



Full wwPDB X-ray Structure Validation Report i

Mar 17, 2022 – 12:13 PM JST

PDB ID : 6IVM
Title : Crystal structure of a membrane protein P143A
Authors : Kittredge, A.; Fukuda, F.; Zhang, Y.; Yang, T.
Deposited on : 2018-12-04
Resolution : 2.95 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

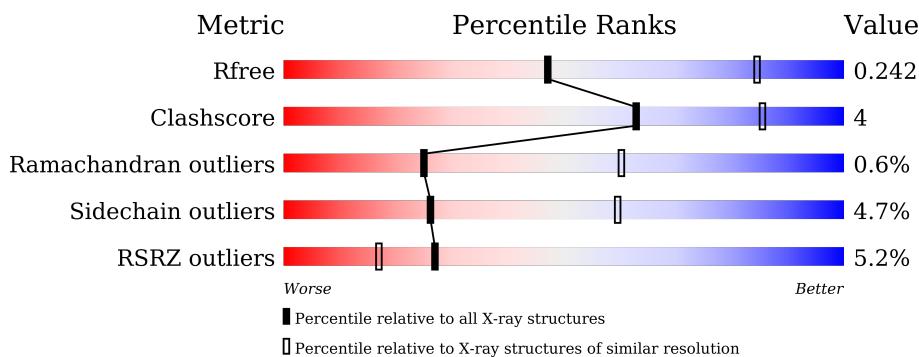
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 10888 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 Ibkestrophin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2151	1393	365	384	9			
1	B	270	Total	C	N	O	S	0	0	0
			2150	1392	365	384	9			
1	C	269	Total	C	N	O	S	0	0	0
			2144	1389	364	382	9			
1	D	269	Total	C	N	O	S	0	0	0
			2141	1387	362	383	9			
1	E	271	Total	C	N	O	S	0	0	0
			2160	1399	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	143	ALA	PRO	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	143	ALA	PRO	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	143	ALA	PRO	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	143	ALA	PRO	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	143	ALA	PRO	engineered mutation	UNP W9BH30

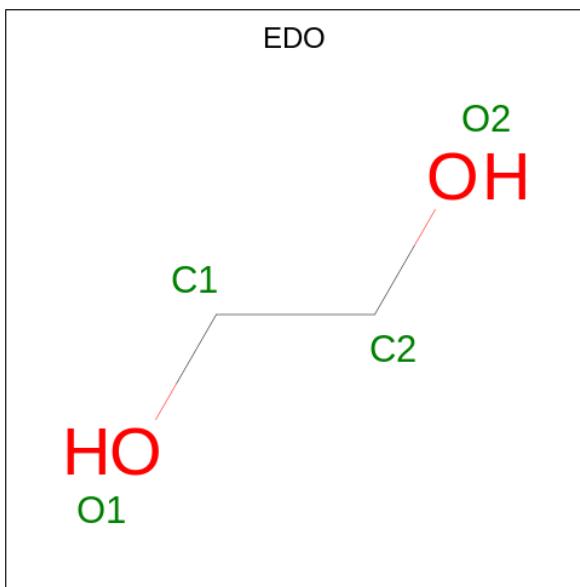
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

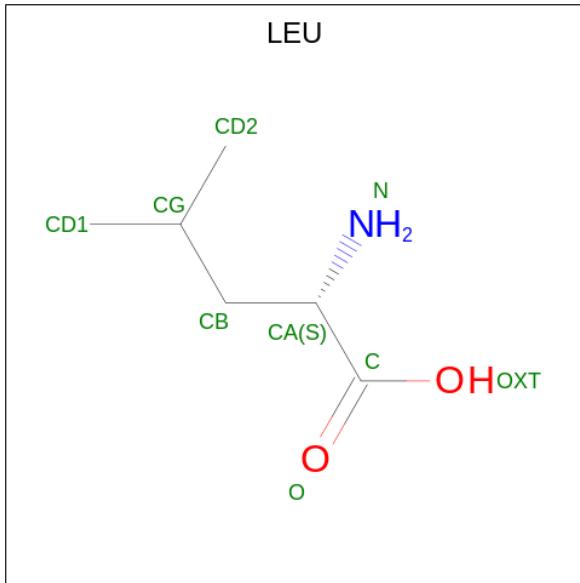
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3 3	0	0
3	B	1	Total Cl 1 1	0	0
3	C	2	Total Cl 2 2	0	0
3	D	3	Total Cl 3 3	0	0
3	E	3	Total Cl 3 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



