Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:26 AM GMT

PDB ID	:	3IGQ
Title	:	Crystal structure of the extracellular domain of a bacterial pentameric ligand-gated ion channel
Authors	:	Nury, H.; Delarue, M.
Deposited on	:	2009-07-28
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/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:

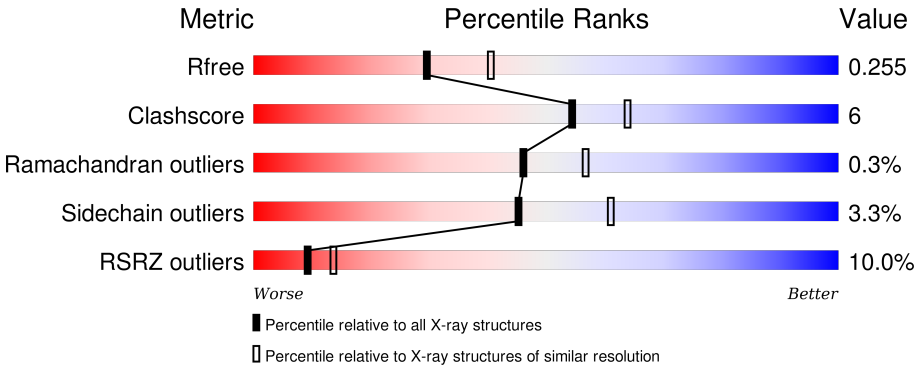
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	201	10% 78% 10% 12%
1	B	201	5% 82% 7% 10%
1	C	201	8% 73% 14% • 8%
1	D	201	9% 69% 16% • 13%
1	E	201	9% 72% 15% • 10%

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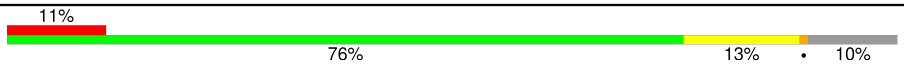
Mol	Chain	Length	Quality of chain
1	F	201	

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	ACY	F	701	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9053 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 Glr4197 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1411	903	235	271	2			
1	B	180	Total	C	N	O	S	0	0	0
			1440	920	240	278	2			
1	C	184	Total	C	N	O	S	0	0	0
			1468	938	244	285	1			
1	D	174	Total	C	N	O	S	0	0	0
			1396	894	233	267	2			
1	E	180	Total	C	N	O	S	0	0	0
			1440	924	240	274	2			
1	F	181	Total	C	N	O	S	0	0	0
			1448	927	244	275	2			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
A	116	GLY	PHE	ENGINEERED	UNP Q7NDN8
A	119	THR	TYR	ENGINEERED	UNP Q7NDN8
A	120	GLU	PRO	ENGINEERED	UNP Q7NDN8
A	121	SER	PHE	ENGINEERED	UNP Q7NDN8
A	194	GLY	-	EXPRESSION TAG	UNP Q7NDN8
A	195	GLY	-	EXPRESSION TAG	UNP Q7NDN8
A	196	HIS	-	EXPRESSION TAG	UNP Q7NDN8
A	197	HIS	-	EXPRESSION TAG	UNP Q7NDN8
A	198	HIS	-	EXPRESSION TAG	UNP Q7NDN8
A	199	HIS	-	EXPRESSION TAG	UNP Q7NDN8
A	200	HIS	-	EXPRESSION TAG	UNP Q7NDN8
A	201	HIS	-	EXPRESSION TAG	UNP Q7NDN8
B	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
B	116	GLY	PHE	ENGINEERED	UNP Q7NDN8
B	119	THR	TYR	ENGINEERED	UNP Q7NDN8
B	120	GLU	PRO	ENGINEERED	UNP Q7NDN8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	121	SER	PHE	ENGINEERED	UNP Q7NDN8
B	194	GLY	-	EXPRESSION TAG	UNP Q7NDN8
B	195	GLY	-	EXPRESSION TAG	UNP Q7NDN8
B	196	HIS	-	EXPRESSION TAG	UNP Q7NDN8
B	197	HIS	-	EXPRESSION TAG	UNP Q7NDN8
B	198	HIS	-	EXPRESSION TAG	UNP Q7NDN8
B	199	HIS	-	EXPRESSION TAG	UNP Q7NDN8
B	200	HIS	-	EXPRESSION TAG	UNP Q7NDN8
B	201	HIS	-	EXPRESSION TAG	UNP Q7NDN8
C	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
C	116	GLY	PHE	ENGINEERED	UNP Q7NDN8
C	119	THR	TYR	ENGINEERED	UNP Q7NDN8
C	120	GLU	PRO	ENGINEERED	UNP Q7NDN8
C	121	SER	PHE	ENGINEERED	UNP Q7NDN8
C	194	GLY	-	EXPRESSION TAG	UNP Q7NDN8
C	195	GLY	-	EXPRESSION TAG	UNP Q7NDN8
C	196	HIS	-	EXPRESSION TAG	UNP Q7NDN8
C	197	HIS	-	EXPRESSION TAG	UNP Q7NDN8
C	198	HIS	-	EXPRESSION TAG	UNP Q7NDN8
C	199	HIS	-	EXPRESSION TAG	UNP Q7NDN8
C	200	HIS	-	EXPRESSION TAG	UNP Q7NDN8
C	201	HIS	-	EXPRESSION TAG	UNP Q7NDN8
D	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
D	116	GLY	PHE	ENGINEERED	UNP Q7NDN8
D	119	THR	TYR	ENGINEERED	UNP Q7NDN8
D	120	GLU	PRO	ENGINEERED	UNP Q7NDN8
D	121	SER	PHE	ENGINEERED	UNP Q7NDN8
D	194	GLY	-	EXPRESSION TAG	UNP Q7NDN8
D	195	GLY	-	EXPRESSION TAG	UNP Q7NDN8
D	196	HIS	-	EXPRESSION TAG	UNP Q7NDN8
D	197	HIS	-	EXPRESSION TAG	UNP Q7NDN8
D	198	HIS	-	EXPRESSION TAG	UNP Q7NDN8
D	199	HIS	-	EXPRESSION TAG	UNP Q7NDN8
D	200	HIS	-	EXPRESSION TAG	UNP Q7NDN8
D	201	HIS	-	EXPRESSION TAG	UNP Q7NDN8
E	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
E	116	GLY	PHE	ENGINEERED	UNP Q7NDN8
E	119	THR	TYR	ENGINEERED	UNP Q7NDN8
E	120	GLU	PRO	ENGINEERED	UNP Q7NDN8
E	121	SER	PHE	ENGINEERED	UNP Q7NDN8
E	194	GLY	-	EXPRESSION TAG	UNP Q7NDN8
E	195	GLY	-	EXPRESSION TAG	UNP Q7NDN8

