



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 25, 2018 – 06:46 PM EST

PDB ID : 5OSA
Title : GLIC-GABAAR alpha1 chimera crystallized at pH4.6
Authors : Lavery, D.C.; Gold, M.G.; Smart, T.G.
Deposited on : 2017-08-17
Resolution : 2.75 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

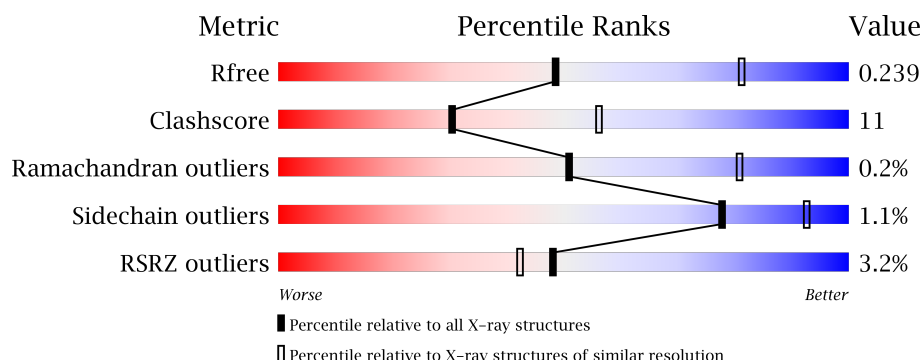
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	336	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>7%</div> </div> </div>
1	B	336	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>7%</div> </div> </div>
1	C	336	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>7%</div> </div> </div>
1	D	336	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>7%</div> </div> </div>
1	E	336	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>7%</div> </div> </div>

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
2	ACT	A	502	-	-	-	X
2	ACT	B	501	-	-	X	-
2	ACT	C	501	-	-	X	X
2	ACT	D	501	-	-	-	X
2	ACT	D	502	-	-	-	X
2	ACT	E	501	-	-	X	-
4	D12	B	503	-	-	-	X
4	D12	D	505	-	-	-	X
4	D12	E	504	-	-	-	X
5	Y01	A	507	-	-	-	X
5	Y01	B	505	-	-	-	X
5	Y01	C	505	-	-	-	X
5	Y01	D	506	-	-	-	X
5	Y01	E	505	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13261 atoms, of which 459 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 Proton-gated ion channel, Gamma-aminobutyric acid receptor subunit alpha-2, Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2489	1627	400	456	6			
1	B	313	Total	C	N	O	S	0	0	0
			2495	1630	403	456	6			
1	C	313	Total	C	N	O	S	0	0	0
			2495	1630	403	456	6			
1	D	313	Total	C	N	O	S	0	0	0
			2489	1627	400	456	6			
1	E	313	Total	C	N	O	S	0	0	0
			2489	1627	400	456	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	VAL	GLY	conflict	UNP P26048
A	312	SER	-	linker	UNP P26048
A	313	GLN	-	linker	UNP P26048
A	314	PRO	-	linker	UNP P26048
A	315	ALA	-	linker	UNP P26048
A	316	ARG	-	linker	UNP P26048
A	317	ALA	-	linker	UNP P26048
A	318	ALA	-	linker	UNP P26048
A	429	HIS	-	expression tag	UNP A0A093IEU4
A	430	HIS	-	expression tag	UNP A0A093IEU4
A	431	HIS	-	expression tag	UNP A0A093IEU4
A	432	HIS	-	expression tag	UNP A0A093IEU4
A	433	HIS	-	expression tag	UNP A0A093IEU4
A	434	HIS	-	expression tag	UNP A0A093IEU4
A	435	HIS	-	expression tag	UNP A0A093IEU4
A	436	HIS	-	expression tag	UNP A0A093IEU4
B	258	VAL	GLY	conflict	UNP P26048
B	312	SER	-	linker	UNP P26048

