



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:29 PM UTC

PDB ID : 6IVK / pdb_00006ivk
Title : Crystal structure of a membrane protein G175A
Authors : Kittredge, A.; Fukuda, F.; Zhang, Y.; Yang, T.
Deposited on : 2018-12-04
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

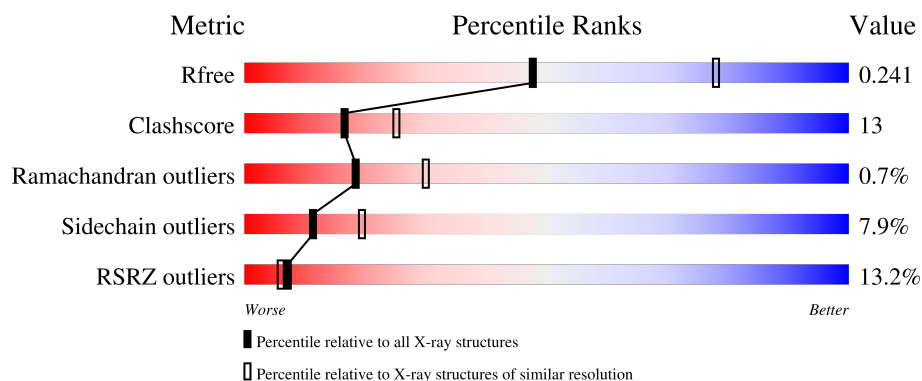
1 Overall quality at a glance

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	10% 68% 20% • 10%
1	B	297	15% 64% 23% • 8%
1	C	297	10% 69% 18% • 9%
1	D	297	13% 68% 20% • 10%
1	E	297	12% 63% 25% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACY	A	306	-	-	-	X
5	CL	C	305	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10934 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ibestrophin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2136	1384	361	382	9			
1	B	272	Total	C	N	O	S	0	0	0
			2168	1406	367	386	9			
1	C	270	Total	C	N	O	S	0	0	0
			2147	1389	365	384	9			
1	D	268	Total	C	N	O	S	0	0	0
			2136	1384	361	382	9			
1	E	271	Total	C	N	O	S	0	0	0
			2163	1402	365	387	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP W9BH30
A	-1	ASN	-	expression tag	UNP W9BH30
A	0	ALA	-	expression tag	UNP W9BH30
A	175	ALA	GLY	engineered mutation	UNP W9BH30
B	-2	SER	-	expression tag	UNP W9BH30
B	-1	ASN	-	expression tag	UNP W9BH30
B	0	ALA	-	expression tag	UNP W9BH30
B	175	ALA	GLY	engineered mutation	UNP W9BH30
C	-2	SER	-	expression tag	UNP W9BH30
C	-1	ASN	-	expression tag	UNP W9BH30
C	0	ALA	-	expression tag	UNP W9BH30
C	175	ALA	GLY	engineered mutation	UNP W9BH30
D	-2	SER	-	expression tag	UNP W9BH30
D	-1	ASN	-	expression tag	UNP W9BH30
D	0	ALA	-	expression tag	UNP W9BH30
D	175	ALA	GLY	engineered mutation	UNP W9BH30
E	-2	SER	-	expression tag	UNP W9BH30
E	-1	ASN	-	expression tag	UNP W9BH30
E	0	ALA	-	expression tag	UNP W9BH30

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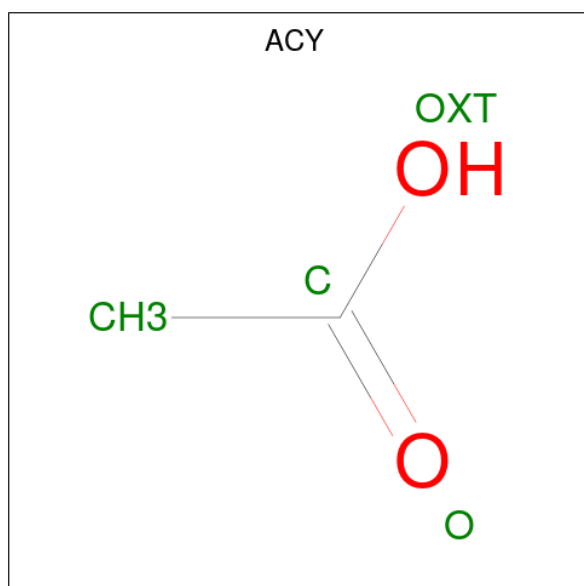
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Chain	Residue	Modelled	Actual	Comment	Reference
E	175	ALA	GLY	engineered mutation	UNP W9BH30

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

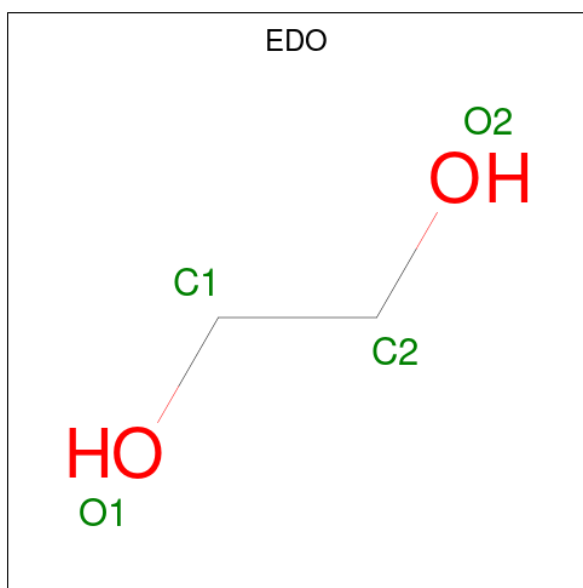
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Zn 4 4	0	0
2	B	2	Total Zn 2 2	0	0
2	C	4	Total Zn 4 4	0	0
2	D	4	Total Zn 4 4	0	0
2	E	2	Total Zn 2 2	0	0

