



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:04 AM UTC

PDB ID : 6IVM / pdb_00006ivm
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

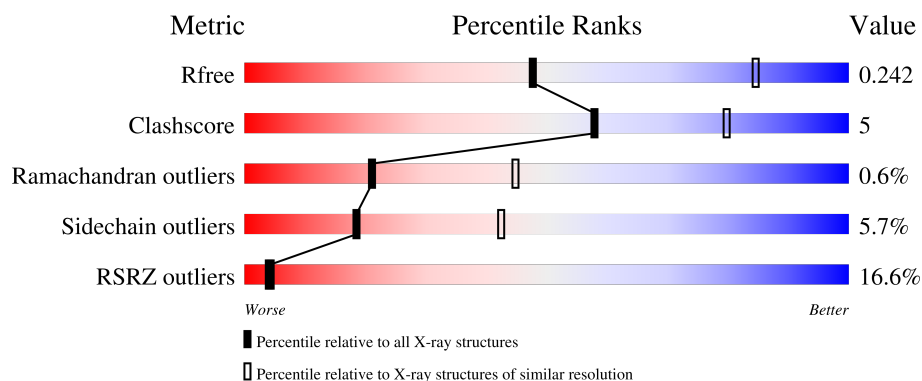
1 Overall quality at a glance

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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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.

Mol	Chain	Length	Quality of chain
1	A	297	12% 76% 14% 9%
1	B	297	14% 77% 11% 9%
1	C	297	14% 77% 12% 9%
1	D	297	20% 77% 11% 9%
1	E	297	15% 78% 12% 9%

2 Entry composition

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 Ibestrophin.

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	143	ALA	PRO	engineered mutation	UNP W9BH30

- Molecule 2 is ZINC ION (CCD ID: 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 (CCD ID: CL) (formula: Cl).

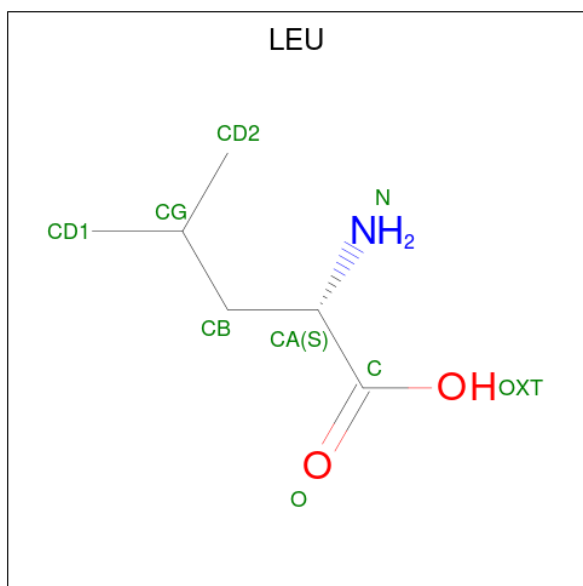
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3 3	0	0
3	B	1	Total Cl 1 1	0	0
3	C	2	Total Cl 2 2	0	0
3	D	3	Total Cl 3 3	0	0
3	E	3	Total Cl 3 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



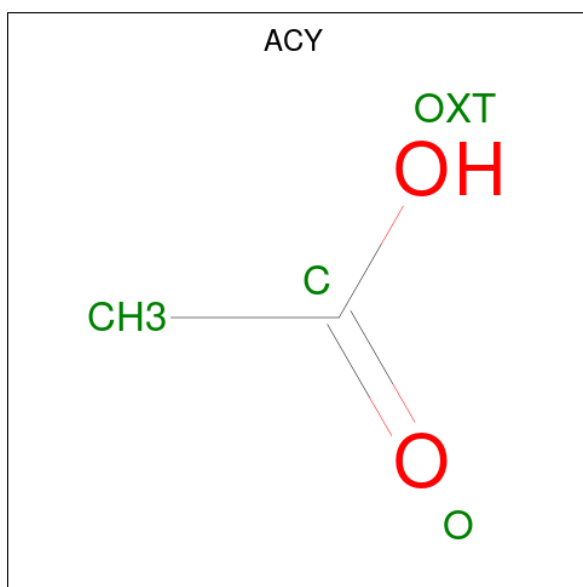
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is LEUCINE (CCD ID: LEU) (formula: $C_6H_{13}NO_2$).