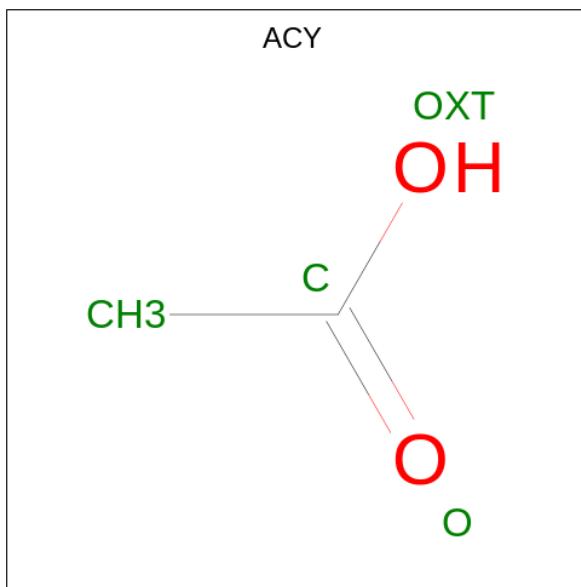
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is LEUCINE (three-letter code: LEU) (formula: C₆H₁₃NO₂).



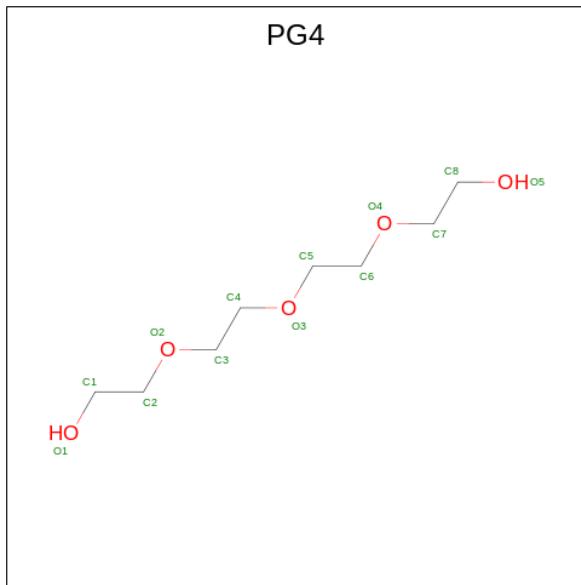
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 8 6 1 1	0	0

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

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

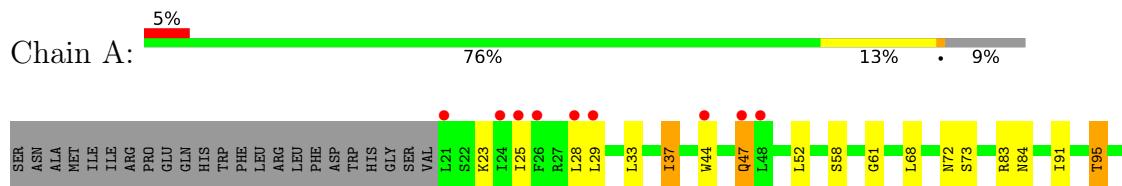
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	20	Total O 20 20	0	0
9	B	16	Total O 16 16	0	0
9	C	18	Total O 18 18	0	0
9	D	10	Total O 10 10	0	0
9	E	15	Total O 15 15	0	0

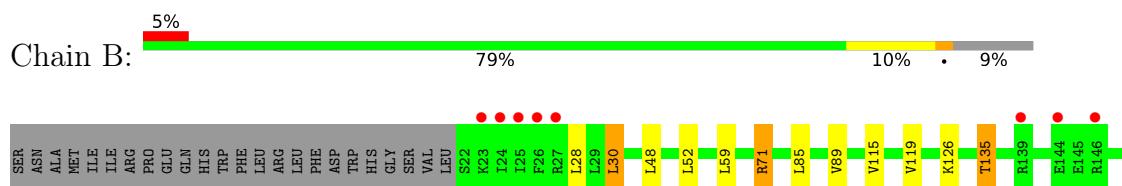
3 Residue-property plots

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.

