Full wwPDB X-ray Structure Validation Report (i)

Mar 17, 2022 – 12:15 PM JST

PDB ID	:	6IVK
Title	:	Crystal structure of a membrane protein G175A
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:

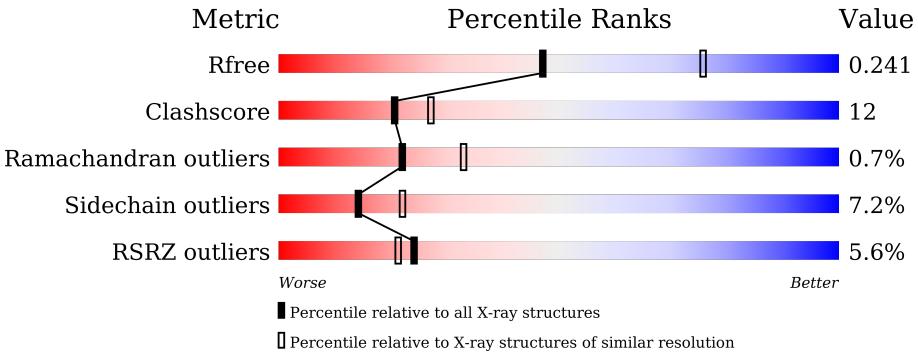
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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% 69% 18% • 10%
1	B	297	7% 67% 21% • 8%
1	C	297	7% 71% 17% • 9%
1	D	297	6% 69% 20% • 10%
1	E	297	2% 65% 24% • 9%

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
5	CL	C	305	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10934 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	268	Total	C	N	O	S	0	0	0
			2136	1384	361	382	9			
1	B	272	Total	C	N	O	S	0	0	0
			2168	1406	367	386	9			
1	C	270	Total	C	N	O	S	0	0	0
			2147	1389	365	384	9			
1	D	268	Total	C	N	O	S	0	0	0
			2136	1384	361	382	9			
1	E	271	Total	C	N	O	S	0	0	0
			2163	1402	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	175	ALA	GLY	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	175	ALA	GLY	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	175	ALA	GLY	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	175	ALA	GLY	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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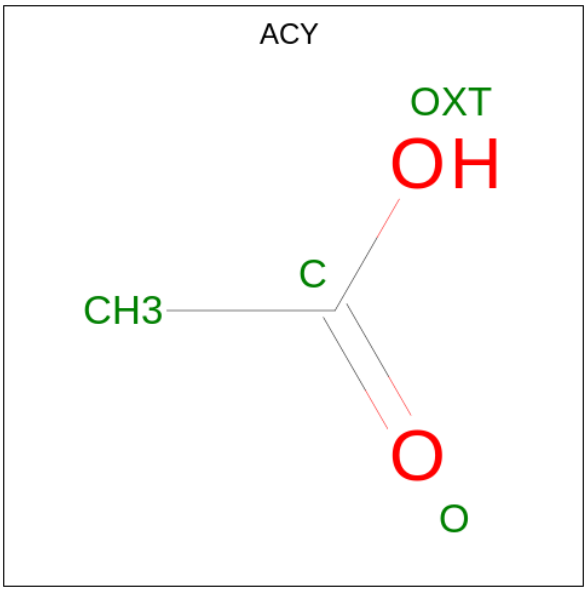
Chain	Residue	Modelled	Actual	Comment	Reference
E	175	ALA	GLY	engineered mutation	UNP W9BH30

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

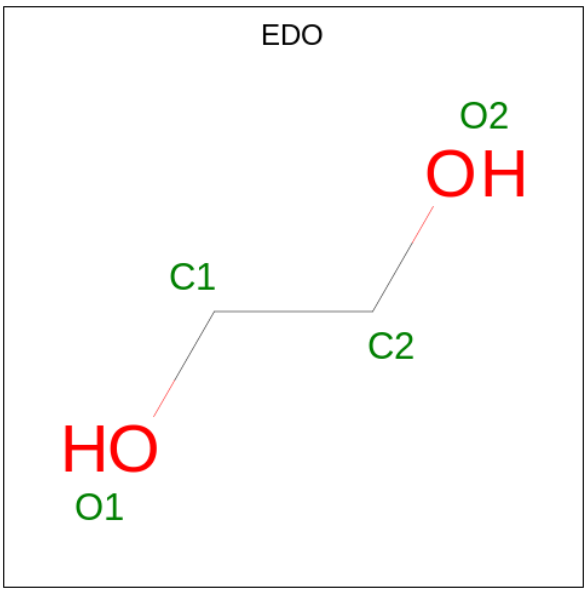
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Zn 4 4	0	0
2	B	2	Total Zn 2 2	0	0
2	C	4	Total Zn 4 4	0	0
2	D	4	Total Zn 4 4	0	0
2	E	2	Total Zn 2 2	0	0

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

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

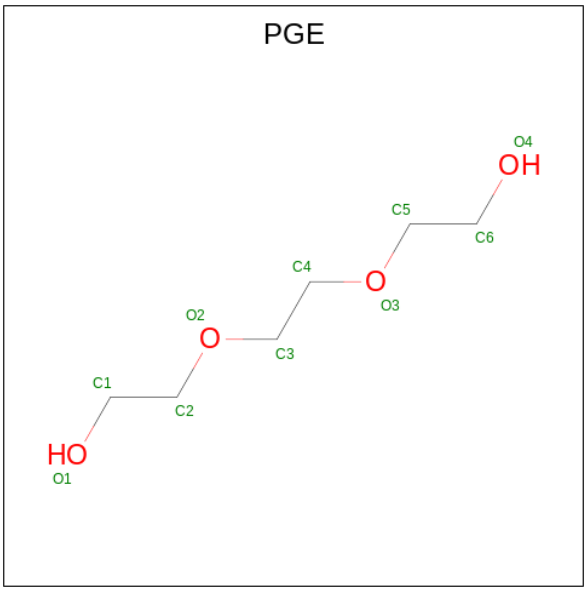


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0

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

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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O 10 6 4	0	0

