Full wwPDB X-ray Structure Validation Report (i)

Mar 17, 2022 – 12:08 PM JST

PDB ID	:	6IVQ
Title	:	Crystal structure of a membrane protein S19A
Authors	:	Kittredge, A.; Fukuda, F.; Zhang, Y.; Yang, T.
Deposited on	:	2018-12-04
Resolution	:	2.65 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

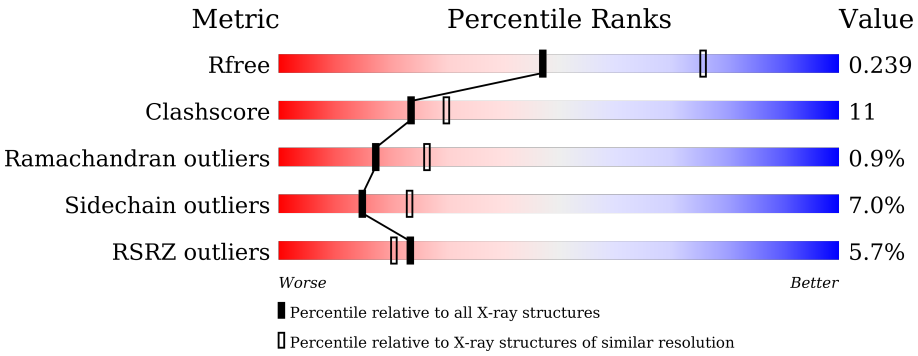
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	297	3% 70% 18% • 9%
1	B	297	6% 63% 24% • 9%
1	C	297	8% 71% 17% • 9%
1	D	297	7% 71% 16% • 9%
1	E	297	2% 66% 22% •• 9%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10898 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 Ibestrophin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2153	1395	365	384	9			
1	B	271	Total	C	N	O	S	0	0	0
			2160	1400	366	385	9			
1	C	269	Total	C	N	O	S	0	0	0
			2146	1391	364	382	9			
1	D	269	Total	C	N	O	S	0	0	0
			2143	1389	362	383	9			
1	E	271	Total	C	N	O	S	0	0	0
			2162	1401	365	387	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP W9BH30
A	-1	ASN	-	expression tag	UNP W9BH30
A	0	ALA	-	expression tag	UNP W9BH30
A	19	ALA	SER	engineered mutation	UNP W9BH30
B	-2	SER	-	expression tag	UNP W9BH30
B	-1	ASN	-	expression tag	UNP W9BH30
B	0	ALA	-	expression tag	UNP W9BH30
B	19	ALA	SER	engineered mutation	UNP W9BH30
C	-2	SER	-	expression tag	UNP W9BH30
C	-1	ASN	-	expression tag	UNP W9BH30
C	0	ALA	-	expression tag	UNP W9BH30
C	19	ALA	SER	engineered mutation	UNP W9BH30
D	-2	SER	-	expression tag	UNP W9BH30
D	-1	ASN	-	expression tag	UNP W9BH30
D	0	ALA	-	expression tag	UNP W9BH30
D	19	ALA	SER	engineered mutation	UNP W9BH30
E	-2	SER	-	expression tag	UNP W9BH30
E	-1	ASN	-	expression tag	UNP W9BH30
E	0	ALA	-	expression tag	UNP W9BH30

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Chain	Residue	Modelled	Actual	Comment	Reference
E	19	ALA	SER	engineered mutation	UNP W9BH30

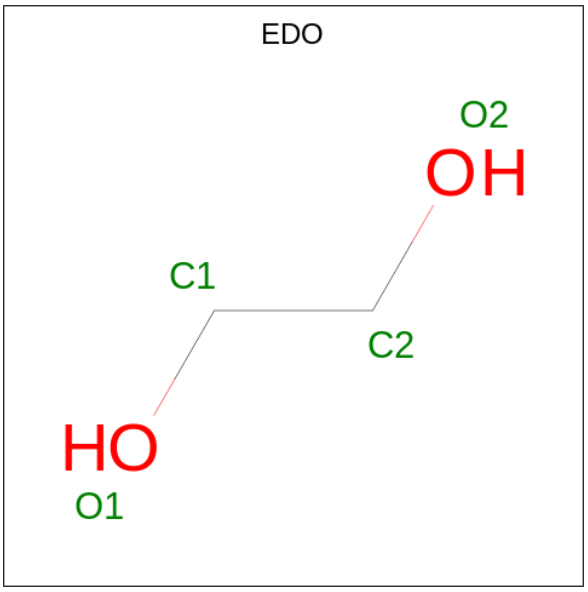
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

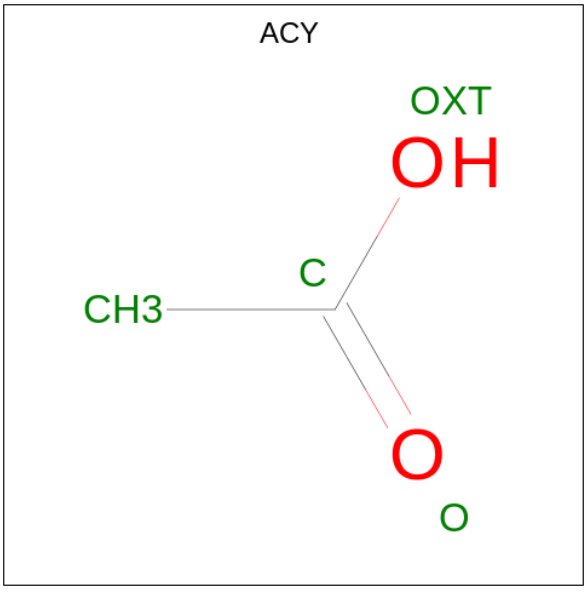
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3 3	0	0
3	B	1	Total Cl 1 1	0	0
3	C	3	Total Cl 3 3	0	0
3	D	3	Total Cl 3 3	0	0
3	E	2	Total Cl 2 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).

