



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:43 PM UTC

PDB ID : 6IVN / pdb_00006ivn
Title : Crystal structure of a membrane protein G264A
Authors : Kittredge, A.; Fukuda, F.; Zhang, Y.; Yang, T.
Deposited on : 2018-12-04
Resolution : 3.10 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

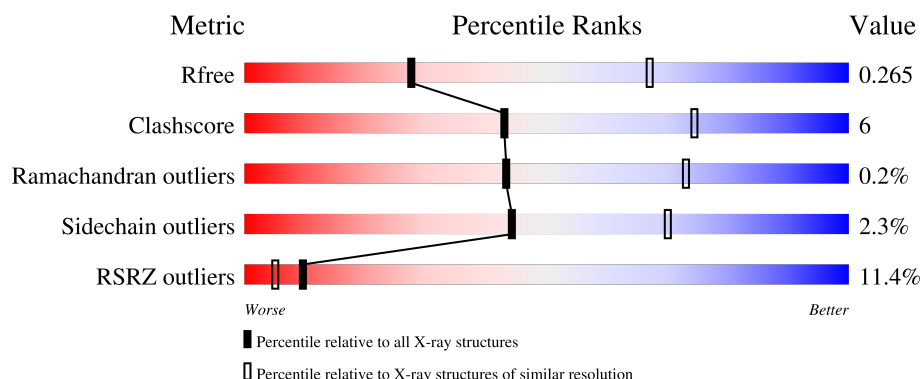
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	7% 75% 15% • 8%
1	B	297	9% 78% 13% 9%
1	C	297	10% 76% 13% • 9%
1	D	297	13% 79% 11% 10%
1	E	297	12% 78% 12% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10832 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	273	Total	C	N	O	S	0	0	0
			2178	1411	368	390	9			
1	B	270	Total	C	N	O	S	0	0	0
			2153	1395	365	384	9			
1	C	269	Total	C	N	O	S	0	0	0
			2141	1386	364	382	9			
1	D	268	Total	C	N	O	S	0	0	0
			2130	1378	361	382	9			
1	E	272	Total	C	N	O	S	0	0	0
			2168	1406	367	386	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	264	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	264	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	264	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	264	ALA	GLY	engineered mutation	UNP W9BH30
E	-2	SER	-	expression tag	UNP W9BH30
E	-1	ASN	-	expression tag	UNP W9BH30
E	0	ALA	-	expression tag	UNP W9BH30

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Chain	Residue	Modelled	Actual	Comment	Reference
E	264	ALA	GLY	engineered mutation	UNP W9BH30

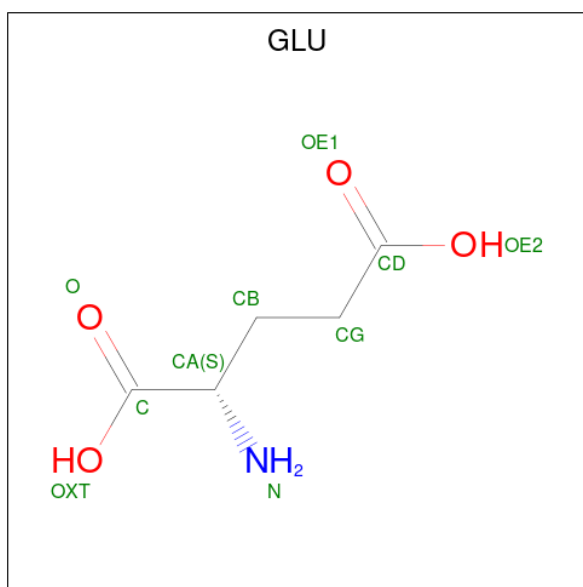
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Zn 3 3	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	1	Total Zn 1 1	0	0