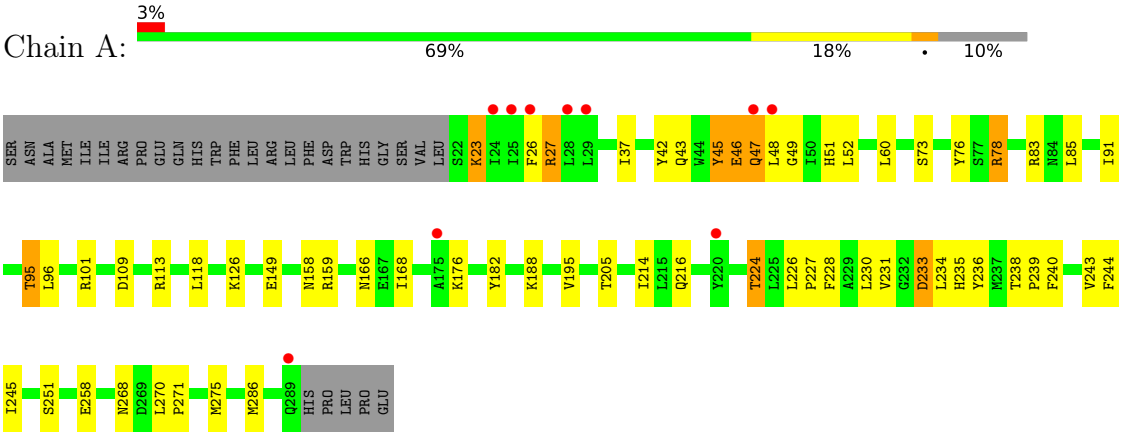
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	30	Total O 30 30	0	0
7	B	31	Total O 31 31	0	0
7	C	22	Total O 22 22	0	0
7	D	22	Total O 22 22	0	0
7	E	19	Total O 19 19	0	0

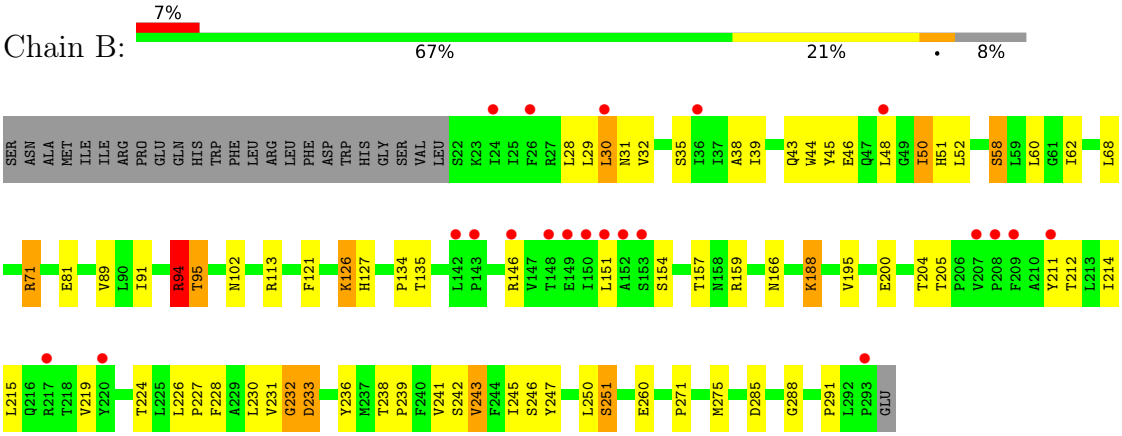
3 Residue-property plots (i)

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.