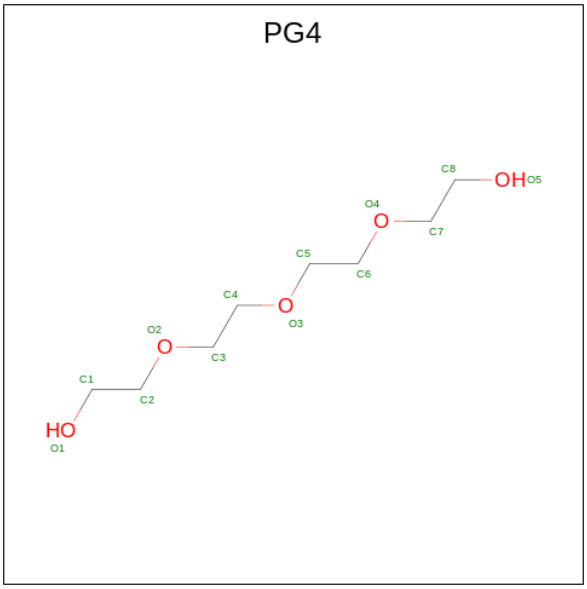


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Na 1 1	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C O 13 8 5	0	0

- Molecule 8 is water.

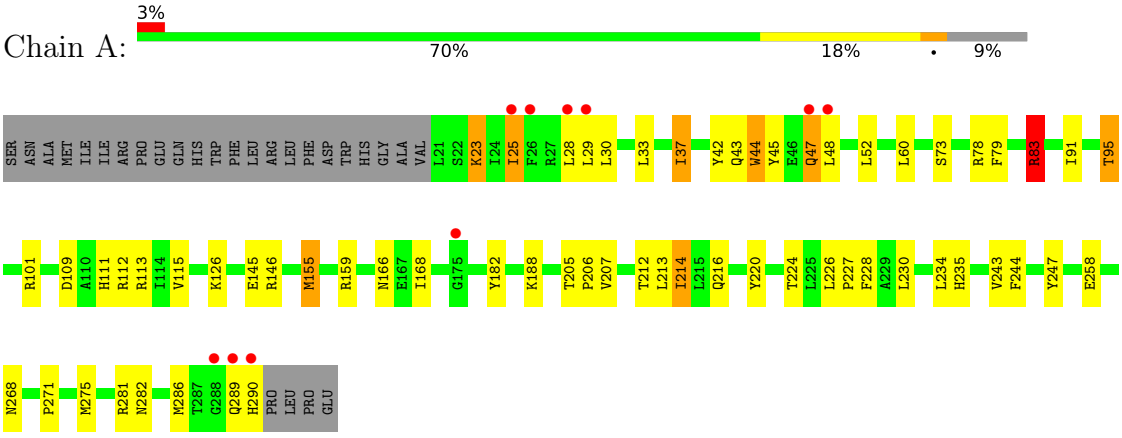
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	17	Total O 17 17	0	0
8	B	18	Total O 18 18	0	0
8	C	18	Total O 18 18	0	0
8	D	9	Total O 9 9	0	0
8	E	17	Total O 17 17	0	0

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.

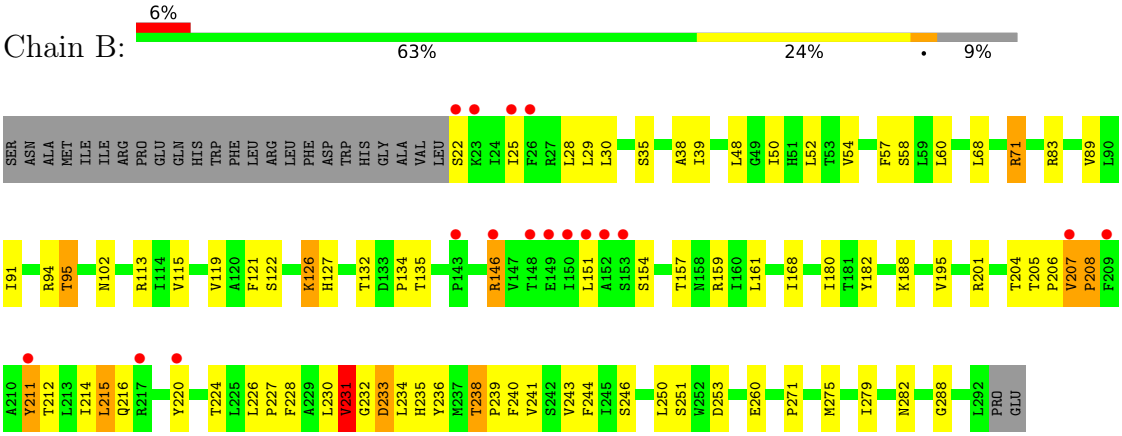
• Molecule 1: Ibestrophin

Chain A:



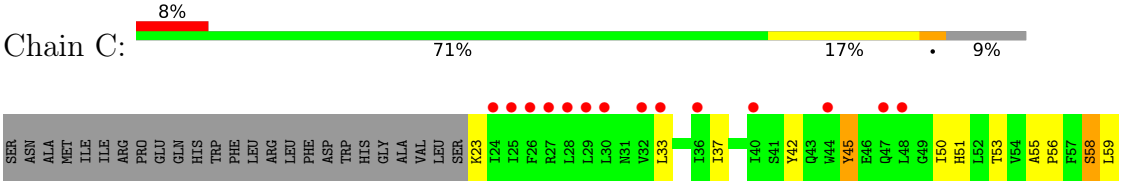
• Molecule 1: Ibestrophin

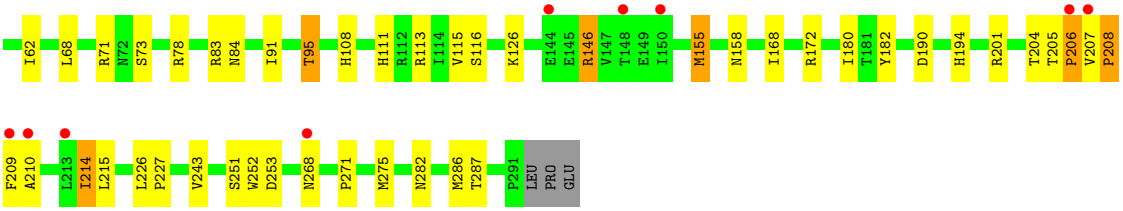
Chain B:



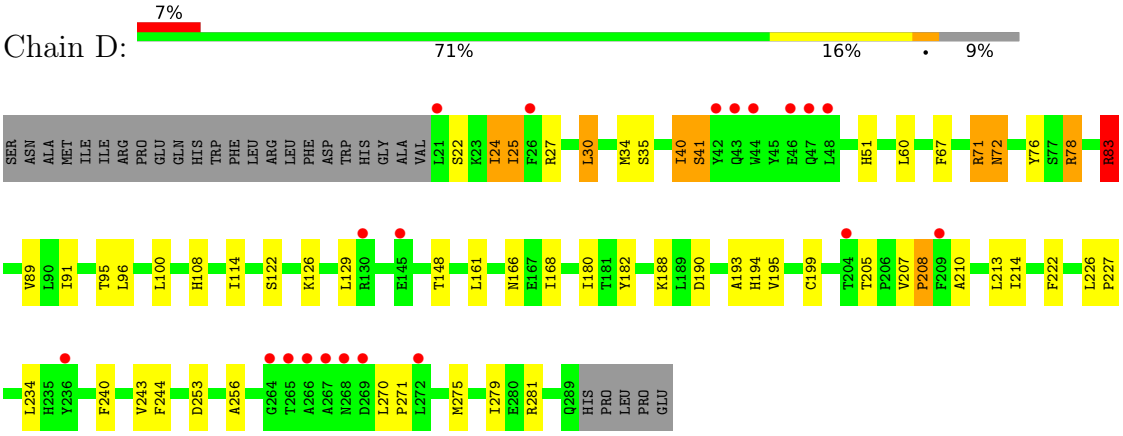
• Molecule 1: Ibestrophin

Chain C:

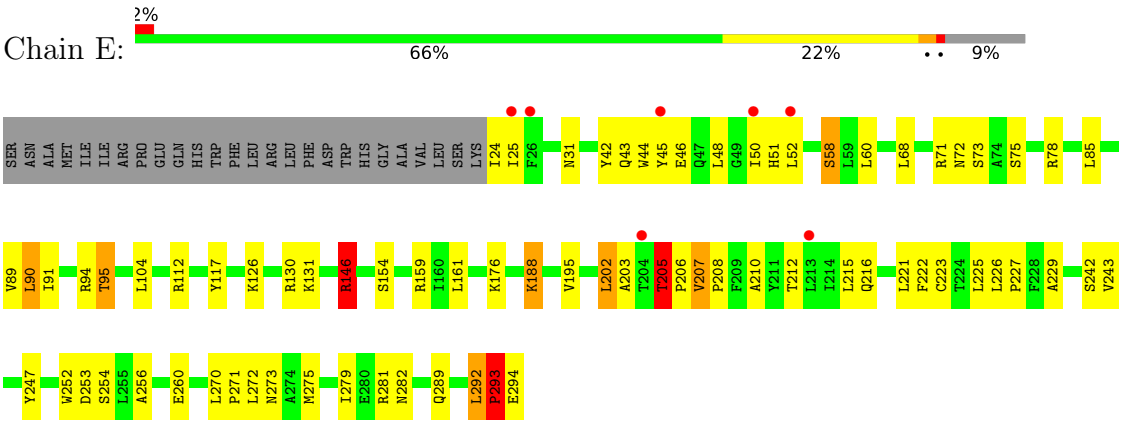




• Molecule 1: Ibestrophin



• Molecule 1: Ibestrophin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.70Å 159.64Å 161.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 2.65 48.61 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.61-2.65) 99.8 (48.61-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.201 , 0.239 0.201 , 0.239	Depositor DCC
R_{free} test set	4278 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10898	wwPDB-VP
Average B, all atoms (Å^2)	75.0	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: NA, CL, PG4, ZN, EDO, ACY

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	0.38	0/2200	0.77	1/2994 (0.0%)
1	B	0.36	0/2208	0.73	0/3006
1	C	0.34	0/2194	0.69	0/2987
1	D	0.34	0/2189	0.65	1/2979 (0.0%)
1	E	0.41	1/2211 (0.0%)	0.91	3/3011 (0.1%)
All	All	0.37	1/11002 (0.0%)	0.75	5/14977 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	2
1	D	0	2
1	E	0	3
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	293	PRO	C-N	7.90	1.52	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	293	PRO	O-C-N	-21.58	88.17	122.70
1	E	293	PRO	C-N-CA	13.17	154.61	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	293	PRO	CA-C-N	13.05	145.92	117.20
1	A	83	ARG	CG-CD-NE	-6.21	98.76	111.80
1	D	83	ARG	CG-CD-NE	5.04	122.39	111.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ARG	Sidechain
1	A	281	ARG	Sidechain
1	A	83	ARG	Sidechain
1	B	113	ARG	Sidechain
1	B	159	ARG	Sidechain
1	B	94	ARG	Sidechain
1	C	113	ARG	Sidechain
1	C	146	ARG	Sidechain
1	D	281	ARG	Sidechain
1	D	71	ARG	Sidechain
1	E	146	ARG	Sidechain
1	E	159	ARG	Sidechain
1	E	293	PRO	Mainchain

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	2153	0	2199	59	0
1	B	2160	0	2206	67	0
1	C	2146	0	2190	37	0
1	D	2143	0	2192	43	0
1	E	2162	0	2201	70	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	3	0	0	0	0
3	A	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	3	0	0	2	0
3	D	3	0	0	1	0
3	E	2	0	0	0	0
4	A	4	0	6	0	0
5	B	4	0	3	1	0
5	E	4	0	3	1	0
6	D	1	0	0	0	0
7	E	13	0	18	1	0
8	A	17	0	0	0	0
8	B	18	0	0	0	0
8	C	18	0	0	0	0
8	D	9	0	0	0	0
8	E	17	0	0	0	0
All	All	10898	0	11018	244	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.