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

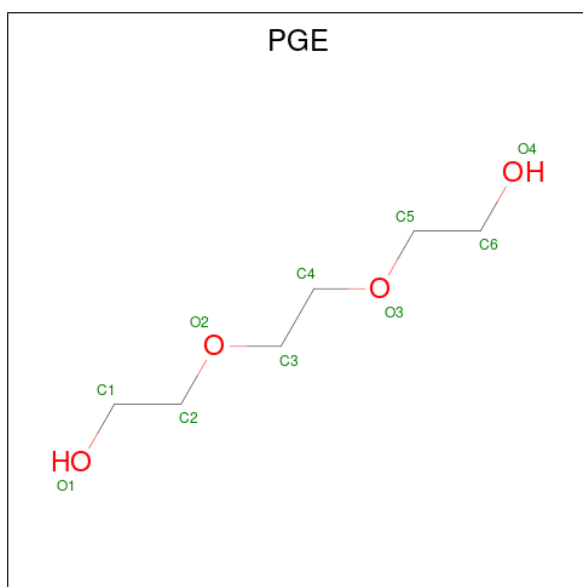


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

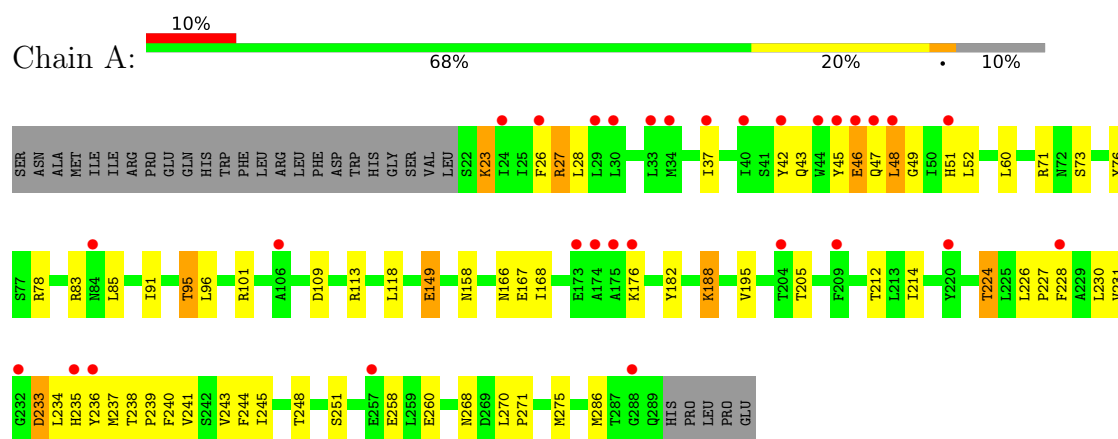
- Molecule 7 is water.

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

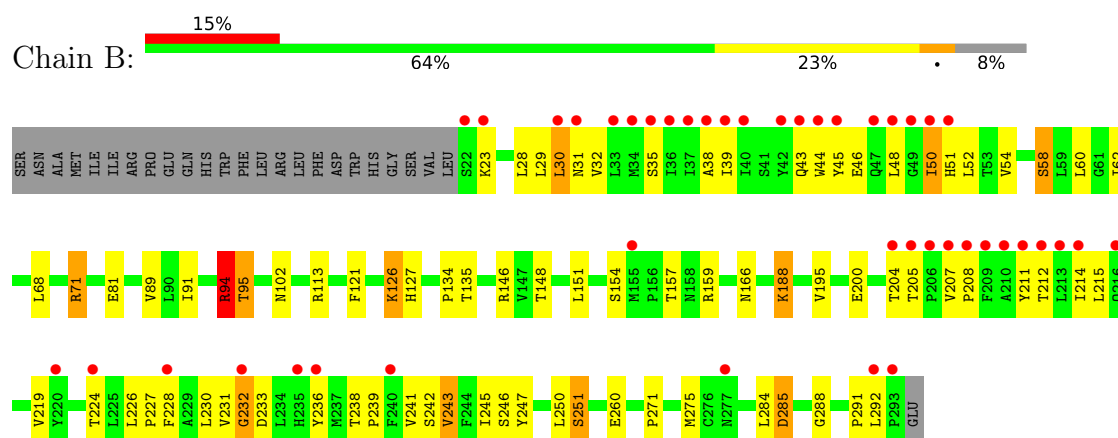
3 Residue-property plots [i](#)

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.