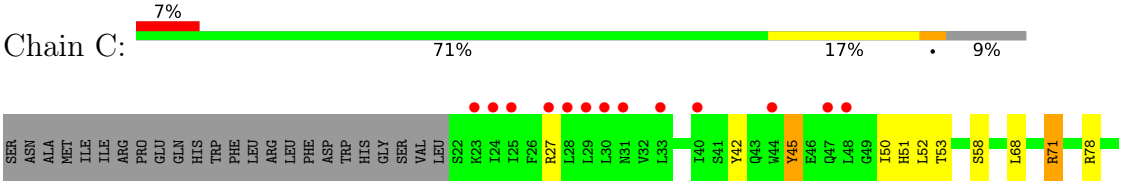
• Molecule 1: Ibestrophin

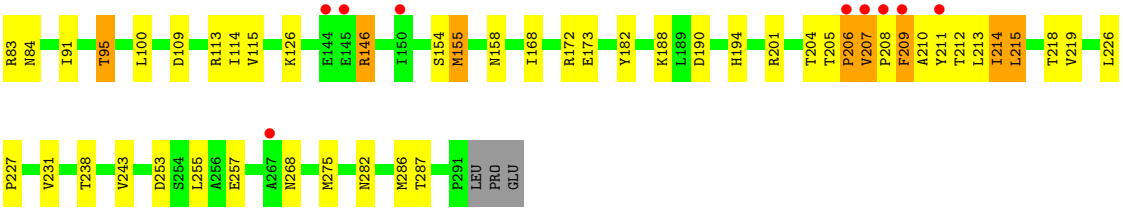


• Molecule 1: Ibestrophin

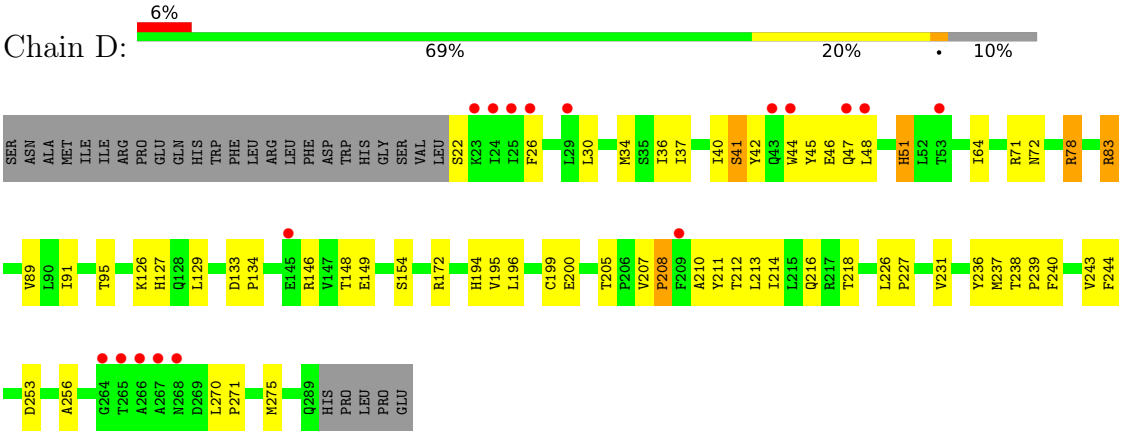


• Molecule 1: Ibestrophin

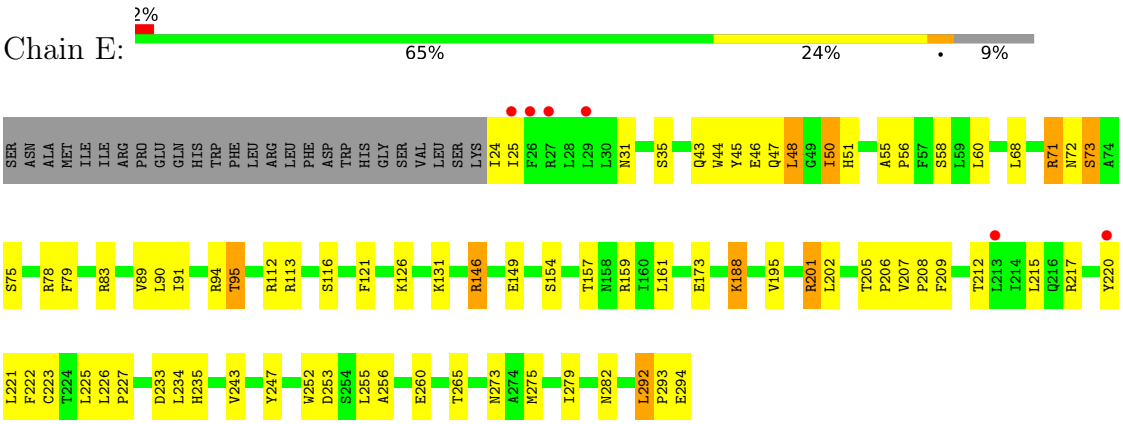




• Molecule 1: Ibestrophin



• 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	113.55Å 159.42Å 161.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.64 – 2.65 48.64 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.64-2.65) 100.0 (48.64-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.201 , 0.241 0.201 , 0.241	Depositor DCC
R_{free} test set	4277 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	65.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10934	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: CL, EDO, ZN, ACY, PGE

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	0.36	0/2182	0.74	1/2970 (0.0%)
1	B	0.36	0/2217	0.71	0/3020
1	C	0.35	0/2194	0.70	1/2988 (0.0%)
1	D	0.33	0/2182	0.65	1/2970 (0.0%)
1	E	0.37	0/2212	0.74	1/3013 (0.0%)
All	All	0.35	0/10987	0.71	4/14961 (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	B	0	3
1	C	0	2
1	E	0	2
All	All	0	7

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	D	78	ARG	CB-CA-C	6.20	122.81	110.40
1	E	201	ARG	CB-CA-C	5.70	121.81	110.40
1	C	206	PRO	C-N-CA	5.07	134.36	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	113	ARG	Sidechain
1	B	159	ARG	Sidechain
1	B	94	ARG	Sidechain
1	C	146	ARG	Sidechain
1	C	172	ARG	Sidechain
1	E	112	ARG	Sidechain
1	E	159	ARG	Sidechain

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	2136	0	2183	73	0
1	B	2168	0	2215	63	0
1	C	2147	0	2190	61	0
1	D	2136	0	2183	36	0
1	E	2163	0	2203	81	1
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	2	0	0	0	0
3	A	8	0	6	0	0
3	B	4	0	3	1	0
3	E	4	0	3	0	0
4	A	4	0	6	0	0
4	E	4	0	6	0	0
5	A	3	0	0	1	0
5	B	1	0	0	1	0
5	C	2	0	0	2	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
6	E	10	0	14	1	0
7	A	30	0	0	2	0
7	B	31	0	0	1	0
7	C	22	0	0	0	0
7	D	22	0	0	2	1
7	E	19	0	0	1	0
All	All	10934	0	11012	269	1

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 12.