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

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

- Molecule 4 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			10	5	1	4		

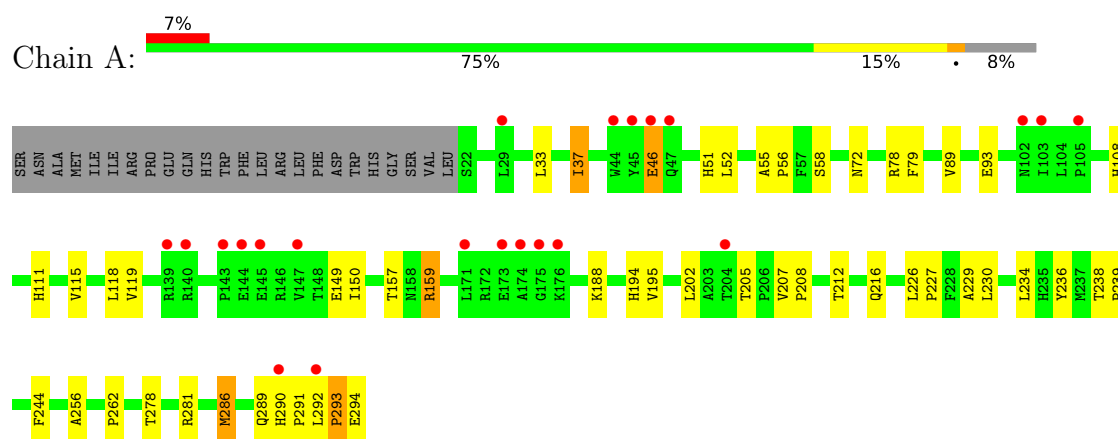
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	4	Total	O	0	0
			4	4		
5	C	6	Total	O	0	0
			6	6		
5	D	5	Total	O	0	0
			5	5		
5	E	5	Total	O	0	0
			5	5		

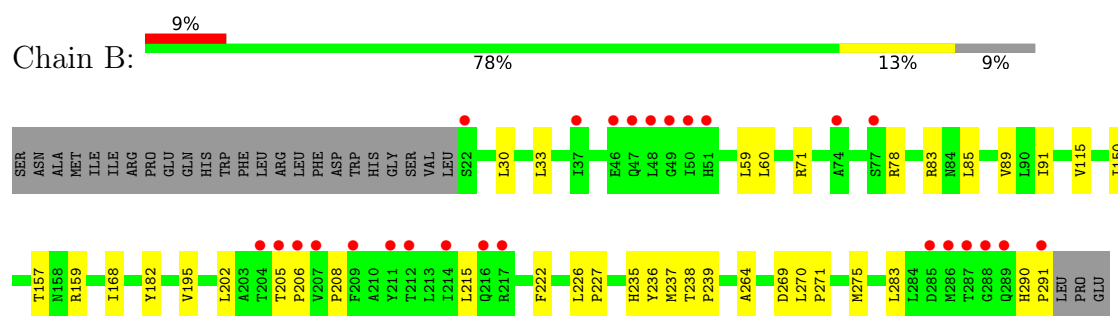
3 Residue-property plots [i](#)

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.