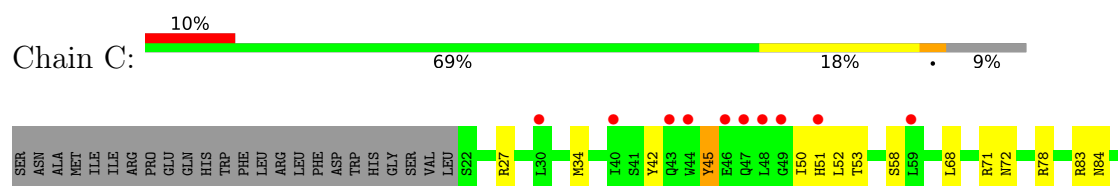
• Molecule 1: Ibestrophin

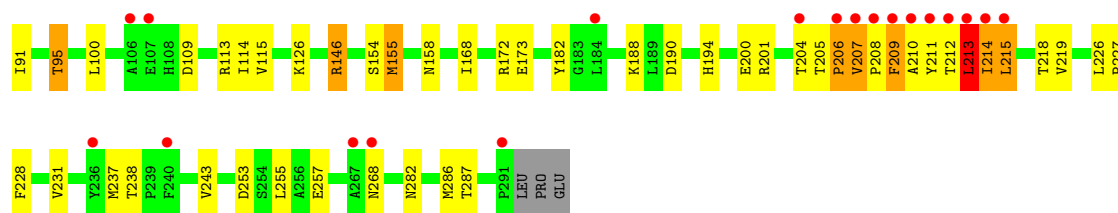


• Molecule 1: Ibestrophin

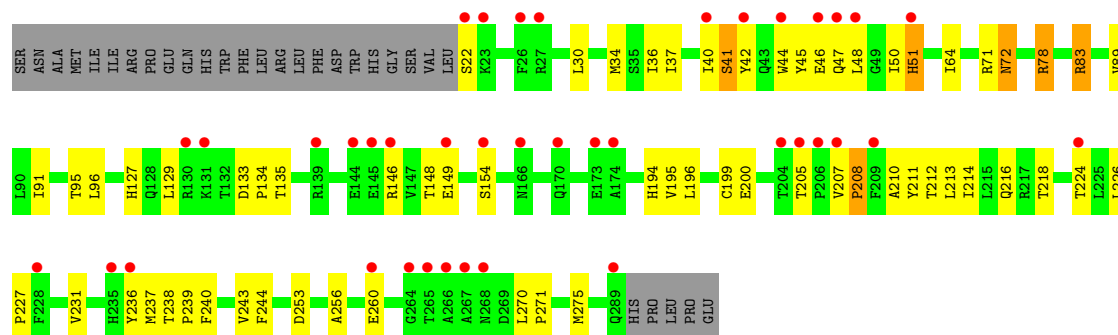


• Molecule 1: Ibestrophin

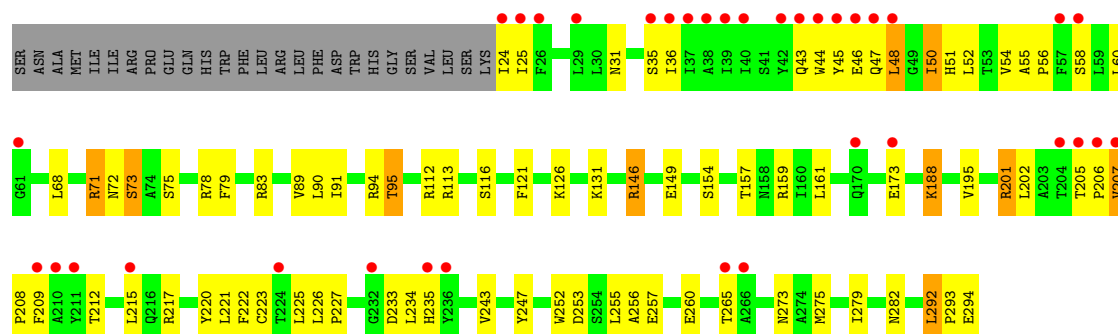




● Molecule 1: Ibestrophin



● 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	113.55Å 159.42Å 161.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.64 – 2.65 48.64 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.64-2.65) 99.9 (48.64-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.201 , 0.241 0.201 , 0.241	Depositor DCC
R_{free} test set	4277 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10934	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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: PGE, ZN, CL, ACY, 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	0.53	0/2182	1.14	3/2970 (0.1%)
1	B	0.54	0/2217	1.11	1/3020 (0.0%)
1	C	0.54	0/2194	1.11	6/2988 (0.2%)
1	D	0.50	0/2182	1.06	1/2970 (0.0%)
1	E	0.57	0/2212	1.17	3/3013 (0.1%)
All	All	0.54	0/10987	1.12	14/14961 (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	B	0	3
1	C	0	2
1	E	0	2
All	All	0	7

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	78	ARG	CB-CA-C	7.03	122.81	110.85
1	C	206	PRO	CA-C-N	6.61	134.36	122.13
1	C	206	PRO	C-N-CA	6.61	134.36	122.13
1	E	201	ARG	CB-CA-C	6.45	121.81	110.85
1	A	167	GLU	CA-C-N	5.31	127.97	120.42
1	A	167	GLU	C-N-CA	5.31	127.97	120.42
1	C	206	PRO	O-C-N	5.22	128.75	122.23
1	E	207	VAL	CA-C-N	5.21	124.52	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	207	VAL	C-N-CA	5.21	124.52	118.85
1	C	213	LEU	N-CA-C	-5.18	105.63	111.28
1	C	72	ASN	CB-CA-C	5.16	120.18	110.63
1	B	148	THR	CB-CA-C	5.15	120.02	109.67
1	A	212	THR	CB-CA-C	5.09	120.45	110.67
1	C	200	GLU	CB-CA-C	-5.04	102.96	110.88

There are no chirality outliers.