All (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:C:207:VAL:HG22	1:C:208:PRO:CD	1.56	1.36
1:C:207:VAL:CG2	1:C:208:PRO:HD2	1.70	1.21
1:D:133:ASP:OD2	7:D:401:HOH:O	1.54	1.19
1:C:210:ALA:O	1:C:214:ILE:HG13	1.45	1.14
1:D:51:HIS:HB2	7:D:419:HOH:O	1.48	1.10
1:E:207:VAL:H	1:E:208:PRO:HD2	1.25	1.01
1:E:205:THR:HB	1:E:206:PRO:HA	1.39	1.01
1:E:207:VAL:N	1:E:208:PRO:HD2	1.77	1.00
1:A:83:ARG:CZ	1:E:205:THR:HG22	1.91	0.99
1:A:83:ARG:HH12	1:E:205:THR:CG2	1.75	0.98
1:A:83:ARG:NH1	1:E:205:THR:HG22	1.82	0.95
1:E:201:ARG:O	1:E:205:THR:HG23	1.67	0.94
1:A:83:ARG:NH1	1:E:205:THR:CG2	2.30	0.93
1:A:149:GLU:HG2	1:B:291:PRO:HG3	1.51	0.92
1:E:207:VAL:H	1:E:208:PRO:CD	1.82	0.90
1:A:49:GLY:HA3	1:B:236:TYR:CD2	2.07	0.90
1:E:44:TRP:O	1:E:48:LEU:HD13	1.73	0.88
1:E:207:VAL:N	1:E:208:PRO:CD	2.39	0.86
1:C:207:VAL:HG22	1:C:208:PRO:HD2	0.86	0.85
1:A:83:ARG:HH12	1:E:205:THR:HG21	1.38	0.85
1:A:83:ARG:NH2	1:E:205:THR:HG22	1.93	0.84
1:D:83:ARG:HG2	1:D:270:LEU:HD21	1.57	0.84
1:E:206:PRO:HB2	1:E:208:PRO:HD2	1.58	0.84
1:D:78:ARG:NH1	1:D:205:THR:O	2.11	0.83
1:A:27:ARG:HH21	1:A:27:ARG:CG	1.93	0.82
1:B:35:SER:OG	1:B:239:PRO:HA	1.82	0.80
1:C:210:ALA:O	1:C:214:ILE:CG1	2.30	0.80
1:C:214:ILE:O	1:C:218:THR:HB	1.82	0.79
1:B:28:LEU:HD22	1:B:243:VAL:HG22	1.66	0.77
1:C:155:MET:HG2	1:C:158:ASN:HB2	1.65	0.77
1:C:207:VAL:HG22	1:C:208:PRO:HD3	1.66	0.76
1:C:207:VAL:CG2	1:C:208:PRO:CD	2.46	0.76
1:B:271:PRO:HG2	1:B:275:MET:HE3	1.67	0.75
1:A:49:GLY:HA3	1:B:236:TYR:HD2	1.49	0.75
1:D:271:PRO:HD2	1:D:275:MET:HE1	1.69	0.74
1:C:42:TYR:O	1:C:45:TYR:HB2	1.87	0.74
1:E:94:ARG:HH21	1:E:282:ASN:HD21	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD12	1:A:228:PHE:HB3	1.72	0.72
1:E:205:THR:CB	1:E:206:PRO:HA	2.17	0.71
1:C:91:ILE:O	1:C:95:THR:HG23	1.91	0.70
1:A:52:LEU:CD1	1:A:228:PHE:HB3	2.21	0.70
1:B:29:LEU:C	1:B:31:ASN:H	1.94	0.70
1:E:60:LEU:HD23	1:E:222:PHE:HD1	1.57	0.69
1:C:68:LEU:HD21	1:C:215:LEU:HD12	1.75	0.69
1:E:226:LEU:N	1:E:227:PRO:HD2	2.08	0.68
1:A:168:ILE:HG22	1:A:182:TYR:CE1	2.28	0.68
1:A:49:GLY:CA	1:B:236:TYR:HD2	2.06	0.68
1:C:213:LEU:C	1:C:213:LEU:HD23	2.13	0.68
1:D:91:ILE:O	1:D:95:THR:HG23	1.95	0.67
1:E:91:ILE:O	1:E:95:THR:HG23	1.94	0.67
1:A:258:GLU:CD	1:A:268:ASN:HD22	1.98	0.67
1:C:214:ILE:O	1:C:218:THR:CB	2.43	0.67
1:B:91:ILE:O	1:B:95:THR:HG23	1.95	0.66
1:E:205:THR:HB	1:E:206:PRO:CA	2.21	0.66
1:A:27:ARG:HH21	1:A:27:ARG:HG3	1.61	0.65
1:C:190:ASP:OD1	5:C:305:CL:CL	2.53	0.64
1:E:292:LEU:HD22	1:E:293:PRO:HD2	1.80	0.63
1:B:71:ARG:HH22	1:B:212:THR:HG22	1.62	0.63
1:E:24:ILE:HG23	1:E:25:ILE:H	1.62	0.63
1:A:91:ILE:O	1:A:95:THR:HG23	1.97	0.63
1:B:44:TRP:O	1:B:48:LEU:HD12	1.99	0.63
1:A:109:ASP:HB3	1:A:113:ARG:HH12	1.64	0.61
1:C:213:LEU:CD2	1:E:247:TYR:OH	2.48	0.61
1:A:83:ARG:NH2	1:E:205:THR:CG2	2.62	0.61
1:E:72:ASN:HD22	1:E:256:ALA:HB2	1.66	0.60
1:D:226:LEU:N	1:D:227:PRO:HD2	2.16	0.60
1:D:30:LEU:O	1:D:34:MET:HG2	2.01	0.60
1:E:235:HIS:NE2	7:E:401:HOH:O	1.99	0.60
1:A:27:ARG:HH21	1:A:27:ARG:HG2	1.66	0.60
1:C:205:THR:HG23	1:C:205:THR:O	2.02	0.60
1:B:51:HIS:NE2	7:B:401:HOH:O	2.27	0.59
1:E:94:ARG:HH21	1:E:282:ASN:ND2	2.00	0.59
1:A:49:GLY:HA3	1:B:236:TYR:CE2	2.38	0.59
1:A:83:ARG:HH22	1:E:205:THR:CG2	2.16	0.58
1:B:231:VAL:HG13	1:B:232:GLY:N	2.18	0.58
1:B:71:ARG:HH12	1:B:212:THR:HG23	1.68	0.58
1:A:46:GLU:O	1:A:46:GLU:HG3	2.03	0.58
1:B:39:ILE:HD13	1:B:236:TYR:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:HIS:HA	1:E:91:ILE:HD13	1.86	0.57
1:E:75:SER:OG	1:E:260:GLU:HG3	2.03	0.57
1:C:207:VAL:HG23	1:E:79:PHE:CE2	2.39	0.57
1:E:207:VAL:HG23	1:E:208:PRO:HD3	1.87	0.57
1:A:76:TYR:CE1	1:E:207:VAL:HG21	2.39	0.56
1:C:226:LEU:N	1:C:227:PRO:HD2	2.19	0.56
1:E:90:LEU:HD13	1:E:279:ILE:HD13	1.87	0.56
1:A:96:LEU:HD23	1:A:118:LEU:HD11	1.87	0.56
1:A:42:TYR:O	1:A:45:TYR:HB2	2.05	0.56
1:B:200:GLU:O	1:B:204:THR:HG23	2.06	0.56
1:E:73:SER:HA	6:E:305:PGE:H52	1.88	0.56
