wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 08:52 am BST

PDB ID	:	4X5T
Title	:	alpha 1 glycine receptor transmembrane structure fused to the extracellular domain of GLIC
Authors	:	Sauguet, L.; Corringer, P.J.; Huon, C.; Delarue, M.
Deposited on	:	2014-12-05
Resolution	:	3.50 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 following versions of software and data (see references (1)) were used in the production of this report:

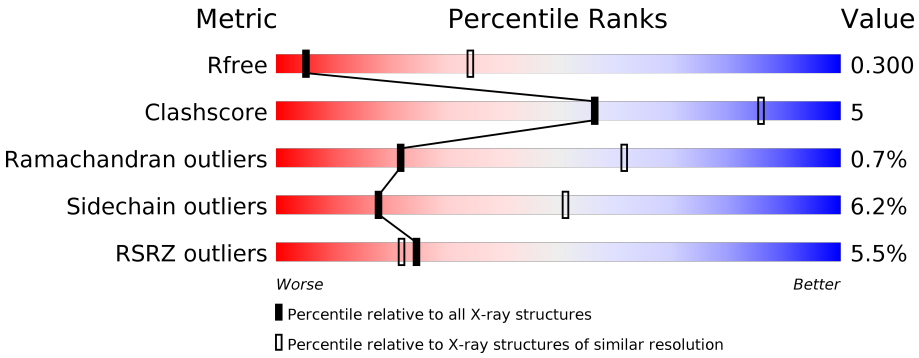
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	330	10% 79% 13% • 7%
1	B	330	3% 79% 13% • 7%
1	C	330	4% 81% 10% • 7%
1	D	330	2% 81% 11% • 7%
1	E	330	7% 80% 10% • 8%

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
3	CL	C	503	-	-	-	X
4	ACT	D	503	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11485 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 Proton-gated ion channel,GLRA1 protein,GLRA1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2307	1484	385	431	7			
1	B	308	Total	C	N	O	S	0	0	0
			2293	1474	384	428	7			
1	C	308	Total	C	N	O	S	0	0	0
			2302	1481	384	430	7			
1	D	308	Total	C	N	O	S	0	1	0
			2294	1473	385	429	7			
1	E	304	Total	C	N	O	S	0	0	0
			2257	1449	379	422	7			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	PHE	TYR	conflict	UNP Q7NDN8
A	121	MET	PHE	conflict	UNP Q7NDN8
A	311	SER	-	linker	UNP Q14C71
A	312	GLN	-	linker	UNP Q14C71
A	313	PRO	-	linker	UNP Q14C71
A	411	PHE	-	expression tag	UNP Q14C71
A	412	GLY	-	expression tag	UNP Q14C71
A	413	PHE	-	expression tag	UNP Q14C71
A	414	GLY	-	expression tag	UNP Q14C71
A	415	GLY	-	expression tag	UNP Q14C71
A	416	HIS	-	expression tag	UNP Q14C71
A	417	HIS	-	expression tag	UNP Q14C71
A	418	HIS	-	expression tag	UNP Q14C71
A	419	HIS	-	expression tag	UNP Q14C71
A	420	HIS	-	expression tag	UNP Q14C71
A	421	HIS	-	expression tag	UNP Q14C71
A	422	HIS	-	expression tag	UNP Q14C71
A	423	HIS	-	expression tag	UNP Q14C71
A	424	HIS	-	expression tag	UNP Q14C71