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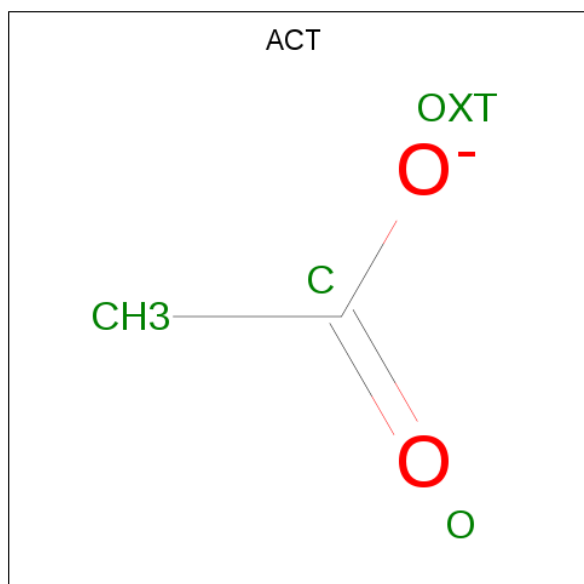
Chain	Residue	Modelled	Actual	Comment	Reference
B	313	GLN	-	linker	UNP P26048
B	314	PRO	-	linker	UNP P26048
B	315	ALA	-	linker	UNP P26048
B	316	ARG	-	linker	UNP P26048
B	317	ALA	-	linker	UNP P26048
B	318	ALA	-	linker	UNP P26048
B	429	HIS	-	expression tag	UNP A0A093IEU4
B	430	HIS	-	expression tag	UNP A0A093IEU4
B	431	HIS	-	expression tag	UNP A0A093IEU4
B	432	HIS	-	expression tag	UNP A0A093IEU4
B	433	HIS	-	expression tag	UNP A0A093IEU4
B	434	HIS	-	expression tag	UNP A0A093IEU4
B	435	HIS	-	expression tag	UNP A0A093IEU4
B	436	HIS	-	expression tag	UNP A0A093IEU4
C	258	VAL	GLY	conflict	UNP P26048
C	312	SER	-	linker	UNP P26048
C	313	GLN	-	linker	UNP P26048
C	314	PRO	-	linker	UNP P26048
C	315	ALA	-	linker	UNP P26048
C	316	ARG	-	linker	UNP P26048
C	317	ALA	-	linker	UNP P26048
C	318	ALA	-	linker	UNP P26048
C	429	HIS	-	expression tag	UNP A0A093IEU4
C	430	HIS	-	expression tag	UNP A0A093IEU4
C	431	HIS	-	expression tag	UNP A0A093IEU4
C	432	HIS	-	expression tag	UNP A0A093IEU4
C	433	HIS	-	expression tag	UNP A0A093IEU4
C	434	HIS	-	expression tag	UNP A0A093IEU4
C	435	HIS	-	expression tag	UNP A0A093IEU4
C	436	HIS	-	expression tag	UNP A0A093IEU4
D	258	VAL	GLY	conflict	UNP P26048
D	312	SER	-	linker	UNP P26048
D	313	GLN	-	linker	UNP P26048
D	314	PRO	-	linker	UNP P26048
D	315	ALA	-	linker	UNP P26048
D	316	ARG	-	linker	UNP P26048
D	317	ALA	-	linker	UNP P26048
D	318	ALA	-	linker	UNP P26048
D	429	HIS	-	expression tag	UNP A0A093IEU4
D	430	HIS	-	expression tag	UNP A0A093IEU4
D	431	HIS	-	expression tag	UNP A0A093IEU4
D	432	HIS	-	expression tag	UNP A0A093IEU4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	433	HIS	-	expression tag	UNP A0A093IEU4
D	434	HIS	-	expression tag	UNP A0A093IEU4
D	435	HIS	-	expression tag	UNP A0A093IEU4
D	436	HIS	-	expression tag	UNP A0A093IEU4
E	258	VAL	GLY	conflict	UNP P26048
E	312	SER	-	linker	UNP P26048
E	313	GLN	-	linker	UNP P26048
E	314	PRO	-	linker	UNP P26048
E	315	ALA	-	linker	UNP P26048
E	316	ARG	-	linker	UNP P26048
E	317	ALA	-	linker	UNP P26048
E	318	ALA	-	linker	UNP P26048
E	429	HIS	-	expression tag	UNP A0A093IEU4
E	430	HIS	-	expression tag	UNP A0A093IEU4
E	431	HIS	-	expression tag	UNP A0A093IEU4
E	432	HIS	-	expression tag	UNP A0A093IEU4
E	433	HIS	-	expression tag	UNP A0A093IEU4
E	434	HIS	-	expression tag	UNP A0A093IEU4
E	435	HIS	-	expression tag	UNP A0A093IEU4
E	436	HIS	-	expression tag	UNP A0A093IEU4