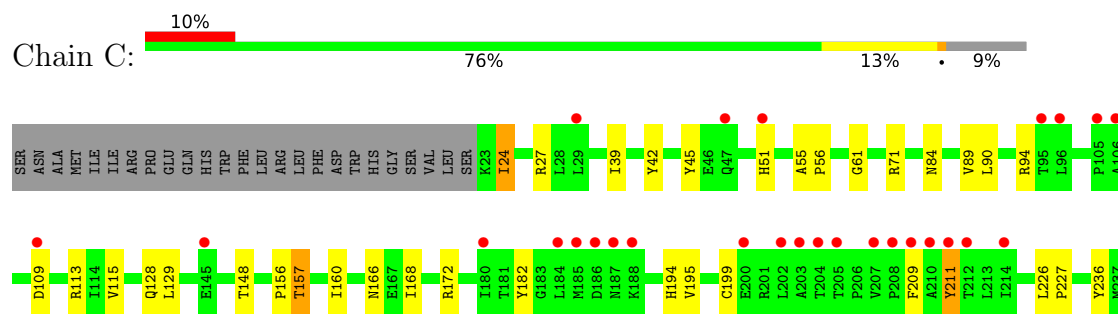
• Molecule 1: Ibestrophin



• Molecule 1: Ibestrophin

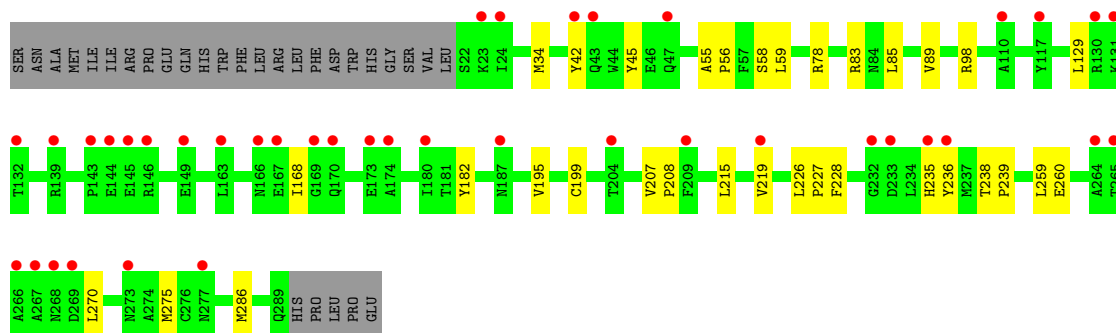
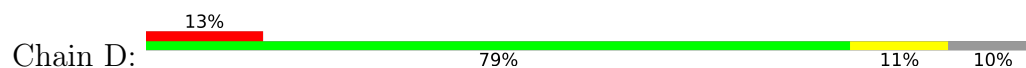


• Molecule 1: Ibestrophin

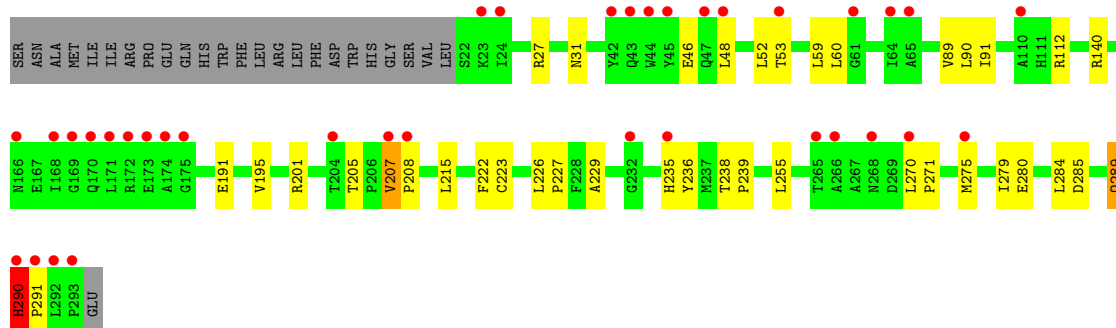
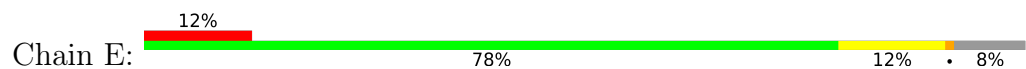




● Molecule 1: Ibestrophin



● 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	114.15Å 160.94Å 160.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 3.10 48.56 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.56-3.10) 97.9 (48.56-3.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.213 , 0.265 0.213 , 0.265	Depositor DCC
R_{free} test set	2676 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	98.2	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10832	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.45	0/2227	1.00	0/3032
1	B	0.44	0/2201	1.00	0/2997
1	C	0.44	0/2188	0.99	0/2980
1	D	0.43	0/2175	1.00	0/2961
1	E	0.46	0/2217	1.02	0/3020
All	All	0.44	0/11008	1.00	0/14990

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2178	0	2221	34	0
1	B	2153	0	2197	26	0
1	C	2141	0	2185	27	0
1	D	2130	0	2176	25	0
1	E	2168	0	2215	36	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3	0	0	0	0
2	E	1	0	0	0	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	1	0	0	0	0
4	E	10	0	5	0	0
5	A	7	0	0	0	0
5	B	4	0	0	0	0
5	C	6	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
All	All	10832	0	10999	135	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 6.