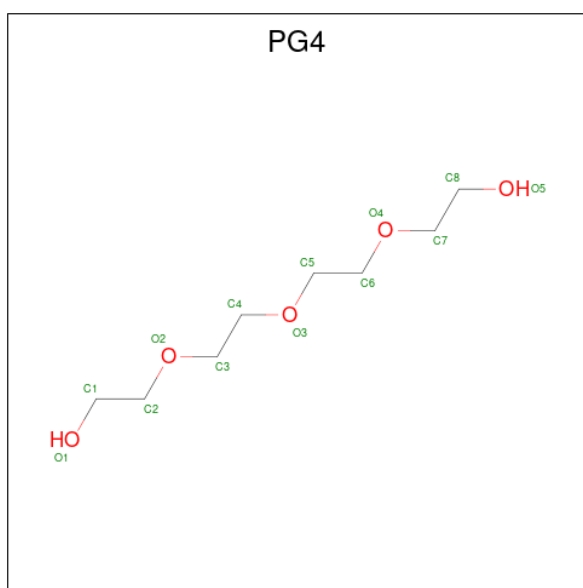
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 6 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

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

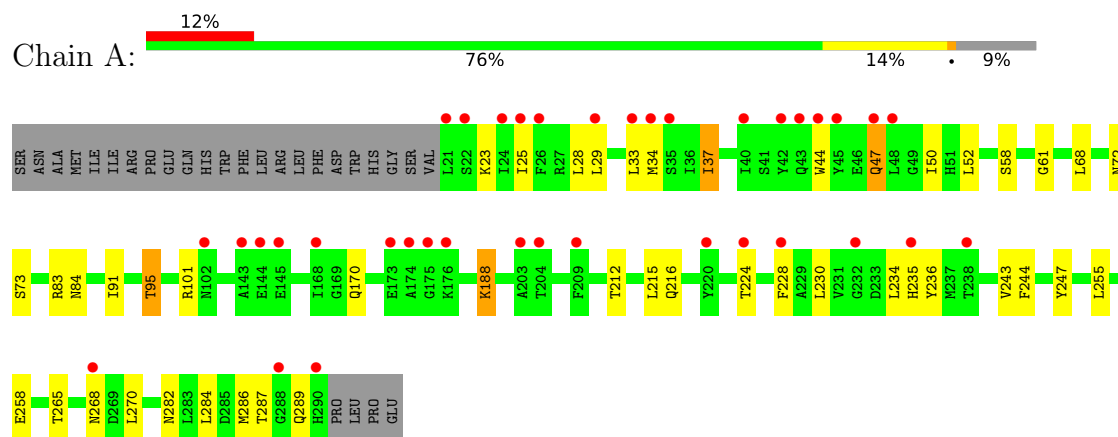
- Molecule 9 is water.

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

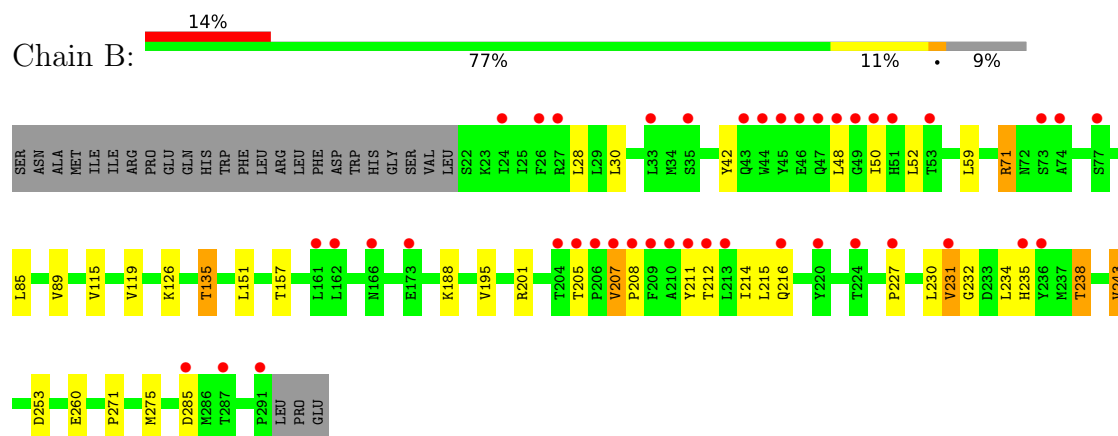
3 Residue-property plots [i](#)

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.

