



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:25 AM UTC

PDB ID : 6IVQ / pdb_00006ivq
Title : Crystal structure of a membrane protein S19A
Authors : Kittredge, A.; Fukuda, F.; Zhang, Y.; Yang, T.
Deposited on : 2018-12-04
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

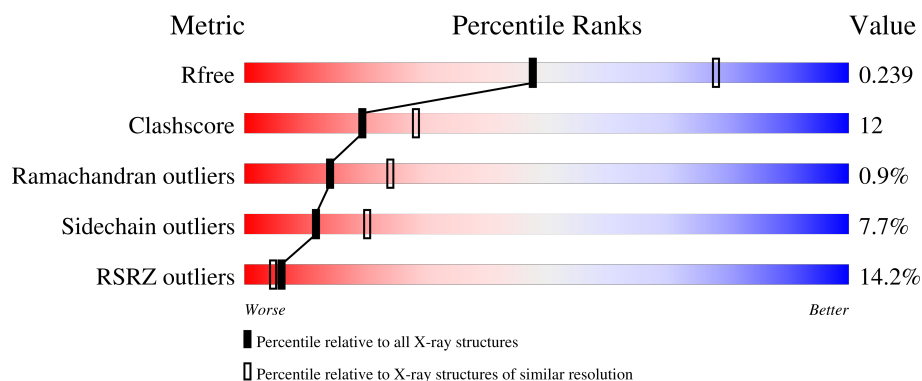
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	11% 69% 18% • • 9%
1	B	297	11% 62% 25% • 9%
1	C	297	9% 70% 18% • 9%
1	D	297	18% 70% 17% • 9%
1	E	297	15% 64% 23% • • 9%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10898 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ibestrophin.

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

There are 20 discrepancies between the modelled and reference sequences:

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

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

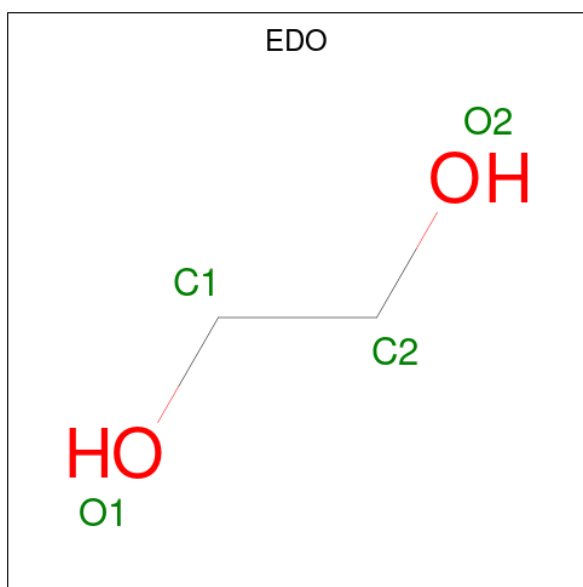
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

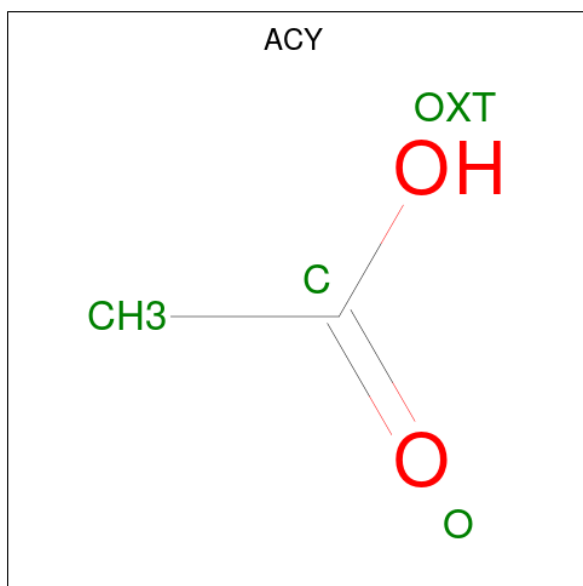
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3 3	0	0
3	B	1	Total Cl 1 1	0	0
3	C	3	Total Cl 3 3	0	0
3	D	3	Total Cl 3 3	0	0
3	E	2	Total Cl 2 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (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 ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).

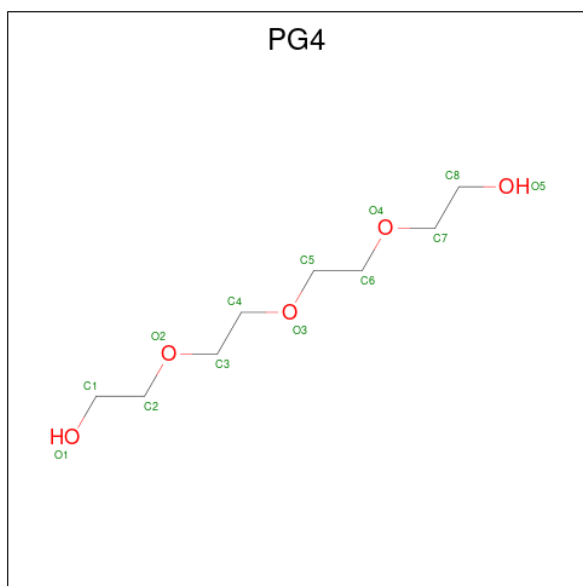


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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