All (135) 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:E:207:VAL:HG23	1:E:208:PRO:HD3	1.50	0.94
1:C:236:TYR:O	1:C:239:PRO:HD2	1.75	0.86
1:E:290:HIS:HB3	1:E:291:PRO:CD	2.08	0.83
1:D:236:TYR:O	1:D:239:PRO:HD2	1.82	0.79
1:B:235:HIS:O	1:B:238:THR:OG1	2.01	0.76
1:A:46:GLU:HG3	1:A:51:HIS:NE2	2.02	0.75
1:A:236:TYR:O	1:A:239:PRO:HD2	1.88	0.74
1:B:236:TYR:O	1:B:239:PRO:HD2	1.91	0.71
1:E:236:TYR:O	1:E:239:PRO:HD2	1.90	0.70
1:E:290:HIS:CB	1:E:291:PRO:HD3	2.25	0.67
1:E:290:HIS:CB	1:E:291:PRO:CD	2.74	0.65
1:C:115:VAL:HG21	1:C:287:THR:HG21	1.78	0.65
1:E:290:HIS:ND1	1:E:291:PRO:HD3	2.12	0.64
1:E:290:HIS:CG	1:E:291:PRO:HD3	2.34	0.62
1:A:89:VAL:HG22	1:A:195:VAL:HG11	1.82	0.62
1:E:290:HIS:HB3	1:E:291:PRO:HD3	1.80	0.62
1:D:235:HIS:O	1:D:238:THR:OG1	2.16	0.61
1:A:212:THR:O	1:A:216:GLN:HB2	2.02	0.60
1:D:129:LEU:HD21	1:D:199:CYS:HB3	1.83	0.60
1:C:226:LEU:N	1:C:227:PRO:HD2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:HIS:HA	1:E:91:ILE:HD13	1.85	0.59
1:E:226:LEU:N	1:E:227:PRO:HD2	2.18	0.59
1:D:78:ARG:HD3	1:D:207:VAL:HG22	1.84	0.59
1:D:89:VAL:CG2	1:D:195:VAL:HG11	2.33	0.59
1:E:207:VAL:HG23	1:E:208:PRO:CD	2.29	0.59
1:A:33:LEU:O	1:A:37:ILE:HG23	2.01	0.59
1:C:55:ALA:HB3	1:C:56:PRO:HD3	1.84	0.59
1:D:83:ARG:HG2	1:D:270:LEU:HD21	1.83	0.59
1:E:290:HIS:HB3	1:E:291:PRO:HD2	1.83	0.59
1:C:211:TYR:CE1	1:E:255:LEU:HD21	2.37	0.58
1:B:270:LEU:HD22	1:B:275:MET:HE1	1.86	0.57
1:A:292:LEU:N	1:A:293:PRO:HD3	2.19	0.57
1:E:235:HIS:O	1:E:238:THR:OG1	2.12	0.56
1:D:42:TYR:HA	1:D:45:TYR:CD1	2.42	0.55
1:D:207:VAL:HG21	1:D:260:GLU:HG2	1.89	0.55
1:A:58:SER:HA	1:E:59:LEU:HD13	1.91	0.53
1:A:205:THR:HG21	1:B:83:ARG:HG2	1.91	0.53
1:C:51:HIS:ND1	1:E:235:HIS:HD2	2.07	0.53
1:C:89:VAL:CG2	1:C:195:VAL:HG11	2.40	0.52
1:B:226:LEU:N	1:B:227:PRO:HD2	2.25	0.52
1:D:168:ILE:HG22	1:D:182:TYR:CD1	2.44	0.51
1:A:226:LEU:N	1:A:227:PRO:HD2	2.25	0.51
1:B:89:VAL:CG2	1:B:195:VAL:HG11	2.40	0.51
1:A:115:VAL:O	1:A:119:VAL:HG23	2.10	0.50
1:C:89:VAL:HG22	1:C:195:VAL:HG11	1.92	0.50
1:A:238:THR:N	1:A:239:PRO:HD2	2.26	0.50
1:D:34:MET:HE3	1:D:228:PHE:HE1	1.76	0.49
1:A:72:ASN:OD1	1:A:256:ALA:HB2	2.13	0.49
1:A:150:ILE:HA	1:A:159:ARG:HG2	1.95	0.48
1:D:226:LEU:N	1:D:227:PRO:HD2	2.28	0.48
1:D:55:ALA:HB3	1:D:56:PRO:HD3	1.95	0.48
1:B:271:PRO:HD2	1:B:275:MET:HE3	1.96	0.47
1:B:78:ARG:NH2	1:B:202:LEU:O	2.47	0.47
1:E:236:TYR:C	1:E:238:THR:H	2.22	0.47
1:C:61:GLY:HA3	1:D:59:LEU:HD11	1.97	0.47
1:B:271:PRO:O	1:B:275:MET:HG3	2.15	0.47
1:C:71:ARG:NH2	1:C:253:ASP:OD1	2.48	0.47
1:E:191:GLU:O	1:E:195:VAL:HG23	2.15	0.47
1:B:60:LEU:HD23	1:B:222:PHE:HD1	1.79	0.46
1:E:60:LEU:HD23	1:E:222:PHE:HD1	1.80	0.46
1:C:129:LEU:HD21	1:C:199:CYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:HIS:ND1	1:A:290:HIS:C	2.73	0.46
1:A:108:HIS:CG	1:A:291:PRO:HG3	2.51	0.46
1:E:201:ARG:O	1:E:205:THR:HB	2.15	0.46
1:A:108:HIS:HA	1:A:111:HIS:ND1	2.31	0.45
1:A:236:TYR:C	1:A:238:THR:H	2.23	0.45
1:E:275:MET:O	1:E:279:ILE:HG22	2.17	0.45
1:C:115:VAL:HG21	1:C:287:THR:CG2	2.46	0.45
1:E:31:ASN:ND2	1:E:223:CYS:O	2.50	0.45
1:B:238:THR:N	1:B:239:PRO:HD2	2.31	0.45
1:C:90:LEU:O	1:C:94:ARG:HG3	2.16	0.45
1:B:236:TYR:C	1:B:238:THR:H	2.24	0.45