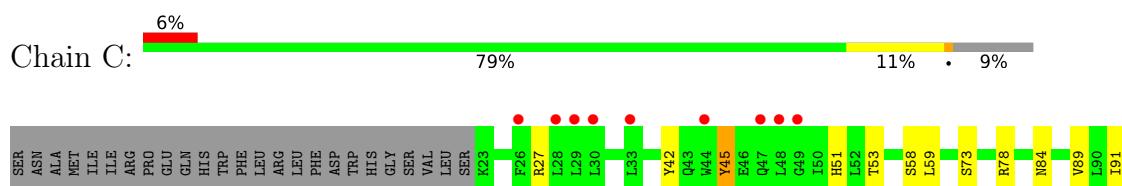
- Molecule 1: Ibvestrophin



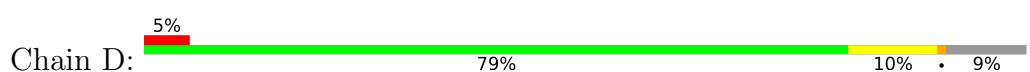
- Molecule 1: Ibvestrophin



- Molecule 1: Ibvestrophin

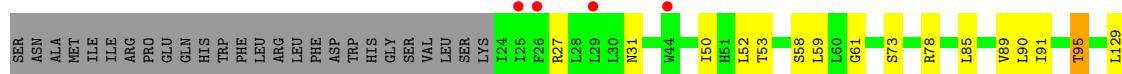
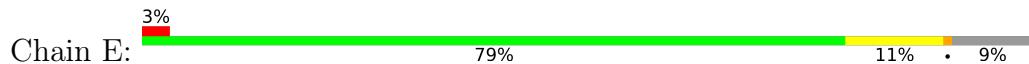


- Molecule 1: Ibvestrophin





- 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	113.97 Å 158.81 Å 161.68 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 2.95 48.01 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.72-2.95) 97.2 (48.01-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	2.04 (at 2.96 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R , R_{free}	0.208 , 0.243 0.208 , 0.242	Depositor DCC
R_{free} test set	2867 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10888	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ACY, ZN, PG4, CL, EDO

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	0.50	0/2197	0.70	0/2989
1	B	0.50	0/2197	0.73	1/2990 (0.0%)
1	C	0.47	0/2191	0.68	0/2982
1	D	0.47	0/2186	0.68	0/2974
1	E	0.50	0/2208	0.71	2/3006 (0.1%)
All	All	0.49	0/10979	0.70	3/14941 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	292	LEU	CA-CB-CG	6.15	129.45	115.30
1	B	30	LEU	CA-CB-CG	5.68	128.37	115.30
1	E	90	LEU	CA-CB-CG	5.24	127.35	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2151	0	2197	24	0
1	B	2150	0	2193	17	0
1	C	2144	0	2188	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2141	0	2190	17	0
1	E	2160	0	2199	33	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
4	A	4	0	6	0	0
5	B	8	0	10	1	0
6	B	4	0	3	0	0
6	C	4	0	3	1	0
7	C	13	0	18	1	0
8	D	1	0	0	0	0
9	A	20	0	0	0	0
9	B	16	0	0	0	0
9	C	18	0	0	0	0
9	D	10	0	0	0	0
9	E	15	0	0	0	0
All	All	10888	0	11007	93	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 4.