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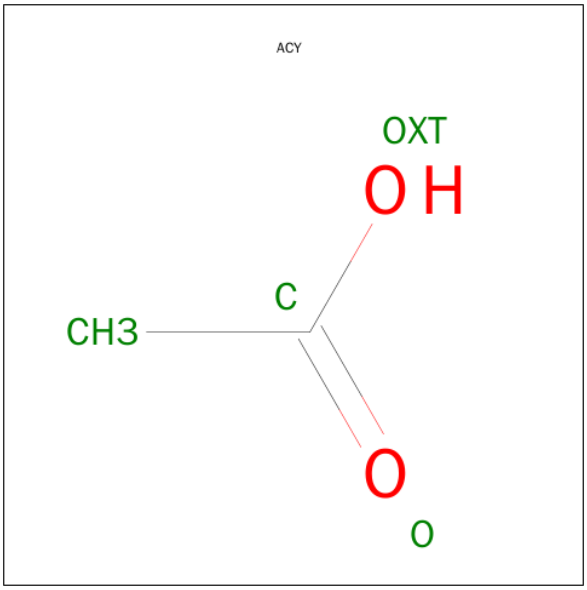
Chain	Residue	Modelled	Actual	Comment	Reference
E	196	HIS	-	EXPRESSION TAG	UNP Q7NDN8
E	197	HIS	-	EXPRESSION TAG	UNP Q7NDN8
E	198	HIS	-	EXPRESSION TAG	UNP Q7NDN8
E	199	HIS	-	EXPRESSION TAG	UNP Q7NDN8
E	200	HIS	-	EXPRESSION TAG	UNP Q7NDN8
E	201	HIS	-	EXPRESSION TAG	UNP Q7NDN8
F	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
F	116	GLY	PHE	ENGINEERED	UNP Q7NDN8
F	119	THR	TYR	ENGINEERED	UNP Q7NDN8
F	120	GLU	PRO	ENGINEERED	UNP Q7NDN8
F	121	SER	PHE	ENGINEERED	UNP Q7NDN8
F	194	GLY	-	EXPRESSION TAG	UNP Q7NDN8
F	195	GLY	-	EXPRESSION TAG	UNP Q7NDN8
F	196	HIS	-	EXPRESSION TAG	UNP Q7NDN8
F	197	HIS	-	EXPRESSION TAG	UNP Q7NDN8
F	198	HIS	-	EXPRESSION TAG	UNP Q7NDN8
F	199	HIS	-	EXPRESSION TAG	UNP Q7NDN8
F	200	HIS	-	EXPRESSION TAG	UNP Q7NDN8
F	201	HIS	-	EXPRESSION TAG	UNP Q7NDN8

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Hg 1 1	0	0
4	E	1	Total Hg 1 1	0	0
4	B	1	Total Hg 1 1	0	0
4	C	1	Total Hg 1 1	0	0
4	A	1	Total Hg 1 1	0	0
4	F	1	Total Hg 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is water.