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

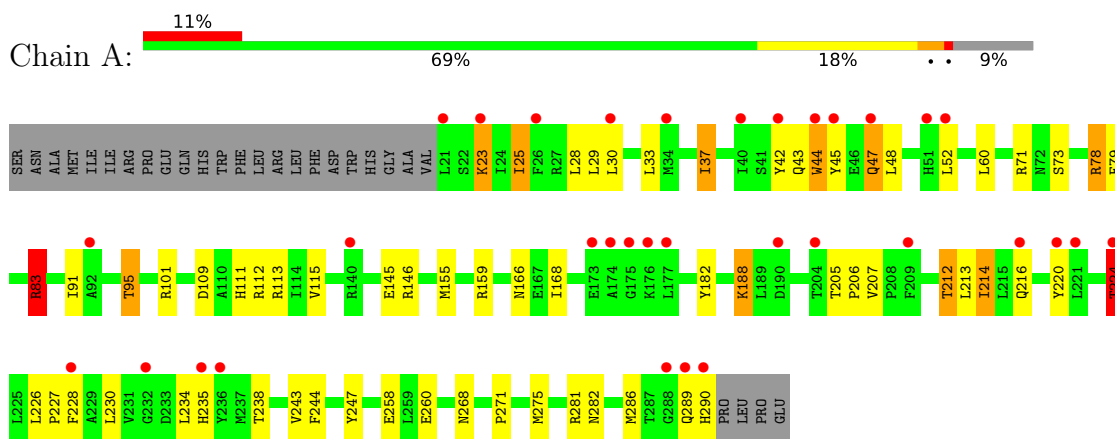
- Molecule 8 is water.