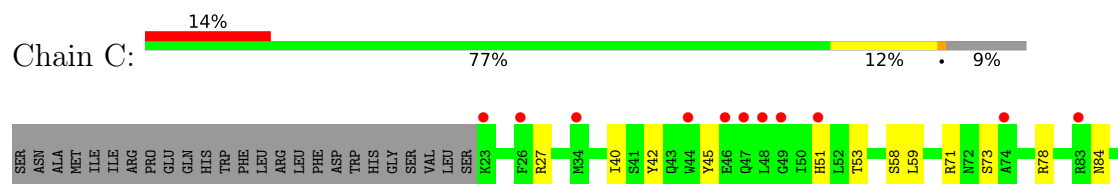
• Molecule 1: Ibestrophin

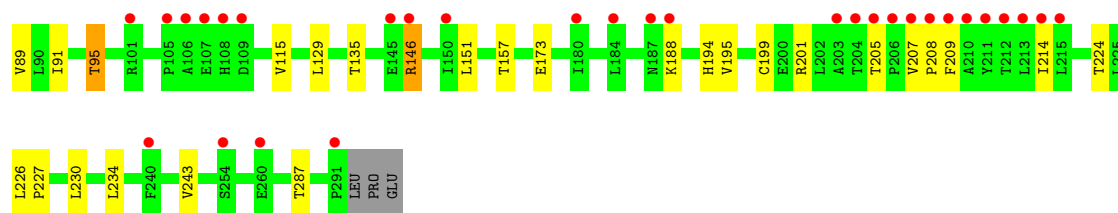


• Molecule 1: Ibestrophin

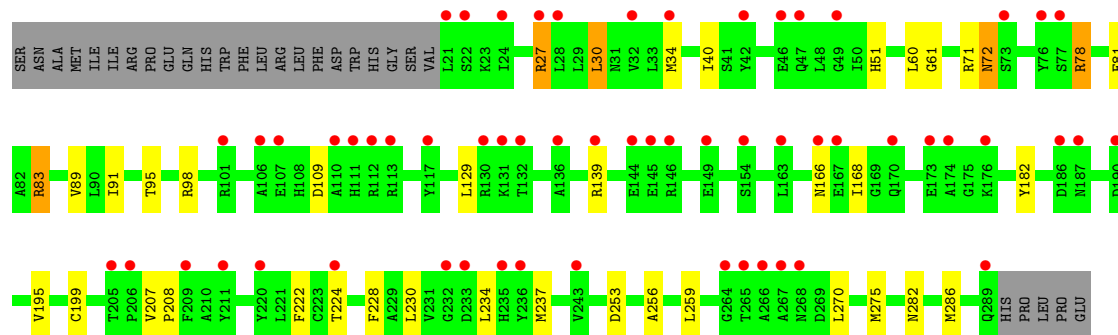
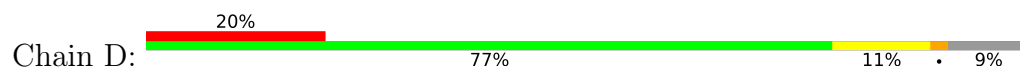


• Molecule 1: Ibestrophin

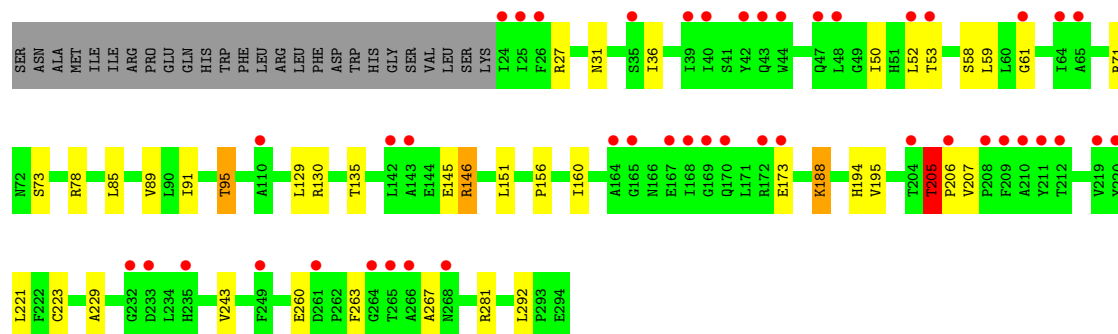
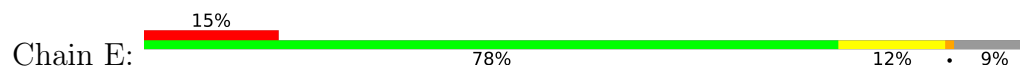