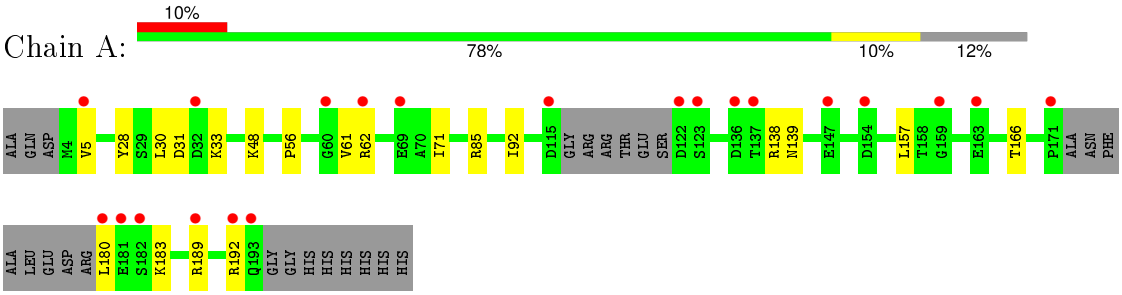
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	69	Total O 69 69	0	0
6	B	55	Total O 55 55	0	0
6	C	79	Total O 79 79	0	0
6	D	69	Total O 69 69	0	0
6	E	59	Total O 59 59	0	0
6	F	77	Total O 77 77	0	0

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 errors 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.

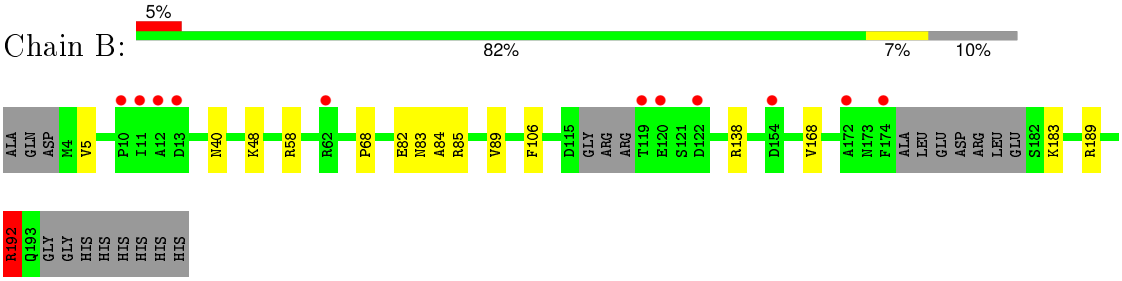
- Molecule 1: Glr4197 protein

Chain A:



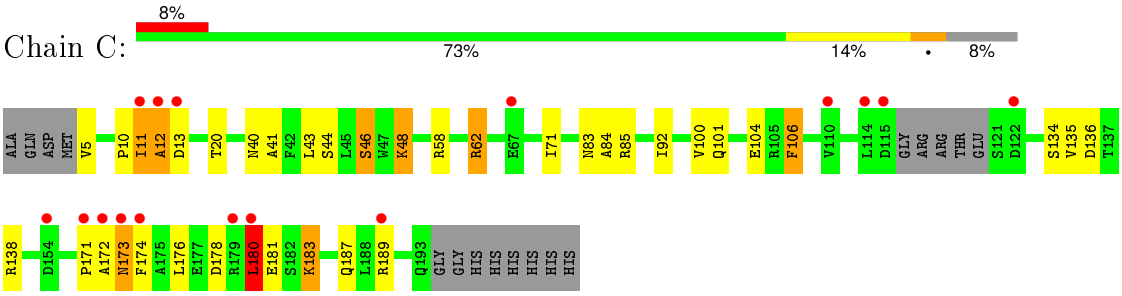
- Molecule 1: Glr4197 protein

Chain B:



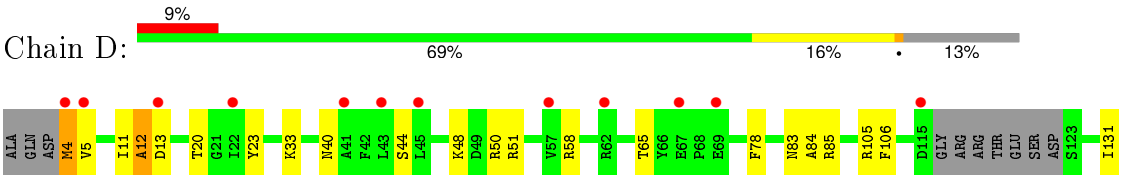
- Molecule 1: Glr4197 protein

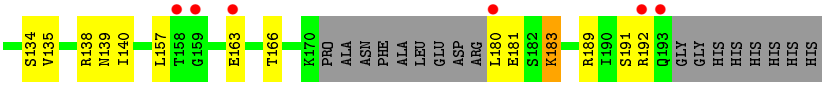
Chain C:



- Molecule 1: Glr4197 protein

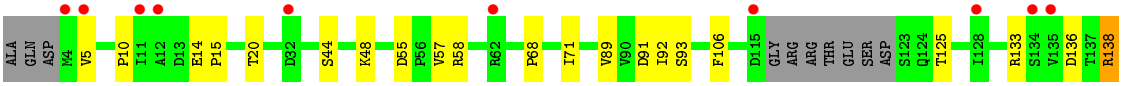
Chain D:

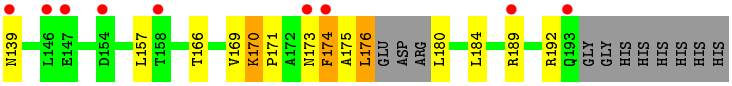




• Molecule 1: Glr4197 protein

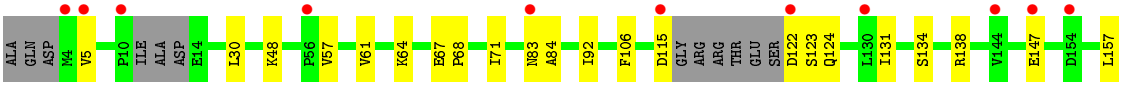
Chain E:

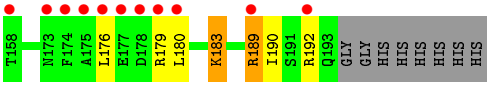




• Molecule 1: Glr4197 protein

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	84.45Å 130.24Å 113.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 24.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-2.30) 99.7 (24.89-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.207 , 0.255 0.206 , 0.255	Depositor DCC
R_{free} test set	2845 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 56198 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9053	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 6.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, ACY, HG, 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	0.92	0/1439	1.30	8/1960 (0.4%)
1	B	0.87	3/1469 (0.2%)	0.93	6/2001 (0.3%)
1	C	0.94	2/1498 (0.1%)	0.99	5/2043 (0.2%)
1	D	1.06	6/1423 (0.4%)	1.34	15/1937 (0.8%)
1	E	0.90	1/1469 (0.1%)	1.10	11/2001 (0.5%)
1	F	1.01	4/1477 (0.3%)	1.01	8/2011 (0.4%)
All	All	0.95	16/8775 (0.2%)	1.12	53/11953 (0.4%)

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	C	0	1
1	D	0	2
All	All	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	106	PHE	CE2-CZ	-9.97	1.18	1.37
1	F	106	PHE	CE2-CZ	-9.66	1.19	1.37
1	D	106	PHE	CE1-CZ	-9.14	1.20	1.37
1	F	106	PHE	CG-CD1	-9.04	1.25	1.38
1	D	85	ARG	CZ-NH1	-9.01	1.21	1.33
1	F	106	PHE	CE1-CZ	-9.00	1.20	1.37
1	D	85	ARG	CZ-NH2	-8.82	1.21	1.33
1	D	106	PHE	CG-CD2	-8.14	1.26	1.38
1	F	106	PHE	CG-CD2	-8.06	1.26	1.38
1	D	106	PHE	CG-CD1	-7.69	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	SER	CB-OG	-5.75	1.34	1.42
1	E	106	PHE	CE2-CZ	-5.59	1.26	1.37
1	B	106	PHE	CE1-CZ	-5.59	1.26	1.37
1	C	106	PHE	CG-CD2	-5.43	1.30	1.38
1	B	168	VAL	CB-CG1	-5.39	1.41	1.52
1	B	106	PHE	CG-CD1	-5.10	1.31	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	ARG	NE-CZ-NH2	-24.19	108.20	120.30
1	A	138	ARG	NE-CZ-NH1	21.38	130.99	120.30
1	D	192	ARG	NE-CZ-NH1	-18.55	111.03	120.30
1	D	192	ARG	NE-CZ-NH2	18.41	129.50	120.30
1	E	133	ARG	NE-CZ-NH1	-16.64	111.98	120.30
1	E	133	ARG	NE-CZ-NH2	15.52	128.06	120.30
1	D	189	ARG	NE-CZ-NH1	-15.48	112.56	120.30
1	A	189	ARG	NE-CZ-NH1	-14.96	112.82	120.30
1	D	85	ARG	NE-CZ-NH1	14.07	127.34	120.30
1	A	189	ARG	NE-CZ-NH2	14.07	127.34	120.30
1	D	189	ARG	NE-CZ-NH2	12.91	126.75	120.30
1	D	85	ARG	NE-CZ-NH2	12.28	126.44	120.30
1	D	85	ARG	NH1-CZ-NH2	-12.02	106.18	119.40
1	A	138	ARG	CD-NE-CZ	10.57	138.40	123.60
1	F	189	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	D	192	ARG	CD-NE-CZ	8.80	135.91	123.60
1	C	85	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	C	189	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	B	85	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	B	189	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	E	189	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	D	138	ARG	NE-CZ-NH2	7.01	123.81	120.30
1	D	138	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	C	189	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	E	133	ARG	CD-NE-CZ	6.58	132.82	123.60
1	D	51	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	B	189	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	F	138	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	E	138	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	B	138	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	E	192	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	31	ASP	CB-CG-OD1	5.90	123.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	192	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	D	189	ARG	CD-NE-CZ	5.89	131.85	123.60
1	F	189	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	F	106	PHE	CD1-CG-CD2	-5.72	110.86	118.30
1	D	106	PHE	CD1-CG-CD2	-5.72	110.86	118.30
1	D	106	PHE	CB-CG-CD2	5.70	124.79	120.80
1	A	189	ARG	CD-NE-CZ	5.67	131.54	123.60
1	F	106	PHE	CD1-CE1-CZ	5.56	126.77	120.10
1	F	106	PHE	CB-CG-CD2	5.55	124.69	120.80
1	E	189	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	F	138	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	85	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	E	57	VAL	CB-CA-C	-5.19	101.54	111.40
1	B	192	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	13	ASP	CB-CG-OD2	5.10	122.89	118.30
1	F	106	PHE	CB-CG-CD1	5.08	124.35	120.80
1	D	106	PHE	CB-CG-CD1	5.07	124.35	120.80
1	B	192	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	C	138	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	E	138	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	E	170	LYS	CB-CA-C	-5.03	100.34	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	180	LEU	Peptide
1	D	11	ILE	Peptide
1	D	4	MET	Peptide