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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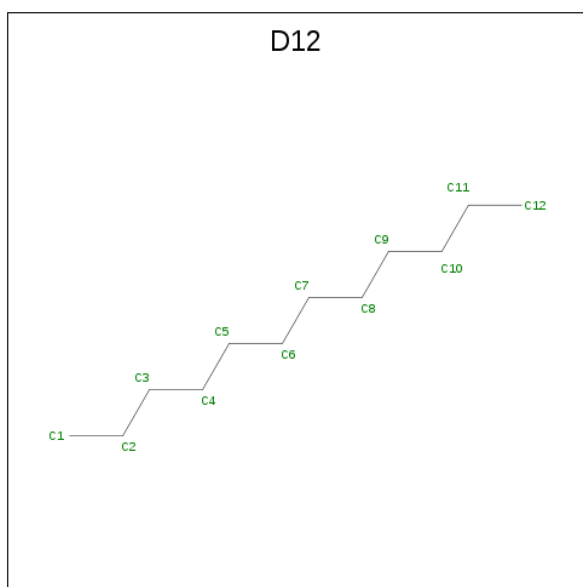
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 7 2 3 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C H O 7 2 3 2	0	0
2	E	1	Total C O 4 2 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	3	Total Cl 3 3	0	0
3	D	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0

- Molecule 4 is DODECANE (three-letter code: D12) (formula: C₁₂H₂₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	H	0	0
			38	12	26		
4	B	1	Total	C	H	0	0
			38	12	26		
4	B	1	Total	C	H	0	0
			38	12	26		
4	C	1	Total	C	H	0	0
			38	12	26		
4	D	1	Total	C	H	0	0
			38	12	26		
4	D	1	Total	C	H	0	0
			38	12	26		
4	E	1	Total	C	H	0	0
			38	12	26		
4	E	1	Total	C	H	0	0
			38	12	26		

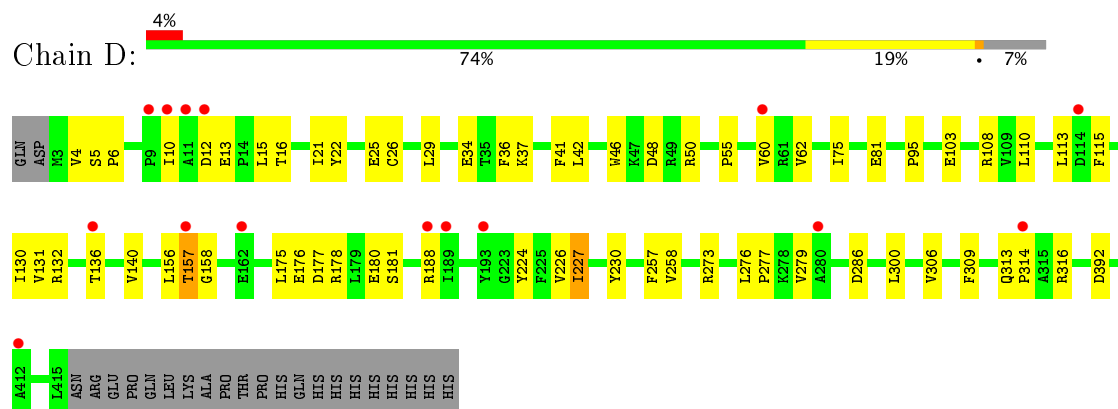
- Molecule 5 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