All (93) 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:A:83:ARG:HH22	1:E:205:THR:HG23	1.00	1.13
1:A:83:ARG:NH2	1:E:205:THR:HG23	1.77	0.98
1:A:83:ARG:HH22	1:E:205:THR:CG2	1.91	0.79
1:E:205:THR:HG22	1:E:206:PRO:HA	1.62	0.79
1:D:83:ARG:HG2	1:D:270:LEU:HD21	1.67	0.75
1:B:135:THR:HG23	1:B:151:LEU:HD11	1.75	0.69
1:E:205:THR:CG2	1:E:206:PRO:HA	2.24	0.67
1:B:234:LEU:HB2	1:B:238:THR:HG22	1.79	0.64
1:D:89:VAL:HG23	1:D:195:VAL:HG11	1.80	0.62
1:A:284:LEU:O	1:A:287:THR:O	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:NH2	1:E:205:THR:CG2	2.58	0.62
6:C:308:ACY:H3	1:E:281:ARG:HD3	1.82	0.61
1:A:91:ILE:O	1:A:95:THR:HG23	2.01	0.60
7:C:307:PG4:H61	1:E:73:SER:HA	1.82	0.60
1:E:130:ARG:HH12	1:E:267:ALA:HB3	1.65	0.60
1:C:115:VAL:HG21	1:C:287:THR:HG21	1.84	0.59
1:E:205:THR:CB	1:E:206:PRO:HA	2.33	0.59
1:B:71:ARG:NH1	1:B:260:GLU:OE2	2.36	0.58
1:A:28:LEU:HD21	1:A:247:TYR:HB2	1.84	0.58
1:E:78:ARG:HH12	1:E:205:THR:HG21	1.69	0.57
1:D:78:ARG:HD3	1:D:207:VAL:HG23	1.86	0.57
1:B:231:VAL:HA	1:B:238:THR:HG21	1.86	0.57
1:B:216:GLN:HG2	1:B:253:ASP:OD2	2.05	0.57
1:E:91:ILE:O	1:E:95:THR:HG23	2.04	0.57
1:C:78:ARG:HH12	1:C:205:THR:HG23	1.70	0.56
1:A:44:TRP:HA	1:A:47:GLN:HG3	1.88	0.55
1:D:72:ASN:ND2	1:D:256:ALA:HB2	2.22	0.55
1:A:212:THR:O	1:A:216:GLN:HB2	2.07	0.55
1:C:91:ILE:O	1:C:95:THR:HG23	2.07	0.54
1:D:129:LEU:HD21	1:D:199:CYS:HB3	1.90	0.54
1:E:50:ILE:O	1:E:50:ILE:HG13	2.10	0.51
1:A:52:LEU:CD1	1:A:228:PHE:HB3	2.42	0.50
1:C:135:THR:HG23	1:C:151:LEU:HD11	1.92	0.50
1:A:91:ILE:HD13	1:E:194:HIS:HA	1.93	0.50
1:C:146:ARG:HH11	1:C:146:ARG:HA	1.76	0.50
1:D:168:ILE:HG22	1:D:182:TYR:CD1	2.47	0.49
1:A:244:PHE:CE1	1:E:221:LEU:HD23	2.47	0.49
1:B:71:ARG:HH12	1:B:212:THR:CG2	2.24	0.49
1:A:170:GLN:HG3	5:B:301:LEU:HD11	1.94	0.49
1:C:42:TYR:O	1:C:45:TYR:HB2	2.12	0.49
1:D:89:VAL:CG2	1:D:195:VAL:HG11	2.43	0.49
1:D:91:ILE:O	1:D:95:THR:HG23	2.13	0.48
1:A:68:LEU:HD23	1:A:215:LEU:HD13	1.96	0.48
1:E:85:LEU:HD22	1:E:195:VAL:HA	1.96	0.48
1:E:31:ASN:ND2	1:E:223:CYS:O	2.42	0.48
1:C:78:ARG:HH12	1:C:205:THR:CG2	2.26	0.47
1:E:205:THR:HB	1:E:206:PRO:HA	1.97	0.47
1:A:236:TYR:HB2	1:E:50:ILE:HG22	1.98	0.46
1:C:230:LEU:HB3	1:C:234:LEU:HD12	1.96	0.46
1:A:33:LEU:O	1:A:37:ILE:HG23	2.15	0.46
1:E:135:THR:HG23	1:E:151:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:THR:HG22	1:E:206:PRO:CA	2.40	0.46