● Molecule 1: Ibestrophin



● Molecule 1: Ibestrophin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.97Å 158.81Å 161.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 2.95 48.72 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.72-2.95) 97.2 (48.72-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.96Å)	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 (4.59%)	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)	0.25 , 23.0	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	0.92	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

5.1 Standard geometry

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

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	0.63	0/2197	1.07	0/2989
1	B	0.64	0/2197	1.11	4/2990 (0.1%)
1	C	0.61	0/2191	1.07	2/2982 (0.1%)
1	D	0.60	0/2186	1.09	0/2974
1	E	0.64	0/2208	1.08	0/3006
All	All	0.63	0/10979	1.08	6/14941 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	ILE	N-CA-C	5.91	115.83	106.32
1	C	207	VAL	CA-C-N	5.38	126.56	119.84
1	C	207	VAL	C-N-CA	5.38	126.56	119.84
1	B	207	VAL	CA-C-N	5.20	126.34	119.84
1	B	207	VAL	C-N-CA	5.20	126.34	119.84
1	B	42	TYR	N-CA-C	5.10	117.58	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2151	0	2197	25	0
1	B	2150	0	2193	18	0
1	C	2144	0	2188	17	0
1	D	2141	0	2190	21	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	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (99) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:271:PRO:HG2	1:B:275:MET:HE3	1.86	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:D:270:LEU:HD22	1:D:275:MET:HE1	1.91	0.52
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:A:34:MET:HE3	1:A:224:THR:HG23	1.94	0.49
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:D:34:MET:HE2	1:D:224:THR:HG23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:HH12	1:C:205:THR:CG2	2.26	0.47
1:D:98:ARG:HB2	1:D:286:MET:HE1	1.97	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
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:D:34:MET:HE3	1:D:228:PHE:HE2	1.82	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: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:HD22	1:B:195:VAL:HA	2.01	0.42
1:B:85:LEU:HB3	1:B:195:VAL:HG13	2.01	0.42
1:C:188:LYS:HA	1:C:188:LYS:HD3	1.93	0.42
1:D:34:MET:HE3	1:D:228:PHE:CE2	2.54	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:129:LEU:HB3	1:E:263:PHE:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	30	53
1	B	268/297 (90%)	252 (94%)	13 (5%)	3 (1%)	11	29
1	C	267/297 (90%)	258 (97%)	7 (3%)	2 (1%)	18	40
1	D	267/297 (90%)	258 (97%)	8 (3%)	1 (0%)	30	53
1	E	269/297 (91%)	259 (96%)	9 (3%)	1 (0%)	30	53
All	All	1339/1485 (90%)	1284 (96%)	47 (4%)	8 (1%)	21	45

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	209	PHE
1	D	208	PRO
1	E	205	THR

5.3.2 Protein sidechains ⓘ

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%)	220 (94%)	14 (6%)	17	40
1	B	234/259 (90%)	220 (94%)	14 (6%)	17	40
1	C	233/259 (90%)	220 (94%)	13 (6%)	19	43
1	D	233/259 (90%)	221 (95%)	12 (5%)	21	46
1	E	235/259 (91%)	222 (94%)	13 (6%)	19	43
All	All	1169/1295 (90%)	1103 (94%)	66 (6%)	18	43