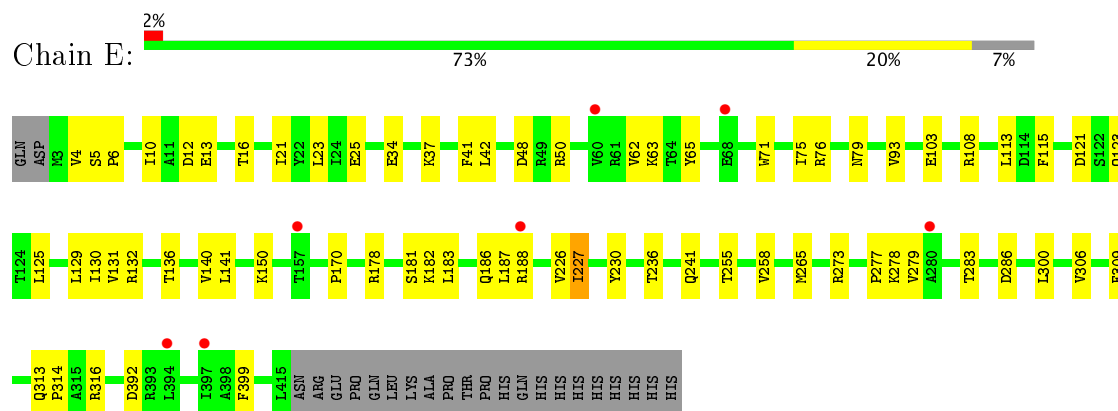
- Molecule 6 is water.



- Molecule 1: Proton-gated ion channel, Gamma-aminobutyric acid receptor subunit alpha-2, Gamma-aminobutyric acid receptor subunit alpha-1



- Molecule 1: Proton-gated ion channel, Gamma-aminobutyric acid receptor subunit alpha-2, Gamma-aminobutyric acid receptor subunit alpha-1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.02Å 133.95Å 162.70Å 90.00° 103.53° 90.00°	Depositor
Resolution (Å)	29.98 – 2.75 95.28 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.98-2.75) 100.0 (95.28-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.73Å)	Xtriage
Refinement program	BUSTER dev_2645, PHENIX dev_2645	Depositor
R, R_{free}	0.203 , 0.229 0.214 , 0.239	Depositor DCC
R_{free} test set	5054 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13261	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: CL, Y01, D12, ACT

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	0.32	0/2554	0.50	0/3499
1	B	0.33	0/2560	0.50	0/3506
1	C	0.33	0/2560	0.51	0/3506
1	D	0.34	0/2554	0.52	0/3499
1	E	0.35	0/2554	0.52	0/3499
All	All	0.33	0/12782	0.51	0/17509

There are no bond length outliers.

There are no bond angle outliers.

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	2489	0	2454	53	0
1	B	2495	0	2465	57	0
1	C	2495	0	2465	58	0
1	D	2489	0	2454	59	0
1	E	2489	0	2454	67	0
2	A	8	3	6	1	0
2	B	4	0	3	3	0
2	C	8	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	8	3	6	1	0
2	E	4	0	3	2	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	12	26	26	0	0
4	B	24	52	52	0	0
4	C	12	26	26	0	0
4	D	24	52	52	0	0
4	E	24	52	52	0	0
5	A	35	49	49	3	0
5	B	35	49	49	1	0
5	C	35	49	49	5	0
5	D	35	49	49	2	0
5	E	35	49	49	1	0
6	A	5	0	0	1	0
6	B	6	0	0	0	0
6	C	6	0	0	0	0
6	D	9	0	0	1	0
6	E	9	0	0	1	0
All	All	12802	459	12769	269	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 11.

The worst 5 of 269 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:E:186:GLN:OE1	1:E:188:ARG:NH2	2.01	0.93
1:A:227:ILE:HD11	1:B:273:ARG:HD2	1.56	0.86
1:D:227:ILE:HD11	1:E:273:ARG:HD2	1.56	0.86
1:A:7:PRO:O	1:A:49:ARG:NH2	2.12	0.83
1:D:37:LYS:HE3	1:D:108:ARG:HD2	1.60	0.82

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	311/336 (93%)	298 (96%)	13 (4%)	0	100	100
1	B	311/336 (93%)	299 (96%)	12 (4%)	0	100	100
1	C	311/336 (93%)	298 (96%)	11 (4%)	2 (1%)	28	59
1	D	311/336 (93%)	299 (96%)	11 (4%)	1 (0%)	44	75
1	E	311/336 (93%)	299 (96%)	12 (4%)	0	100	100
All	All	1555/1680 (93%)	1493 (96%)	59 (4%)	3 (0%)	51	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	157	THR
1	D	157	THR
1	C	63	LYS