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Chain	Residue	Modelled	Actual	Comment	Reference
A	425	HIS	-	expression tag	UNP Q14C71
B	119	PHE	TYR	conflict	UNP Q7NDN8
B	121	MET	PHE	conflict	UNP Q7NDN8
B	311	SER	-	linker	UNP Q14C71
B	312	GLN	-	linker	UNP Q14C71
B	313	PRO	-	linker	UNP Q14C71
B	411	PHE	-	expression tag	UNP Q14C71
B	412	GLY	-	expression tag	UNP Q14C71
B	413	PHE	-	expression tag	UNP Q14C71
B	414	GLY	-	expression tag	UNP Q14C71
B	415	GLY	-	expression tag	UNP Q14C71
B	416	HIS	-	expression tag	UNP Q14C71
B	417	HIS	-	expression tag	UNP Q14C71
B	418	HIS	-	expression tag	UNP Q14C71
B	419	HIS	-	expression tag	UNP Q14C71
B	420	HIS	-	expression tag	UNP Q14C71
B	421	HIS	-	expression tag	UNP Q14C71
B	422	HIS	-	expression tag	UNP Q14C71
B	423	HIS	-	expression tag	UNP Q14C71
B	424	HIS	-	expression tag	UNP Q14C71
B	425	HIS	-	expression tag	UNP Q14C71
C	119	PHE	TYR	conflict	UNP Q7NDN8
C	121	MET	PHE	conflict	UNP Q7NDN8
C	311	SER	-	linker	UNP Q14C71
C	312	GLN	-	linker	UNP Q14C71
C	313	PRO	-	linker	UNP Q14C71
C	411	PHE	-	expression tag	UNP Q14C71
C	412	GLY	-	expression tag	UNP Q14C71
C	413	PHE	-	expression tag	UNP Q14C71
C	414	GLY	-	expression tag	UNP Q14C71
C	415	GLY	-	expression tag	UNP Q14C71
C	416	HIS	-	expression tag	UNP Q14C71
C	417	HIS	-	expression tag	UNP Q14C71
C	418	HIS	-	expression tag	UNP Q14C71
C	419	HIS	-	expression tag	UNP Q14C71
C	420	HIS	-	expression tag	UNP Q14C71
C	421	HIS	-	expression tag	UNP Q14C71
C	422	HIS	-	expression tag	UNP Q14C71
C	423	HIS	-	expression tag	UNP Q14C71
C	424	HIS	-	expression tag	UNP Q14C71
C	425	HIS	-	expression tag	UNP Q14C71
D	119	PHE	TYR	conflict	UNP Q7NDN8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	121	MET	PHE	conflict	UNP Q7NDN8
D	311	SER	-	linker	UNP Q14C71
D	312	GLN	-	linker	UNP Q14C71
D	313	PRO	-	linker	UNP Q14C71
D	411	PHE	-	expression tag	UNP Q14C71
D	412	GLY	-	expression tag	UNP Q14C71
D	413	PHE	-	expression tag	UNP Q14C71
D	414	GLY	-	expression tag	UNP Q14C71
D	415	GLY	-	expression tag	UNP Q14C71
D	416	HIS	-	expression tag	UNP Q14C71
D	417	HIS	-	expression tag	UNP Q14C71
D	418	HIS	-	expression tag	UNP Q14C71
D	419	HIS	-	expression tag	UNP Q14C71
D	420	HIS	-	expression tag	UNP Q14C71
D	421	HIS	-	expression tag	UNP Q14C71
D	422	HIS	-	expression tag	UNP Q14C71
D	423	HIS	-	expression tag	UNP Q14C71
D	424	HIS	-	expression tag	UNP Q14C71
D	425	HIS	-	expression tag	UNP Q14C71
E	119	PHE	TYR	conflict	UNP Q7NDN8
E	121	MET	PHE	conflict	UNP Q7NDN8
E	311	SER	-	linker	UNP Q14C71
E	312	GLN	-	linker	UNP Q14C71
E	313	PRO	-	linker	UNP Q14C71
E	411	PHE	-	expression tag	UNP Q14C71
E	412	GLY	-	expression tag	UNP Q14C71
E	413	PHE	-	expression tag	UNP Q14C71
E	414	GLY	-	expression tag	UNP Q14C71
E	415	GLY	-	expression tag	UNP Q14C71
E	416	HIS	-	expression tag	UNP Q14C71
E	417	HIS	-	expression tag	UNP Q14C71
E	418	HIS	-	expression tag	UNP Q14C71
E	419	HIS	-	expression tag	UNP Q14C71
E	420	HIS	-	expression tag	UNP Q14C71
E	421	HIS	-	expression tag	UNP Q14C71
E	422	HIS	-	expression tag	UNP Q14C71
E	423	HIS	-	expression tag	UNP Q14C71
E	424	HIS	-	expression tag	UNP Q14C71
E	425	HIS	-	expression tag	UNP Q14C71

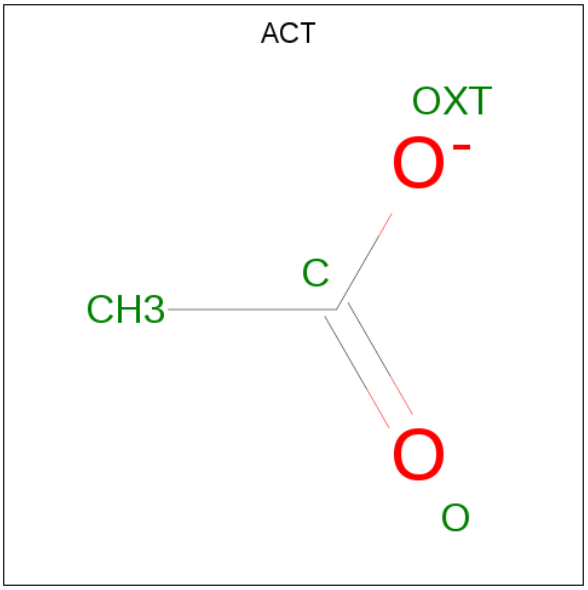
- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