All (66) 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	50	ILE
1	A	73	SER
1	A	84	ASN
1	A	95	THR
1	A	188	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	71	ARG
1	B	126	LYS
1	B	135	THR
1	B	157	THR
1	B	188	LYS
1	B	207	VAL
1	B	211	TYR
1	B	214	ILE
1	B	215	LEU
1	B	231	VAL
1	B	238	THR
1	B	243	VAL
1	C	40	ILE
1	C	51	HIS
1	C	53	THR
1	C	58	SER
1	C	71	ARG
1	C	73	SER
1	C	84	ASN
1	C	95	THR
1	C	146	ARG
1	C	157	THR
1	C	173	GLU
1	C	214	ILE
1	C	243	VAL
1	D	27	ARG
1	D	30	LEU
1	D	40	ILE
1	D	51	HIS
1	D	72	ASN
1	D	78	ARG
1	D	81	GLU
1	D	83	ARG
1	D	109	ASP
1	D	139	ARG
1	D	166	ASN
1	D	282	ASN
1	E	27	ARG
1	E	36	ILE
1	E	53	THR
1	E	71	ARG
1	E	95	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	146	ARG
1	E	173	GLU
1	E	188	LYS
1	E	205	THR
1	E	207	VAL
1	E	243	VAL
1	E	260	GLU
1	E	292	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	47	GLN
1	A	72	ASN
1	A	99	GLN
1	A	102	ASN
1	A	216	GLN
1	A	268	ASN
1	B	31	ASN
1	B	47	GLN
1	B	99	GLN
1	B	166	ASN
1	C	99	GLN
1	C	102	ASN
1	C	166	ASN
1	D	72	ASN
1	D	268	ASN
1	D	289	GLN
1	E	72	ASN
1	E	99	GLN
1	E	166	ASN
1	E	268	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	EDO	A	308	-	3,3,3	0.52	0	2,2,2	0.34	0
6	ACY	C	308	-	3,3,3	1.13	0	3,3,3	1.58	1 (33%)
7	PG4	C	307	-	12,12,12	0.56	0	11,11,11	0.38	0
5	LEU	B	301	-	5,7,8	0.57	0	6,8,10	0.48	0
6	ACY	B	306	2	3,3,3	0.97	0	3,3,3	0.46	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	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	308	ACY	OXT-C-CH3	2.17	124.15	115.05

