



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:29 PM UTC

PDB ID : 6QF5 / pdb_00006qf5
Title : X-Ray structure of human Aquaporin 2 crystallized on a silicon chip
Authors : Lieske, J.; Cerv, M.; Kreida, S.; Barthelmess, M.; Fischer, P.; Pakendorf, T.; Yefanov, O.; Mariani, V.; Seine, T.; Ross, B.H.; Crosas, E.; Lorbeer, O.; Burkhardt, A.; Lane, T.J.; Guenther, S.; Bergtholdt, J.; Schoen, S.; Tornroth-Horsefield, S.; Chapman, H.N.; Meents, A.
Deposited on : 2019-01-09
Resolution : 3.70 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
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

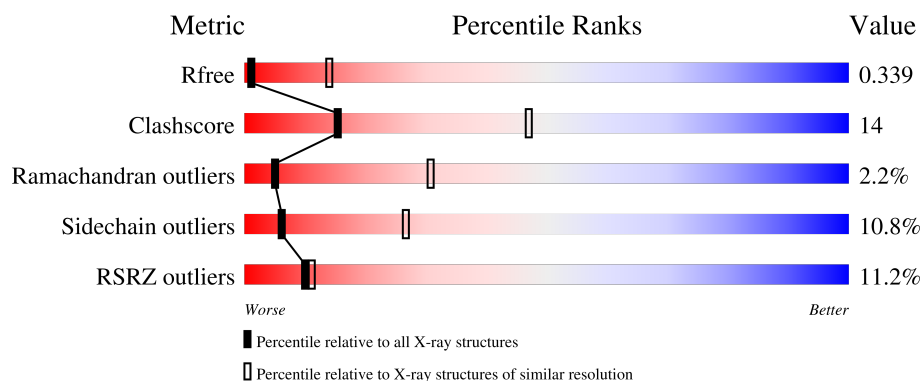
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	242	13% 66% 24% 6%
1	B	242	11% 58% 31% 5% 5%
1	C	242	7% 61% 24% 7% 8%
1	D	242	11% 60% 29% 9%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6616 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 Aquaporin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1678	1096	281	295	6			
1	B	230	Total	C	N	O	S	0	0	0
			1687	1105	283	293	6			
1	C	222	Total	C	N	O	S	0	0	0
			1629	1067	271	285	6			
1	D	220	Total	C	N	O	S	0	0	0
			1614	1059	269	280	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P41181
A	2	SER	-	cloning artifact	UNP P41181
B	1	GLY	-	cloning artifact	UNP P41181
B	2	SER	-	cloning artifact	UNP P41181
C	1	GLY	-	cloning artifact	UNP P41181
C	2	SER	-	cloning artifact	UNP P41181
D	1	GLY	-	cloning artifact	UNP P41181
D	2	SER	-	cloning artifact	UNP P41181

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cd	0	1
			2	2		
2	C	1	Total	Cd	0	0
			1	1		
2	D	1	Total	Cd	0	0
			1	1		

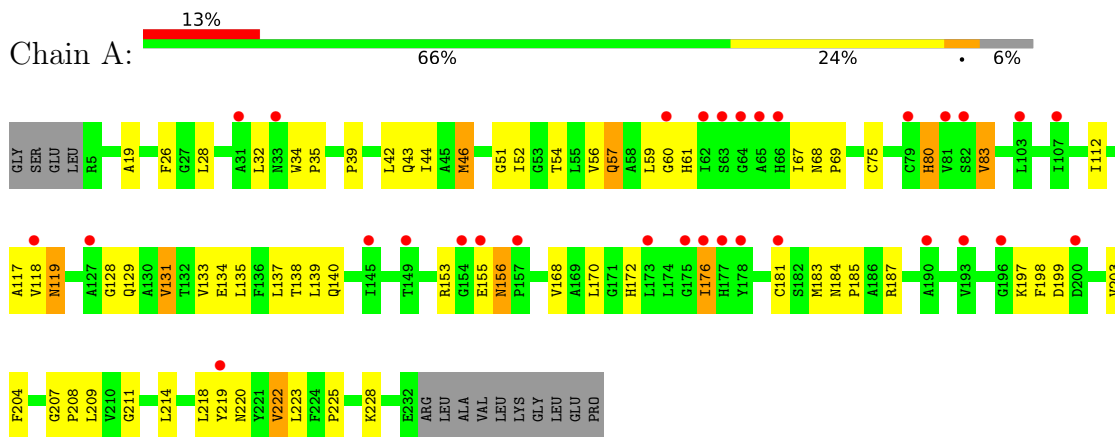
- Molecule 3 is water.

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

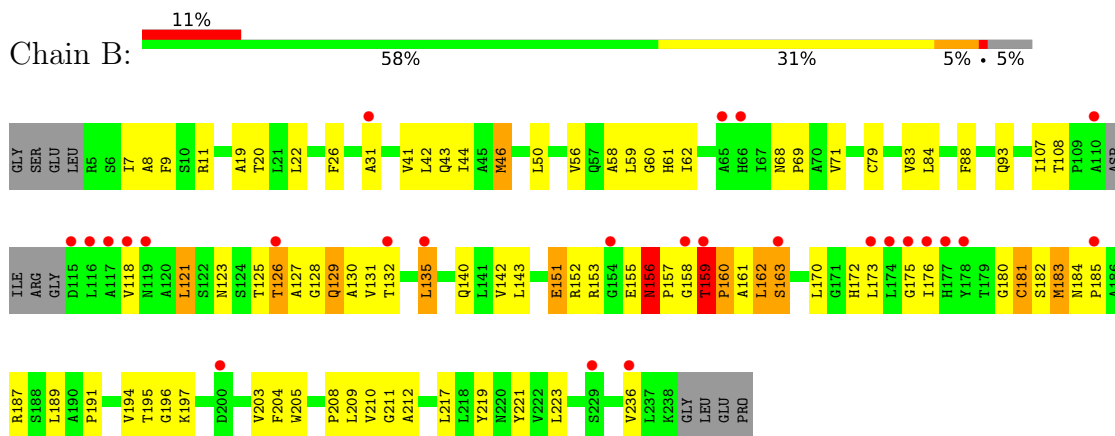
3 Residue-property plots [i](#)

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.