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	1411	0	1409	9	0
1	B	1440	0	1430	6	0
1	C	1468	0	1454	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1396	0	1398	23	1
1	E	1440	0	1441	26	3
1	F	1448	0	1442	17	4
2	A	4	0	3	1	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	1	0
2	E	4	0	3	1	0
2	F	4	0	3	3	0
3	A	1	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
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	69	0	0	4	0
6	B	55	0	0	2	0
6	C	79	0	0	9	0
6	D	69	0	0	3	0
6	E	59	0	0	3	0
6	F	77	0	0	8	0
All	All	9053	0	8592	111	4

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 6.

All (111) 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:F:147:GLU:HG2	6:F:270:HOH:O	1.48	1.11
1:E:169:VAL:HG22	1:E:184:LEU:CD2	1.82	1.08
2:F:701:ACY:H1	6:F:234:HOH:O	1.70	0.92
1:D:135:VAL:O	1:D:180:LEU:HD23	1.69	0.90
1:E:10:PRO:HD3	1:E:138:ARG:HD3	1.66	0.78
1:E:169:VAL:HG22	1:E:184:LEU:HD21	1.68	0.75
1:E:169:VAL:HG22	1:E:184:LEU:HD23	1.69	0.74
1:F:189:ARG:CG	6:F:280:HOH:O	2.36	0.72
1:D:139:ASN:HD22	1:D:180:LEU:N	1.89	0.70
1:E:173:ASN:O	1:E:174:PHE:HD1	1.74	0.69
1:E:15:PRO:HA	1:E:139:ASN:O	1.93	0.69
1:D:135:VAL:O	1:D:180:LEU:CD2	2.39	0.68
1:E:173:ASN:O	1:E:174:PHE:CD1	2.48	0.67
2:F:701:ACY:H2	6:F:208:HOH:O	1.93	0.66
2:D:701:ACY:H2	6:D:225:HOH:O	1.96	0.65
1:C:187:GLN:OE1	6:C:375:HOH:O	2.14	0.65
1:C:171:PRO:HG2	1:C:183:LYS:HG2	1.79	0.65
1:D:134:SER:CB	1:D:180:LEU:HB3	2.27	0.64
1:C:40:ASN:HB2	6:C:288:HOH:O	1.96	0.64
1:C:62:ARG:NE	6:C:252:HOH:O	2.14	0.63
1:E:175:ALA:O	1:E:176:LEU:HB2	1.98	0.63
1:D:139:ASN:ND2	1:D:180:LEU:N	2.46	0.62
2:A:701:ACY:H2	6:A:237:HOH:O	2.01	0.60
1:C:11:ILE:O	1:C:11:ILE:HG22	2.01	0.60
1:F:123:SER:HB2	6:F:280:HOH:O	2.00	0.60
2:E:701:ACY:H2	6:E:213:HOH:O	2.00	0.59
1:A:139:ASN:O	1:A:139:ASN:OD1	2.20	0.59
1:B:192:ARG:HG2	6:B:233:HOH:O	2.02	0.59
1:C:171:PRO:CG	1:C:183:LYS:HG2	2.33	0.58
1:C:5:VAL:O	1:C:5:VAL:HG12	2.03	0.58
1:C:178:ASP:C	1:C:180:LEU:H	2.07	0.58
1:F:5:VAL:HG12	1:F:5:VAL:O	2.04	0.58
1:E:10:PRO:HD3	1:E:138:ARG:CD	2.34	0.57
1:C:10:PRO:HB2	1:C:12:ALA:O	2.03	0.57
1:C:58:ARG:NE	6:C:334:HOH:O	2.37	0.57
1:D:12:ALA:HB1	1:D:13:ASP:HA	1.85	0.57
1:B:5:VAL:O	1:B:5:VAL:HG12	2.05	0.57
1:D:134:SER:HB3	1:D:180:LEU:HB3	1.85	0.57
1:D:163:GLU:OE2	1:D:191:SER:OG	2.21	0.57
1:D:5:VAL:O	1:D:5:VAL:HG12	2.04	0.57
1:E:125:THR:O	6:E:224:HOH:O	2.18	0.55
1:E:5:VAL:HG12	1:E:5:VAL:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PRO:CB	1:A:61:VAL:O	2.56	0.54
1:E:15:PRO:CA	1:E:139:ASN:O	2.57	0.53
1:D:33:LYS:HD3	6:D:217:HOH:O	2.09	0.53
1:F:71:ILE:HD11	1:F:92:ILE:HG21	1.92	0.52
2:F:701:ACY:H3	6:F:350:HOH:O	2.10	0.52