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	C4-C3-O2-C2
7	C	307	PG4	O3-C5-C6-O4
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
7	C	307	PG4	1	0
5	B	301	LEU	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, 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%)	0.59	37 (13%) 6 6	42, 69, 132, 177	0
1	B	270/297 (90%)	0.67	42 (15%) 5 5	42, 76, 127, 154	0
1	C	269/297 (90%)	0.85	41 (15%) 5 5	45, 70, 143, 204	0
1	D	269/297 (90%)	1.23	59 (21%) 2 2	44, 81, 135, 168	0
1	E	271/297 (91%)	0.70	45 (16%) 4 4	44, 68, 135, 175	0
All	All	1349/1485 (90%)	0.81	224 (16%) 4 4	42, 73, 136, 204	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	PHE	18.9
1	C	206	PRO	13.6
1	D	233	ASP	12.3
1	D	145	GLU	11.7
1	D	170	GLN	10.8
1	D	146	ARG	10.5
1	B	46	GLU	9.9
1	E	266	ALA	9.4
1	C	106	ALA	9.1
1	C	207	VAL	8.7
1	C	208	PRO	8.7
1	D	173	GLU	7.7
1	D	265	THR	7.7
1	D	166	ASN	7.6
1	D	46	GLU	7.3
1	D	131	LYS	7.1
1	D	236	TYR	7.0
1	E	204	THR	6.8
1	D	149	GLU	6.7
1	A	175	GLY	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	204	THR	6.6
1	C	210	ALA	6.4
1	B	47	GLN	6.2
1	D	167	GLU	6.1
1	C	204	THR	6.0
1	A	21	LEU	6.0
1	B	51	HIS	6.0
1	A	47	GLN	5.8
1	E	42	TYR	5.3
1	C	51	HIS	5.3
1	E	264	GLY	5.3
1	D	130	ARG	5.1
1	A	145	GLU	5.1
1	B	49	GLY	5.1
1	E	265	THR	5.1
1	B	211	TYR	5.1
1	B	207	VAL	4.9
1	E	235	HIS	4.9
1	C	105	PRO	4.8
1	C	26	PHE	4.7
1	C	205	THR	4.6
1	C	109	ASP	4.6
1	D	187	ASN	4.6
1	D	112	ARG	4.5
1	C	291	PRO	4.5
1	D	174	ALA	4.5
1	E	206	PRO	4.5
1	D	113	ARG	4.5
1	D	21	LEU	4.4
1	D	209	PHE	4.4
1	C	211	TYR	4.4
1	D	106	ALA	4.3
1	B	77	SER	4.3
1	B	210	ALA	4.3
1	D	264	GLY	4.3
1	D	107	GLU	4.3
1	C	184	LEU	4.2
1	B	44	TRP	4.2
1	D	232	GLY	4.2
1	E	211	TYR	4.1
1	E	26	PHE	4.1
1	B	73	SER	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	48	LEU	4.1
1	E	208	PRO	4.1
1	D	144	GLU	4.1
1	B	204	THR	4.0
1	C	47	GLN	4.0
1	D	24	ILE	4.0
1	D	42	TYR	4.0
1	C	240	PHE	3.9
1	C	212	THR	3.9
1	D	163	LEU	3.9
1	E	61	GLY	3.9
1	E	64	ILE	3.8
1	D	235	HIS	3.8
1	B	216	GLN	3.8
1	A	44	TRP	3.8
1	E	24	ILE	3.8
1	E	170	GLN	3.7
1	E	173	GLU	3.7
1	A	34	MET	3.7
1	D	154	SER	3.5
1	D	220	TYR	3.5
1	A	25	ILE	3.5
1	D	206	PRO	3.5
1	E	168	ILE	3.4
1	B	212	THR	3.4
1	B	213	LEU	3.4
1	E	39	ILE	3.4
1	B	209	PHE	3.4
1	B	48	LEU	3.4
1	A	174	ALA	3.4
1	D	110	ALA	3.4
1	E	210	ALA	3.3
1	B	285	ASP	3.3
1	B	166	ASN	3.3
1	D	101	ARG	3.3
1	B	50	ILE	3.3
1	D	73	SER	3.3
1	D	139	ARG	3.3
1	C	260	GLU	3.3
1	D	243	VAL	3.3
1	A	232	GLY	3.3
1	A	24	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	26	PHE	3.2
1	D	289	GLN	3.2
1	B	53	THR	3.2
1	A	40	ILE	3.2
1	A	144	GLU	3.1
1	B	220	TYR	3.1
1	D	47	GLN	3.0
1	E	25	ILE	3.0
1	D	28	LEU	3.0
1	D	186	ASP	3.0
1	E	44	TRP	3.0
1	B	45	TYR	2.9
1	C	215	LEU	2.9
1	A	48	LEU	2.9
1	D	22	SER	2.9
1	D	76	TYR	2.9
1	D	117	TYR	2.9
1	D	32	VAL	2.9
1	A	228	PHE	2.9
1	B	162	LEU	2.9
1	A	288	GLY	2.8
1	E	232	GLY	2.8
1	B	43	GLN	2.8
1	B	287	THR	2.8
1	A	235	HIS	2.8
1	B	35	SER	2.8
1	D	49	GLY	2.8
1	C	107	GLU	2.8
1	D	77	SER	2.8
1	C	187	ASN	2.7
1	A	143	ALA	2.7
1	E	143	ALA	2.7
1	C	46	GLU	2.7
1	E	65	ALA	2.7