1:B:115:VAL:O	1:B:119:VAL:HG23	2.16	0.45
1:C:194:HIS:HA	1:E:91:ILE:HD13	1.98	0.45
1:B:28:LEU:HD22	1:B:243:VAL:HG22	1.99	0.45
1:E:145:GLU:HB3	1:E:146:ARG:HH21	1.81	0.45
1:E:52:LEU:HB3	1:E:229:ALA:HA	1.99	0.44
1:A:58:SER:HA	1:E:59:LEU:HD13	1.99	0.44
1:C:59:LEU:HD13	1:E:58:SER:HA	2.00	0.44
1:D:271:PRO:HD2	1:D:275:MET:HE3	1.99	0.44
1:B:71:ARG:HH12	1:B:212:THR:HG22	1.83	0.44
1:D:60:LEU:HD23	1:D:222:PHE:HD1	1.82	0.44
1:E:95:THR:OG1	1:E:188:LYS:HD2	2.18	0.44
1:A:83:ARG:HG2	1:A:270:LEU:HD21	2.00	0.44
1:A:188:LYS:HD3	1:A:188:LYS:HA	1.72	0.44
1:B:59:LEU:HD11	1:D:61:GLY:HA3	2.00	0.43
1:A:230:LEU:HB3	1:A:234:LEU:HD12	2.01	0.43
1:C:27:ARG:HH12	1:C:224:THR:HG23	1.84	0.43
1:D:71:ARG:NH2	1:D:253:ASP:OD1	2.48	0.43
1:A:258:GLU:HG2	1:A:268:ASN:HD22	1.84	0.43
1:C:129:LEU:HD21	1:C:199:CYS:HB3	2.00	0.42
1:B:85:LEU:HB3	1:B:195:VAL:HG13	2.01	0.42
1:B:85:LEU:HD22	1:B:195:VAL:HA	2.01	0.42
1:C:188:LYS:HA	1:C:188:LYS:HD3	1.93	0.42
1:D:230:LEU:HB3	1:D:234:LEU:HD12	2.01	0.42
1:B:227:PRO:HA	1:B:230:LEU:HB2	2.00	0.42
1:C:226:LEU:N	1:C:227:PRO:HD2	2.35	0.42
1:B:201:ARG:O	1:B:205:THR:HB	2.19	0.42
1:B:89:VAL:CG2	1:B:195:VAL:HG11	2.50	0.42
1:A:72:ASN:HD22	1:A:255:LEU:HD23	1.84	0.41
1:A:101:ARG:HD2	1:A:286:MET:O	2.20	0.41
1:D:168:ILE:HG22	1:D:182:TYR:CE1	2.55	0.41
1:E:130:ARG:NH1	1:E:267:ALA:HB3	2.35	0.41
1:B:208:PRO:HG2	1:D:259:LEU:HD21	2.02	0.41
1:A:61:GLY:HA3	1:E:59:LEU:HD11	2.03	0.41
1:E:156:PRO:O	1:E:160:ILE:HG13	2.21	0.41
1:E:89:VAL:HG23	1:E:195:VAL:HG11	2.03	0.41
1:C:59:LEU:HD11	1:E:61:GLY:HA3	2.03	0.40
1:D:27:ARG:HH11	1:D:30:LEU:HD22	1.86	0.40
1:B:52:LEU:HD11	1:D:237:MET:HE2	2.03	0.40
1:C:89:VAL:CG2	1:C:195:VAL:HG11	2.51	0.40
1:C:201:ARG:O	1:C:205:THR:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:LEU:HB3	1:E:263:PHE:HB3	2.04	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%)	257 (96%)	10 (4%)	1 (0%)	34 69
1	B	268/297 (90%)	252 (94%)	13 (5%)	3 (1%)	14 46
1	C	267/297 (90%)	258 (97%)	7 (3%)	2 (1%)	22 56
1	D	267/297 (90%)	258 (97%)	8 (3%)	1 (0%)	34 69
1	E	269/297 (91%)	259 (96%)	9 (3%)	1 (0%)	34 69
All	All	1339/1485 (90%)	1284 (96%)	47 (4%)	8 (1%)	25 60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	208	PRO
1	B	285	ASP
1	A	235	HIS
1	B	235	HIS
1	B	232	GLY
1	C	209	PHE
1	D	208	PRO
1	E	205	THR