All (7) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2136	0	2183	77	0
1	B	2168	0	2215	67	0
1	C	2147	0	2190	63	0
1	D	2136	0	2183	39	0
1	E	2163	0	2203	83	1
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	2	0	0	0	0
3	A	8	0	6	0	0
3	B	4	0	3	1	0
3	E	4	0	3	0	0
4	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	4	0	6	0	0
5	A	3	0	0	1	0
5	B	1	0	0	1	0
5	C	2	0	0	2	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
6	E	10	0	14	1	0
7	A	30	0	0	2	0
7	B	31	0	0	1	0
7	C	22	0	0	0	0
7	D	22	0	0	2	1
7	E	19	0	0	1	0
All	All	10934	0	11012	282	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (282) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:VAL:HG22	1:C:208:PRO:CD	1.56	1.36
1:C:207:VAL:CG2	1:C:208:PRO:HD2	1.70	1.21
1:D:133:ASP:OD2	7:D:401:HOH:O	1.54	1.19
1:C:210:ALA:O	1:C:214:ILE:HG13	1.45	1.14
1:D:51:HIS:HB2	7:D:419:HOH:O	1.48	1.10
1:E:207:VAL:H	1:E:208:PRO:HD2	1.25	1.01
1:E:205:THR:HB	1:E:206:PRO:HA	1.39	1.01
1:E:207:VAL:N	1:E:208:PRO:HD2	1.77	1.00
1:A:83:ARG:CZ	1:E:205:THR:HG22	1.91	0.99
1:A:83:ARG:HH12	1:E:205:THR:CG2	1.75	0.98
1:A:83:ARG:NH1	1:E:205:THR:HG22	1.82	0.95
1:E:201:ARG:O	1:E:205:THR:HG23	1.67	0.94
1:A:83:ARG:NH1	1:E:205:THR:CG2	2.30	0.93
1:A:149:GLU:HG2	1:B:291:PRO:HG3	1.51	0.92
1:E:207:VAL:H	1:E:208:PRO:CD	1.82	0.90
1:A:49:GLY:HA3	1:B:236:TYR:CD2	2.07	0.90
1:E:44:TRP:O	1:E:48:LEU:HD13	1.73	0.88
1:E:207:VAL:N	1:E:208:PRO:CD	2.39	0.86
1:C:207:VAL:HG22	1:C:208:PRO:HD2	0.86	0.85
1:A:83:ARG:HH12	1:E:205:THR:HG21	1.38	0.85
1:A:83:ARG:NH2	1:E:205:THR:HG22	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ARG:HG2	1:D:270:LEU:HD21	1.57	0.84
1:E:206:PRO:HB2	1:E:208:PRO:HD2	1.58	0.84
1:D:78:ARG:NH1	1:D:205:THR:O	2.11	0.83
1:A:27:ARG:HH21	1:A:27:ARG:CG	1.93	0.82
1:B:35:SER:OG	1:B:239:PRO:HA	1.82	0.80
1:C:210:ALA:O	1:C:214:ILE:CG1	2.30	0.80
1:C:214:ILE:O	1:C:218:THR:HB	1.82	0.79
1:B:28:LEU:HD22	1:B:243:VAL:HG22	1.66	0.77
1:C:155:MET:HG2	1:C:158:ASN:HB2	1.65	0.77
1:C:207:VAL:HG22	1:C:208:PRO:HD3	1.66	0.76
1:C:207:VAL:CG2	1:C:208:PRO:CD	2.46	0.76
1:B:271:PRO:HG2	1:B:275:MET:HE3	1.67	0.75
1:B:29:LEU:C	1:B:31:ASN:H	1.94	0.75
1:A:49:GLY:HA3	1:B:236:TYR:HD2	1.49	0.75
1:C:42:TYR:O	1:C:45:TYR:HB2	1.87	0.74
1:E:94:ARG:HH21	1:E:282:ASN:HD21	1.36	0.73
1:C:213:LEU:C	1:C:213:LEU:HD23	2.13	0.72
1:A:52:LEU:HD12	1:A:228:PHE:HB3	1.72	0.72
1:A:258:GLU:CD	1:A:268:ASN:HD22	1.98	0.72
1:E:205:THR:CB	1:E:206:PRO:HA	2.17	0.71
1:C:91:ILE:O	1:C:95:THR:HG23	1.91	0.70
1:A:52:LEU:CD1	1:A:228:PHE:HB3	2.21	0.70
1:E:60:LEU:HD23	1:E:222:PHE:HD1	1.57	0.69
1:C:68:LEU:HD21	1:C:215:LEU:HD12	1.75	0.69
1:E:226:LEU:N	1:E:227:PRO:HD2	2.08	0.68
1:A:168:ILE:HG22	1:A:182:TYR:CE1	2.28	0.68
1:B:51:HIS:NE2	7:B:401:HOH:O	2.27	0.68
1:A:49:GLY:CA	1:B:236:TYR:HD2	2.06	0.68
1:D:91:ILE:O	1:D:95:THR:HG23	1.95	0.67
1:E:91:ILE:O	1:E:95:THR:HG23	1.94	0.67
1:C:214:ILE:O	1:C:218:THR:CB	2.43	0.67
1:B:91:ILE:O	1:B:95:THR:HG23	1.95	0.66
1:E:205:THR:HB	1:E:206:PRO:CA	2.21	0.66
1:A:27:ARG:HH21	1:A:27:ARG:HG3	1.61	0.65
1:C:190:ASP:OD1	5:C:305:CL:CL	2.53	0.64
1:E:292:LEU:HD22	1:E:293:PRO:HD2	1.80	0.63
1:B:71:ARG:HH22	1:B:212:THR:HG22	1.62	0.63
1:E:24:ILE:HG23	1:E:25:ILE:H	1.62	0.63
1:A:91:ILE:O	1:A:95:THR:HG23	1.97	0.63
1:B:44:TRP:O	1:B:48:LEU:HD12	1.99	0.63
1:A:109:ASP:HB3	1:A:113:ARG:HH12	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:LEU:CD2	1:E:247:TYR:OH	2.48	0.61
1:A:83:ARG:NH2	1:E:205:THR:CG2	2.62	0.61
1:E:72:ASN:HD22	1:E:256:ALA:HB2	1.66	0.60
1:D:226:LEU:N	1:D:227:PRO:HD2	2.16	0.60
1:D:30:LEU:O	1:D:34:MET:HG2	2.01	0.60
1:E:235:HIS:NE2	7:E:401:HOH:O	1.99	0.60
1:A:27:ARG:HH21	1:A:27:ARG:HG2	1.66	0.60
1:C:205:THR:HG23	1:C:205:THR:O	2.02	0.60
1:E:94:ARG:HH21	1:E:282:ASN:ND2	2.00	0.59
1:A:49:GLY:HA3	1:B:236:TYR:CE2	2.38	0.59
1:A:83:ARG:HH22	1:E:205:THR:CG2	2.16	0.58
1:B:231:VAL:HG13	1:B:232:GLY:N	2.18	0.58
1:B:71:ARG:HH12	1:B:212:THR:HG23	1.68	0.58
1:A:46:GLU:O	1:A:46:GLU:HG3	2.03	0.58
1:B:39:ILE:HD13	1:B:236:TYR:HA	1.85	0.58
1:C:194:HIS:HA	1:E:91:ILE:HD13	1.86	0.57
1:E:75:SER:OG	1:E:260:GLU:HG3	2.03	0.57
1:C:207:VAL:HG23	1:E:79:PHE:CE2	2.39	0.57
1:E:207:VAL:HG23	1:E:208:PRO:HD3	1.87	0.57
1:A:76:TYR:CE1	1:E:207:VAL:HG21	2.39	0.56
1:A:271:PRO:HD2	1:A:275:MET:HE3	1.87	0.56
1:C:226:LEU:N	1:C:227:PRO:HD2	2.19	0.56
1:E:90:LEU:HD13	1:E:279:ILE:HD13	1.87	0.56
1:A:96:LEU:HD23	1:A:118:LEU:HD11	1.87	0.56
1:A:42:TYR:O	1:A:45:TYR:HB2	2.05	0.56
1:B:29:LEU:C	1:B:31:ASN:N	2.60	0.56
1:B:200:GLU:O	1:B:204:THR:HG23	2.06	0.56
1:E:73:SER:HA	6:E:305:PGE:H52	1.88	0.56
1:C:68:LEU:CD2	1:C:215:LEU:HD12	2.36	0.55