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

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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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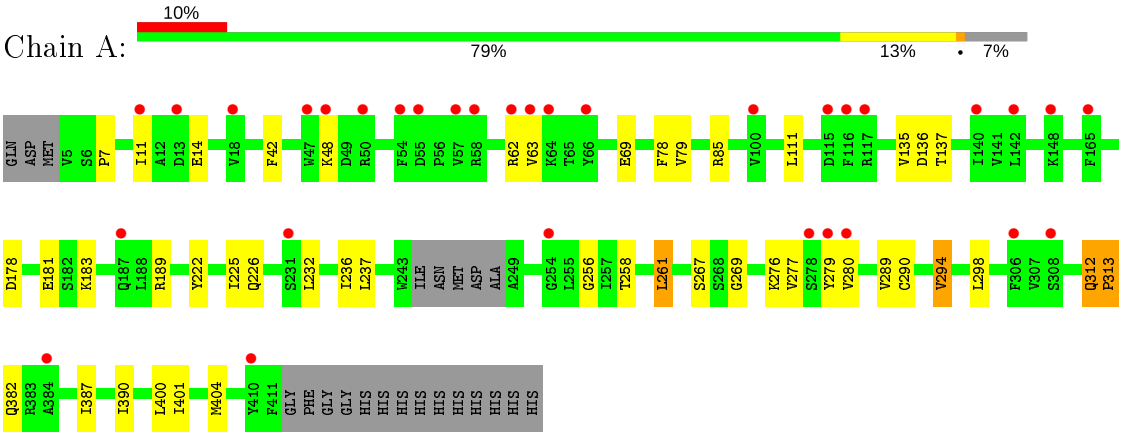
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

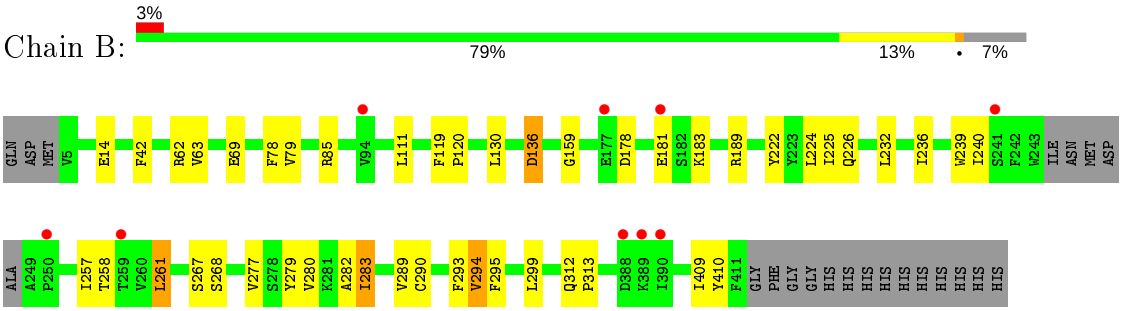
- Molecule 1: Proton-gated ion channel,GLRA1 protein,GLRA1 protein

Chain A:



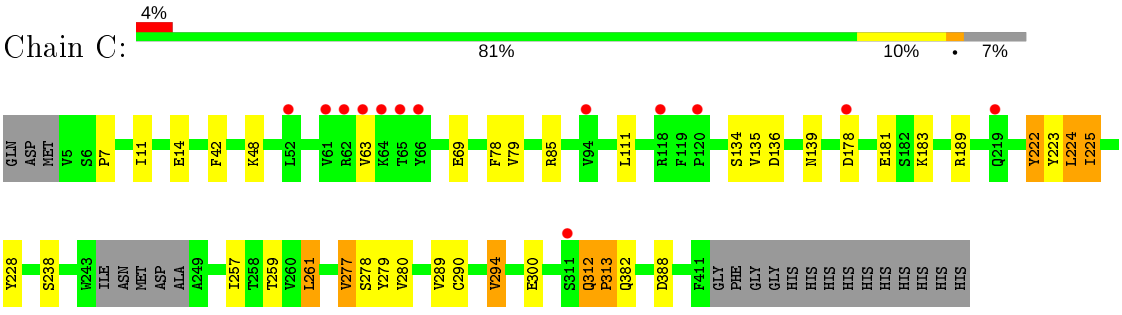
- Molecule 1: Proton-gated ion channel,GLRA1 protein,GLRA1 protein

