	1.12
1:A:114[B]:ARG:HH11	1:A:114[B]:ARG:HG3	0.98	1.07
1:A:114[B]:ARG:HH11	1:A:114[B]:ARG:CG	1.79	0.94
1:E:114[B]:ARG:HH11	1:E:114[B]:ARG:HG3	1.29	0.94
1:A:114[B]:ARG:HG3	1:A:114[B]:ARG:NH1	1.78	0.88
1:B:114[B]:ARG:HG3	1:B:114[B]:ARG:NH1	1.92	0.75
1:E:114[B]:ARG:HH11	1:E:114[B]:ARG:CG	2.01	0.74
1:A:206:LYS:HE2	1:B:181:ASP:OD1	1.90	0.72
1:B:114[B]:ARG:HH11	1:B:114[B]:ARG:CG	1.97	0.71
1:A:114[B]:ARG:CG	1:A:114[B]:ARG:NH1	2.44	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114[B]:ARG:NH1	1:B:114[B]:ARG:CG	2.58	0.65
1:E:225:ARG:HH21	1:E:225:ARG:HG2	1.64	0.63
1:D:189:SER:O	1:D:224:ARG:NE	2.32	0.63
1:E:114[B]:ARG:HG3	1:E:114[B]:ARG:NH1	2.08	0.60
1:E:225:ARG:HG2	1:E:225:ARG:NH2	2.19	0.57
1:C:165:VAL:HG21	1:D:123:ILE:HG21	1.87	0.56
1:E:114[B]:ARG:CG	1:E:114[B]:ARG:NH1	2.63	0.56
1:C:153[A]:GLU:OE1	1:C:153[A]:GLU:HA	2.07	0.54
1:E:76:ARG:HD2	5:E:421:HOH:O	2.08	0.53
1:C:205:TYR:HB2	1:C:208:THR:O	2.09	0.52
1:D:205:TYR:HB2	1:D:208:THR:O	2.12	0.50
1:D:152:GLU:HG2	1:D:225:ARG:NH1	2.31	0.46
1:D:60:VAL:HG22	1:D:67:VAL:HG22	1.98	0.45
1:A:106:ASP:HB2	1:B:121:PRO:HG2	1.99	0.45
1:A:123:ILE:HG21	1:E:165:VAL:HG21	1.98	0.45
1:B:60:VAL:HG22	1:B:67:VAL:HG22	1.99	0.43
1:D:224:ARG:HG3	1:D:224:ARG:NH1	2.34	0.43
1:E:112:SER:O	3:E:301:ACT:H1	2.18	0.43
1:E:60:VAL:HG22	1:E:67:VAL:HG22	2.00	0.43
1:B:227:GLY:O	1:B:229:GLY:HA2	2.19	0.43
1:C:245:HIS:N	1:C:245:HIS:HD1	2.17	0.43
1:A:112:SER:O	3:A:302:ACT:H1	2.19	0.43
1:B:227:GLY:C	1:B:229:GLY:HA2	2.44	0.42
1:C:112:SER:O	3:C:603:ACT:H1	2.19	0.42
1:E:74:ARG:HD3	1:E:133[B]:MET:HE1	2.01	0.42
1:E:41:THR:HB	5:E:437:HOH:O	2.19	0.42
1:C:60:VAL:HG22	1:C:67:VAL:HG22	2.01	0.42
1:D:189:SER:O	1:D:224:ARG:HD2	2.20	0.42
1:C:165:VAL:HG21	1:D:123:ILE:CG2	2.50	0.41
1:A:113:THR:O	1:B:139:ARG:HD2	2.21	0.41
1:D:189:SER:O	1:D:224:ARG:CD	2.69	0.41
1:D:76:ARG:NH1	1:D:133[A]:MET:HE2	2.36	0.41
1:B:106:ASP:HB2	1:C:121:PRO:HG2	2.02	0.40

All (2) 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)
5:C:718:HOH:O	5:C:718:HOH:O[2_575]	1.50	0.70
1:B:179:GLN:NE2	1:C:201:GLN:OE1[3_745]	2.18	0.02