1:A:230:LEU:HB3	1:A:234:LEU:HD12	1.87	0.55
1:D:37:ILE:O	1:D:41:SER:HB3	2.06	0.55
1:A:42:TYR:HA	1:A:45:TYR:CD1	2.41	0.55
1:B:215:LEU:O	1:B:219:VAL:HG23	2.07	0.55
1:C:207:VAL:CB	1:C:208:PRO:HD2	2.33	0.55
1:A:83:ARG:NH1	1:E:205:THR:HG21	2.09	0.54
1:C:208:PRO:O	1:C:210:ALA:N	2.35	0.54
1:D:236:TYR:O	1:D:239:PRO:HD2	2.08	0.54
1:C:215:LEU:O	1:C:219:VAL:HG23	2.07	0.54
1:B:60:LEU:HD21	1:D:244:PHE:CE2	2.43	0.54
1:C:78:ARG:HH12	1:C:205:THR:CG2	2.21	0.54
1:D:83:ARG:HG2	1:D:270:LEU:CD2	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:HH12	1:C:205:THR:HG23	1.73	0.54
1:E:71:ARG:HH12	1:E:212:THR:HG23	1.74	0.53
1:A:47:GLN:HE21	1:A:47:GLN:HA	1.74	0.53
1:E:94:ARG:HE	1:E:282:ASN:HD22	1.57	0.53
1:C:42:TYR:HA	1:C:45:TYR:CD1	2.44	0.53
1:C:68:LEU:CD2	1:C:215:LEU:CD1	2.87	0.53
1:A:258:GLU:CD	1:A:268:ASN:ND2	2.66	0.53
1:D:240:PHE:O	1:D:243:VAL:HG12	2.09	0.53
1:B:246:SER:O	1:B:250:LEU:HD12	2.10	0.52
1:B:29:LEU:HA	1:B:32:VAL:HG23	1.91	0.52
1:B:227:PRO:HA	1:B:230:LEU:HB2	1.90	0.52
1:B:236:TYR:C	1:B:238:THR:H	2.18	0.52
1:A:78:ARG:NH1	1:A:205:THR:O	2.42	0.52
1:A:101:ARG:HD2	1:A:286:MET:O	2.09	0.52
1:B:231:VAL:HG13	1:B:232:GLY:H	1.72	0.52
1:B:224:THR:O	1:B:227:PRO:HD2	2.09	0.52
1:D:71:ARG:HD2	1:D:71:ARG:C	2.34	0.52
1:A:258:GLU:OE1	1:A:268:ASN:ND2	2.43	0.52
1:A:42:TYR:CE2	1:A:235:HIS:CE1	2.98	0.52
1:A:43:GLN:C	1:A:45:TYR:H	2.17	0.52
1:E:226:LEU:N	1:E:227:PRO:CD	2.73	0.52
1:B:29:LEU:O	1:B:31:ASN:N	2.43	0.52
1:E:48:LEU:CD1	1:E:48:LEU:N	2.73	0.52
1:A:236:TYR:CB	1:E:50:ILE:HG22	2.39	0.52
1:D:196:LEU:O	1:D:200:GLU:HG3	2.10	0.51
1:A:76:TYR:HE1	1:E:207:VAL:HG21	1.75	0.51
1:E:233:ASP:C	1:E:234:LEU:HD23	2.36	0.51
1:A:236:TYR:HB3	1:E:50:ILE:HG22	1.92	0.51
1:A:231:VAL:C	1:A:233:ASP:H	2.19	0.51
1:D:36:ILE:HG13	1:D:37:ILE:N	2.26	0.51
1:C:83:ARG:HG2	1:D:205:THR:HG21	1.91	0.50
1:B:89:VAL:CG2	1:B:195:VAL:HG11	2.41	0.50
1:C:205:THR:OG1	1:E:83:ARG:HD3	2.11	0.50
1:C:68:LEU:HG	1:C:215:LEU:HD11	1.94	0.50
1:E:24:ILE:HG23	1:E:25:ILE:N	2.25	0.50
1:A:95:THR:HG21	5:A:308:CL:CL	2.48	0.50
1:B:231:VAL:O	1:B:233:ASP:N	2.45	0.49
1:E:78:ARG:NH2	1:E:205:THR:OG1	2.42	0.49
1:A:76:TYR:HE1	1:E:207:VAL:CG2	2.25	0.49
1:B:39:ILE:CD1	1:B:236:TYR:HA	2.42	0.49
1:B:71:ARG:HG3	1:B:215:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:MET:HE3	1:C:228:PHE:HE1	1.78	0.49
1:D:231:VAL:HA	1:D:238:THR:OG1	2.12	0.49
1:A:49:GLY:C	1:B:236:TYR:HD2	2.20	0.49
1:E:71:ARG:HD3	1:E:260:GLU:OE2	2.13	0.48
1:E:47:GLN:OE1	1:E:47:GLN:HA	2.14	0.48
1:A:23:LYS:O	1:A:23:LYS:HD3	2.14	0.48
1:C:78:ARG:NH1	1:C:205:THR:HG23	2.28	0.48
1:D:207:VAL:O	1:D:208:PRO:C	2.56	0.48
1:C:50:ILE:O	1:C:50:ILE:HG13	2.14	0.48
1:A:224:THR:O	1:A:227:PRO:HD2	2.13	0.48
1:B:135:THR:HG23	1:B:151:LEU:HD11	1.96	0.47
1:B:204:THR:OG1	1:B:205:THR:N	2.47	0.47
1:E:146:ARG:NH2	1:E:149:GLU:OE2	2.48	0.47
1:A:271:PRO:O	1:A:275:MET:HG3	2.15	0.47
1:C:204:THR:C	1:C:206:PRO:HD3	2.40	0.47
1:E:31:ASN:ND2	1:E:223:CYS:O	2.47	0.47
1:C:205:THR:OG1	1:E:83:ARG:CD	2.63	0.47
1:E:94:ARG:HE	1:E:282:ASN:ND2	2.12	0.47
1:C:115:VAL:HG21	1:C:287:THR:HG21	1.97	0.47
1:A:226:LEU:N	1:A:227:PRO:HD2	2.31	0.46
1:E:126:LYS:HE3	1:E:273:ASN:OD1	2.15	0.46
1:E:71:ARG:NH1	1:E:212:THR:HG23	2.30	0.46
1:B:45:TYR:HB3	1:B:50:ILE:O	2.16	0.46
1:B:127:HIS:CD2	1:B:134:PRO:HA	2.51	0.46
1:B:146:ARG:HA	1:B:146:ARG:HD3	1.78	0.46
1:E:55:ALA:N	1:E:56:PRO:HD2	2.30	0.46
1:A:42:TYR:HE2	1:A:235:HIS:CE1	2.32	0.46
1:B:226:LEU:N	1:B:227:PRO:CD	2.79	0.46
1:D:271:PRO:HG2	1:D:275:MET:HE3	1.98	0.46
1:D:64:ILE:HD11	1:D:218:THR:HG22	1.97	0.45
1:A:23:LYS:O	1:A:26:PHE:HB3	2.16	0.45
1:A:46:GLU:HB2	1:A:51:HIS:NE2	2.31	0.45
1:A:188:LYS:HA	1:A:188:LYS:HD3	1.63	0.45
1:A:27:ARG:HG3	1:A:27:ARG:NH2	2.27	0.45
1:A:27:ARG:CG	1:A:27:ARG:NH2	2.63	0.45
1:D:89:VAL:CG2	1:D:195:VAL:HG11	2.47	0.45
1:C:213:LEU:C	1:C:213:LEU:CD2	2.85	0.45
1:C:213:LEU:HD23	1:E:247:TYR:OH	2.17	0.45
1:D:89:VAL:HG23	1:D:195:VAL:HG11	1.99	0.45
1:C:213:LEU:HD21	1:E:247:TYR:OH	2.16	0.45
1:E:217:ARG:HA	1:E:220:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HH22	1:E:205:THR:HG23	1.81	0.44
1:D:212:THR:HG23	1:D:216:GLN:HG3	1.99	0.44
1:A:60:LEU:HD13	1:B:245:ILE:HG12	1.99	0.44
1:B:43:GLN:O	1:B:46:GLU:HB2	2.17	0.44
1:A:109:ASP:HB3	1:A:113:ARG:NH1	2.31	0.44
1:C:27:ARG:HD2	1:C:27:ARG:HA	1.88	0.44
1:D:71:ARG:NH2	1:D:253:ASP:OD1	2.50	0.44
1:A:83:ARG:HG3	1:A:270:LEU:HD21	1.98	0.44
1:A:235:HIS:ND1	7:A:401:HOH:O	2.36	0.44
1:A:237:MET:HE3	1:E:52:LEU:HD21	2.00	0.44
1:D:129:LEU:HD21	1:D:199:CYS:HB3	2.00	0.44
1:B:29:LEU:O	1:B:32:VAL:N	2.49	0.44
1:B:247:TYR:O	1:B:251:SER:HB2	2.18	0.44