1:C:68:LEU:CD2	1:C:215:LEU:HD12	2.36	0.55
1:A:230:LEU:HB3	1:A:234:LEU:HD12	1.87	0.55
1:D:37:ILE:O	1:D:41:SER:HB3	2.06	0.55
1:A:42:TYR:HA	1:A:45:TYR:CD1	2.41	0.55
1:B:29:LEU:C	1:B:31:ASN:N	2.60	0.55
1:B:215:LEU:O	1:B:219:VAL:HG23	2.07	0.55
1:C:207:VAL:CB	1:C:208:PRO:HD2	2.33	0.55
1:A:83:ARG:NH1	1:E:205:THR:HG21	2.09	0.54
1:C:208:PRO:O	1:C:210:ALA:N	2.35	0.54
1:D:236:TYR:O	1:D:239:PRO:HD2	2.08	0.54
1:C:215:LEU:O	1:C:219:VAL:HG23	2.07	0.54
1:B:60:LEU:HD21	1:D:244:PHE:CE2	2.43	0.54
1:C:78:ARG:HH12	1:C:205:THR:CG2	2.21	0.54
1:D:83:ARG:HG2	1:D:270:LEU:CD2	2.35	0.54
1:C:78:ARG:HH12	1:C:205:THR:HG23	1.73	0.54
1:E:71:ARG:HH12	1:E:212:THR:HG23	1.74	0.53
1:A:47:GLN:HE21	1:A:47:GLN:HA	1.74	0.53
1:E:94:ARG:HE	1:E:282:ASN:HD22	1.57	0.53
1:C:42:TYR:HA	1:C:45:TYR:CD1	2.44	0.53
1:C:68:LEU:CD2	1:C:215:LEU:CD1	2.87	0.53
1:D:240:PHE:O	1:D:243:VAL:HG12	2.09	0.53
1:B:246:SER:O	1:B:250:LEU:HD12	2.10	0.52
1:B:29:LEU:HA	1:B:32:VAL:HG23	1.91	0.52
1:B:227:PRO:HA	1:B:230:LEU:HB2	1.90	0.52
1:A:78:ARG:NH1	1:A:205:THR:O	2.42	0.52
1:A:101:ARG:HD2	1:A:286:MET:O	2.09	0.52
1:B:231:VAL:HG13	1:B:232:GLY:H	1.72	0.52
1:B:224:THR:O	1:B:227:PRO:HD2	2.09	0.52
1:A:258:GLU:OE1	1:A:268:ASN:ND2	2.43	0.52
1:A:42:TYR:CE2	1:A:235:HIS:CE1	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:LEU:N	1:E:227:PRO:CD	2.73	0.52
1:B:29:LEU:O	1:B:31:ASN:N	2.43	0.52
1:E:48:LEU:CD1	1:E:48:LEU:N	2.73	0.52
1:A:236:TYR:CB	1:E:50:ILE:HG22	2.39	0.52
1:D:196:LEU:O	1:D:200:GLU:HG3	2.10	0.51
1:A:76:TYR:HE1	1:E:207:VAL:HG21	1.75	0.51
1:A:236:TYR:HB3	1:E:50:ILE:HG22	1.92	0.51
1:D:36:ILE:HG13	1:D:37:ILE:N	2.26	0.51
1:C:83:ARG:HG2	1:D:205:THR:HG21	1.91	0.50
1:B:89:VAL:CG2	1:B:195:VAL:HG11	2.41	0.50
1:B:271:PRO:CG	1:B:275:MET:HE3	2.41	0.50
1:C:205:THR:OG1	1:E:83:ARG:HD3	2.11	0.50
1:C:68:LEU:HG	1:C:215:LEU:HD11	1.94	0.50
1:E:24:ILE:HG23	1:E:25:ILE:N	2.25	0.50
1:A:95:THR:HG21	5:A:308:CL:CL	2.48	0.50
1:B:231:VAL:O	1:B:233:ASP:N	2.45	0.49
1:E:78:ARG:NH2	1:E:205:THR:OG1	2.42	0.49
1:A:76:TYR:HE1	1:E:207:VAL:CG2	2.25	0.49
1:B:39:ILE:CD1	1:B:236:TYR:HA	2.42	0.49
1:B:71:ARG:HG3	1:B:215:LEU:HD12	1.94	0.49
1:D:231:VAL:HA	1:D:238:THR:OG1	2.12	0.49
1:E:71:ARG:HD3	1:E:260:GLU:OE2	2.13	0.48
1:D:71:ARG:HD2	1:D:71:ARG:C	2.34	0.48
1:E:47:GLN:OE1	1:E:47:GLN:HA	2.14	0.48
1:A:23:LYS:O	1:A:23:LYS:HD3	2.14	0.48
1:C:78:ARG:NH1	1:C:205:THR:HG23	2.28	0.48
1:A:258:GLU:CD	1:A:268:ASN:ND2	2.66	0.48
1:C:50:ILE:O	1:C:50:ILE:HG13	2.14	0.48
1:A:224:THR:O	1:A:227:PRO:HD2	2.13	0.48
1:B:236:TYR:C	1:B:238:THR:H	2.18	0.48
1:B:135:THR:HG23	1:B:151:LEU:HD11	1.96	0.47
1:B:204:THR:OG1	1:B:205:THR:N	2.47	0.47
1:A:43:GLN:C	1:A:45:TYR:H	2.17	0.47
1:E:146:ARG:NH2	1:E:149:GLU:OE2	2.48	0.47
1:A:271:PRO:O	1:A:275:MET:HG3	2.15	0.47
1:E:31:ASN:ND2	1:E:223:CYS:O	2.47	0.47
1:C:205:THR:OG1	1:E:83:ARG:CD	2.63	0.47
1:E:94:ARG:HE	1:E:282:ASN:ND2	2.12	0.47
1:C:115:VAL:HG21	1:C:287:THR:HG21	1.97	0.47
1:A:226:LEU:N	1:A:227:PRO:HD2	2.31	0.46
1:E:126:LYS:HE3	1:E:273:ASN:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ARG:NH1	1:E:212:THR:HG23	2.30	0.46
1:E:233:ASP:C	1:E:234:LEU:HD23	2.36	0.46
1:B:45:TYR:HB3	1:B:50:ILE:O	2.16	0.46
1:B:127:HIS:CD2	1:B:134:PRO:HA	2.51	0.46
1:B:146:ARG:HA	1:B:146:ARG:HD3	1.78	0.46
1:E:55:ALA:N	1:E:56:PRO:HD2	2.30	0.46
1:A:231:VAL:C	1:A:233:ASP:H	2.19	0.46
1:A:42:TYR:HE2	1:A:235:HIS:CE1	2.32	0.46
1:B:226:LEU:N	1:B:227:PRO:CD	2.79	0.46
1:D:64:ILE:HD11	1:D:218:THR:HG22	1.97	0.45
1:A:23:LYS:O	1:A:26:PHE:HB3	2.16	0.45
1:A:46:GLU:HB2	1:A:51:HIS:NE2	2.31	0.45
1:A:188:LYS:HA	1:A:188:LYS:HD3	1.63	0.45
1:A:27:ARG:HG3	1:A:27:ARG:NH2	2.27	0.45
1:A:27:ARG:CG	1:A:27:ARG:NH2	2.63	0.45
1:D:89:VAL:CG2	1:D:195:VAL:HG11	2.47	0.45
1:C:213:LEU:HD23	1:E:247:TYR:OH	2.17	0.45
1:D:89:VAL:HG23	1:D:195:VAL:HG11	1.99	0.45
1:C:213:LEU:HD21	1:E:247:TYR:OH	2.16	0.45