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

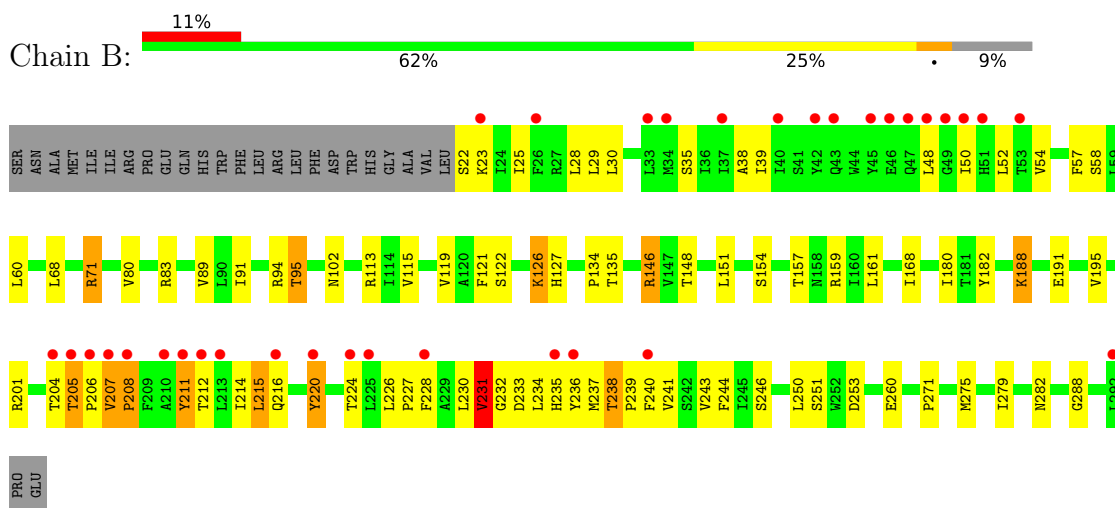
3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.70Å 159.64Å 161.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 2.65 48.61 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.61-2.65) 99.8 (48.61-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.201 , 0.239 0.201 , 0.239	Depositor DCC
R_{free} test set	4278 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 24.5	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	0.93	EDS
Total number of atoms	10898	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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: ACY, PG4, NA, CL, ZN, 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	0.57	0/2200	1.16	4/2994 (0.1%)
1	B	0.55	0/2208	1.14	4/3006 (0.1%)
1	C	0.53	0/2194	1.08	2/2987 (0.1%)
1	D	0.52	0/2189	1.06	0/2979
1	E	0.62	1/2211 (0.0%)	1.32	6/3011 (0.2%)
All	All	0.56	1/11002 (0.0%)	1.16	16/14977 (0.1%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	293	PRO	C-N	13.47	1.52	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	293	PRO	O-C-N	-25.54	88.17	122.64
1	E	293	PRO	CA-C-N	18.29	154.61	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	293	PRO	C-N-CA	18.29	154.61	121.70
1	A	83	ARG	CG-CD-NE	-6.02	98.76	112.00
1	A	224	THR	CB-CA-C	5.74	120.33	110.86
1	B	148	THR	CB-CA-C	5.60	120.95	110.70
1	E	201	ARG	CB-CA-C	5.60	120.37	110.85
1	A	212	THR	CB-CA-C	5.42	120.65	110.63
1	C	209	PHE	CA-CB-CG	5.24	119.04	113.80
1	B	191	GLU	CB-CA-C	5.20	119.41	110.79
1	E	205	THR	CB-CA-C	5.15	120.31	110.17
1	E	238	THR	CA-CB-OG1	-5.09	101.97	109.60
1	B	23	LYS	N-CA-C	-5.08	106.92	113.01
1	A	238	THR	CA-CB-OG1	-5.06	102.02	109.60
1	B	220	TYR	CB-CA-C	5.05	118.88	110.90
1	C	233	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (13) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2153	0	2199	64	0
1	B	2160	0	2206	67	0
1	C	2146	0	2190	39	0
1	D	2143	0	2192	47	0
1	E	2162	0	2201	70	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	3	0	0	0	0
3	A	3	0	0	1	0
3	B	1	0	0	0	0
3	C	3	0	0	2	0
3	D	3	0	0	1	0
3	E	2	0	0	0	0
4	A	4	0	6	0	0
5	B	4	0	3	1	0
5	E	4	0	3	1	0
6	D	1	0	0	0	0
7	E	13	0	18	1	0
8	A	17	0	0	0	0
8	B	18	0	0	0	0
8	C	18	0	0	0	0
8	D	9	0	0	0	0
8	E	17	0	0	0	0
All	All	10898	0	11018	254	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 12.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:HIS:O	1:B:238:THR:HG23	1.38	1.21
1:A:83:ARG:HH22	1:E:205:THR:CG2	1.64	1.10
1:A:83:ARG:NH2	1:E:205:THR:HG23	1.69	1.07
1:A:83:ARG:HH22	1:E:205:THR:HG23	0.84	1.01
1:B:234:LEU:HB2	1:B:238:THR:HG22	1.41	1.00
1:C:78:ARG:HH12	1:C:205:THR:CG2	1.78	0.96
1:E:78:ARG:HH12	1:E:205:THR:HG21	1.28	0.95
1:C:201:ARG:O	1:C:205:THR:HB	1.73	0.86
1:B:71:ARG:HH12	1:B:212:THR:HG22	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ARG:NH1	1:B:260:GLU:OE2	2.11	0.84
1:B:235:HIS:O	1:B:238:THR:CG2	2.24	0.84
1:D:83:ARG:HG2	1:D:270:LEU:HD21	1.61	0.82
1:B:204:THR:O	1:B:206:PRO:HD3	1.80	0.81
1:C:78:ARG:HH12	1:C:205:THR:HG21	1.45	0.81
1:E:94:ARG:HH21	1:E:282:ASN:HD21	1.27	0.80
1:A:101:ARG:HH22	1:A:290:HIS:C	1.91	0.79
1:E:205:THR:HB	1:E:206:PRO:HA	1.64	0.78
1:B:71:ARG:HH12	1:B:212:THR:CG2	1.96	0.78
1:C:155:MET:HG2	1:C:158:ASN:HB2	1.63	0.78
1:B:231:VAL:HA	1:B:238:THR:HG21	1.66	0.77
1:E:205:THR:CB	1:E:206:PRO:HA	2.15	0.76
1:B:211:TYR:O	1:B:215:LEU:HB2	1.84	0.76