1:B:28:LEU:HD23	1:B:28:LEU:HA	1.79	0.44
5:C:305:CL:CL	1:E:188:LYS:HE2	2.55	0.44
1:B:58:SER:O	1:B:62:ILE:HG13	2.17	0.44
1:B:188:LYS:HE2	5:B:304:CL:CL	2.54	0.44
1:D:226:LEU:N	1:D:227:PRO:CD	2.79	0.44
1:C:211:TYR:CE1	1:E:255:LEU:HD21	2.53	0.43
1:A:91:ILE:O	1:A:95:THR:CG2	2.66	0.43
1:B:288:GLY:HA3	3:B:303:ACY:H2	2.00	0.43
1:C:45:TYR:OH	1:C:52:LEU:HD12	2.18	0.43
1:C:71:ARG:NH2	1:C:253:ASP:OD1	2.51	0.43
1:E:68:LEU:HB3	1:E:252:TRP:HD1	1.83	0.43
1:C:282:ASN:O	1:C:286:MET:HG3	2.17	0.43
1:E:95:THR:OG1	1:E:188:LYS:HD2	2.18	0.43
1:E:161:LEU:HD23	1:E:161:LEU:HA	1.84	0.43
1:A:168:ILE:HG22	1:A:182:TYR:CD1	2.54	0.43
1:B:284:LEU:O	1:B:285:ASP:C	2.61	0.43
1:D:271:PRO:HD2	1:D:275:MET:CE	2.48	0.43
1:C:237:MET:O	1:C:238:THR:C	2.61	0.43
1:E:90:LEU:HD12	1:E:94:ARG:CZ	2.49	0.43
1:C:109:ASP:HB3	1:C:113:ARG:HH12	1.83	0.43
1:C:210:ALA:O	1:C:214:ILE:CD1	2.66	0.43
1:C:213:LEU:HD22	1:C:214:ILE:HG12	2.01	0.43
1:D:78:ARG:HD2	1:D:207:VAL:HG23	2.00	0.43
1:A:48:LEU:O	1:B:236:TYR:CE2	2.72	0.43
1:C:205:THR:O	1:C:205:THR:CG2	2.65	0.43
1:E:60:LEU:HD23	1:E:222:PHE:CD1	2.46	0.43
1:B:38:ALA:HB2	1:B:228:PHE:HD1	1.83	0.43
1:E:45:TYR:HB2	1:E:50:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:MET:HE2	1:E:52:LEU:HD11	2.00	0.42
1:B:45:TYR:CE1	1:B:50:ILE:HD11	2.54	0.42
1:C:188:LYS:HA	1:C:188:LYS:HD3	1.89	0.42
1:E:71:ARG:NH2	1:E:253:ASP:OD1	2.52	0.42
1:A:235:HIS:HB3	7:A:401:HOH:O	2.19	0.42
1:D:127:HIS:CD2	1:D:134:PRO:HA	2.54	0.42
1:B:95:THR:OG1	1:B:188:LYS:HD2	2.20	0.42
1:B:241:VAL:O	1:B:241:VAL:HG12	2.20	0.42
1:E:45:TYR:O	1:E:50:ILE:HG12	2.19	0.42
1:B:71:ARG:NH1	1:B:260:GLU:OE2	2.53	0.42
1:A:83:ARG:CZ	1:E:205:THR:CG2	2.73	0.42
1:C:201:ARG:O	1:C:205:THR:HB	2.20	0.42
1:C:255:LEU:HD21	1:D:211:TYR:CE1	2.54	0.42
1:D:34:MET:HE2	1:D:224:THR:HG23	2.01	0.42
1:C:71:ARG:HD2	1:C:71:ARG:C	2.45	0.42
1:E:113:ARG:O	1:E:116:SER:HB2	2.20	0.42
1:A:71:ARG:HD2	1:A:71:ARG:C	2.45	0.42
1:B:238:THR:N	1:B:239:PRO:HD2	2.34	0.42
1:C:231:VAL:HA	1:C:238:THR:OG1	2.20	0.42
1:A:158:ASN:ND2	1:B:94:ARG:HG2	2.34	0.42
1:B:271:PRO:CG	1:B:275:MET:HE3	2.42	0.42
1:C:91:ILE:HD13	1:D:194:HIS:HA	2.00	0.42
1:C:207:VAL:HG23	1:E:79:PHE:CZ	2.55	0.42
1:E:121:PHE:CE1	1:E:157:THR:HG22	2.55	0.42
1:A:166:ASN:ND2	1:B:102:ASN:HD22	2.18	0.41
1:B:166:ASN:HD22	1:B:166:ASN:HA	1.70	0.41
1:A:48:LEU:O	1:B:236:TYR:CD2	2.73	0.41
1:C:210:ALA:HB3	1:E:255:LEU:HD13	2.02	0.41
1:D:146:ARG:NH1	1:D:149:GLU:OE1	2.53	0.41
1:A:239:PRO:HG2	1:A:240:PHE:HD1	1.85	0.41
1:C:168:ILE:HG13	1:C:182:TYR:CE2	2.55	0.41
1:E:146:ARG:HA	1:E:146:ARG:HH21	1.85	0.41
1:B:52:LEU:HD11	1:D:237:MET:HE2	2.03	0.41
1:C:209:PHE:HD1	1:C:209:PHE:HA	1.65	0.41
1:A:244:PHE:CE1	1:E:221:LEU:HD23	2.56	0.41
1:A:214:ILE:HD13	1:B:251:SER:HB3	2.03	0.41
1:D:210:ALA:HA	1:D:213:LEU:HB3	2.03	0.41
1:A:85:LEU:HD22	1:A:195:VAL:HA	2.02	0.41
1:A:239:PRO:HG2	1:A:240:PHE:CD1	2.55	0.41
1:C:100:LEU:HD11	1:C:114:ILE:HD13	2.03	0.41
1:D:271:PRO:HD2	1:D:275:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:THR:N	1:A:239:PRO:HD2	2.36	0.41
1:B:121:PHE:CE1	1:B:157:THR:HG22	2.56	0.41
1:A:245:ILE:HG12	1:E:60:LEU:HD13	2.03	0.40
1:B:231:VAL:O	1:B:232:GLY:C	2.64	0.40
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.94	0.40
1:B:126:LYS:HE2	1:B:126:LYS:HB3	1.79	0.40
1:C:91:ILE:O	1:C:95:THR:CG2	2.65	0.40
1:C:226:LEU:N	1:C:227:PRO:CD	2.83	0.40
1:E:206:PRO:CB	1:E:208:PRO:HD2	2.41	0.40
1:B:207:VAL:O	1:B:208:PRO:C	2.64	0.40
1:D:42:TYR:O	1:D:45:TYR:HB2	2.21	0.40
1:D:212:THR:O	1:D:216:GLN:HB2	2.21	0.40
1:E:89:VAL:CG2	1:E:195:VAL:HG11	2.51	0.40
1:B:207:VAL:HG22	1:B:260:GLU:CD	2.46	0.40
1:D:72:ASN:ND2	1:D:256:ALA:HB2	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:HIS:NE2	7:D:401:HOH:O[2_554]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	266/297 (90%)	253 (95%)	13 (5%)	0	100	100
1	B	270/297 (91%)	245 (91%)	21 (8%)	4 (2%)	8	13
1	C	268/297 (90%)	259 (97%)	7 (3%)	2 (1%)	18	30
1	D	266/297 (90%)	257 (97%)	7 (3%)	2 (1%)	16	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	269/297 (91%)	260 (97%)	7 (3%)	2 (1%)	18	30
All	All	1339/1485 (90%)	1274 (95%)	55 (4%)	10 (1%)	18	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	207	VAL
1	B	30	LEU
1	B	232	GLY
1	E	209	PHE
1	E	43	GLN
1	B	285	ASP
1	C	154	SER
1	D	208	PRO
1	D	214	ILE
1	B	214	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/260 (90%)	215 (92%)	18 (8%)	12	20
1	B	237/260 (91%)	220 (93%)	17 (7%)	13	22
1	C	234/260 (90%)	216 (92%)	18 (8%)	12	20
1	D	233/260 (90%)	217 (93%)	16 (7%)	14	24
1	E	236/260 (91%)	212 (90%)	24 (10%)	7	10
All	All	1173/1300 (90%)	1080 (92%)	93 (8%)	11	19