All (244) 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:235:HIS:O	1:B:238:THR:HG23	1.38	1.21
1:A:83:ARG:HH22	1:E:205:THR:CG2	1.64	1.10
1:A:83:ARG:NH2	1:E:205:THR:HG23	1.69	1.07
1:A:83:ARG:HH22	1:E:205:THR:HG23	0.84	1.01
1:B:234:LEU:HB2	1:B:238:THR:HG22	1.41	1.00
1:C:78:ARG:HH12	1:C:205:THR:CG2	1.78	0.96
1:E:78:ARG:HH12	1:E:205:THR:HG21	1.28	0.95
1:C:201:ARG:O	1:C:205:THR:HB	1.73	0.86
1:B:71:ARG:HH12	1:B:212:THR:HG22	1.42	0.84
1:B:71:ARG:NH1	1:B:260:GLU:OE2	2.11	0.84
1:B:235:HIS:O	1:B:238:THR:CG2	2.24	0.84
1:D:83:ARG:HG2	1:D:270:LEU:HD21	1.61	0.82
1:B:204:THR:O	1:B:206:PRO:HD3	1.80	0.81
1:C:78:ARG:HH12	1:C:205:THR:HG21	1.45	0.81
1:E:94:ARG:HH21	1:E:282:ASN:HD21	1.27	0.80
1:D:271:PRO:HD2	1:D:275:MET:HE1	1.64	0.79
1:E:205:THR:HB	1:E:206:PRO:HA	1.64	0.78
1:A:271:PRO:HD2	1:A:275:MET:HE3	1.65	0.78
1:B:71:ARG:HH12	1:B:212:THR:CG2	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:MET:HG2	1:C:158:ASN:HB2	1.63	0.78
1:B:231:VAL:HA	1:B:238:THR:HG21	1.66	0.77
1:E:205:THR:CB	1:E:206:PRO:HA	2.15	0.76
1:B:211:TYR:O	1:B:215:LEU:HB2	1.84	0.76
1:A:101:ARG:HH22	1:A:290:HIS:C	1.91	0.74
1:B:39:ILE:HD13	1:B:236:TYR:HA	1.70	0.73
1:A:91:ILE:O	1:A:95:THR:HG23	1.88	0.72
1:A:168:ILE:HG22	1:A:182:TYR:CE1	2.24	0.72
1:A:83:ARG:NH2	1:E:205:THR:CG2	2.38	0.72
1:A:258:GLU:HG2	1:A:268:ASN:HD22	1.55	0.71
1:C:42:TYR:O	1:C:45:TYR:HB2	1.89	0.71
1:D:25:ILE:HD13	1:D:25:ILE:N	2.05	0.71
1:C:251:SER:HB3	1:D:214:ILE:HD13	1.74	0.69
1:E:94:ARG:HH21	1:E:282:ASN:ND2	1.89	0.69
1:E:91:ILE:O	1:E:95:THR:HG23	1.91	0.69
1:C:78:ARG:NH1	1:C:205:THR:CG2	2.54	0.69
1:B:236:TYR:O	1:B:239:PRO:HD2	1.93	0.68
1:D:78:ARG:HD3	1:D:207:VAL:HG23	1.76	0.68
1:A:43:GLN:C	1:A:45:TYR:H	1.97	0.67
1:E:78:ARG:NH1	1:E:205:THR:HG21	2.08	0.66
1:A:52:LEU:CD1	1:A:228:PHE:HB3	2.25	0.66
1:A:78:ARG:NH1	1:A:206:PRO:HA	2.11	0.66
1:E:42:TYR:CE1	1:E:46:GLU:HG3	2.31	0.66
1:D:72:ASN:ND2	1:D:256:ALA:HB2	2.10	0.66
1:E:50:ILE:HG13	1:E:50:ILE:O	1.96	0.66
1:B:207:VAL:HG12	1:D:76:TYR:HE1	1.61	0.66
1:D:271:PRO:HD2	1:D:275:MET:CE	2.25	0.65
1:C:205:THR:N	1:C:206:PRO:CD	2.60	0.64
1:A:214:ILE:HD13	1:B:251:SER:HB3	1.80	0.64
1:A:43:GLN:O	1:A:45:TYR:N	2.31	0.64
1:B:224:THR:O	1:B:227:PRO:HD2	1.98	0.64
1:B:39:ILE:CD1	1:B:236:TYR:HA	2.27	0.64
1:A:109:ASP:HB3	1:A:113:ARG:HH12	1.61	0.63
1:B:146:ARG:HA	1:B:146:ARG:HH11	1.62	0.63
1:A:33:LEU:O	1:A:37:ILE:HG23	1.98	0.63
1:D:78:ARG:CD	1:D:207:VAL:HG23	2.28	0.63
1:A:42:TYR:O	1:A:45:TYR:HB2	2.00	0.62
1:C:115:VAL:HG21	1:C:287:THR:HG21	1.80	0.62
1:E:281:ARG:HD3	5:E:307:ACY:H3	1.80	0.61
1:A:235:HIS:ND1	1:E:51:HIS:NE2	2.47	0.61
1:B:35:SER:OG	1:B:239:PRO:HA	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ILE:HG23	1:D:25:ILE:HD13	1.82	0.60
1:E:206:PRO:HB2	1:E:208:PRO:HD2	1.83	0.60
1:A:244:PHE:CE1	1:E:221:LEU:HD23	2.37	0.59
1:A:271:PRO:HD2	1:A:275:MET:CE	2.32	0.59
1:C:91:ILE:O	1:C:95:THR:HG23	2.03	0.59
1:A:166:ASN:ND2	1:B:102:ASN:HD22	2.01	0.59
1:B:238:THR:N	1:B:239:PRO:HD2	2.18	0.59
1:A:52:LEU:HD12	1:A:228:PHE:HB3	1.83	0.58
1:A:282:ASN:O	1:A:286:MET:HG3	2.02	0.58
1:E:207:VAL:H	1:E:208:PRO:HD2	1.68	0.58
1:A:168:ILE:HG22	1:A:182:TYR:CD1	2.38	0.58
1:A:271:PRO:CD	1:A:275:MET:HE3	2.34	0.58
1:C:83:ARG:HG2	1:D:205:THR:HG21	1.85	0.58
1:E:90:LEU:HD13	1:E:279:ILE:HD13	1.86	0.57
1:A:101:ARG:NH2	1:A:290:HIS:C	2.58	0.57
1:B:71:ARG:NH1	1:B:212:THR:HG22	2.17	0.57
1:A:258:GLU:CG	1:A:268:ASN:HD22	2.16	0.57
1:D:91:ILE:O	1:D:95:THR:HG23	2.04	0.57
1:E:205:THR:CG2	1:E:206:PRO:HA	2.35	0.57
1:E:60:LEU:HD23	1:E:222:PHE:HD1	1.70	0.56
1:D:71:ARG:HD2	1:D:71:ARG:C	2.25	0.56
1:A:166:ASN:HD22	1:B:102:ASN:HD22	1.53	0.56
1:E:292:LEU:HD22	1:E:293:PRO:HD2	1.87	0.56
1:D:168:ILE:HG22	1:D:182:TYR:CE2	2.41	0.56
1:E:216:GLN:HG3	1:E:253:ASP:OD2	2.06	0.56
1:A:230:LEU:HB3	1:A:234:LEU:HD12	1.87	0.55
1:C:78:ARG:NH1	1:C:205:THR:HG23	2.22	0.55
1:E:95:THR:OG1	1:E:188:LYS:HD2	2.07	0.55
1:A:23:LYS:HE3	1:A:220:TYR:OH	2.07	0.55
1:C:226:LEU:N	1:C:227:PRO:HD2	2.21	0.54
1:E:205:THR:HG22	1:E:206:PRO:HA	1.89	0.54
1:A:205:THR:HG21	1:B:83:ARG:HG2	1.90	0.54
1:E:24:ILE:HG23	1:E:25:ILE:N	2.21	0.54
1:E:207:VAL:N	1:E:208:PRO:HD2	2.23	0.54
1:C:194:HIS:HA	1:E:91:ILE:HD13	1.90	0.53
1:E:226:LEU:N	1:E:227:PRO:HD2	2.22	0.53
1:B:271:PRO:HD2	1:B:275:MET:HE3	1.90	0.53
1:A:60:LEU:HD21	1:B:244:PHE:CE2	2.44	0.53
1:C:190:ASP:OD1	3:C:306:CL:CL	2.63	0.53
1:E:31:ASN:ND2	1:E:223:CYS:O	2.41	0.53
1:B:135:THR:HG23	1:B:151:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:VAL:O	1:C:208:PRO:C	2.46	0.53
1:E:45:TYR:HB2	1:E:50:ILE:HD11	1.90	0.53
1:E:73:SER:HA	7:E:306:PG4:H61	1.90	0.53
1:E:90:LEU:HD12	1:E:94:ARG:CZ	2.39	0.52
1:C:91:ILE:HD13	1:D:194:HIS:HA	1.91	0.52
1:B:22:SER:HB3	1:B:25:ILE:H	1.74	0.52
1:D:25:ILE:N	1:D:25:ILE:CD1	2.73	0.52
1:E:24:ILE:CG2	1:E:25:ILE:N	2.73	0.52
1:A:101:ARG:HD2	1:A:286:MET:O	2.10	0.52
1:D:71:ARG:NH2	1:D:253:ASP:OD1	2.43	0.51
1:D:226:LEU:N	1:D:227:PRO:HD2	2.24	0.51
1:A:78:ARG:HD3	1:A:207:VAL:HG23	1.93	0.51
1:A:91:ILE:O	1:A:95:THR:CG2	2.58	0.51
1:C:168:ILE:HG13	1:C:182:TYR:CE2	2.44	0.51
1:C:180:ILE:HD12	1:D:180:ILE:HD13	1.92	0.51
1:D:78:ARG:HD3	1:D:207:VAL:CG2	2.39	0.51
1:D:168:ILE:HG22	1:D:182:TYR:CD2	2.46	0.50
1:B:91:ILE:O	1:B:95:THR:HG23	2.11	0.50
1:E:112:ARG:NH1	1:E:289:GLN:HG2	2.26	0.50
1:A:28:LEU:HD21	1:A:247:TYR:HB2	1.95	0.49
1:E:68:LEU:HD23	1:E:215:LEU:HD21	1.93	0.49