1:D:134:SER:OG	1:D:180:LEU:HB3	2.10	0.51
1:F:189:ARG:HG2	6:F:280:HOH:O	2.06	0.51
1:C:11:ILE:O	1:C:12:ALA:CB	2.58	0.51
1:E:10:PRO:CD	1:E:138:ARG:HD3	2.38	0.51
1:E:170:LYS:HB3	1:E:171:PRO:HD2	1.92	0.51
1:D:58:ARG:HH11	1:D:58:ARG:HG2	1.74	0.51
1:C:172:ALA:HA	1:C:174:PHE:HD2	1.75	0.51
1:D:12:ALA:CB	1:D:13:ASP:HA	2.37	0.50
1:C:171:PRO:CD	1:C:183:LYS:O	2.59	0.50
1:B:83:ASN:O	1:B:84:ALA:C	2.49	0.50
1:C:5:VAL:N	6:C:264:HOH:O	2.44	0.50
1:C:5:VAL:N	6:C:304:HOH:O	2.43	0.49
1:A:62:ARG:NE	6:A:429:HOH:O	2.44	0.49
1:F:115:ASP:HB3	1:F:124:GLN:HE22	1.77	0.49
1:F:189:ARG:HD3	6:F:280:HOH:O	2.13	0.49
1:A:5:VAL:HG12	1:A:5:VAL:O	2.12	0.48
1:A:180:LEU:HA	6:A:422:HOH:O	2.13	0.48
1:C:136:ASP:N	6:C:231:HOH:O	2.35	0.48
1:C:71:ILE:HD11	1:C:92:ILE:HG21	1.96	0.48
1:A:33:LYS:HD3	6:A:228:HOH:O	2.14	0.48
1:D:23:TYR:HB2	1:E:174:PHE:HE1	1.78	0.47
1:F:67:GLU:HG3	1:F:68:PRO:HD2	1.96	0.47
1:F:124:GLN:HB2	1:F:190:ILE:CG1	2.44	0.47
1:C:101:GLN:HG3	6:C:299:HOH:O	2.15	0.47
1:C:171:PRO:HD2	1:C:183:LYS:O	2.14	0.46
1:C:11:ILE:HD11	1:C:48:LYS:HG2	1.97	0.46
1:C:83:ASN:O	1:C:84:ALA:C	2.53	0.46
1:C:134:SER:OG	1:C:181:GLU:HB2	2.15	0.46
1:C:135:VAL:HB	6:C:231:HOH:O	2.14	0.46
1:E:71:ILE:HD11	1:E:92:ILE:HG21	1.98	0.46
1:C:43:LEU:HB3	1:C:104:GLU:HG2	1.98	0.46
1:A:71:ILE:HD11	1:A:92:ILE:HG21	1.99	0.45
1:D:40:ASN:HB2	6:D:243:HOH:O	2.16	0.45
1:D:65:THR:HB	1:E:136:ASP:HB3	1.98	0.45
1:B:68:PRO:HG3	1:B:89:VAL:HG21	1.98	0.45
1:A:30:LEU:HB2	1:A:157:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ASN:O	1:D:84:ALA:C	2.55	0.45
1:E:169:VAL:HB	6:E:235:HOH:O	2.17	0.45
1:C:11:ILE:CD1	1:C:48:LYS:HG2	2.47	0.44
1:E:55:ASP:OD2	1:E:58:ARG:CG	2.66	0.44
1:C:41:ALA:HB3	1:C:106:PHE:CZ	2.53	0.44
1:E:68:PRO:HG3	1:E:89:VAL:HG21	1.99	0.44
1:D:139:ASN:HA	1:D:180:LEU:HG	1.99	0.44
1:D:131:ILE:HG22	1:D:183:LYS:HB2	1.98	0.44
1:F:30:LEU:HB2	1:F:157:LEU:HD21	2.00	0.43
1:D:140:ILE:H	1:D:180:LEU:N	2.17	0.43
1:F:61:VAL:HG21	1:F:64:LYS:HG2	2.01	0.43
1:E:93:SER:CB	1:F:176:LEU:HD22	2.48	0.43
1:F:131:ILE:HG22	1:F:183:LYS:HB2	2.01	0.43
1:C:20:THR:HA	1:C:44:SER:O	2.18	0.43
1:E:20:THR:HA	1:E:44:SER:O	2.19	0.42
1:C:172:ALA:HA	1:C:174:PHE:CD2	2.53	0.42
1:E:55:ASP:OD2	1:E:58:ARG:HG2	2.20	0.42
1:D:20:THR:HA	1:D:44:SER:O	2.20	0.42
1:E:91:ASP:OD1	1:F:134:SER:HB2	2.20	0.42
1:B:40:ASN:HB2	6:B:356:HOH:O	2.20	0.42
1:D:78:PHE:CD1	1:D:78:PHE:N	2.88	0.41
1:C:46:SER:HA	1:C:100:VAL:O	2.21	0.41
1:A:28:TYR:OH	1:B:82:GLU:HG3	2.20	0.41
1:F:176:LEU:HD12	1:F:179:ARG:HD2	2.02	0.41
1:C:173:ASN:HB3	1:C:183:LYS:NZ	2.36	0.40
1:E:169:VAL:HG22	1:E:184:LEU:HD22	1.88	0.40
1:F:83:ASN:O	1:F:84:ALA:C	2.58	0.40
1:D:23:TYR:CB	1:E:174:PHE:HE1	2.33	0.40