1:B:271:PRO:HG2	1:B:275:MET:HE3	1.69	0.74
1:B:39:ILE:HD13	1:B:236:TYR:HA	1.70	0.73
1:A:271:PRO:HD2	1:A:275:MET:HE3	1.70	0.72
1:A:91:ILE:O	1:A:95:THR:HG23	1.88	0.72
1:A:168:ILE:HG22	1:A:182:TYR:CE1	2.24	0.72
1:A:83:ARG:NH2	1:E:205:THR:CG2	2.38	0.72
1:A:43:GLN:C	1:A:45:TYR:H	1.97	0.72
1:A:258:GLU:HG2	1:A:268:ASN:HD22	1.55	0.71
1:C:42:TYR:O	1:C:45:TYR:HB2	1.89	0.71
1:D:25:ILE:HD13	1:D:25:ILE:N	2.05	0.71
1:C:251:SER:HB3	1:D:214:ILE:HD13	1.74	0.69
1:E:94:ARG:HH21	1:E:282:ASN:ND2	1.89	0.69
1:E:91:ILE:O	1:E:95:THR:HG23	1.91	0.69
1:C:78:ARG:NH1	1:C:205:THR:CG2	2.54	0.69
1:B:236:TYR:O	1:B:239:PRO:HD2	1.93	0.68
1:D:78:ARG:HD3	1:D:207:VAL:HG23	1.76	0.68
1:D:271:PRO:HD2	1:D:275:MET:HE3	1.76	0.67
1:E:78:ARG:NH1	1:E:205:THR:HG21	2.08	0.66
1:A:52:LEU:CD1	1:A:228:PHE:HB3	2.25	0.66
1:A:78:ARG:NH1	1:A:206:PRO:HA	2.11	0.66
1:E:42:TYR:CE1	1:E:46:GLU:HG3	2.31	0.66
1:D:72:ASN:ND2	1:D:256:ALA:HB2	2.10	0.66
1:E:50:ILE:HG13	1:E:50:ILE:O	1.96	0.66
1:B:207:VAL:HG12	1:D:76:TYR:HE1	1.61	0.66
1:D:271:PRO:HD2	1:D:275:MET:CE	2.25	0.65
1:A:271:PRO:CD	1:A:275:MET:HE3	2.27	0.65
1:C:205:THR:N	1:C:206:PRO:CD	2.60	0.64
1:A:214:ILE:HD13	1:B:251:SER:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLN:O	1:A:45:TYR:N	2.31	0.64
1:B:224:THR:O	1:B:227:PRO:HD2	1.98	0.64
1:B:39:ILE:CD1	1:B:236:TYR:HA	2.27	0.64
1:A:109:ASP:HB3	1:A:113:ARG:HH12	1.61	0.63
1:B:146:ARG:HA	1:B:146:ARG:HH11	1.62	0.63
1:A:33:LEU:O	1:A:37:ILE:HG23	1.98	0.63
1:D:78:ARG:CD	1:D:207:VAL:HG23	2.28	0.63
1:A:42:TYR:O	1:A:45:TYR:HB2	2.00	0.62
1:C:115:VAL:HG21	1:C:287:THR:HG21	1.80	0.62
1:D:71:ARG:HD2	1:D:71:ARG:C	2.25	0.61
1:E:281:ARG:HD3	5:E:307:ACY:H3	1.80	0.61
1:A:235:HIS:ND1	1:E:51:HIS:NE2	2.47	0.61
1:B:35:SER:OG	1:B:239:PRO:HA	1.99	0.60
1:D:24:ILE:HG23	1:D:25:ILE:HD13	1.82	0.60
1:A:101:ARG:NH2	1:A:290:HIS:C	2.58	0.60
1:E:206:PRO:HB2	1:E:208:PRO:HD2	1.83	0.60
1:A:244:PHE:CE1	1:E:221:LEU:HD23	2.37	0.59
1:A:271:PRO:HD2	1:A:275:MET:CE	2.32	0.59
1:C:91:ILE:O	1:C:95:THR:HG23	2.03	0.59
1:A:166:ASN:ND2	1:B:102:ASN:HD22	2.01	0.59
1:B:238:THR:N	1:B:239:PRO:HD2	2.18	0.59
1:A:52:LEU:HD12	1:A:228:PHE:HB3	1.83	0.58
1:A:282:ASN:O	1:A:286:MET:HG3	2.02	0.58
1:E:207:VAL:H	1:E:208:PRO:HD2	1.68	0.58
1:A:168:ILE:HG22	1:A:182:TYR:CD1	2.38	0.58
1:C:83:ARG:HG2	1:D:205:THR:HG21	1.85	0.58
1:E:90:LEU:HD13	1:E:279:ILE:HD13	1.86	0.57
1:C:207:VAL:O	1:C:208:PRO:C	2.46	0.57
1:D:34:MET:HE3	1:D:228:PHE:HE2	1.70	0.57
1:B:71:ARG:NH1	1:B:212:THR:HG22	2.17	0.57
1:A:258:GLU:CG	1:A:268:ASN:HD22	2.16	0.57
1:D:91:ILE:O	1:D:95:THR:HG23	2.04	0.57
1:E:205:THR:CG2	1:E:206:PRO:HA	2.35	0.57
1:E:60:LEU:HD23	1:E:222:PHE:HD1	1.70	0.56
1:A:166:ASN:HD22	1:B:102:ASN:HD22	1.53	0.56
1:E:292:LEU:HD22	1:E:293:PRO:HD2	1.87	0.56
1:D:168:ILE:HG22	1:D:182:TYR:CE2	2.41	0.56
1:E:216:GLN:HG3	1:E:253:ASP:OD2	2.06	0.56
1:A:230:LEU:HB3	1:A:234:LEU:HD12	1.87	0.55
1:C:78:ARG:NH1	1:C:205:THR:HG23	2.22	0.55
1:E:95:THR:OG1	1:E:188:LYS:HD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:HE3	1:A:220:TYR:OH	2.07	0.55
1:C:226:LEU:N	1:C:227:PRO:HD2	2.21	0.54
1:E:205:THR:HG22	1:E:206:PRO:HA	1.89	0.54
1:A:205:THR:HG21	1:B:83:ARG:HG2	1.90	0.54
1:E:24:ILE:HG23	1:E:25:ILE:N	2.21	0.54
1:E:207:VAL:N	1:E:208:PRO:HD2	2.23	0.54
1:C:194:HIS:HA	1:E:91:ILE:HD13	1.90	0.53
1:E:226:LEU:N	1:E:227:PRO:HD2	2.22	0.53
1:A:60:LEU:HD21	1:B:244:PHE:CE2	2.44	0.53
1:C:190:ASP:OD1	3:C:306:CL:CL	2.63	0.53
1:E:31:ASN:ND2	1:E:223:CYS:O	2.41	0.53