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	234/259 (90%)	221 (94%)	13 (6%)	21 53
1	B	234/259 (90%)	220 (94%)	14 (6%)	19 50
1	C	233/259 (90%)	222 (95%)	11 (5%)	26 59
1	D	233/259 (90%)	224 (96%)	9 (4%)	32 65
1	E	235/259 (91%)	227 (97%)	8 (3%)	37 69
All	All	1169/1295 (90%)	1114 (95%)	55 (5%)	26 59

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	25	ILE
1	A	29	LEU
1	A	37	ILE
1	A	47	GLN
1	A	73	SER
1	A	84	ASN
1	A	95	THR
1	A	126	LYS
1	A	243	VAL
1	A	265	THR
1	A	282	ASN
1	A	289	GLN
1	B	30	LEU
1	B	48	LEU
1	B	71	ARG
1	B	126	LYS
1	B	135	THR
1	B	157	THR
1	B	172	ARG
1	B	188	LYS
1	B	207	VAL
1	B	211	TYR

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Mol	Chain	Res	Type
1	B	215	LEU
1	B	231	VAL
1	B	238	THR
1	B	243	VAL
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	126	LYS
1	C	146	ARG
1	C	157	THR
1	C	243	VAL
1	D	27	ARG
1	D	51	HIS
1	D	72	ASN
1	D	81	GLU
1	D	83	ARG
1	D	109	ASP
1	D	126	LYS
1	D	139	ARG
1	D	166	ASN
1	E	27	ARG
1	E	53	THR
1	E	95	THR
1	E	146	ARG
1	E	188	LYS
1	E	205	THR
1	E	207	VAL
1	E	243	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	268	ASN
1	B	166	ASN
1	B	216	GLN
1	C	166	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 35 ligands modelled in this entry, 30 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACY	C	308	-	1,3,3	5.21	1 (100%)	0,3,3	-	-
5	LEU	B	301	-	5,7,8	0.54	0	5,8,10	0.48	0
4	EDO	A	308	-	3,3,3	0.55	0	2,2,2	0.31	0
6	ACY	B	306	2	1,3,3	2.70	1 (100%)	0,3,3	-	-
7	PG4	C	307	-	12,12,12	0.56	0	11,11,11	0.38	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	-
5	LEU	B	301	-	-	3/5/6/8	-
7	PG4	C	307	-	-	6/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	308	ACY	CH3-C	5.21	1.55	1.48
6	B	306	ACY	CH3-C	2.70	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	LEU	O-C-CA-CB
7	C	307	PG4	O2-C3-C4-O3
7	C	307	PG4	O1-C1-C2-O2
5	B	301	LEU	CA-CB-CG-CD1
5	B	301	LEU	CA-CB-CG-CD2
7	C	307	PG4	C8-C7-O4-C6
7	C	307	PG4	O3-C5-C6-O4
7	C	307	PG4	C4-C3-O2-C2
4	A	308	EDO	O1-C1-C2-O2
7	C	307	PG4	C6-C5-O3-C4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	308	ACY	1	0
5	B	301	LEU	1	0
7	C	307	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 [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	270/297 (90%)	-0.02	14 (5%) 27 17	42, 69, 132, 177	0
1	B	270/297 (90%)	-0.04	14 (5%) 27 17	42, 76, 127, 154	0
1	C	269/297 (90%)	0.08	17 (6%) 20 11	45, 70, 143, 204	0
1	D	269/297 (90%)	0.03	16 (5%) 22 13	44, 81, 135, 168	0
1	E	271/297 (91%)	-0.14	9 (3%) 46 30	44, 68, 135, 175	0
All	All	1349/1485 (90%)	-0.02	70 (5%) 27 17	42, 73, 136, 204	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	PHE	14.9
1	C	206	PRO	7.5
1	A	47	GLN	7.3
1	C	26	PHE	5.9
1	C	207	VAL	5.8