1:C:42:TYR:HA	1:C:45:TYR:CD1	2.52	0.45
1:D:207:VAL:O	1:D:208:PRO:C	2.60	0.45
1:D:238:THR:N	1:D:239:PRO:HD2	2.32	0.45
1:E:112:ARG:HH11	1:E:289:GLN:NE2	2.15	0.45
1:A:78:ARG:HD3	1:A:207:VAL:HG23	1.99	0.45
1:A:278:THR:HA	1:A:281:ARG:HH21	1.81	0.45
1:E:52:LEU:HB3	1:E:229:ALA:HA	1.99	0.45
1:B:264:ALA:HB3	1:B:269:ASP:OD2	2.17	0.44
1:D:168:ILE:HG22	1:D:182:TYR:HD1	1.80	0.44
1:E:89:VAL:HG22	1:E:195:VAL:HG11	1.98	0.44
1:C:266:ALA:HB3	1:C:269:ASP:OD2	2.18	0.44
1:A:52:LEU:HD11	1:B:237:MET:HE2	1.98	0.44
1:A:194:HIS:HA	1:B:91:ILE:HD13	2.00	0.44
1:B:85:LEU:HD22	1:B:195:VAL:HA	2.00	0.44
1:B:30:LEU:HA	1:B:33:LEU:HD12	2.00	0.44
1:C:42:TYR:O	1:C:45:TYR:HB2	2.18	0.44
1:C:71:ARG:HG2	1:C:211:TYR:HE2	1.82	0.43
1:E:140:ARG:HH22	1:E:280:GLU:CD	2.26	0.43
1:C:109:ASP:HB3	1:C:113:ARG:HH12	1.84	0.43
1:C:128:GLN:OE1	1:C:157:THR:OG1	2.35	0.43
1:B:150:ILE:HA	1:B:159:ARG:HG2	2.01	0.43
1:D:85:LEU:HD22	1:D:195:VAL:HA	1.99	0.43
1:E:270:LEU:N	1:E:271:PRO:HD2	2.34	0.43
1:C:236:TYR:C	1:C:238:THR:H	2.26	0.43
1:D:215:LEU:O	1:D:219:VAL:HG23	2.18	0.43
1:C:168:ILE:HG22	1:C:182:TYR:CD1	2.53	0.43
1:C:39:ILE:HD11	1:C:239:PRO:HD3	2.00	0.42
1:A:230:LEU:HB3	1:A:234:LEU:HD12	2.01	0.42
1:B:115:VAL:HG13	1:B:283:LEU:HB3	2.01	0.42
1:A:79:PHE:CD1	1:A:262:PRO:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ARG:HG2	1:C:211:TYR:CE2	2.54	0.42
1:E:226:LEU:N	1:E:227:PRO:CD	2.81	0.42
1:A:149:GLU:CD	1:B:291:PRO:HG2	2.44	0.42
1:B:290:HIS:HA	1:B:291:PRO:HD3	1.93	0.42
1:A:93:GLU:HG2	1:A:118:LEU:HD22	2.00	0.42
1:E:205:THR:O	1:E:205:THR:HG23	2.19	0.42
1:A:188:LYS:HD3	1:A:188:LYS:HA	1.80	0.42
1:A:55:ALA:N	1:A:56:PRO:CD	2.83	0.42
1:B:168:ILE:HG22	1:B:182:TYR:CD1	2.55	0.42
1:D:78:ARG:CD	1:D:207:VAL:HG22	2.49	0.42
1:E:238:THR:N	1:E:239:PRO:HD2	2.34	0.42
1:A:286:MET:HE3	1:A:286:MET:HB3	1.79	0.41
1:E:112:ARG:NH1	1:E:289:GLN:NE2	2.68	0.41
1:A:78:ARG:HG2	1:A:202:LEU:HD22	2.02	0.41
1:B:205:THR:HB	1:D:83:ARG:CZ	2.50	0.41
1:E:27:ARG:HH11	1:E:27:ARG:HB3	1.84	0.41
1:E:89:VAL:CG2	1:E:195:VAL:HG11	2.51	0.41
1:B:89:VAL:HG22	1:B:195:VAL:HG11	2.01	0.41
1:C:24:ILE:HG12	1:C:27:ARG:NH2	2.35	0.41
1:B:59:LEU:HD13	1:D:58:SER:HA	2.02	0.41
1:A:207:VAL:O	1:A:208:PRO:C	2.62	0.41
1:E:284:LEU:HD13	1:E:290:HIS:O	2.20	0.41
1:A:244:PHE:CE2	1:E:60:LEU:HD21	2.56	0.41
1:B:208:PRO:HG2	1:D:259:LEU:HD21	2.02	0.41
1:D:98:ARG:HB2	1:D:286:MET:HE1	2.03	0.41
1:A:52:LEU:HB3	1:A:229:ALA:HA	2.03	0.41
1:C:156:PRO:O	1:C:160:ILE:HG13	2.20	0.41
1:A:292:LEU:N	1:A:293:PRO:CD	2.82	0.41
1:D:270:LEU:HD22	1:D:275:MET:HE1	2.02	0.41
1:D:89:VAL:HG23	1:D:195:VAL:HG11	2.00	0.41
1:E:46:GLU:C	1:E:48:LEU:H	2.29	0.41
1:A:111:HIS:O	1:A:115:VAL:HG23	2.21	0.40
1:C:226:LEU:N	1:C:227:PRO:CD	2.84	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	271/297 (91%)	262 (97%)	8 (3%)	1 (0%)	30	61
1	B	268/297 (90%)	264 (98%)	3 (1%)	1 (0%)	30	61
1	C	267/297 (90%)	259 (97%)	8 (3%)	0	100	100
1	D	266/297 (90%)	265 (100%)	1 (0%)	0	100	100
1	E	270/297 (91%)	261 (97%)	8 (3%)	1 (0%)	30	61
All	All	1342/1485 (90%)	1311 (98%)	28 (2%)	3 (0%)	43	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	290	HIS
1	B	206	PRO
1	A	293	PRO