1:E:217:ARG:HA	1:E:220:TYR:HB2	1.99	0.45
1:A:83:ARG:HH22	1:E:205:THR:HG23	1.81	0.44
1:D:212:THR:HG23	1:D:216:GLN:HG3	1.99	0.44
1:A:60:LEU:HD13	1:B:245:ILE:HG12	1.99	0.44
1:B:43:GLN:O	1:B:46:GLU:HB2	2.17	0.44
1:A:109:ASP:HB3	1:A:113:ARG:NH1	2.31	0.44
1:C:27:ARG:HD2	1:C:27:ARG:HA	1.88	0.44
1:D:71:ARG:NH2	1:D:253:ASP:OD1	2.50	0.44
1:A:83:ARG:HG3	1:A:270:LEU:HD21	1.98	0.44
1:A:49:GLY:C	1:B:236:TYR:HD2	2.20	0.44
1:A:235:HIS:ND1	7:A:401:HOH:O	2.36	0.44
1:B:52:LEU:HD11	1:D:237:MET:HE2	1.99	0.44
1:D:129:LEU:HD21	1:D:199:CYS:HB3	2.00	0.44
1:B:29:LEU:O	1:B:32:VAL:N	2.49	0.44
1:B:247:TYR:O	1:B:251:SER:HB2	2.18	0.44
1:B:28:LEU:HD23	1:B:28:LEU:HA	1.79	0.44
5:C:305:CL:CL	1:E:188:LYS:HE2	2.55	0.44
1:B:58:SER:O	1:B:62:ILE:HG13	2.17	0.44
1:B:188:LYS:HE2	5:B:304:CL:CL	2.54	0.44
1:D:226:LEU:N	1:D:227:PRO:CD	2.79	0.44
1:C:211:TYR:CE1	1:E:255:LEU:HD21	2.53	0.43
1:A:91:ILE:O	1:A:95:THR:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:VAL:O	1:D:208:PRO:C	2.56	0.43
1:B:288:GLY:HA3	3:B:303:ACY:H2	2.00	0.43
1:C:45:TYR:OH	1:C:52:LEU:HD12	2.18	0.43
1:C:71:ARG:NH2	1:C:253:ASP:OD1	2.51	0.43
1:E:68:LEU:HB3	1:E:252:TRP:HD1	1.83	0.43
1:C:282:ASN:O	1:C:286:MET:HG3	2.17	0.43
1:E:95:THR:OG1	1:E:188:LYS:HD2	2.18	0.43
1:E:161:LEU:HD23	1:E:161:LEU:HA	1.84	0.43
1:A:168:ILE:HG22	1:A:182:TYR:CD1	2.54	0.43
1:E:90:LEU:HD12	1:E:94:ARG:CZ	2.49	0.43
1:C:109:ASP:HB3	1:C:113:ARG:HH12	1.83	0.43
1:C:210:ALA:O	1:C:214:ILE:CD1	2.66	0.43
1:C:213:LEU:HD22	1:C:214:ILE:HG12	2.01	0.43
1:D:78:ARG:HD2	1:D:207:VAL:HG23	2.00	0.43
1:A:48:LEU:O	1:B:236:TYR:CE2	2.72	0.43
1:C:205:THR:O	1:C:205:THR:CG2	2.65	0.43
1:E:60:LEU:HD23	1:E:222:PHE:CD1	2.46	0.43
1:B:38:ALA:HB2	1:B:228:PHE:HD1	1.83	0.43
1:E:45:TYR:HB2	1:E:50:ILE:HD11	2.01	0.43
1:B:45:TYR:CE1	1:B:50:ILE:HD11	2.54	0.42
1:C:188:LYS:HA	1:C:188:LYS:HD3	1.89	0.42
1:E:71:ARG:NH2	1:E:253:ASP:OD1	2.52	0.42
1:A:235:HIS:HB3	7:A:401:HOH:O	2.19	0.42
1:D:127:HIS:CD2	1:D:134:PRO:HA	2.54	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	2.20	0.42
1:C:83:ARG:NE	1:C:275:MET:HE2	2.34	0.42
1:E:45:TYR:O	1:E:50:ILE:HG12	2.19	0.42
1:B:71:ARG:NH1	1:B:260:GLU:OE2	2.53	0.42
1:C:204:THR:C	1:C:206:PRO:HD3	2.40	0.42
1:A:83:ARG:CZ	1:E:205:THR:CG2	2.73	0.42
1:C:201:ARG:O	1:C:205:THR:HB	2.20	0.42
1:C:255:LEU:HD21	1:D:211:TYR:CE1	2.54	0.42
1:E:113:ARG:O	1:E:116:SER:HB2	2.20	0.42
1:B:238:THR:N	1:B:239:PRO:HD2	2.34	0.42
1:C:231:VAL:HA	1:C:238:THR:OG1	2.20	0.42
1:A:158:ASN:ND2	1:B:94:ARG:HG2	2.34	0.42
1:C:91:ILE:HD13	1:D:194:HIS:HA	2.00	0.42
1:C:207:VAL:HG23	1:E:79:PHE:CZ	2.55	0.42
1:E:121:PHE:CE1	1:E:157:THR:HG22	2.55	0.42
1:A:166:ASN:ND2	1:B:102:ASN:HD22	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ASN:HD22	1:B:166:ASN:HA	1.70	0.41
1:A:48:LEU:O	1:B:236:TYR:CD2	2.73	0.41
1:C:210:ALA:HB3	1:E:255:LEU:HD13	2.02	0.41
1:D:146:ARG:NH1	1:D:149:GLU:OE1	2.53	0.41
1:A:239:PRO:HG2	1:A:240:PHE:HD1	1.85	0.41
1:C:168:ILE:HG13	1:C:182:TYR:CE2	2.55	0.41
1:E:146:ARG:HA	1:E:146:ARG:HH21	1.85	0.41
1:C:209:PHE:HD1	1:C:209:PHE:HA	1.65	0.41
1:A:244:PHE:CE1	1:E:221:LEU:HD23	2.56	0.41
1:A:214:ILE:HD13	1:B:251:SER:HB3	2.03	0.41
1:D:210:ALA:HA	1:D:213:LEU:HB3	2.03	0.41
1:A:85:LEU:HD22	1:A:195:VAL:HA	2.02	0.41
1:A:239:PRO:HG2	1:A:240:PHE:CD1	2.55	0.41
1:C:100:LEU:HD11	1:C:114:ILE:HD13	2.03	0.41
1:C:213:LEU:C	1:C:213:LEU:CD2	2.85	0.41
1:A:238:THR:N	1:A:239:PRO:HD2	2.36	0.41
1:B:121:PHE:CE1	1:B:157:THR:HG22	2.56	0.41
1:A:245:ILE:HG12	1:E:60:LEU:HD13	2.03	0.40
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.94	0.40
1:B:126:LYS:HE2	1:B:126:LYS:HB3	1.79	0.40
1:C:91:ILE:O	1:C:95:THR:CG2	2.65	0.40
1:C:226:LEU:N	1:C:227:PRO:CD	2.83	0.40
1:E:206:PRO:CB	1:E:208:PRO:HD2	2.41	0.40
1:D:42:TYR:O	1:D:45:TYR:HB2	2.21	0.40
1:D:212:THR:O	1:D:216:GLN:HB2	2.21	0.40
1:E:89:VAL:CG2	1:E:195:VAL:HG11	2.51	0.40
1:D:72:ASN:ND2	1:D:256:ALA:HB2	2.37	0.40