1:B:227:PRO:HA	1:B:230:LEU:HB2	1.95	0.49
1:E:117:TYR:OH	1:E:146:ARG:HG2	2.13	0.49
1:A:212:THR:O	1:A:216:GLN:HB2	2.11	0.49
1:B:28:LEU:HD22	1:B:243:VAL:HG22	1.94	0.49
1:B:234:LEU:CB	1:B:238:THR:HG22	2.30	0.49
1:C:271:PRO:HD2	1:C:275:MET:HE3	1.95	0.48
1:D:240:PHE:O	1:D:243:VAL:HG12	2.13	0.48
1:A:48:LEU:O	1:B:236:TYR:CE2	2.66	0.48
1:D:207:VAL:O	1:D:208:PRO:C	2.52	0.48
1:B:25:ILE:O	1:B:29:LEU:HG	2.12	0.48
1:A:44:TRP:HA	1:A:47:GLN:HG3	1.95	0.48
1:A:30:LEU:HD23	1:A:30:LEU:O	2.14	0.47
1:C:68:LEU:HD23	1:C:215:LEU:HD21	1.96	0.47
1:A:145:GLU:HB3	1:A:146:ARG:HH21	1.79	0.47
1:E:202:LEU:C	1:E:205:THR:OG1	2.52	0.47
1:B:127:HIS:CD2	1:B:134:PRO:HA	2.50	0.47
1:C:50:ILE:O	1:C:50:ILE:HG13	2.15	0.47
1:A:43:GLN:C	1:A:45:TYR:N	2.67	0.47
1:B:240:PHE:O	1:B:243:VAL:HG12	2.15	0.47
1:D:89:VAL:HG23	1:D:195:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ILE:HG13	1:B:182:TYR:CE1	2.49	0.47
1:B:216:GLN:HG2	1:B:253:ASP:OD2	2.15	0.47
1:C:95:THR:HG21	3:C:304:CL:CL	2.52	0.47
1:E:42:TYR:HE1	1:E:46:GLU:HG3	1.76	0.47
1:E:270:LEU:HB3	1:E:271:PRO:HD3	1.95	0.47
1:E:85:LEU:HD22	1:E:195:VAL:HA	1.97	0.47
1:B:205:THR:HG21	1:D:83:ARG:HD3	1.97	0.46
1:E:24:ILE:CG2	1:E:25:ILE:H	2.28	0.46
1:D:30:LEU:O	1:D:34:MET:HG2	2.15	0.46
1:A:224:THR:O	1:A:227:PRO:HD2	2.16	0.46
1:B:122:SER:OG	1:B:279:ILE:HD13	2.16	0.46
1:A:226:LEU:N	1:A:227:PRO:HD2	2.31	0.46
1:E:126:LYS:HG3	1:E:272:LEU:HD23	1.97	0.46
1:A:230:LEU:HB3	1:A:234:LEU:CD1	2.46	0.45
1:A:214:ILE:CD1	1:B:251:SER:HB3	2.43	0.45
1:B:246:SER:O	1:B:250:LEU:HD12	2.17	0.45
1:B:201:ARG:O	1:B:205:THR:HB	2.16	0.45
1:E:126:LYS:HE3	1:E:273:ASN:OD1	2.16	0.45
1:C:58:SER:O	1:C:62:ILE:HG13	2.17	0.45
1:C:214:ILE:HG13	1:E:247:TYR:OH	2.17	0.45
1:E:104:LEU:HD21	1:E:176:LYS:O	2.16	0.45
1:E:94:ARG:HE	1:E:282:ASN:ND2	2.15	0.45
1:E:226:LEU:N	1:E:227:PRO:CD	2.80	0.45
1:D:190:ASP:O	1:D:193:ALA:HB3	2.16	0.44
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.79	0.44
1:B:271:PRO:CD	1:B:275:MET:HE3	2.47	0.44
1:E:72:ASN:ND2	1:E:256:ALA:HB2	2.33	0.44
1:B:71:ARG:HH22	1:B:212:THR:HG22	1.82	0.44
1:E:44:TRP:O	1:E:48:LEU:HG	2.17	0.44
1:E:75:SER:OG	1:E:260:GLU:HG3	2.18	0.44
1:A:258:GLU:CD	1:A:268:ASN:ND2	2.71	0.44
1:B:226:LEU:HG	1:B:230:LEU:CD1	2.47	0.44
1:C:204:THR:C	1:C:206:PRO:HD2	2.38	0.44
1:E:89:VAL:HG23	1:E:195:VAL:HG11	1.99	0.44
1:E:207:VAL:N	1:E:208:PRO:CD	2.81	0.44
1:B:60:LEU:HD21	1:D:244:PHE:CE2	2.53	0.44
1:C:55:ALA:HB3	1:C:56:PRO:HD3	1.99	0.44
1:C:252:TRP:CH2	1:D:67:PHE:HB3	2.53	0.43
1:A:60:LEU:HD21	1:B:244:PHE:CD2	2.53	0.43
1:A:155:MET:HG2	1:B:282:ASN:OD1	2.18	0.43
1:E:205:THR:CB	1:E:206:PRO:CA	2.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:PHE:CE1	1:B:157:THR:HG22	2.53	0.43
1:D:60:LEU:HD23	1:D:222:PHE:HD1	1.84	0.43
1:E:161:LEU:HD23	1:E:161:LEU:HA	1.82	0.43
1:E:68:LEU:HB3	1:E:252:TRP:HD1	1.83	0.43
1:E:71:ARG:NH2	1:E:253:ASP:OD1	2.51	0.43
1:C:108:HIS:HA	1:C:111:HIS:ND1	2.34	0.43
1:A:166:ASN:ND2	1:B:102:ASN:ND2	2.65	0.43
1:B:52:LEU:HD23	1:D:234:LEU:HD22	2.01	0.43
1:A:78:ARG:NH1	1:A:205:THR:O	2.52	0.42
1:D:108:HIS:HB3	3:D:306:CL:CL	2.56	0.42
1:A:188:LYS:HA	1:A:188:LYS:HD3	1.66	0.42
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.89	0.42
1:C:71:ARG:HD2	1:C:71:ARG:C	2.39	0.42
1:E:203:ALA:C	1:E:205:THR:H	2.20	0.42
1:B:127:HIS:ND1	1:B:132:THR:OG1	2.52	0.42
1:B:238:THR:N	1:B:239:PRO:CD	2.81	0.42
1:D:89:VAL:CG2	1:D:195:VAL:HG11	2.49	0.42
1:C:180:ILE:HD12	1:D:180:ILE:CD1	2.49	0.42
1:D:71:ARG:HD2	1:D:71:ARG:O	2.19	0.42
1:A:95:THR:HG21	3:A:305:CL:CL	2.56	0.42
1:C:282:ASN:O	1:C:286:MET:HG3	2.19	0.42
1:A:111:HIS:O	1:A:115:VAL:HG23	2.20	0.42
1:B:220:TYR:O	1:B:224:THR:HG23	2.19	0.42
1:E:207:VAL:HG23	1:E:208:PRO:HD3	2.01	0.42
1:B:95:THR:OG1	1:B:188:LYS:HD2	2.20	0.42
1:B:241:VAL:O	1:B:241:VAL:HG12	2.19	0.42
1:B:89:VAL:CG2	1:B:195:VAL:HG11	2.49	0.42
1:E:89:VAL:CG2	1:E:195:VAL:HG11	2.50	0.42
1:E:43:GLN:HG3	1:E:44:TRP:H	1.85	0.41
1:A:109:ASP:HB3	1:A:113:ARG:NH1	2.34	0.41
1:B:288:GLY:HA3	5:B:304:ACY:H3	2.03	0.41
1:C:71:ARG:NH2	1:C:253:ASP:OD1	2.53	0.41
1:B:207:VAL:O	1:B:208:PRO:O	2.39	0.41
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.94	0.41
1:E:72:ASN:HD22	1:E:256:ALA:HB2	1.86	0.41
1:A:47:GLN:H	1:A:47:GLN:HG2	1.52	0.41
1:D:275:MET:O	1:D:279:ILE:HG13	2.21	0.41
1:E:208:PRO:O	1:E:210:ALA:N	2.48	0.41
1:A:25:ILE:O	1:A:29:LEU:HD12	2.21	0.41
1:B:54:VAL:O	1:B:57:PHE:N	2.49	0.41
1:C:205:THR:HG23	1:C:205:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ILE:HG13	1:D:41:SER:N	2.36	0.41
1:D:100:LEU:HD11	1:D:114:ILE:HG21	2.03	0.41
1:E:52:LEU:HB3	1:E:229:ALA:HA	2.03	0.41
1:B:180:ILE:CD1	1:D:180:ILE:HD12	2.51	0.41
1:B:226:LEU:N	1:B:227:PRO:HD2	2.36	0.41
1:D:188:LYS:HA	1:D:188:LYS:HD3	1.94	0.41
1:E:205:THR:HB	1:E:206:PRO:CA	2.43	0.41
1:E:279:ILE:HD12	1:E:279:ILE:HA	1.90	0.41
1:B:38:ALA:HB2	1:B:228:PHE:CD1	2.56	0.40
1:C:208:PRO:O	1:C:210:ALA:N	2.53	0.40
1:D:129:LEU:HD21	1:D:199:CYS:HB3	2.03	0.40
1:D:210:ALA:O	1:D:214:ILE:HG13	2.22	0.40
1:E:112:ARG:HH12	1:E:289:GLN:HG2	1.85	0.40
1:B:231:VAL:O	1:B:233:ASP:N	2.55	0.40
1:B:115:VAL:O	1:B:119:VAL:HG23	2.21	0.40
1:C:59:LEU:HD13	1:E:58:SER:HA	2.02	0.40
1:C:268:ASN:ND2	1:D:208:PRO:HB3	2.36	0.40
1:E:202:LEU:C	1:E:205:THR:HG1	2.24	0.40
1:A:79:PHE:CE1	1:E:207:VAL:HG12	2.57	0.40
1:B:126:LYS:HB3	1:B:126:LYS:HE2	1.78	0.40