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	238/260 (92%)	231 (97%)	7 (3%)	37	66
1	B	235/260 (90%)	232 (99%)	3 (1%)	61	77
1	C	233/260 (90%)	224 (96%)	9 (4%)	28	60
1	D	232/260 (89%)	232 (100%)	0	100	100
1	E	237/260 (91%)	230 (97%)	7 (3%)	36	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1175/1300 (90%)	1149 (98%)	26 (2%)	44 71

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ILE
1	A	46	GLU
1	A	157	THR
1	A	159	ARG
1	A	286	MET
1	A	289	GLN
1	A	294	GLU
1	B	71	ARG
1	B	157	THR
1	B	215	LEU
1	C	24	ILE
1	C	84	ASN
1	C	148	THR
1	C	157	THR
1	C	166	ASN
1	C	172	ARG
1	C	209	PHE
1	C	211	TYR
1	C	268	ASN
1	E	53	THR
1	E	90	LEU
1	E	207	VAL
1	E	215	LEU
1	E	285	ASP
1	E	289	GLN
1	E	290	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	102	ASN
1	A	158	ASN
1	A	166	ASN
1	A	216	GLN
1	A	273	ASN

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Mol	Chain	Res	Type
1	A	289	GLN
1	B	31	ASN
1	B	43	GLN
1	B	216	GLN
1	C	31	ASN
1	C	166	ASN
1	C	216	GLN
1	D	31	ASN
1	D	72	ASN
1	D	166	ASN
1	D	282	ASN
1	E	31	ASN
1	E	47	GLN
1	E	166	ASN
1	E	216	GLN
1	E	235	HIS
1	E	268	ASN
1	E	289	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 25 are monoatomic - leaving 1 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	GLU	E	301	-	8,9,9	1.14	1 (12%)	8,11,11	1.47	1 (12%)