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	271/302 (90%)	268 (99%)	3 (1%)	78	92
1	B	272/302 (90%)	268 (98%)	4 (2%)	70	90
1	C	272/302 (90%)	269 (99%)	3 (1%)	78	92
1	D	271/302 (90%)	268 (99%)	3 (1%)	78	92
1	E	271/302 (90%)	269 (99%)	2 (1%)	87	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1357/1510 (90%)	1342 (99%)	15 (1%)	78 92

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	227	ILE
1	C	26	CYS
1	D	227	ILE
1	B	151	ASN
1	D	136	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	151	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 7 are monoatomic - leaving 21 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
2	ACT	A	501	-	1,3,3	7.19	1 (100%)	0,3,3	0.00	-
2	ACT	A	502	-	1,3,3	7.45	1 (100%)	0,3,3	0.00	-
4	D12	A	506	-	11,11,11	0.40	0	10,10,10	0.63	0
5	Y01	A	507	-	35,38,38	0.58	0	54,57,57	1.32	9 (16%)
2	ACT	B	501	-	1,3,3	6.90	1 (100%)	0,3,3	0.00	-
4	D12	B	503	-	11,11,11	0.38	0	10,10,10	0.67	0
4	D12	B	504	-	11,11,11	0.37	0	10,10,10	0.70	0
5	Y01	B	505	-	35,38,38	0.56	0	54,57,57	1.32	7 (12%)
2	ACT	C	501	-	1,3,3	6.46	1 (100%)	0,3,3	0.00	-
2	ACT	C	502	-	1,3,3	7.69	1 (100%)	0,3,3	0.00	-
4	D12	C	504	-	11,11,11	0.36	0	10,10,10	0.70	0
5	Y01	C	505	-	35,38,38	0.54	0	54,57,57	1.37	8 (14%)
2	ACT	D	501	-	1,3,3	7.11	1 (100%)	0,3,3	0.00	-
2	ACT	D	502	-	1,3,3	7.35	1 (100%)	0,3,3	0.00	-
4	D12	D	504	-	11,11,11	0.38	0	10,10,10	0.69	0
4	D12	D	505	-	11,11,11	0.36	0	10,10,10	0.67	0
5	Y01	D	506	-	35,38,38	0.56	0	54,57,57	1.26	8 (14%)
2	ACT	E	501	-	1,3,3	7.10	1 (100%)	0,3,3	0.00	-
4	D12	E	503	-	11,11,11	0.36	0	10,10,10	0.74	0
4	D12	E	504	-	11,11,11	0.36	0	10,10,10	0.71	0
5	Y01	E	505	-	35,38,38	0.57	0	54,57,57	1.29	6 (11%)

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
2	ACT	A	501	-	-	0/0/0/0	0/0/0/0
2	ACT	A	502	-	-	0/0/0/0	0/0/0/0
4	D12	A	506	-	-	0/9/9/9	0/0/0/0
5	Y01	A	507	-	-	0/17/77/77	0/4/4/4
2	ACT	B	501	-	-	0/0/0/0	0/0/0/0
4	D12	B	503	-	-	0/9/9/9	0/0/0/0
4	D12	B	504	-	-	0/9/9/9	0/0/0/0
5	Y01	B	505	-	-	0/17/77/77	0/4/4/4
2	ACT	C	501	-	-	0/0/0/0	0/0/0/0
2	ACT	C	502	-	-	0/0/0/0	0/0/0/0
4	D12	C	504	-	-	0/9/9/9	0/0/0/0
5	Y01	C	505	-	-	0/17/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACT	D	501	-	-	0/0/0/0	0/0/0/0
2	ACT	D	502	-	-	0/0/0/0	0/0/0/0
4	D12	D	504	-	-	0/9/9/9	0/0/0/0
4	D12	D	505	-	-	0/9/9/9	0/0/0/0
5	Y01	D	506	-	-	0/17/77/77	0/4/4/4
2	ACT	E	501	-	-	0/0/0/0	0/0/0/0
4	D12	E	503	-	-	0/9/9/9	0/0/0/0
4	D12	E	504	-	-	0/9/9/9	0/0/0/0
5	Y01	E	505	-	-	0/17/77/77	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	ACT	CH3-C	6.46	1.57	1.48
2	B	501	ACT	CH3-C	6.90	1.57	1.48
2	E	501	ACT	CH3-C	7.10	1.57	1.48
2	D	501	ACT	CH3-C	7.11	1.57	1.48
2	A	501	ACT	CH3-C	7.19	1.58	1.48