All (4) 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)
1:E:14:GLU:CB	1:F:189:ARG:NH2[4_456]	1.80	0.40
1:D:50:ARG:NH2	1:F:57:VAL:CG1[1_455]	1.81	0.39
1:E:14:GLU:CA	1:F:189:ARG:NH2[4_456]	1.84	0.36
1:E:14:GLU:N	1:F:189:ARG:NH2[4_456]	2.08	0.12

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	170/201 (85%)	161 (95%)	9 (5%)	0	100 100
1	B	174/201 (87%)	167 (96%)	7 (4%)	0	100 100
1	C	180/201 (90%)	171 (95%)	7 (4%)	2 (1%)	17 18
1	D	168/201 (84%)	160 (95%)	7 (4%)	1 (1%)	30 36
1	E	174/201 (87%)	164 (94%)	10 (6%)	0	100 100
1	F	175/201 (87%)	169 (97%)	6 (3%)	0	100 100
All	All	1041/1206 (86%)	992 (95%)	46 (4%)	3 (0%)	46 57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	12	ALA
1	D	12	ALA
1	C	11	ILE

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	161/180 (89%)	157 (98%)	4 (2%)	55 73
1	B	164/180 (91%)	160 (98%)	4 (2%)	57 74
1	C	166/180 (92%)	160 (96%)	6 (4%)	42 57
1	D	159/180 (88%)	152 (96%)	7 (4%)	35 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	163/180 (91%)	157 (96%)	6 (4%)	41 55
1	F	163/180 (91%)	158 (97%)	5 (3%)	47 64
All	All	976/1080 (90%)	944 (97%)	32 (3%)	45 61

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	166	THR
1	A	183	LYS
1	A	192	ARG
1	B	48	LYS
1	B	58	ARG
1	B	183	LYS
1	B	192	ARG
1	C	48	LYS
1	C	62	ARG
1	C	173	ASN
1	C	176	LEU
1	C	180	LEU
1	C	183	LYS
1	D	4	MET
1	D	48	LYS
1	D	105	ARG
1	D	157	LEU
1	D	166	THR
1	D	181	GLU
1	D	183	LYS
1	E	48	LYS
1	E	157	LEU
1	E	166	THR
1	E	174	PHE
1	E	176	LEU
1	E	180	LEU
1	F	48	LYS
1	F	122	ASP
1	F	180	LEU
1	F	183	LYS
1	F	192	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	139	ASN
1	F	139	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 24 ligands modelled in this entry, 18 are monoatomic - leaving 6 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	ACY	A	701	-	1,3,3	1.07	0	0,3,3	0.00	-
2	ACY	B	701	-	1,3,3	1.52	0	0,3,3	0.00	-
2	ACY	C	701	-	1,3,3	1.53	0	0,3,3	0.00	-
2	ACY	D	701	-	1,3,3	0.35	0	0,3,3	0.00	-
2	ACY	E	701	-	1,3,3	0.42	0	0,3,3	0.00	-
2	ACY	F	701	-	1,3,3	1.02	0	0,3,3	0.00	-

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	ACY	A	701	-	-	0/0/0/0	0/0/0/0
2	ACY	B	701	-	-	0/0/0/0	0/0/0/0
2	ACY	C	701	-	-	0/0/0/0	0/0/0/0
2	ACY	D	701	-	-	0/0/0/0	0/0/0/0
2	ACY	E	701	-	-	0/0/0/0	0/0/0/0
2	ACY	F	701	-	-	0/0/0/0	0/0/0/0