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	GLU	E	301	-	-	5/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	301	GLU	OXT-C	-2.26	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	301	GLU	OXT-C-O	-3.40	116.36	124.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	301	GLU	N-CA-CB-CG
4	E	301	GLU	C-CA-CB-CG
4	E	301	GLU	OXT-C-CA-N
4	E	301	GLU	CA-CB-CG-CD
4	E	301	GLU	O-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	273/297 (91%)	0.38	22 (8%) 18 10	58, 93, 154, 206	0
1	B	270/297 (90%)	0.31	26 (9%) 13 7	59, 88, 159, 197	0
1	C	269/297 (90%)	0.56	30 (11%) 10 5	60, 92, 159, 191	0
1	D	268/297 (90%)	0.94	40 (14%) 5 3	62, 96, 144, 173	0
1	E	272/297 (91%)	0.60	36 (13%) 7 4	58, 88, 170, 201	0
All	All	1352/1485 (91%)	0.56	154 (11%) 10 5	58, 92, 155, 206	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	265	THR	16.2
1	D	170	GLN	9.2
1	C	204	THR	8.5
1	D	173	GLU	8.1
1	B	291	PRO	8.1
1	C	106	ALA	7.3
1	D	145	GLU	7.3
1	E	47	GLN	6.9
1	D	166	ASN	6.9
1	E	170	GLN	6.7
1	D	146	ARG	6.7
1	C	105	PRO	6.4
1	C	207	VAL	6.4
1	B	285	ASP	6.3
1	C	211	TYR	6.2
1	A	144	GLU	6.1
1	A	175	GLY	6.0
1	B	47	GLN	6.0
1	B	288	GLY	6.0
1	E	48	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	48	LEU	5.6
1	D	264	ALA	5.5
1	D	233	ASP	5.5
1	C	210	ALA	5.5
1	E	173	GLU	5.4
1	E	290	HIS	5.3
1	B	46	GLU	5.3
1	D	174	ALA	5.2
1	B	49	GLY	5.1
1	D	232	GLY	5.1
1	C	209	PHE	5.0
1	C	187	ASN	5.0
1	D	167	GLU	4.8
1	E	268	ASN	4.7
1	D	236	TYR	4.7
1	C	184	LEU	4.6
1	D	273	ASN	4.6
1	D	42	TYR	4.6
1	D	130	ARG	4.6
1	C	205	THR	4.6
1	C	214	ILE	4.5
1	E	172	ARG	4.5
1	B	287	THR	4.4
1	C	208	PRO	4.4
1	E	166	ASN	4.3
1	A	47	GLN	4.3
1	D	149	GLU	4.1
1	C	109	ASP	4.0
1	A	145	GLU	4.0
1	B	51	HIS	4.0
1	E	204	THR	3.9
1	D	131	LYS	3.8
1	E	45	TYR	3.8
1	C	47	GLN	3.7
1	E	207	VAL	3.7
1	B	211	TYR	3.7
1	D	110	ALA	3.7
1	E	265	THR	3.6
1	E	42	TYR	3.6
1	D	266	ALA	3.6
1	B	207	VAL	3.5
1	A	292	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	235	HIS	3.5
1	E	235	HIS	3.4
1	A	143	PRO	3.4
1	C	188	LYS	3.3
1	E	270	LEU	3.3
1	C	185	MET	3.3
1	D	204	THR	3.3
1	D	187	ASN	3.2
1	D	269	ASP	3.2
1	D	23	LYS	3.2
1	B	77	SER	3.2
1	C	29	LEU	3.1
1	B	212	THR	3.1
1	D	47	GLN	3.1
1	D	267	ALA	3.1
1	A	102	ASN	3.1
1	C	96	LEU	3.1
1	B	216	GLN	3.0
1	B	209	PHE	3.0
1	E	53	THR	3.0
1	D	117	TYR	3.0
1	E	232	GLY	3.0
1	C	51	HIS	2.9
1	C	200	GLU	2.9
1	E	168	ILE	2.9
1	E	110	ALA	2.9