All (1) 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:51:HIS:NE2	7:D:401:HOH:O[2_554]	2.19	0.01

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	266/297 (90%)	253 (95%)	13 (5%)	0	100	100
1	B	270/297 (91%)	245 (91%)	21 (8%)	4 (2%)	10	15
1	C	268/297 (90%)	259 (97%)	7 (3%)	2 (1%)	22	33
1	D	266/297 (90%)	257 (97%)	7 (3%)	2 (1%)	19	29
1	E	269/297 (91%)	260 (97%)	7 (3%)	2 (1%)	22	33
All	All	1339/1485 (90%)	1274 (95%)	55 (4%)	10 (1%)	22	33

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	207	VAL
1	B	30	LEU
1	B	232	GLY
1	E	209	PHE
1	E	43	GLN
1	B	285	ASP
1	C	154	SER
1	D	208	PRO
1	D	214	ILE
1	B	214	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	233/260 (90%)	217 (93%)	16 (7%)	15	24
1	B	237/260 (91%)	222 (94%)	15 (6%)	18	28
1	C	234/260 (90%)	216 (92%)	18 (8%)	13	20
1	D	233/260 (90%)	219 (94%)	14 (6%)	19	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	236/260 (91%)	215 (91%)	21 (9%)	9 14
All	All	1173/1300 (90%)	1089 (93%)	84 (7%)	14 22

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	27	ARG
1	A	37	ILE
1	A	45	TYR
1	A	46	GLU
1	A	47	GLN
1	A	73	SER
1	A	95	THR
1	A	126	LYS
1	A	159	ARG
1	A	176	LYS
1	A	216	GLN
1	A	224	THR
1	A	233	ASP
1	A	243	VAL
1	A	251	SER
1	B	30	LEU
1	B	50	ILE
1	B	58	SER
1	B	71	ARG
1	B	81	GLU
1	B	94	ARG
1	B	95	THR
1	B	126	LYS
1	B	154	SER
1	B	188	LYS
1	B	211	TYR
1	B	233	ASP
1	B	242	SER
1	B	243	VAL
1	B	251	SER
1	C	45	TYR
1	C	51	HIS
1	C	53	THR
1	C	58	SER
1	C	71	ARG

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Mol	Chain	Res	Type
1	C	84	ASN
1	C	95	THR
1	C	126	LYS
1	C	146	ARG
1	C	155	MET
1	C	173	GLU
1	C	209	PHE
1	C	212	THR
1	C	214	ILE
1	C	215	LEU
1	C	243	VAL
1	C	257	GLU
1	C	268	ASN
1	D	22	SER
1	D	26	PHE
1	D	40	ILE
1	D	41	SER
1	D	44	TRP
1	D	46	GLU
1	D	47	GLN
1	D	48	LEU
1	D	51	HIS
1	D	83	ARG
1	D	126	LYS
1	D	148	THR
1	D	154	SER
1	D	172	ARG
1	E	35	SER
1	E	46	GLU
1	E	48	LEU
1	E	50	ILE
1	E	58	SER
1	E	71	ARG
1	E	73	SER
1	E	95	THR
1	E	131	LYS
1	E	146	ARG
1	E	154	SER
1	E	173	GLU
1	E	188	LYS
1	E	202	LEU
1	E	215	LEU