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	268/297 (90%)	260 (97%)	5 (2%)	3 (1%)	14	21
1	B	269/297 (91%)	252 (94%)	14 (5%)	3 (1%)	14	21
1	C	267/297 (90%)	257 (96%)	7 (3%)	3 (1%)	14	21
1	D	267/297 (90%)	258 (97%)	8 (3%)	1 (0%)	34	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	269/297 (91%)	260 (97%)	7 (3%)	2 (1%)	22 33
All	All	1340/1485 (90%)	1287 (96%)	41 (3%)	12 (1%)	17 26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	TRP
1	A	214	ILE
1	E	293	PRO
1	B	208	PRO
1	B	232	GLY
1	C	209	PHE
1	A	213	LEU
1	C	208	PRO
1	E	205	THR
1	D	208	PRO
1	C	206	PRO
1	B	231	VAL

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	235/259 (91%)	224 (95%)	11 (5%)	26 40
1	B	236/259 (91%)	220 (93%)	16 (7%)	16 24
1	C	234/259 (90%)	217 (93%)	17 (7%)	14 21
1	D	234/259 (90%)	215 (92%)	19 (8%)	11 17
1	E	236/259 (91%)	217 (92%)	19 (8%)	11 17
All	All	1175/1295 (91%)	1093 (93%)	82 (7%)	15 23