1	D	209	PHE	2.9
1	E	175	GLY	2.9
1	E	275	MET	2.9
1	E	293	PRO	2.8
1	C	291	PRO	2.8
1	A	29	LEU	2.8
1	A	103	ILE	2.8
1	A	176	LYS	2.8
1	A	147	VAL	2.7
1	E	169	GLY	2.7
1	D	139	ARG	2.7
1	A	44	TRP	2.7
1	C	145	GLU	2.6
1	C	212	THR	2.6
1	E	23	LYS	2.6
1	B	214	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	169	GLY	2.6
1	D	163	LEU	2.6
1	E	61	GLY	2.6
1	E	171	LEU	2.6
1	A	46	GLU	2.5
1	C	186	ASP	2.4
1	B	206	PRO	2.4
1	D	143	PRO	2.4
1	D	268	ASN	2.4
1	C	180	ILE	2.4
1	B	205	THR	2.4
1	E	266	ALA	2.4
1	A	173	GLU	2.4
1	A	139	ARG	2.4
1	D	144	GLU	2.4
1	E	44	TRP	2.4
1	D	132	THR	2.3
1	A	174	ALA	2.3
1	B	289	GLN	2.3
1	B	22	SER	2.3
1	A	140	ARG	2.3
1	E	208	PRO	2.3
1	C	95	THR	2.3
1	D	277	ASN	2.3
1	E	291	PRO	2.2
1	C	203	ALA	2.2
1	A	45	TYR	2.2
1	D	219	VAL	2.2
1	A	204	THR	2.2
1	C	268	ASN	2.2
1	E	292	LEU	2.2
1	A	290	HIS	2.2
1	D	43	GLN	2.2
1	E	43	GLN	2.2
1	B	74	ALA	2.2
1	B	50	ILE	2.2
1	C	202	LEU	2.1
1	C	257	GLU	2.1
1	A	105	PRO	2.1
1	D	180	ILE	2.1
1	B	204	THR	2.1
1	B	217	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	2.1
1	D	24	ILE	2.1
1	E	64	ILE	2.0
1	B	286	MET	2.0
1	E	174	ALA	2.0
1	B	37	ILE	2.0
1	E	24	ILE	2.0
1	E	65	ALA	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
2	ZN	D	303	1/1	0.79	0.11	205,205,205,205	0
2	ZN	C	307	1/1	0.83	0.09	173,173,173,173	0
4	GLU	E	301	10/10	0.88	0.20	105,110,113,114	0
2	ZN	D	302	1/1	0.92	0.10	112,112,112,112	0
3	CL	A	304	1/1	0.94	0.09	116,116,116,116	0
3	CL	D	306	1/1	0.95	0.09	115,115,115,115	0
3	CL	C	305	1/1	0.96	0.15	102,102,102,102	0
3	CL	B	305	1/1	0.97	0.09	100,100,100,100	0
3	CL	B	304	1/1	0.97	0.13	94,94,94,94	0
3	CL	D	305	1/1	0.98	0.05	97,97,97,97	0
3	CL	C	304	1/1	0.98	0.12	91,91,91,91	0
3	CL	E	303	1/1	0.98	0.05	86,86,86,86	0
3	CL	C	306	1/1	0.98	0.07	97,97,97,97	0
2	ZN	D	301	1/1	0.99	0.03	106,106,106,106	0
2	ZN	A	302	1/1	0.99	0.03	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	303	1/1	0.99	0.03	101,101,101,101	0
3	CL	D	304	1/1	0.99	0.04	103,103,103,103	0
2	ZN	B	301	1/1	0.99	0.04	133,133,133,133	0
2	ZN	C	303	1/1	0.99	0.03	85,85,85,85	0
2	ZN	A	301	1/1	0.99	0.06	80,80,80,80	0
3	CL	B	306	1/1	0.99	0.04	95,95,95,95	0
2	ZN	C	302	1/1	1.00	0.06	80,80,80,80	0
2	ZN	B	302	1/1	1.00	0.02	79,79,79,79	0
2	ZN	E	302	1/1	1.00	0.01	82,82,82,82	0
2	ZN	B	303	1/1	1.00	0.02	85,85,85,85	0
2	ZN	C	301	1/1	1.00	0.04	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.