1:B:135:THR:HG23	1:B:151:LEU:HD11	1.90	0.53
1:D:207:VAL:O	1:D:208:PRO:C	2.52	0.53
1:E:202:LEU:C	1:E:205:THR:OG1	2.52	0.53
1:E:45:TYR:HB2	1:E:50:ILE:HD11	1.90	0.53
1:E:73:SER:HA	7:E:306:PG4:H61	1.90	0.53
1:E:90:LEU:HD12	1:E:94:ARG:CZ	2.39	0.52
1:C:91:ILE:HD13	1:D:194:HIS:HA	1.91	0.52
1:B:22:SER:HB3	1:B:25:ILE:H	1.74	0.52
1:D:25:ILE:N	1:D:25:ILE:CD1	2.73	0.52
1:E:24:ILE:CG2	1:E:25:ILE:N	2.73	0.52
1:A:101:ARG:HD2	1:A:286:MET:O	2.10	0.52
1:D:71:ARG:NH2	1:D:253:ASP:OD1	2.43	0.51
1:D:226:LEU:N	1:D:227:PRO:HD2	2.24	0.51
1:A:78:ARG:HD3	1:A:207:VAL:HG23	1.93	0.51
1:A:91:ILE:O	1:A:95:THR:CG2	2.58	0.51
1:C:168:ILE:HG13	1:C:182:TYR:CE2	2.44	0.51
1:C:180:ILE:HD12	1:D:180:ILE:HD13	1.92	0.51
1:D:78:ARG:HD3	1:D:207:VAL:CG2	2.39	0.51
1:D:34:MET:HE3	1:D:228:PHE:CE2	2.46	0.51
1:D:168:ILE:HG22	1:D:182:TYR:CD2	2.46	0.50
1:B:91:ILE:O	1:B:95:THR:HG23	2.11	0.50
1:E:112:ARG:NH1	1:E:289:GLN:HG2	2.26	0.50
1:A:28:LEU:HD21	1:A:247:TYR:HB2	1.95	0.49
1:E:68:LEU:HD23	1:E:215:LEU:HD21	1.93	0.49
1:A:43:GLN:C	1:A:45:TYR:N	2.67	0.49
1:B:227:PRO:HA	1:B:230:LEU:HB2	1.95	0.49
1:E:117:TYR:OH	1:E:146:ARG:HG2	2.13	0.49
1:A:212:THR:O	1:A:216:GLN:HB2	2.11	0.49
1:B:28:LEU:HD22	1:B:243:VAL:HG22	1.94	0.49
1:A:258:GLU:CD	1:A:268:ASN:ND2	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:CB	1:B:238:THR:HG22	2.30	0.49
1:C:204:THR:C	1:C:206:PRO:HD2	2.38	0.48
1:D:240:PHE:O	1:D:243:VAL:HG12	2.13	0.48
1:A:48:LEU:O	1:B:236:TYR:CE2	2.66	0.48
1:A:52:LEU:HD21	1:B:237:MET:HE2	1.95	0.48
1:B:25:ILE:O	1:B:29:LEU:HG	2.12	0.48
1:E:203:ALA:C	1:E:205:THR:H	2.20	0.48
1:A:44:TRP:HA	1:A:47:GLN:HG3	1.95	0.48
1:C:271:PRO:HD2	1:C:275:MET:HE3	1.96	0.48
1:A:30:LEU:HD23	1:A:30:LEU:O	2.14	0.47
1:C:68:LEU:HD23	1:C:215:LEU:HD21	1.96	0.47
1:A:145:GLU:HB3	1:A:146:ARG:HH21	1.79	0.47
1:B:127:HIS:CD2	1:B:134:PRO:HA	2.50	0.47
1:A:271:PRO:HG2	1:A:275:MET:HE3	1.96	0.47
1:C:71:ARG:HD2	1:C:71:ARG:C	2.39	0.47
1:B:240:PHE:O	1:B:243:VAL:HG12	2.15	0.47
1:D:89:VAL:HG23	1:D:195:VAL:HG11	1.97	0.47
1:B:168:ILE:HG13	1:B:182:TYR:CE1	2.49	0.47
1:B:216:GLN:HG2	1:B:253:ASP:OD2	2.15	0.47
1:C:95:THR:HG21	3:C:304:CL:CL	2.52	0.47
1:D:271:PRO:HD2	1:D:275:MET:HE1	1.97	0.47
1:E:42:TYR:HE1	1:E:46:GLU:HG3	1.76	0.47
1:E:270:LEU:HB3	1:E:271:PRO:HD3	1.95	0.47
1:E:85:LEU:HD22	1:E:195:VAL:HA	1.97	0.47
1:B:205:THR:HG21	1:D:83:ARG:HD3	1.97	0.46
1:E:24:ILE:CG2	1:E:25:ILE:H	2.28	0.46
1:D:30:LEU:O	1:D:34:MET:HG2	2.15	0.46
1:A:224:THR:O	1:A:227:PRO:HD2	2.16	0.46
1:B:122:SER:OG	1:B:279:ILE:HD13	2.16	0.46
1:A:226:LEU:N	1:A:227:PRO:HD2	2.31	0.46
1:E:126:LYS:HG3	1:E:272:LEU:HD23	1.97	0.46
1:A:230:LEU:HB3	1:A:234:LEU:CD1	2.46	0.45
1:A:214:ILE:CD1	1:B:251:SER:HB3	2.43	0.45
1:B:246:SER:O	1:B:250:LEU:HD12	2.17	0.45
1:B:201:ARG:O	1:B:205:THR:HB	2.16	0.45
1:E:126:LYS:HE3	1:E:273:ASN:OD1	2.16	0.45
1:C:58:SER:O	1:C:62:ILE:HG13	2.17	0.45
1:C:214:ILE:HG13	1:E:247:TYR:OH	2.17	0.45
1:E:104:LEU:HD21	1:E:176:LYS:O	2.16	0.45
1:E:202:LEU:C	1:E:205:THR:HG1	2.24	0.45
1:C:50:ILE:O	1:C:50:ILE:HG13	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:ARG:HE	1:E:282:ASN:ND2	2.15	0.45
1:E:226:LEU:N	1:E:227:PRO:CD	2.80	0.45
1:D:190:ASP:O	1:D:193:ALA:HB3	2.16	0.44
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.79	0.44
1:D:34:MET:HE2	1:D:224:THR:HG23	1.99	0.44
1:E:72:ASN:ND2	1:E:256:ALA:HB2	2.33	0.44
1:B:71:ARG:HH22	1:B:212:THR:HG22	1.82	0.44
1:E:44:TRP:O	1:E:48:LEU:HG	2.17	0.44
1:E:75:SER:OG	1:E:260:GLU:HG3	2.18	0.44