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	205/249 (82%)	200 (98%)	5 (2%)	0	100	100
1	B	210/249 (84%)	206 (98%)	4 (2%)	0	100	100
1	C	212/249 (85%)	207 (98%)	4 (2%)	1 (0%)	24	46
1	D	208/249 (84%)	204 (98%)	4 (2%)	0	100	100
1	E	208/249 (84%)	204 (98%)	4 (2%)	0	100	100
All	All	1043/1245 (84%)	1021 (98%)	21 (2%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	248	HIS

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	189/222 (85%)	183 (97%)	6 (3%)	34	62
1	B	192/222 (86%)	185 (96%)	7 (4%)	31	58
1	C	196/222 (88%)	190 (97%)	6 (3%)	35	63
1	D	193/222 (87%)	186 (96%)	7 (4%)	31	58
1	E	191/222 (86%)	184 (96%)	7 (4%)	30	57
All	All	961/1110 (87%)	928 (97%)	33 (3%)	32	60

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	133	MET
1	A	171	ILE
1	A	203	GLN
1	A	206	LYS
1	A	225	ARG
1	B	20	GLN
1	B	34	SER
1	B	59	LYS
1	B	74	ARG
1	B	133	MET
1	B	171	ILE
1	B	203	GLN
1	C	20	GLN
1	C	59	LYS
1	C	171	ILE
1	C	203	GLN
1	C	208	THR
1	C	245	HIS
1	D	20	GLN
1	D	60	VAL
1	D	171	ILE
1	D	203	GLN
1	D	206	LYS
1	D	224	ARG
1	D	225	ARG
1	E	20	GLN
1	E	133[A]	MET
1	E	133[B]	MET
1	E	171	ILE
1	E	203	GLN
1	E	206	LYS
1	E	225	ARG

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

Mol	Chain	Res	Type
1	A	20	GLN
1	A	65	ASN
1	A	201	GLN
1	B	20	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	55	GLN
1	B	179	GLN
1	B	201	GLN
1	C	20	GLN
1	C	179	GLN
1	C	248	HIS
1	D	20	GLN
1	D	55	GLN
1	D	65	ASN
1	E	20	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	ACT	A	302	-	3,3,3	0.81	0	3,3,3	0.82	0
3	ACT	C	603	-	3,3,3	0.79	0	3,3,3	0.97	0
3	ACT	B	603	-	3,3,3	0.81	0	3,3,3	0.88	0
4	GLY	C	601	-	4,4,4	1.26	1 (25%)	3,4,4	1.85	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GLY	B	601	-	4,4,4	1.17	1 (25%)	3,4,4	2.03	2 (66%)
4	GLY	E	302	-	4,4,4	1.05	0	3,4,4	1.54	1 (33%)
3	ACT	D	603	-	3,3,3	0.97	0	3,3,3	0.47	0
4	GLY	D	601	-	4,4,4	1.13	1 (25%)	3,4,4	1.96	2 (66%)
3	ACT	E	301	-	3,3,3	0.89	0	3,3,3	0.88	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	GLY	D	601	-	-	2/2/2/2	-
4	GLY	B	601	-	-	2/2/2/2	-
4	GLY	C	601	-	-	2/2/2/2	-
4	GLY	E	302	-	-	0/2/2/2	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	GLY	OXT-C	-2.36	1.23	1.30
4	B	601	GLY	OXT-C	-2.26	1.23	1.30
4	D	601	GLY	OXT-C	-2.22	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	GLY	OXT-C-O	-2.71	116.35	123.33
4	D	601	GLY	OXT-C-O	-2.65	116.52	123.33
4	C	601	GLY	OXT-C-O	-2.65	116.52	123.33
4	B	601	GLY	OXT-C-CA	2.22	122.19	113.38
4	D	601	GLY	OXT-C-CA	2.11	121.79	113.38
4	E	302	GLY	OXT-C-CA	2.08	121.63	113.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	GLY	O-C-CA-N
4	B	601	GLY	OXT-C-CA-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	601	GLY	O-C-CA-N
4	D	601	GLY	OXT-C-CA-N
4	C	601	GLY	O-C-CA-N
4	C	601	GLY	OXT-C-CA-N