1	D	268	ASN	5.8
1	A	25	ILE	5.5
1	E	26	PHE	5.2
1	A	290	HIS	5.2
1	C	47	GLN	5.1
1	E	204	THR	5.0
1	D	265	THR	4.8
1	D	48	LEU	4.7
1	D	47	GLN	4.7
1	C	48	LEU	4.6
1	D	44	TRP	4.6
1	D	209	PHE	4.5
1	C	208	PRO	4.4
1	A	48	LEU	4.4
1	B	209	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	26	PHE	4.2
1	A	29	LEU	4.1
1	A	28	LEU	4.0
1	B	211	TYR	4.0
1	D	236	TYR	3.9
1	E	266	ALA	3.7
1	A	24	ILE	3.7
1	D	267	ALA	3.6
1	D	21	LEU	3.6
1	B	204	THR	3.5
1	C	49	GLY	3.5
1	B	220	TYR	3.4
1	D	46	GLU	3.4
1	C	210	ALA	3.3
1	C	29	LEU	3.3
1	A	289	GLN	3.2
1	E	265	THR	3.2
1	D	266	ALA	3.1
1	E	44	TRP	3.0
1	A	175	GLY	3.0
1	B	144	GLU	3.0
1	A	44	TRP	3.0
1	B	26	PHE	2.9
1	B	152	ALA	2.8
1	D	43	GLN	2.8
1	B	25	ILE	2.7
1	D	22	SER	2.7
1	E	25	ILE	2.7
1	B	139	ARG	2.6
1	C	33	LEU	2.6
1	A	21	LEU	2.5
1	E	264	GLY	2.5
1	D	264	GLY	2.5
1	C	44	TRP	2.5
1	B	150	ILE	2.5
1	B	146	ARG	2.4
1	C	268	ASN	2.4
1	A	288	GLY	2.4
1	C	291	PRO	2.4
1	B	27	ARG	2.4
1	E	29	LEU	2.3
1	C	145	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	28	LEU	2.3
1	D	144	GLU	2.2
1	A	204	THR	2.2
1	E	236	TYR	2.2
1	D	26	PHE	2.2
1	B	23	LYS	2.1
1	B	24	ILE	2.1
1	C	30	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	C	306	1/1	0.71	0.16	161,161,161,161	0
2	ZN	E	306	1/1	0.78	0.15	170,170,170,170	0
5	LEU	B	301	8/9	0.83	0.30	103,108,112,112	0
7	PG4	C	307	13/13	0.84	0.32	78,93,107,108	0
6	ACY	C	308	4/4	0.87	0.27	46,51,57,59	0
2	ZN	D	303	1/1	0.91	0.14	121,121,121,121	0
2	ZN	D	302	1/1	0.94	0.12	110,110,110,110	0
6	ACY	B	306	4/4	0.94	0.19	72,79,88,89	0
4	EDO	A	308	4/4	0.96	0.25	63,69,75,80	0
8	NA	D	307	1/1	0.96	0.40	86,86,86,86	0
2	ZN	A	304	1/1	0.99	0.08	79,79,79,79	0
2	ZN	E	301	1/1	0.99	0.07	58,58,58,58	0
2	ZN	E	302	1/1	0.99	0.15	58,58,58,58	0
2	ZN	B	302	1/1	0.99	0.13	123,123,123,123	0
3	CL	A	307	1/1	0.99	0.07	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	D	304	1/1	0.99	0.09	90,90,90,90	0
3	CL	D	305	1/1	0.99	0.08	91,91,91,91	0
3	CL	E	304	1/1	0.99	0.09	73,73,73,73	0
2	ZN	B	303	1/1	0.99	0.10	77,77,77,77	0
2	ZN	B	304	1/1	0.99	0.12	63,63,63,63	0
2	ZN	C	302	1/1	0.99	0.15	78,78,78,78	0
2	ZN	A	301	1/1	0.99	0.12	67,67,67,67	0
2	ZN	D	301	1/1	0.99	0.09	80,80,80,80	0
2	ZN	A	302	1/1	0.99	0.10	77,77,77,77	0
2	ZN	C	301	1/1	1.00	0.15	61,61,61,61	0
3	CL	D	306	1/1	1.00	0.09	81,81,81,81	0
3	CL	E	303	1/1	1.00	0.07	63,63,63,63	0
3	CL	A	305	1/1	1.00	0.13	71,71,71,71	0
3	CL	E	305	1/1	1.00	0.17	98,98,98,98	0
3	CL	A	306	1/1	1.00	0.14	92,92,92,92	0
2	ZN	A	303	1/1	1.00	0.06	73,73,73,73	0
3	CL	B	305	1/1	1.00	0.10	82,82,82,82	0
3	CL	C	304	1/1	1.00	0.17	64,64,64,64	0
3	CL	C	305	1/1	1.00	0.09	83,83,83,83	0
2	ZN	C	303	1/1	1.00	0.11	67,67,67,67	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.