1:B:226:LEU:HG	1:B:230:LEU:CD1	2.47	0.44
1:E:89:VAL:HG23	1:E:195:VAL:HG11	1.99	0.44
1:E:207:VAL:N	1:E:208:PRO:CD	2.81	0.44
1:B:60:LEU:HD21	1:D:244:PHE:CE2	2.53	0.44
1:C:55:ALA:HB3	1:C:56:PRO:HD3	1.99	0.44
1:C:252:TRP:CH2	1:D:67:PHE:HB3	2.53	0.43
1:A:44:TRP:H	1:A:44:TRP:CD1	2.36	0.43
1:A:60:LEU:HD21	1:B:244:PHE:CD2	2.53	0.43
1:A:71:ARG:HD2	1:A:71:ARG:C	2.44	0.43
1:A:155:MET:HG2	1:B:282:ASN:OD1	2.18	0.43
1:B:271:PRO:CG	1:B:275:MET:HE3	2.42	0.43
1:E:205:THR:CB	1:E:206:PRO:CA	2.93	0.43
1:A:271:PRO:CG	1:A:275:MET:HE3	2.48	0.43
1:B:121:PHE:CE1	1:B:157:THR:HG22	2.53	0.43
1:D:60:LEU:HD23	1:D:222:PHE:HD1	1.84	0.43
1:E:161:LEU:HD23	1:E:161:LEU:HA	1.82	0.43
1:E:68:LEU:HB3	1:E:252:TRP:HD1	1.83	0.43
1:E:71:ARG:NH2	1:E:253:ASP:OD1	2.51	0.43
1:C:108:HIS:HA	1:C:111:HIS:ND1	2.34	0.43
1:A:166:ASN:ND2	1:B:102:ASN:ND2	2.65	0.43
1:B:52:LEU:HD23	1:D:234:LEU:HD22	2.01	0.43
1:A:78:ARG:NH1	1:A:205:THR:O	2.52	0.42
1:D:108:HIS:HB3	3:D:306:CL:CL	2.56	0.42
1:A:188:LYS:HA	1:A:188:LYS:HD3	1.66	0.42
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.89	0.42
1:B:238:THR:N	1:B:239:PRO:CD	2.81	0.42
1:D:89:VAL:CG2	1:D:195:VAL:HG11	2.49	0.42
1:C:180:ILE:HD12	1:D:180:ILE:CD1	2.49	0.42
1:D:71:ARG:HD2	1:D:71:ARG:O	2.19	0.42
1:A:95:THR:HG21	3:A:305:CL:CL	2.56	0.42
1:C:282:ASN:O	1:C:286:MET:HG3	2.19	0.42
1:A:111:HIS:O	1:A:115:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:TYR:O	1:B:224:THR:HG23	2.19	0.42
1:E:207:VAL:HG23	1:E:208:PRO:HD3	2.01	0.42
1:B:95:THR:OG1	1:B:188:LYS:HD2	2.20	0.42
1:B:241:VAL:O	1:B:241:VAL:HG12	2.19	0.42
1:C:237:MET:O	1:C:238:THR:C	2.63	0.42
1:B:89:VAL:CG2	1:B:195:VAL:HG11	2.49	0.42
1:E:89:VAL:CG2	1:E:195:VAL:HG11	2.50	0.42
1:E:43:GLN:HG3	1:E:44:TRP:H	1.85	0.41
1:A:109:ASP:HB3	1:A:113:ARG:NH1	2.34	0.41
1:B:288:GLY:HA3	5:B:304:ACY:H3	2.03	0.41
1:C:71:ARG:NH2	1:C:253:ASP:OD1	2.53	0.41
1:B:207:VAL:O	1:B:208:PRO:O	2.39	0.41
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.94	0.41
1:E:72:ASN:HD22	1:E:256:ALA:HB2	1.86	0.41
1:A:47:GLN:H	1:A:47:GLN:HG2	1.52	0.41
1:D:275:MET:O	1:D:279:ILE:HG13	2.21	0.41
1:E:208:PRO:O	1:E:210:ALA:N	2.48	0.41
1:A:25:ILE:O	1:A:29:LEU:HD12	2.21	0.41
1:B:54:VAL:O	1:B:57:PHE:N	2.49	0.41
1:C:205:THR:HG23	1:C:205:THR:O	2.21	0.41
1:D:40:ILE:HG13	1:D:41:SER:N	2.36	0.41
1:D:100:LEU:HD11	1:D:114:ILE:HG21	2.03	0.41
1:E:52:LEU:HB3	1:E:229:ALA:HA	2.03	0.41
1:B:180:ILE:CD1	1:D:180:ILE:HD12	2.51	0.41
1:B:226:LEU:N	1:B:227:PRO:HD2	2.36	0.41
1:D:188:LYS:HA	1:D:188:LYS:HD3	1.94	0.41
1:E:205:THR:HB	1:E:206:PRO:CA	2.43	0.41
1:E:279:ILE:HD12	1:E:279:ILE:HA	1.90	0.41
1:B:38:ALA:HB2	1:B:228:PHE:CD1	2.56	0.40
1:C:208:PRO:O	1:C:210:ALA:N	2.53	0.40
1:D:129:LEU:HD21	1:D:199:CYS:HB3	2.03	0.40
1:D:210:ALA:O	1:D:214:ILE:HG13	2.22	0.40
1:E:112:ARG:HH12	1:E:289:GLN:HG2	1.85	0.40
1:B:231:VAL:O	1:B:233:ASP:N	2.55	0.40
1:C:110:ALA:O	1:C:111:HIS:C	2.65	0.40
1:B:115:VAL:O	1:B:119:VAL:HG23	2.21	0.40
1:C:59:LEU:HD13	1:E:58:SER:HA	2.02	0.40
1:C:268:ASN:ND2	1:D:208:PRO:HB3	2.36	0.40
1:A:79:PHE:CE1	1:E:207:VAL:HG12	2.57	0.40
1:B:126:LYS:HB3	1:B:126:LYS:HE2	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/297 (90%)	260 (97%)	5 (2%)	3 (1%)	11	19
1	B	269/297 (91%)	252 (94%)	14 (5%)	3 (1%)	11	19
1	C	267/297 (90%)	257 (96%)	7 (3%)	3 (1%)	11	19
1	D	267/297 (90%)	258 (97%)	8 (3%)	1 (0%)	30	45
1	E	269/297 (91%)	260 (97%)	7 (3%)	2 (1%)	18	30
All	All	1340/1485 (90%)	1287 (96%)	41 (3%)	12 (1%)	14	24