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	25	ILE
1	A	37	ILE
1	A	47	GLN
1	A	73	SER
1	A	95	THR
1	A	126	LYS
1	A	155	MET
1	A	159	ARG
1	A	243	VAL
1	A	289	GLN
1	B	30	LEU
1	B	48	LEU
1	B	50	ILE
1	B	58	SER
1	B	71	ARG
1	B	95	THR
1	B	126	LYS
1	B	146	ARG
1	B	154	SER
1	B	207	VAL
1	B	211	TYR
1	B	214	ILE
1	B	215	LEU
1	B	231	VAL
1	B	233	ASP
1	B	238	THR
1	C	23	LYS
1	C	33	LEU
1	C	37	ILE
1	C	45	TYR
1	C	51	HIS
1	C	53	THR
1	C	58	SER
1	C	73	SER
1	C	84	ASN
1	C	95	THR
1	C	116	SER
1	C	126	LYS
1	C	146	ARG
1	C	155	MET
1	C	172	ARG
1	C	214	ILE

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Mol	Chain	Res	Type
1	C	243	VAL
1	D	22	SER
1	D	24	ILE
1	D	25	ILE
1	D	27	ARG
1	D	30	LEU
1	D	35	SER
1	D	40	ILE
1	D	41	SER
1	D	51	HIS
1	D	72	ASN
1	D	78	ARG
1	D	83	ARG
1	D	96	LEU
1	D	122	SER
1	D	126	LYS
1	D	148	THR
1	D	161	LEU
1	D	166	ASN
1	D	213	LEU
1	E	58	SER
1	E	90	LEU
1	E	95	THR
1	E	130	ARG
1	E	131	LYS
1	E	146	ARG
1	E	154	SER
1	E	188	LYS
1	E	202	LEU
1	E	205	THR
1	E	207	VAL
1	E	212	THR
1	E	225	LEU
1	E	242	SER
1	E	243	VAL
1	E	254	SER
1	E	275	MET
1	E	292	LEU
1	E	294	GLU

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	47	GLN
1	A	84	ASN
1	A	158	ASN
1	A	166	ASN
1	A	268	ASN
1	B	31	ASN
1	B	43	GLN
1	B	166	ASN
1	C	166	ASN
1	D	72	ASN
1	D	289	GLN
1	E	166	ASN
1	E	268	ASN
1	E	282	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 30 are monoatomic - leaving 4 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	EDO	A	308	-	3,3,3	0.60	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ACY	E	307	2	1,3,3	6.30	1 (100%)	0,3,3	-	-
5	ACY	B	304	2	1,3,3	6.04	1 (100%)	0,3,3	-	-
7	PG4	E	306	-	12,12,12	0.71	0	11,11,11	0.57	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	EDO	A	308	-	-	1/1/1/1	-
7	PG4	E	306	-	-	7/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	307	ACY	CH3-C	6.30	1.56	1.48
5	B	304	ACY	CH3-C	6.04	1.56	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	306	PG4	C1-C2-O2-C3
4	A	308	EDO	O1-C1-C2-O2
7	E	306	PG4	C8-C7-O4-C6
7	E	306	PG4	C6-C5-O3-C4
7	E	306	PG4	O2-C3-C4-O3
7	E	306	PG4	O3-C5-C6-O4
7	E	306	PG4	O1-C1-C2-O2
7	E	306	PG4	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	307	ACY	1	0
5	B	304	ACY	1	0
7	E	306	PG4	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