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	507	Y01	CAQ-CBG-CBD	-3.00	114.29	119.07
5	D	506	Y01	CAC-CBB-CBE	-2.93	108.36	112.95
5	D	506	Y01	CAM-CAL-CAX	-2.84	107.80	112.66
5	C	505	Y01	CAC-CBB-CAO	-2.79	105.95	110.35
5	A	507	Y01	CAM-CAL-CAX	-2.77	107.92	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ACT	1	0
5	A	507	Y01	3	0
2	B	501	ACT	3	0
5	B	505	Y01	1	0
2	C	501	ACT	2	0
5	C	505	Y01	5	0
2	D	501	ACT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	506	Y01	2	0
2	E	501	ACT	2	0
5	E	505	Y01	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	313/336 (93%)	0.48	12 (3%) 41 35	59, 84, 131, 217	0
1	B	313/336 (93%)	0.47	9 (2%) 52 46	58, 81, 121, 214	0
1	C	313/336 (93%)	0.36	7 (2%) 62 57	59, 84, 133, 262	0
1	D	313/336 (93%)	0.46	15 (4%) 31 25	59, 82, 116, 202	0
1	E	313/336 (93%)	0.41	7 (2%) 62 57	57, 80, 121, 218	0
All	All	1565/1680 (93%)	0.44	50 (3%) 48 42	57, 82, 124, 262	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	ILE	5.8
1	C	157	THR	4.8
1	A	12	ASP	4.1
1	E	60	VAL	4.0
1	B	32	LYS	4.0

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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	Y01	C	505	35/35	0.85	0.56	14.48	109,163,180,182	0
5	Y01	D	506	35/35	0.80	0.45	11.29	116,166,200,200	0
4	D12	E	504	12/12	0.80	0.52	9.46	105,131,150,150	0
5	Y01	A	507	35/35	0.88	0.42	7.51	125,161,174,175	0
5	Y01	B	505	35/35	0.82	0.51	7.38	115,170,189,191	0
4	D12	B	503	12/12	0.78	0.40	6.80	111,137,149,149	0
4	D12	D	505	12/12	0.84	0.49	5.90	118,142,156,156	0
5	Y01	E	505	35/35	0.86	0.30	5.88	116,150,168,170	0
2	ACT	D	502	4/4	0.89	0.37	4.88	123,126,150,150	0
2	ACT	A	502	4/4	0.91	0.30	3.78	116,118,139,139	0
2	ACT	D	501	4/4	0.97	0.23	2.94	69,71,72,73	0
2	ACT	C	501	4/4	0.98	0.28	2.83	74,74,78,84	0
2	ACT	C	502	4/4	0.85	0.25	1.82	109,112,113,113	0
2	ACT	B	501	4/4	0.97	0.23	1.62	78,78,82,90	0
4	D12	D	504	12/12	0.82	0.26	1.28	100,124,132,133	0
2	ACT	E	501	4/4	0.97	0.23	0.57	64,72,72,77	0
4	D12	C	504	12/12	0.89	0.20	0.46	96,119,138,138	0
4	D12	B	504	12/12	0.85	0.17	-0.14	85,114,125,126	0
4	D12	E	503	12/12	0.80	0.21	-0.20	83,108,121,123	0
4	D12	A	506	12/12	0.77	0.16	-0.88	103,128,133,133	0
2	ACT	A	501	4/4	0.97	0.18	-1.09	67,77,77,80	0
3	CL	C	503	1/1	0.98	0.17	-1.68	73,73,73,73	0
3	CL	A	503	1/1	0.95	0.17	-1.89	67,67,67,67	0
3	CL	E	502	1/1	0.97	0.15	-2.13	69,69,69,69	0
3	CL	B	502	1/1	0.95	0.16	-3.11	76,76,76,76	0
3	CL	D	503	1/1	0.94	0.15	-6.43	71,71,71,71	0
3	CL	A	504	1/1	0.82	0.28	-	110,110,110,110	0
3	CL	A	505	1/1	0.70	0.29	-	116,116,116,116	0

6.5 Other polymers ⓘ

There are no such residues in this entry.