All (12) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/259 (91%)	222 (94%)	13 (6%)	19	33
1	B	236/259 (91%)	218 (92%)	18 (8%)	12	21
1	C	234/259 (90%)	216 (92%)	18 (8%)	12	20
1	D	234/259 (90%)	216 (92%)	18 (8%)	12	20
1	E	236/259 (91%)	212 (90%)	24 (10%)	7	10
All	All	1175/1295 (91%)	1084 (92%)	91 (8%)	12	20

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	25	ILE
1	A	37	ILE
1	A	47	GLN
1	A	73	SER
1	A	78	ARG
1	A	95	THR
1	A	159	ARG
1	A	188	LYS
1	A	224	THR
1	A	243	VAL
1	A	260	GLU
1	A	289	GLN
1	B	30	LEU
1	B	48	LEU
1	B	50	ILE
1	B	58	SER
1	B	71	ARG
1	B	80	VAL
1	B	95	THR
1	B	126	LYS
1	B	146	ARG
1	B	154	SER
1	B	188	LYS
1	B	205	THR
1	B	207	VAL
1	B	211	TYR
1	B	214	ILE
1	B	215	LEU
1	B	231	VAL
1	B	238	THR

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Mol	Chain	Res	Type
1	C	23	LYS
1	C	25	ILE
1	C	37	ILE
1	C	45	TYR
1	C	51	HIS
1	C	53	THR
1	C	58	SER
1	C	84	ASN
1	C	95	THR
1	C	116	SER
1	C	146	ARG
1	C	155	MET
1	C	172	ARG
1	C	173	GLU
1	C	205	THR
1	C	213	LEU
1	C	214	ILE
1	C	243	VAL
1	D	24	ILE
1	D	25	ILE
1	D	27	ARG
1	D	30	LEU
1	D	35	SER
1	D	40	ILE
1	D	41	SER
1	D	51	HIS
1	D	72	ASN
1	D	83	ARG
1	D	95	THR
1	D	96	LEU
1	D	122	SER
1	D	148	THR
1	D	161	LEU
1	D	166	ASN
1	D	213	LEU
1	D	265	THR
1	E	32	VAL
1	E	36	ILE
1	E	58	SER
1	E	71	ARG
1	E	90	LEU
1	E	95	THR