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	270/297 (90%)	-0.19	10 (3%)	41	38	39, 60, 126, 151	0
1	B	271/297 (91%)	-0.12	17 (6%)	20	17	39, 69, 122, 157	0
1	C	269/297 (90%)	0.10	23 (8%)	10	8	41, 65, 138, 203	0
1	D	269/297 (90%)	0.04	20 (7%)	14	12	46, 75, 127, 157	0
1	E	271/297 (91%)	-0.21	7 (2%)	56	52	41, 62, 115, 160	0
All	All	1350/1485 (90%)	-0.08	77 (5%)	23	20	39, 66, 126, 203	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	PHE	20.1
1	E	26	PHE	6.0
1	C	26	PHE	5.9
1	C	206	PRO	5.8
1	D	43	GLN	5.4
1	D	47	GLN	5.2
1	A	25	ILE	5.1
1	C	47	GLN	5.0
1	D	44	TRP	4.8
1	B	22	SER	4.7
1	E	204	THR	4.6
1	C	48	LEU	4.6
1	D	236	TYR	4.5
1	D	265	THR	4.5
1	D	268	ASN	4.4
1	D	48	LEU	4.2
1	B	152	ALA	4.2
1	D	267	ALA	4.2
1	B	211	TYR	4.1
1	A	29	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	24	ILE	3.9
1	D	209	PHE	3.9
1	C	207	VAL	3.8
1	D	264	GLY	3.7
1	C	210	ALA	3.7
1	C	40	ILE	3.6
1	A	26	PHE	3.5
1	C	29	LEU	3.5
1	B	150	ILE	3.4
1	C	27	ARG	3.2
1	C	44	TRP	3.2
1	A	48	LEU	3.2
1	C	30	LEU	3.2
1	A	175	GLY	3.1
1	B	146	ARG	3.1
1	B	148	THR	2.9
1	A	47	GLN	2.9
1	A	289	GLN	2.9
1	B	26	PHE	2.9
1	D	204	THR	2.8
1	C	32	VAL	2.8
1	D	130	ARG	2.8
1	C	150	ILE	2.8
1	D	21	LEU	2.8
1	C	213	LEU	2.7
1	D	46	GLU	2.7
1	B	217	ARG	2.6
1	E	25	ILE	2.6
1	D	145	GLU	2.6
1	A	290	HIS	2.6
1	B	23	LYS	2.6
1	B	207	VAL	2.6
1	B	209	PHE	2.6
1	C	28	LEU	2.5
1	C	25	ILE	2.5
1	B	153	SER	2.5
1	D	26	PHE	2.5
1	B	143	PRO	2.5
1	D	42	TYR	2.5
1	D	269	ASP	2.4
1	C	33	LEU	2.4
1	A	28	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	50	ILE	2.4
1	C	36	ILE	2.3
1	B	151	LEU	2.3
1	A	288	GLY	2.3
1	E	45	TYR	2.3
1	E	52	LEU	2.3
1	B	149	GLU	2.3
1	C	148	THR	2.2
1	E	213	LEU	2.2
1	B	220	TYR	2.1
1	D	272	LEU	2.1
1	C	268	ASN	2.1
1	B	25	ILE	2.1
1	D	266	ALA	2.1
1	C	144	GLU	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 monosaccharides 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, 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
7	PG4	E	306	13/13	0.77	0.32	72,83,96,102	0
5	ACY	E	307	4/4	0.86	0.28	44,50,50,51	0
2	ZN	D	304	1/1	0.87	0.18	128,128,128,128	0
2	ZN	E	305	1/1	0.88	0.14	177,177,177,177	0
4	EDO	A	308	4/4	0.89	0.24	60,72,74,78	0
5	ACY	B	304	4/4	0.91	0.17	55,57,58,68	0
2	ZN	C	307	1/1	0.92	0.11	140,140,140,140	0
2	ZN	B	301	1/1	0.93	0.16	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	D	303	1/1	0.96	0.07	98,98,98,98	0
6	NA	D	308	1/1	0.97	0.35	74,74,74,74	0
2	ZN	D	301	1/1	0.99	0.12	70,70,70,70	0
3	CL	A	305	1/1	0.99	0.12	64,64,64,64	0
3	CL	A	306	1/1	0.99	0.06	76,76,76,76	0
3	CL	A	307	1/1	0.99	0.09	78,78,78,78	0
3	CL	C	305	1/1	0.99	0.10	78,78,78,78	0
3	CL	D	306	1/1	0.99	0.08	91,91,91,91	0
3	CL	E	303	1/1	0.99	0.08	69,69,69,69	0
3	CL	E	304	1/1	0.99	0.12	66,66,66,66	0
2	ZN	D	302	1/1	0.99	0.08	77,77,77,77	0
2	ZN	A	302	1/1	0.99	0.13	77,77,77,77	0
2	ZN	A	303	1/1	0.99	0.07	68,68,68,68	0
2	ZN	E	301	1/1	0.99	0.08	58,58,58,58	0
2	ZN	E	302	1/1	0.99	0.16	54,54,54,54	0
3	CL	C	306	1/1	1.00	0.11	86,86,86,86	0
3	CL	D	305	1/1	1.00	0.09	84,84,84,84	0
2	ZN	A	304	1/1	1.00	0.08	66,66,66,66	0
3	CL	D	307	1/1	1.00	0.13	80,80,80,80	0
2	ZN	A	301	1/1	1.00	0.13	61,61,61,61	0
2	ZN	B	302	1/1	1.00	0.12	56,56,56,56	0
2	ZN	C	301	1/1	1.00	0.16	60,60,60,60	0
2	ZN	C	302	1/1	1.00	0.14	73,73,73,73	0
3	CL	B	303	1/1	1.00	0.12	86,86,86,86	0
3	CL	C	304	1/1	1.00	0.17	63,63,63,63	0
2	ZN	C	303	1/1	1.00	0.12	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.