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	ACT	1	0
3	C	603	ACT	1	0
3	E	301	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	224:ARG	C	225:ARG	N	3.29

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	A	206/249 (82%)	-0.11	7 (3%) 48 42	9, 25, 56, 80	2 (0%)
1	B	211/249 (84%)	-0.01	10 (4%) 36 30	9, 23, 59, 88	3 (1%)
1	C	212/249 (85%)	-0.05	14 (6%) 24 19	9, 22, 62, 95	4 (1%)
1	D	208/249 (83%)	-0.01	10 (4%) 35 30	8, 26, 59, 105	4 (1%)
1	E	206/249 (82%)	0.10	12 (5%) 29 23	11, 27, 65, 119	4 (1%)
All	All	1043/1245 (83%)	-0.02	53 (5%) 33 28	8, 25, 61, 119	17 (1%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	GLY	7.3
1	E	205	TYR	6.4
1	D	208	THR	6.3
1	E	206	LYS	5.9
1	B	226	ALA	5.5
1	D	207	GLY	5.4
1	D	209	GLY	5.3
1	E	207	GLY	5.2
1	A	208	THR	4.6
1	C	249	HIS	4.6
1	C	226	ALA	4.5
1	C	33	ARG	4.3
1	A	207	GLY	3.8
1	C	245	HIS	3.8
1	D	205	TYR	3.7
1	E	208	THR	3.6
1	D	225	ARG	3.6
1	C	207	GLY	3.5
1	D	231	PHE	3.1
1	A	33	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	209	GLY	3.1
1	B	206	LYS	3.1
1	E	209	GLY	3.0
1	E	204	HIS	2.9
1	D	33	ARG	2.8
1	A	225	ARG	2.8
1	C	248	HIS	2.8
1	D	224	ARG	2.8
1	C	206	LYS	2.7
1	B	209	GLY	2.7
1	E	210	GLU	2.7
1	A	224	ARG	2.6
1	B	33	ARG	2.6
1	E	33	ARG	2.6
1	E	225	ARG	2.6
1	C	208	THR	2.5
1	E	43	ASP	2.5
1	C	246	HIS	2.5
1	C	20	GLN	2.5
1	D	206	LYS	2.4
1	B	20	GLN	2.4
1	B	229	GLY	2.4
1	C	35	PRO	2.4
1	C	34	SER	2.3
1	E	20	GLN	2.3
1	D	34	SER	2.2
1	E	34	SER	2.2
1	A	206	LYS	2.2
1	C	247	HIS	2.2
1	C	225	ARG	2.2
1	B	34	SER	2.1
1	B	207	GLY	2.1
1	B	87[A]	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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
4	GLY	C	601	5/5	0.78	0.21	54,56,57,61	0
4	GLY	D	601	5/5	0.83	0.18	45,50,52,55	0
4	GLY	E	302	5/5	0.84	0.20	57,60,64,65	0
3	ACT	D	603	4/4	0.88	0.15	23,24,24,24	0
4	GLY	B	601	5/5	0.91	0.14	42,47,49,50	0
3	ACT	A	302	4/4	0.92	0.12	28,29,29,29	0
3	ACT	C	603	4/4	0.93	0.14	31,31,32,32	0
3	ACT	B	603	4/4	0.93	0.10	27,29,29,30	0
3	ACT	E	301	4/4	0.94	0.11	26,28,28,30	0
2	CL	A	301	1/1	0.96	0.06	38,38,38,38	0
2	CL	D	602	1/1	0.97	0.05	32,32,32,32	0
2	CL	B	602	1/1	0.97	0.04	26,26,26,26	0
2	CL	E	303	1/1	0.98	0.04	32,32,32,32	0
2	CL	C	602	1/1	0.98	0.04	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.