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Mol	Chain	Res	Type
1	E	96	LEU
1	E	130	ARG
1	E	131	LYS
1	E	146	ARG
1	E	154	SER
1	E	188	LYS
1	E	202	LEU
1	E	205	THR
1	E	207	VAL
1	E	212	THR
1	E	225	LEU
1	E	243	VAL
1	E	254	SER
1	E	272	LEU
1	E	275	MET
1	E	279	ILE
1	E	292	LEU
1	E	294	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	47	GLN
1	A	84	ASN
1	A	158	ASN
1	A	166	ASN
1	A	268	ASN
1	B	43	GLN
1	B	166	ASN
1	C	99	GLN
1	C	102	ASN
1	C	166	ASN
1	C	268	ASN
1	D	72	ASN
1	E	31	ASN
1	E	43	GLN
1	E	166	ASN
1	E	282	ASN
1	E	289	GLN

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 34 ligands modelled in this entry, 30 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	A	308	-	3,3,3	0.56	0	2,2,2	0.37	0
5	ACY	E	307	2	3,3,3	1.36	0	3,3,3	2.38	2 (66%)
7	PG4	E	306	-	12,12,12	0.71	0	11,11,11	0.57	0
5	ACY	B	304	2	3,3,3	1.31	0	3,3,3	1.66	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	308	-	-	1/1/1/1	-
7	PG4	E	306	-	-	7/10/10/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	E	307	ACY	OXT-C-O	-3.17	110.26	122.03
5	E	307	ACY	OXT-C-CH3	2.61	125.98	115.05
5	B	304	ACY	OXT-C-CH3	2.04	123.59	115.05
5	B	304	ACY	OXT-C-O	-2.03	114.51	122.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	307	ACY	1	0
7	E	306	PG4	1	0
5	B	304	ACY	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%)	0.39	33 (12%) 8 7	39, 60, 126, 151	0
1	B	271/297 (91%)	0.38	34 (12%) 8 6	39, 69, 122, 157	0
1	C	269/297 (90%)	0.57	27 (10%) 12 10	41, 65, 138, 203	0
1	D	269/297 (90%)	1.06	53 (19%) 3 2	46, 75, 127, 157	0
1	E	271/297 (91%)	0.50	45 (16%) 4 3	41, 62, 115, 160	0
All	All	1350/1485 (90%)	0.58	192 (14%) 6 5	39, 66, 126, 203	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	PHE	10.5
1	C	47	GLN	10.2
1	D	145	GLU	10.2
1	E	204	THR	10.1
1	D	173	GLU	9.3
1	D	265	THR	7.5
1	D	130	ARG	7.5
1	C	291	PRO	7.2
1	D	131	LYS	6.9
1	D	170	GLN	6.8
1	D	233	ASP	6.4
1	A	175	GLY	6.3
1	C	51	HIS	6.2
1	B	46	GLU	6.1
1	C	210	ALA	6.0
1	D	146	ARG	6.0
1	E	42	TYR	5.9
1	D	46	GLU	5.9
1	D	236	TYR	5.9
1	D	264	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	21	LEU	5.8
1	C	106	ALA	5.6
1	C	26	PHE	5.6
1	A	21	LEU	5.6
1	D	166	ASN	5.0
1	B	292	LEU	5.0
1	B	207	VAL	5.0
1	A	290	HIS	4.9
1	C	207	VAL	4.9
1	A	288	GLY	4.8
1	B	211	TYR	4.8
1	C	204	THR	4.7
1	D	42	TYR	4.6
1	D	174	ALA	4.6
1	A	228	PHE	4.6
1	E	61	GLY	4.5
1	E	206	PRO	4.5
1	E	208	PRO	4.5
1	B	34	MET	4.5
1	C	206	PRO	4.4
1	E	209	PHE	4.4
1	D	220	TYR	4.4
1	D	47	GLN	4.3
1	D	235	HIS	4.3
1	A	232	GLY	4.3
1	D	268	ASN	4.2
1	B	204	THR	4.2
1	D	132	THR	4.1
1	E	58	SER	4.1
1	C	48	LEU	4.0
1	E	235	HIS	4.0
1	B	210	ALA	4.0
1	C	240	PHE	4.0
1	D	267	ALA	4.0
1	D	266	ALA	3.9
1	B	49	GLY	3.9
1	D	51	HIS	3.9
1	C	44	TRP	3.8
1	B	48	LEU	3.8
1	C	49	GLY	3.8
1	D	204	THR	3.7
1	D	209	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	64	ILE	3.7
1	A	174	ALA	3.7
1	D	149	GLU	3.7
1	C	213	LEU	3.6
1	A	44	TRP	3.6
1	E	266	ALA	3.5
1	B	40	ILE	3.5
1	B	26	PHE	3.5
1	A	45	TYR	3.5
1	E	39	ILE	3.5
1	B	51	HIS	3.5
1	C	46	GLU	3.4
1	D	206	PRO	3.4
1	D	269	ASP	3.4
1	A	204	THR	3.3
1	C	184	LEU	3.3
1	D	232	GLY	3.3
1	D	289	GLN	3.3
1	A	235	HIS	3.2
1	E	38	ALA	3.2
1	D	207	VAL	3.2
1	D	44	TRP	3.1
1	E	210	ALA	3.1
1	C	105	PRO	3.1
1	E	170	GLN	3.1
1	C	40	ILE	3.1
1	E	264	GLY	3.0
1	D	144	GLU	3.0
1	B	216	GLN	3.0
1	E	173	GLU	3.0
1	A	42	TYR	3.0
1	E	47	GLN	3.0
1	E	261	ASP	3.0
1	E	211	TYR	3.0
1	E	236	TYR	3.0
1	C	208	PRO	2.9
1	B	212	THR	2.9
1	B	224	THR	2.9
1	D	23	LYS	2.9
1	B	45	TYR	2.9
1	B	37	ILE	2.9
1	B	205	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	209	PHE	2.9
1	C	268	ASN	2.9
1	D	273	ASN	2.9
1	B	220	TYR	2.9
1	E	265	THR	2.8
1	A	173	GLU	2.8
1	E	44	TRP	2.8
1	A	47	GLN	2.7
1	B	33	LEU	2.7
1	E	35	SER	2.7
1	A	34	MET	2.7
1	D	231	VAL	2.7
1	D	211	TYR	2.7
1	B	50	ILE	2.7
1	E	37	ILE	2.7
1	B	228	PHE	2.7
1	E	45	TYR	2.7
1	E	25	ILE	2.7
1	D	224	THR	2.6
1	D	27	ARG	2.6
1	E	43	GLN	2.6
1	E	172	ARG	2.6
1	A	289	GLN	2.6
1	E	48	LEU	2.6
1	A	51	HIS	2.6
1	B	42	TYR	2.5
1	B	53	THR	2.5
1	B	236	TYR	2.5
1	B	208	PRO	2.5
1	B	23	LYS	2.5
1	B	213	LEU	2.5
1	A	190	ASP	2.4
1	C	27	ARG	2.4
1	D	112	ARG	2.4
1	D	24	ILE	2.4
1	D	167	GLU	2.4
1	C	43	GLN	2.4
1	E	174	ALA	2.4
1	E	40	ILE	2.4
1	B	206	PRO	2.4
1	E	232	GLY	2.4
1	D	243	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	220	TYR	2.4
1	C	30	LEU	2.4
1	B	235	HIS	2.4
1	A	26	PHE	2.3
1	E	57	PHE	2.3
1	B	225	LEU	2.3
1	E	207	VAL	2.3
1	C	211	TYR	2.3
1	E	222	PHE	2.3
1	A	52	LEU	2.3
1	A	177	LEU	2.3
1	A	224	THR	2.2
1	D	205	THR	2.2
1	A	30	LEU	2.2
1	E	205	THR	2.2
1	A	236	TYR	2.2
1	D	187	ASN	2.2
1	B	47	GLN	2.2
1	D	186	ASP	2.2
1	D	288	GLY	2.2
1	E	34	MET	2.2
1	D	48	LEU	2.2
1	D	169	GLY	2.2
1	E	252	TRP	2.1
1	D	221	LEU	2.1
1	A	92	ALA	2.1
1	C	266	ALA	2.1
1	E	31	ASN	2.1
1	E	49	GLY	2.1
1	D	40	ILE	2.1
1	E	24	ILE	2.1
1	E	249	PHE	2.1
1	A	216	GLN	2.1
1	D	43	GLN	2.1
1	E	26	PHE	2.1
1	C	59	LEU	2.1
1	E	213	LEU	2.1
1	A	40	ILE	2.1
1	B	240	PHE	2.1
1	E	228	PHE	2.1
1	A	23	LYS	2.0
1	A	221	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	43	GLN	2.0
1	D	129	LEU	2.0
1	A	176	LYS	2.0
1	A	140	ARG	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 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($\text{\AA}^2$)	Q<0.9
5	ACY	E	307	4/4	0.62	0.27	44,50,50,51	0
5	ACY	B	304	4/4	0.64	0.23	55,57,58,68	0
2	ZN	C	307	1/1	0.76	0.13	140,140,140,140	0
2	ZN	E	305	1/1	0.87	0.21	177,177,177,177	0
6	NA	D	308	1/1	0.90	0.30	74,74,74,74	0
7	PG4	E	306	13/13	0.90	0.21	72,83,96,102	0
2	ZN	D	304	1/1	0.94	0.12	128,128,128,128	0
2	ZN	D	303	1/1	0.94	0.06	98,98,98,98	0
3	CL	C	306	1/1	0.96	0.16	86,86,86,86	0
4	EDO	A	308	4/4	0.96	0.12	60,72,74,78	0
2	ZN	B	301	1/1	0.96	0.09	117,117,117,117	0
3	CL	D	306	1/1	0.97	0.09	91,91,91,91	0
3	CL	B	303	1/1	0.97	0.15	86,86,86,86	0
3	CL	E	304	1/1	0.98	0.07	66,66,66,66	0
3	CL	A	305	1/1	0.98	0.13	64,64,64,64	0
3	CL	C	305	1/1	0.98	0.08	78,78,78,78	0
3	CL	A	306	1/1	0.98	0.05	76,76,76,76	0
3	CL	D	305	1/1	0.98	0.05	84,84,84,84	0
3	CL	A	307	1/1	0.98	0.06	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	E	302	1/1	0.99	0.07	54,54,54,54	0
2	ZN	C	302	1/1	0.99	0.03	73,73,73,73	0
2	ZN	A	304	1/1	0.99	0.02	66,66,66,66	0
3	CL	C	304	1/1	0.99	0.12	63,63,63,63	0
3	CL	D	307	1/1	0.99	0.06	80,80,80,80	0
3	CL	E	303	1/1	0.99	0.03	69,69,69,69	0
2	ZN	A	303	1/1	1.00	0.01	68,68,68,68	0
2	ZN	C	303	1/1	1.00	0.01	62,62,62,62	0
2	ZN	A	301	1/1	1.00	0.02	61,61,61,61	0
2	ZN	D	301	1/1	1.00	0.01	70,70,70,70	0
2	ZN	D	302	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	B	302	1/1	1.00	0.04	56,56,56,56	0
2	ZN	E	301	1/1	1.00	0.02	58,58,58,58	0
2	ZN	C	301	1/1	1.00	0.04	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.