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	27	ARG

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Mol	Chain	Res	Type
1	A	28	LEU
1	A	37	ILE
1	A	46	GLU
1	A	48	LEU
1	A	73	SER
1	A	95	THR
1	A	149	GLU
1	A	176	LYS
1	A	188	LYS
1	A	224	THR
1	A	233	ASP
1	A	241	VAL
1	A	243	VAL
1	A	248	THR
1	A	251	SER
1	A	260	GLU
1	B	23	LYS
1	B	30	LEU
1	B	50	ILE
1	B	54	VAL
1	B	58	SER
1	B	71	ARG
1	B	81	GLU
1	B	94	ARG
1	B	95	THR
1	B	126	LYS
1	B	154	SER
1	B	188	LYS
1	B	211	TYR
1	B	242	SER
1	B	243	VAL
1	B	251	SER
1	B	292	LEU
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	126	LYS
1	C	146	ARG
1	C	155	MET

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Mol	Chain	Res	Type
1	C	173	GLU
1	C	209	PHE
1	C	212	THR
1	C	213	LEU
1	C	214	ILE
1	C	215	LEU
1	C	243	VAL
1	C	257	GLU
1	C	268	ASN
1	D	22	SER
1	D	40	ILE
1	D	41	SER
1	D	44	TRP
1	D	46	GLU
1	D	47	GLN
1	D	48	LEU
1	D	50	ILE
1	D	51	HIS
1	D	72	ASN
1	D	83	ARG
1	D	96	LEU
1	D	135	THR
1	D	148	THR
1	D	154	SER
1	D	260	GLU
1	E	35	SER
1	E	36	ILE
1	E	46	GLU
1	E	48	LEU
1	E	50	ILE
1	E	54	VAL
1	E	58	SER
1	E	71	ARG
1	E	73	SER
1	E	95	THR
1	E	131	LYS
1	E	146	ARG
1	E	154	SER
1	E	173	GLU
1	E	188	LYS
1	E	202	LEU
1	E	215	LEU

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Mol	Chain	Res	Type
1	E	225	LEU
1	E	243	VAL
1	E	257	GLU
1	E	265	THR
1	E	275	MET
1	E	292	LEU
1	E	294	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	47	GLN
1	A	158	ASN
1	A	166	ASN
1	A	216	GLN
1	A	235	HIS
1	A	268	ASN
1	B	166	ASN
1	C	31	ASN
1	C	268	ASN
1	D	47	GLN
1	D	72	ASN
1	D	99	GLN
1	D	166	ASN
1	E	72	ASN
1	E	99	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 26 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACY	A	305	2	3,3,3	0.78	0	3,3,3	1.16	0
3	ACY	A	306	-	3,3,3	0.87	0	3,3,3	0.91	0
4	EDO	A	307	-	3,3,3	0.55	0	2,2,2	0.23	0
3	ACY	E	303	2	3,3,3	1.59	1 (33%)	3,3,3	1.68	1 (33%)
6	PGE	E	305	-	9,9,9	0.73	0	8,8,8	0.77	0
3	ACY	B	303	2	3,3,3	1.24	0	3,3,3	1.12	0
4	EDO	E	304	-	3,3,3	0.99	0	2,2,2	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	E	304	-	-	1/1/1/1	-
4	EDO	A	307	-	-	1/1/1/1	-
6	PGE	E	305	-	-	5/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	303	ACY	CH3-C	2.01	1.57	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	303	ACY	OXT-C-O	-2.43	113.03	122.03