Chain B:



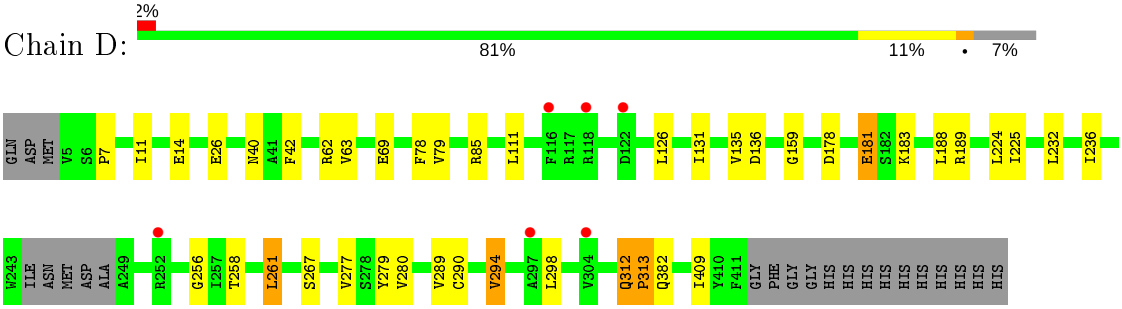
- Molecule 1: Proton-gated ion channel,GLRA1 protein,GLRA1 protein

Chain C:



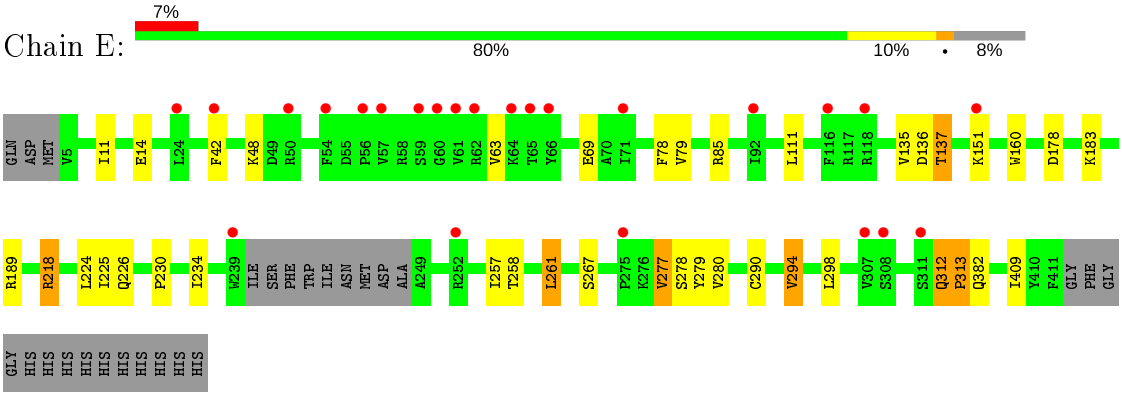
- Molecule 1: Proton-gated ion channel,GLRA1 protein,GLRA1 protein

Chain D:



• Molecule 1: Proton-gated ion channel,GLRA1 protein,GLRA1 protein

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.89Å 132.30Å 190.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.50 47.63 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-3.50) 99.8 (47.63-3.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.254 , 0.270 0.275 , 0.300	Depositor DCC
R_{free} test set	1949 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	149.9	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 167.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	11485	wwPDB-VP
Average B, all atoms (Å^2)	186.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, CL, 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	0.47	0/2355	0.70	0/3220
1	B	0.51	0/2341	0.72	0/3203
1	C	0.53	0/2351	0.71	0/3216
1	D	0.51	0/2341	0.71	0/3204
1	E	0.51	0/2302	0.72	0/3148
All	All	0.51	0/11690	0.71	0/15991

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

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	2307	0	2207	29	0
1	B	2293	0	2173	28	0
1	C	2302	0	2182	27	0
1	D	2294	0	2169	32	0
1	E	2257	0	2149	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2	0	0	0	0
2	E	1	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	E	1	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	3	0
4	E	4	0	3	0	0
All	All	11485	0	10895	112	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 5.