1	E	172	ARG	2.7
1	C	49	GLY	2.7
1	D	205	THR	2.7
1	E	268	ASN	2.7
1	D	190	ASP	2.7
1	E	35	SER	2.7
1	B	235	HIS	2.6
1	A	45	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	208	PRO	2.6
1	E	169	GLY	2.6
1	A	203	ALA	2.6
1	B	236	TYR	2.6
1	D	224	THR	2.6
1	A	43	GLN	2.6
1	D	34	MET	2.6
1	E	209	PHE	2.6
1	B	27	ARG	2.5
1	B	24	ILE	2.5
1	A	209	PHE	2.5
1	A	173	GLU	2.5
1	C	74	ALA	2.5
1	B	26	PHE	2.5
1	B	74	ALA	2.5
1	B	291	PRO	2.5
1	D	211	TYR	2.5
1	C	146	ARG	2.5
1	E	47	GLN	2.5
1	B	205	THR	2.5
1	C	180	ILE	2.4
1	C	254	SER	2.4
1	D	268	ASN	2.4
1	C	101	ARG	2.4
1	B	206	PRO	2.4
1	E	142	LEU	2.4
1	E	219	VAL	2.4
1	C	83	ARG	2.4
1	D	176	LYS	2.4
1	E	212	THR	2.4
1	A	33	LEU	2.4
1	B	227	PRO	2.4
1	C	188	LYS	2.3
1	E	165	GLY	2.3
1	E	261	ASP	2.3
1	B	173	GLU	2.3
1	D	267	ALA	2.3
1	B	161	LEU	2.3
1	A	168	ILE	2.3
1	C	150	ILE	2.3
1	E	249	PHE	2.3
1	A	290	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	220	TYR	2.3
1	C	44	TRP	2.3
1	E	53	THR	2.3
1	E	167	GLU	2.3
1	D	266	ALA	2.2
1	E	110	ALA	2.2
1	B	231	VAL	2.2
1	E	48	LEU	2.2
1	B	224	THR	2.2
1	A	268	ASN	2.2
1	E	40	ILE	2.2
1	A	35	SER	2.2
1	A	176	LYS	2.2
1	D	27	ARG	2.2
1	D	111	HIS	2.2
1	C	145	GLU	2.2
1	D	136	ALA	2.2
1	E	164	ALA	2.2
1	C	213	LEU	2.1
1	A	42	TYR	2.1
1	E	43	GLN	2.1
1	C	23	LYS	2.1
1	E	233	ASP	2.1
1	A	29	LEU	2.1
1	C	203	ALA	2.1
1	E	220	TYR	2.1
1	C	108	HIS	2.1
1	B	33	LEU	2.1
1	A	238	THR	2.1
1	C	214	ILE	2.1
1	A	22	SER	2.1
1	E	52	LEU	2.1
1	D	132	THR	2.1
1	C	34	MET	2.0
1	A	102	ASN	2.0
1	A	224	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
6	ACY	C	308	4/4	0.59	0.31	46,51,57,59	0
2	ZN	C	306	1/1	0.66	0.15	161,161,161,161	0
6	ACY	B	306	4/4	0.76	0.25	72,79,88,89	0
5	LEU	B	301	8/9	0.87	0.23	103,108,112,112	0
8	NA	D	307	1/1	0.87	0.43	86,86,86,86	0
2	ZN	E	306	1/1	0.89	0.16	170,170,170,170	0
7	PG4	C	307	13/13	0.91	0.20	78,93,107,108	0
2	ZN	D	302	1/1	0.94	0.09	110,110,110,110	0
4	EDO	A	308	4/4	0.95	0.13	63,69,75,80	0
2	ZN	D	303	1/1	0.96	0.08	121,121,121,121	0
3	CL	B	305	1/1	0.96	0.10	82,82,82,82	0
3	CL	A	305	1/1	0.97	0.07	71,71,71,71	0
2	ZN	B	302	1/1	0.97	0.08	123,123,123,123	0
3	CL	D	304	1/1	0.97	0.09	90,90,90,90	0
3	CL	C	304	1/1	0.98	0.14	64,64,64,64	0
3	CL	A	307	1/1	0.98	0.06	96,96,96,96	0
3	CL	D	305	1/1	0.98	0.12	91,91,91,91	0
3	CL	D	306	1/1	0.99	0.05	81,81,81,81	0
3	CL	E	304	1/1	0.99	0.06	73,73,73,73	0
3	CL	E	305	1/1	0.99	0.07	98,98,98,98	0
2	ZN	B	304	1/1	0.99	0.06	63,63,63,63	0
2	ZN	E	302	1/1	0.99	0.06	58,58,58,58	0
2	ZN	D	301	1/1	0.99	0.03	80,80,80,80	0
3	CL	C	305	1/1	0.99	0.10	83,83,83,83	0
2	ZN	C	302	1/1	0.99	0.06	78,78,78,78	0
3	CL	A	306	1/1	0.99	0.04	92,92,92,92	0
3	CL	E	303	1/1	1.00	0.02	63,63,63,63	0
2	ZN	A	304	1/1	1.00	0.04	79,79,79,79	0
2	ZN	A	301	1/1	1.00	0.01	67,67,67,67	0
2	ZN	B	303	1/1	1.00	0.02	77,77,77,77	0
2	ZN	A	302	1/1	1.00	0.02	77,77,77,77	0
2	ZN	E	301	1/1	1.00	0.01	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	301	1/1	1.00	0.05	61,61,61,61	0
2	ZN	A	303	1/1	1.00	0.01	73,73,73,73	0
2	ZN	C	303	1/1	1.00	0.02	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.