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Mol	Chain	Res	Type
1	E	225	LEU
1	E	243	VAL
1	E	265	THR
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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	158	ASN
1	A	166	ASN
1	A	216	GLN
1	A	235	HIS
1	A	268	ASN
1	B	166	ASN
1	C	128	GLN
1	D	47	GLN
1	D	72	ASN
1	D	166	ASN
1	E	72	ASN
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 33 ligands modelled in this entry, 26 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ACY	B	303	2	1,3,3	5.17	1 (100%)	0,3,3	-	-
3	ACY	E	303	2	1,3,3	6.50	1 (100%)	0,3,3	-	-
6	PGE	E	305	-	9,9,9	0.72	0	8,8,8	0.78	0
4	EDO	A	307	-	3,3,3	0.58	0	2,2,2	0.18	0
3	ACY	A	306	-	1,3,3	2.73	1 (100%)	0,3,3	-	-
3	ACY	A	305	2	1,3,3	2.23	1 (100%)	0,3,3	-	-
4	EDO	E	304	-	3,3,3	1.02	0	2,2,2	0.64	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
6	PGE	E	305	-	-	5/7/7/7	-
4	EDO	A	307	-	-	1/1/1/1	-
4	EDO	E	304	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	303	ACY	CH3-C	6.50	1.57	1.48
3	B	303	ACY	CH3-C	5.17	1.55	1.48
3	A	306	ACY	CH3-C	2.73	1.52	1.48
3	A	305	ACY	CH3-C	2.23	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	305	PGE	O2-C3-C4-O3
4	E	304	EDO	O1-C1-C2-O2
6	E	305	PGE	O3-C5-C6-O4
6	E	305	PGE	O1-C1-C2-O2
4	A	307	EDO	O1-C1-C2-O2
6	E	305	PGE	C4-C3-O2-C2
6	E	305	PGE	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	ACY	1	0
6	E	305	PGE	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	268/297 (90%)	-0.14	10 (3%)	41	38	37, 57, 116, 165	0
1	B	272/297 (91%)	0.02	21 (7%)	13	10	37, 65, 122, 160	0
1	C	270/297 (90%)	0.04	22 (8%)	12	9	37, 61, 135, 175	0
1	D	268/297 (90%)	-0.04	17 (6%)	20	17	41, 71, 122, 145	0
1	E	271/297 (91%)	-0.10	6 (2%)	62	57	36, 59, 114, 146	0
All	All	1349/1485 (90%)	-0.04	76 (5%)	24	21	36, 63, 124, 175	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	26	PHE	6.6
1	A	25	ILE	6.0
1	A	29	LEU	5.3
1	A	26	PHE	5.2
1	D	48	LEU	5.1
1	B	211	TYR	5.0
1	E	25	ILE	4.8
1	A	289	GLN	4.8
1	B	150	ILE	4.8
1	D	26	PHE	4.6
1	C	48	LEU	4.5
1	C	209	PHE	4.4
1	D	268	ASN	4.3
1	C	47	GLN	4.3
1	A	24	ILE	4.2
1	D	47	GLN	4.2
1	E	29	LEU	4.2
1	B	220	TYR	3.7
1	B	207	VAL	3.7
1	B	26	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	207	VAL	3.6
1	D	44	TRP	3.5
1	C	30	LEU	3.3
1	B	24	ILE	3.3
1	B	217	ARG	3.3
1	C	44	TRP	3.3
1	D	25	ILE	3.2
1	B	209	PHE	3.2
1	B	153	SER	3.2
1	D	209	PHE	3.1
1	D	267	ALA	3.1
1	B	148	THR	3.0
1	C	211	TYR	3.0
1	A	28	LEU	3.0
1	A	175	ALA	3.0
1	E	27	ARG	3.0
1	A	47	GLN	2.9
1	D	264	GLY	2.9
1	E	213	LEU	2.9
1	B	152	ALA	2.9
1	B	146	ARG	2.8
1	B	293	PRO	2.8
1	C	40	ILE	2.8
1	D	265	THR	2.8
1	E	220	TYR	2.8
1	B	36	ILE	2.8
1	C	23	LYS	2.8
1	C	145	GLU	2.7
1	C	27	ARG	2.7
1	D	24	ILE	2.7
1	C	206	PRO	2.6
1	C	267	ALA	2.6
1	B	143	PRO	2.5
1	D	43	GLN	2.5
1	C	33	LEU	2.4
1	D	23	LYS	2.4
1	B	208	PRO	2.4
1	C	29	LEU	2.4
1	B	48	LEU	2.3
1	C	25	ILE	2.3
1	C	208	PRO	2.2
1	C	150	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	149	GLU	2.2
1	A	48	LEU	2.2
1	B	30	LEU	2.2
1	D	266	ALA	2.1
1	D	145	GLU	2.1
1	D	29	LEU	2.1
1	B	151	LEU	2.1
1	C	24	ILE	2.1
1	A	220	TYR	2.1
1	D	53	THR	2.1
1	C	144	GLU	2.0
1	B	142	LEU	2.0
1	C	31	ASN	2.0
1	C	28	LEU	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
3	ACY	A	306	4/4	0.73	0.30	98,105,109,116	0
6	PGE	E	305	10/10	0.79	0.32	74,87,104,104	0
4	EDO	E	304	4/4	0.82	0.27	62,64,69,72	0
2	ZN	C	304	1/1	0.87	0.09	139,139,139,139	0
3	ACY	E	303	4/4	0.90	0.24	41,46,49,50	0
3	ACY	A	305	4/4	0.91	0.12	86,88,99,103	0
4	EDO	A	307	4/4	0.91	0.20	63,71,76,81	0
3	ACY	B	303	4/4	0.92	0.18	52,53,57,65	0
2	ZN	D	303	1/1	0.97	0.11	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	302	1/1	0.99	0.11	69,69,69,69	0
2	ZN	D	301	1/1	0.99	0.09	67,67,67,67	0
2	ZN	D	302	1/1	0.99	0.10	72,72,72,72	0
2	ZN	A	304	1/1	0.99	0.09	68,68,68,68	0
2	ZN	D	304	1/1	0.99	0.15	125,125,125,125	0
2	ZN	E	301	1/1	0.99	0.09	55,55,55,55	0
5	CL	A	309	1/1	0.99	0.08	73,73,73,73	0
5	CL	D	306	1/1	0.99	0.08	79,79,79,79	0
5	CL	E	306	1/1	0.99	0.10	65,65,65,65	0
5	CL	E	307	1/1	0.99	0.10	63,63,63,63	0
2	ZN	E	302	1/1	0.99	0.14	50,50,50,50	0
2	ZN	C	301	1/1	1.00	0.16	55,55,55,55	0
2	ZN	C	302	1/1	1.00	0.13	74,74,74,74	0
5	CL	A	308	1/1	1.00	0.12	62,62,62,62	0
2	ZN	C	303	1/1	1.00	0.12	58,58,58,58	0
5	CL	A	310	1/1	1.00	0.08	70,70,70,70	0
5	CL	B	304	1/1	1.00	0.11	81,81,81,81	0
5	CL	C	305	1/1	1.00	0.12	84,84,84,84	0
5	CL	C	306	1/1	1.00	0.16	57,57,57,57	0
5	CL	D	305	1/1	1.00	0.10	76,76,76,76	0
2	ZN	A	303	1/1	1.00	0.06	63,63,63,63	0
2	ZN	A	301	1/1	1.00	0.13	58,58,58,58	0
2	ZN	B	301	1/1	1.00	0.16	126,126,126,126	0
2	ZN	B	302	1/1	1.00	0.12	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.