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	305	PGE	1	0
3	B	303	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	268/297 (90%)	0.34	30 (11%) 10 8	37, 57, 116, 165	0
1	B	272/297 (91%)	0.49	44 (16%) 4 3	37, 65, 122, 160	0
1	C	270/297 (90%)	0.50	29 (10%) 11 9	37, 61, 135, 175	0
1	D	268/297 (90%)	0.63	39 (14%) 6 4	41, 71, 122, 145	0
1	E	271/297 (91%)	0.40	36 (13%) 7 6	36, 59, 114, 146	0
All	All	1349/1485 (90%)	0.47	178 (13%) 7 6	36, 63, 124, 175	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	204	THR	7.7
1	D	145	GLU	7.7
1	E	206	PRO	7.5
1	C	47	GLN	6.7
1	A	175	ALA	6.0
1	C	44	TRP	5.8
1	C	209	PHE	5.8
1	C	51	HIS	5.6
1	D	48	LEU	5.5
1	C	211	TYR	5.4
1	E	205	THR	5.3
1	D	47	GLN	5.3
1	B	207	VAL	5.1
1	C	291	PRO	4.9
1	E	42	TYR	4.8
1	C	214	ILE	4.8
1	B	211	TYR	4.8
1	C	210	ALA	4.7
1	C	207	VAL	4.7
1	D	173	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	214	ILE	4.6
1	E	25	ILE	4.5
1	A	47	GLN	4.5
1	C	106	ALA	4.5
1	B	48	LEU	4.5
1	B	204	THR	4.4
1	C	213	LEU	4.3
1	B	205	THR	4.3
1	C	206	PRO	4.2
1	E	26	PHE	4.2
1	E	235	HIS	4.2
1	E	209	PHE	4.1
1	B	210	ALA	4.1
1	A	45	TYR	4.0
1	E	44	TRP	4.0
1	C	48	LEU	4.0
1	B	40	ILE	3.9
1	D	51	HIS	3.9
1	C	204	THR	3.9
1	D	204	THR	3.8
1	D	267	ALA	3.8
1	C	240	PHE	3.8
1	D	139	ARG	3.7
1	C	208	PRO	3.7
1	E	47	GLN	3.7
1	D	131	LYS	3.6
1	D	46	GLU	3.6
1	A	174	ALA	3.6
1	D	44	TRP	3.6
1	D	174	ALA	3.6
1	A	26	PHE	3.5
1	D	268	ASN	3.5
1	B	34	MET	3.4
1	D	265	THR	3.4
1	A	173	GLU	3.4
1	E	170	GLN	3.4
1	A	44	TRP	3.4
1	A	40	ILE	3.4
1	B	37	ILE	3.4
1	E	58	SER	3.3
1	D	170	GLN	3.3
1	E	43	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	61	GLY	3.3
1	E	210	ALA	3.3
1	D	209	PHE	3.3
1	B	38	ALA	3.3
1	C	40	ILE	3.3
1	A	228	PHE	3.2
1	A	48	LEU	3.2
1	B	47	GLN	3.2
1	E	265	THR	3.2
1	B	35	SER	3.2
1	C	184	LEU	3.2
1	A	42	TYR	3.1
1	D	27	ARG	3.0
1	A	204	THR	3.0
1	E	39	ILE	3.0
1	A	209	PHE	3.0
1	C	268	ASN	3.0
1	B	236	TYR	3.0
1	D	236	TYR	2.9
1	E	45	TYR	2.9
1	E	211	TYR	2.9
1	D	266	ALA	2.9
1	A	46	GLU	2.9
1	D	130	ARG	2.9
1	B	43	GLN	2.9
1	B	44	TRP	2.9
1	E	24	ILE	2.8
1	B	33	LEU	2.8
1	C	212	THR	2.8
1	D	207	VAL	2.8
1	A	84	ASN	2.8
1	B	277	ASN	2.8
1	B	293	PRO	2.8
1	D	146	ARG	2.8
1	C	43	GLN	2.8
1	A	106	ALA	2.8
1	B	224	THR	2.8
1	A	236	TYR	2.8
1	B	39	ILE	2.7
1	D	264	GLY	2.7
1	B	208	PRO	2.7
1	C	46	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	224	THR	2.7
1	B	212	THR	2.7
1	D	289	GLN	2.7
1	A	34	MET	2.6
1	D	144	GLU	2.6
1	B	209	PHE	2.6
1	B	228	PHE	2.6
1	B	51	HIS	2.6
1	B	23	LYS	2.6
1	B	22	SER	2.6
1	A	29	LEU	2.6
1	A	220	TYR	2.6
1	E	173	GLU	2.5
1	B	206	PRO	2.5
1	B	49	GLY	2.5
1	A	24	ILE	2.5
1	D	260	GLU	2.5
1	D	224	THR	2.5
1	E	40	ILE	2.5
1	A	51	HIS	2.5
1	A	288	GLY	2.5
1	B	42	TYR	2.5
1	B	220	TYR	2.5
1	B	30	LEU	2.4
1	E	36	ILE	2.4
1	D	154	SER	2.4
1	E	46	GLU	2.4
1	E	232	GLY	2.4
1	E	266	ALA	2.4
1	B	213	LEU	2.4
1	D	22	SER	2.4
1	C	49	GLY	2.4
1	B	235	HIS	2.4
1	B	45	TYR	2.4
1	B	216	GLN	2.4
1	E	57	PHE	2.4
1	E	48	LEU	2.3
1	D	149	GLU	2.3
1	B	31	ASN	2.3
1	C	107	GLU	2.3
1	D	166	ASN	2.3
1	C	215	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	236	TYR	2.3
1	E	207	VAL	2.3
1	B	36	ILE	2.2
1	E	29	LEU	2.2
1	D	40	ILE	2.2
1	C	236	TYR	2.2
1	A	33	LEU	2.2
1	A	37	ILE	2.2
1	A	257	GLU	2.2
1	D	42	TYR	2.2
1	A	176	LYS	2.2
1	A	232	GLY	2.2
1	C	30	LEU	2.2
1	D	26	PHE	2.2
1	E	38	ALA	2.2
1	B	292	LEU	2.2
1	E	215	LEU	2.2
1	B	50	ILE	2.2
1	D	205	THR	2.1
1	D	206	PRO	2.1
1	B	155	MET	2.1
1	E	37	ILE	2.1
1	C	267	ALA	2.1
1	C	59	LEU	2.1
1	D	23	LYS	2.0
1	A	235	HIS	2.0
1	B	240	PHE	2.0
1	D	228	PHE	2.0
1	E	35	SER	2.0
1	A	30	LEU	2.0
1	D	235	HIS	2.0
1	B	232	GLY	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 ⓘ

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
3	ACY	A	306	4/4	0.29	0.42	98,105,109,116	0
3	ACY	E	303	4/4	0.65	0.25	41,46,49,50	0
3	ACY	B	303	4/4	0.74	0.24	52,53,57,65	0
3	ACY	A	305	4/4	0.76	0.32	86,88,99,103	0
2	ZN	C	304	1/1	0.82	0.10	139,139,139,139	0
6	PGE	E	305	10/10	0.85	0.25	74,87,104,104	0
4	EDO	E	304	4/4	0.87	0.20	62,64,69,72	0
5	CL	D	306	1/1	0.96	0.08	79,79,79,79	0
2	ZN	D	303	1/1	0.96	0.08	89,89,89,89	0
5	CL	C	305	1/1	0.97	0.10	84,84,84,84	0
4	EDO	A	307	4/4	0.97	0.13	63,71,76,81	0
5	CL	B	304	1/1	0.97	0.17	81,81,81,81	0
2	ZN	B	301	1/1	0.98	0.07	126,126,126,126	0
2	ZN	D	304	1/1	0.98	0.06	125,125,125,125	0
5	CL	D	305	1/1	0.98	0.07	76,76,76,76	0
5	CL	A	308	1/1	0.98	0.11	62,62,62,62	0
5	CL	E	306	1/1	0.98	0.05	65,65,65,65	0
5	CL	E	307	1/1	0.98	0.08	63,63,63,63	0
5	CL	A	309	1/1	0.98	0.06	73,73,73,73	0
5	CL	C	306	1/1	0.99	0.08	57,57,57,57	0
2	ZN	C	302	1/1	0.99	0.02	74,74,74,74	0
5	CL	A	310	1/1	0.99	0.05	70,70,70,70	0
2	ZN	D	302	1/1	1.00	0.02	72,72,72,72	0
2	ZN	A	304	1/1	1.00	0.02	68,68,68,68	0
2	ZN	A	301	1/1	1.00	0.02	58,58,58,58	0
2	ZN	E	301	1/1	1.00	0.02	55,55,55,55	0
2	ZN	E	302	1/1	1.00	0.03	50,50,50,50	0
2	ZN	B	302	1/1	1.00	0.04	55,55,55,55	0
2	ZN	C	301	1/1	1.00	0.03	55,55,55,55	0
2	ZN	A	302	1/1	1.00	0.02	69,69,69,69	0
2	ZN	C	303	1/1	1.00	0.01	58,58,58,58	0
2	ZN	A	303	1/1	1.00	0.01	63,63,63,63	0
2	ZN	D	301	1/1	1.00	0.01	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.