The worst 5 of 112 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:C:238:SER:HB2	1:C:259:THR:HG21	1.45	0.95
1:B:258:THR:HG21	1:C:257:ILE:HG22	1.56	0.88
1:B:225:ILE:HD13	1:C:280:VAL:CG1	2.12	0.80
1:A:280:VAL:CG1	1:E:225:ILE:HD13	2.19	0.73
1:D:258:THR:HG21	1:E:257:ILE:HG22	1.73	0.71

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	304/330 (92%)	282 (93%)	20 (7%)	2 (1%)	22 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	304/330 (92%)	281 (92%)	22 (7%)	1 (0%)	41	75
1	C	304/330 (92%)	282 (93%)	19 (6%)	3 (1%)	15	54
1	D	305/330 (92%)	282 (92%)	20 (7%)	3 (1%)	15	54
1	E	300/330 (91%)	278 (93%)	20 (7%)	2 (1%)	22	61
All	All	1517/1650 (92%)	1405 (93%)	101 (7%)	11 (1%)	22	61

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	312[A]	GLN
1	D	312[B]	GLN
1	D	313	PRO
1	A	313	PRO
1	C	312	GLN

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	235/294 (80%)	222 (94%)	13 (6%)	21	54
1	B	230/294 (78%)	212 (92%)	18 (8%)	12	42
1	C	232/294 (79%)	219 (94%)	13 (6%)	21	54
1	D	229/294 (78%)	216 (94%)	13 (6%)	20	53
1	E	227/294 (77%)	212 (93%)	15 (7%)	16	49
All	All	1153/1470 (78%)	1081 (94%)	72 (6%)	18	51

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	48	LYS
1	C	261	LEU
1	E	224	LEU
1	C	69	GLU

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Mol	Chain	Res	Type
1	C	181	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	187	GLN
1	E	226	GLN
1	D	226	GLN
1	B	187	GLN
1	D	187	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
4	ACT	C	504	-	1,3,3	2.63	1 (100%)	0,3,3	0.00	-
4	ACT	A	503	-	1,3,3	5.28	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ACT	B	504	-	1,3,3	5.98	1 (100%)	0,3,3	0.00	-
4	ACT	D	503	-	1,3,3	3.64	1 (100%)	0,3,3	0.00	-
4	ACT	E	503	-	1,3,3	3.50	1 (100%)	0,3,3	0.00	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	ACT	CH3-C	5.98	1.56	1.48
4	A	503	ACT	CH3-C	5.28	1.55	1.48
4	D	503	ACT	CH3-C	3.64	1.53	1.48
4	E	503	ACT	CH3-C	3.50	1.53	1.48
4	C	504	ACT	CH3-C	2.63	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	503	ACT	3	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

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, 95^{th} 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	308/330 (93%)	0.36	32 (10%) 6 7	113, 206, 272, 284	0
1	B	308/330 (93%)	0.13	9 (2%) 51 45	101, 181, 270, 286	0
1	C	308/330 (93%)	0.19	13 (4%) 36 32	93, 180, 264, 281	0
1	D	308/330 (93%)	0.04	6 (1%) 66 61	95, 174, 256, 272	0
1	E	304/330 (92%)	0.30	24 (7%) 12 13	104, 188, 284, 293	0
All	All	1536/1650 (93%)	0.20	84 (5%) 25 22	93, 185, 272, 293	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	66	TYR	6.5
1	E	66	TYR	5.9
1	A	279	TYR	5.1
1	A	116	PHE	5.0
1	B	390	ILE	4.8

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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
3	CL	C	503	1/1	0.18	0.48	120,120,120,120	0
3	CL	B	503	1/1	0.61	0.34	120,120,120,120	0
3	CL	A	502	1/1	0.62	0.23	120,120,120,120	0
3	CL	C	502	1/1	0.67	0.36	120,120,120,120	0
2	NI	D	502	1/1	0.76	0.25	120,120,120,120	0
3	CL	E	502	1/1	0.77	0.28	120,120,120,120	0
3	CL	B	502	1/1	0.83	0.26	120,120,120,120	0
2	NI	B	501	1/1	0.87	0.28	120,120,120,120	0
2	NI	D	501	1/1	0.90	0.24	120,120,120,120	0
4	ACT	B	504	4/4	0.91	1.34	120,120,120,129	0
2	NI	C	501	1/1	0.91	0.34	120,120,120,120	0
2	NI	E	501	1/1	0.95	0.39	120,120,120,120	0
4	ACT	A	503	4/4	0.95	0.97	124,124,124,127	0
4	ACT	C	504	4/4	0.97	0.27	121,121,121,122	0
2	NI	A	501	1/1	0.97	0.34	120,120,120,120	0
4	ACT	E	503	4/4	0.98	0.41	121,121,121,122	0
4	ACT	D	503	4/4	0.98	0.48	120,120,121,129	0

6.5 Other polymers

There are no such residues in this entry.