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.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	ACY	1	0
2	D	701	ACY	1	0
2	E	701	ACY	1	0
2	F	701	ACY	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	176/201 (87%)	0.54	21 (11%) 6 9	36, 49, 67, 76	0
1	B	180/201 (89%)	0.42	11 (6%) 25 33	37, 48, 72, 85	0
1	C	184/201 (91%)	0.61	16 (8%) 13 18	36, 49, 73, 92	0
1	D	174/201 (86%)	0.53	18 (10%) 9 13	36, 48, 66, 78	0
1	E	180/201 (89%)	0.51	19 (10%) 8 12	36, 48, 70, 78	0
1	F	181/201 (90%)	0.73	22 (12%) 5 9	36, 48, 72, 81	0
All	All	1075/1206 (89%)	0.56	107 (9%) 9 14	36, 48, 71, 92	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	180	LEU	12.0
1	C	174	PHE	8.6
1	A	137	THR	7.7
1	C	179	ARG	6.1
1	B	119	THR	5.9
1	A	122	ASP	5.9
1	C	172	ALA	5.8
1	F	175	ALA	5.8
1	A	180	LEU	5.7
1	B	13	ASP	5.5
1	C	173	ASN	5.5
1	B	12	ALA	5.4
1	A	115	ASP	5.4
1	F	189	ARG	5.3
1	F	178	ASP	4.9
1	B	120	GLU	4.9
1	D	5	VAL	4.8
1	A	182	SER	4.8
1	E	193	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	176	LEU	4.2
1	B	174	PHE	4.1
1	F	173	ASN	4.1
1	C	11	ILE	4.1
1	F	147	GLU	4.0
1	A	136	ASP	3.9
1	F	115	ASP	3.9
1	D	4	MET	3.8
1	C	122	ASP	3.8
1	F	154	ASP	3.7
1	F	4	MET	3.7
1	A	171	PRO	3.7
1	E	11	ILE	3.6
1	D	57	VAL	3.6
1	B	122	ASP	3.5
1	E	139	ASN	3.5
1	D	62	ARG	3.4
1	B	172	ALA	3.3
1	F	5	VAL	3.2
1	C	115	ASP	3.2
1	E	4	MET	3.2
1	A	193	GLN	3.2
1	E	62	ARG	3.1
1	A	192	ARG	3.1
1	A	154	ASP	3.0
1	C	189	ARG	3.0
1	B	62	ARG	3.0
1	E	147	GLU	3.0
1	F	177	GLU	3.0
1	D	163	GLU	2.9
1	F	192	ARG	2.9
1	F	10	PRO	2.9
1	E	174	PHE	2.9
1	F	130	LEU	2.9
1	A	147	GLU	2.9
1	C	67	GLU	2.8
1	C	13	ASP	2.8
1	A	5	VAL	2.8
1	B	11	ILE	2.8
1	F	180	LEU	2.7
1	A	62	ARG	2.7
1	F	122	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	193	GLN	2.6
1	D	159	GLY	2.6
1	E	158	THR	2.6
1	A	69	GLU	2.5
1	B	154	ASP	2.5
1	E	134	SER	2.5
1	F	56	PRO	2.5
1	E	173	ASN	2.5
1	C	171	PRO	2.4
1	F	179	ARG	2.4
1	E	5	VAL	2.4
1	D	43	LEU	2.3
1	E	32	ASP	2.3
1	D	41	ALA	2.3
1	A	163	GLU	2.3
1	C	114	LEU	2.3
1	D	180	LEU	2.3
1	F	158	THR	2.2
1	D	192	ARG	2.2
1	E	189	ARG	2.2
1	A	159	GLY	2.2
1	D	69	GLU	2.2
1	D	13	ASP	2.2
1	D	45	LEU	2.2
1	D	22	ILE	2.2
1	E	115	ASP	2.2
1	E	146	LEU	2.2
1	F	83	ASN	2.2
1	D	67	GLU	2.2
1	E	135	VAL	2.1
1	B	10	PRO	2.1
1	C	110	VAL	2.1
1	A	123	SER	2.1
1	E	128	ILE	2.1
1	A	181	GLU	2.1
1	E	12	ALA	2.1
1	C	154	ASP	2.1
1	E	154	ASP	2.1
1	F	174	PHE	2.0
1	D	115	ASP	2.0
1	A	60	GLY	2.0
1	A	189	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	144	VAL	2.0
1	C	12	ALA	2.0
1	A	32	ASP	2.0
1	D	158	THR	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 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	ACY	C	701	4/4	0.90	0.18	1.48	53,54,54,55	0
2	ACY	D	701	4/4	0.97	0.18	0.67	53,53,54,54	0
2	ACY	A	701	4/4	0.90	0.15	0.39	53,54,54,55	0
2	ACY	E	701	4/4	0.92	0.14	-0.15	53,53,54,55	0
3	NA	B	801	1/1	0.91	0.14	-0.44	56,56,56,56	0
2	ACY	F	701	4/4	0.93	0.15	-0.46	52,53,54,54	0
3	NA	A	801	1/1	0.92	0.14	-0.48	56,56,56,56	0
2	ACY	B	701	4/4	0.94	0.11	-0.56	53,53,54,54	0
5	CL	F	901	1/1	1.00	0.15	-0.81	40,40,40,40	0
3	NA	D	801	1/1	0.88	0.10	-1.17	55,55,55,55	0
3	NA	C	801	1/1	0.89	0.10	-1.35	56,56,56,56	0
3	NA	E	801	1/1	0.95	0.06	-1.43	55,55,55,55	0
3	NA	F	801	1/1	0.95	0.05	-1.64	55,55,55,55	0
5	CL	B	901	1/1	0.98	0.08	-1.69	43,43,43,43	0
5	CL	A	901	1/1	0.99	0.09	-1.76	43,43,43,43	0
5	CL	E	901	1/1	0.99	0.08	-2.41	42,42,42,42	0
5	CL	D	901	1/1	0.98	0.06	-2.44	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	HG	C	700	1/1	0.99	0.04	-2.55	56,56,56,56	0
5	CL	C	901	1/1	0.98	0.09	-2.80	42,42,42,42	0
4	HG	B	700	1/1	1.00	0.05	-3.54	56,56,56,56	0
4	HG	E	700	1/1	1.00	0.04	-3.90	55,55,55,55	0
4	HG	D	700	1/1	0.99	0.02	-4.00	58,58,58,58	0
4	HG	F	700	1/1	1.00	0.05	-4.05	57,57,57,57	0
4	HG	A	700	1/1	1.00	0.03	-5.20	57,57,57,57	0

6.5 Other polymers

There are no such residues in this entry.