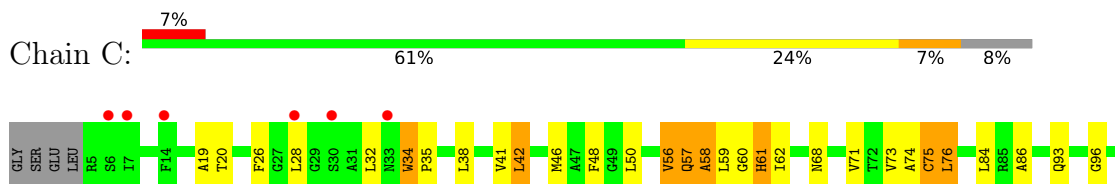
• Molecule 1: Aquaporin-2

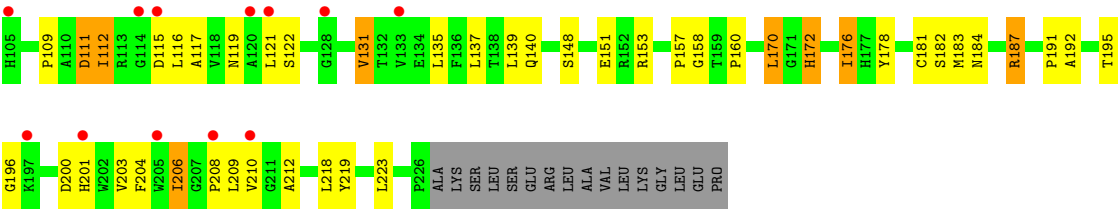


• Molecule 1: Aquaporin-2

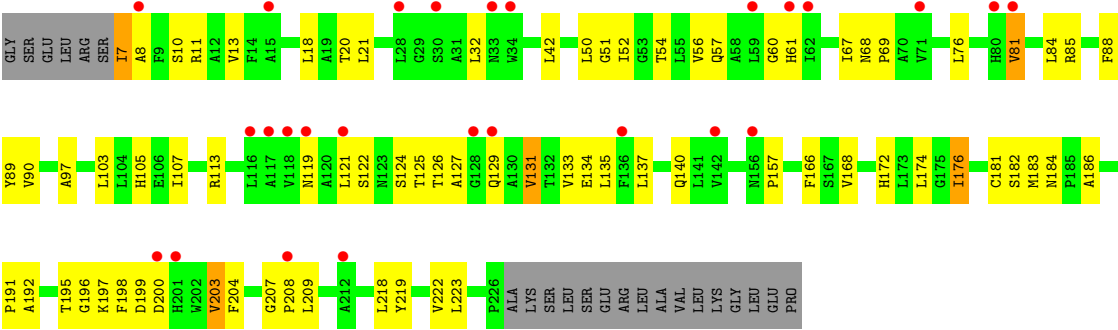


• Molecule 1: Aquaporin-2





● Molecule 1: Aquaporin-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	122.20Å 122.20Å 94.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.89 – 3.70 33.89 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (33.89-3.70) 89.8 (33.89-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.27 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155_9999	Depositor
R, R_{free}	0.282 , 0.336 0.286 , 0.339	Depositor DCC
R_{free} test set	1493 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	93.4	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 140.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.060 for h,-k,-l	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	6616	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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:
CD

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	0.15	0/1719	0.36	0/2352
1	B	0.27	0/1727	0.56	3/2363 (0.1%)
1	C	0.19	0/1670	0.40	0/2288
1	D	0.18	0/1655	0.40	0/2268
All	All	0.20	0/6771	0.44	3/9271 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	GLY	N-CA-C	6.85	121.14	111.42
1	B	162	LEU	CA-C-N	-6.36	111.80	120.44
1	B	162	LEU	C-N-CA	-6.36	111.80	120.44

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	1678	0	1706	45	0
1	B	1687	0	1721	63	0
1	C	1629	0	1650	55	0
1	D	1614	0	1641	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	6616	0	6718	180	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 14.

All (180) 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:56:VAL:O	1:B:60:GLY:HA3	1.41	1.21
1:C:56:VAL:O	1:C:60:GLY:HA3	1.43	1.16
1:B:160:PRO:O	1:B:163:SER:N	1.87	1.07
1:C:172:HIS:O	1:C:176:ILE:HB	1.56	1.06
1:D:172:HIS:O	1:D:176:ILE:HB	1.55	1.06
1:A:56:VAL:O	1:A:60:GLY:HA3	1.57	1.04
1:B:160:PRO:HG2	1:B:163:SER:HB2	1.45	0.99
1:B:59:LEU:O	1:B:62:ILE:N	2.10	0.85
1:A:172:HIS:O	1:A:176:ILE:HB	1.76	0.84
1:D:56:VAL:O	1:D:60:GLY:HA3	1.83	0.79
1:A:129:GLN:HB3	1:D:107:ILE:HG23	1.65	0.79
1:B:131:VAL:HG22	1:B:203:VAL:HG13	1.65	0.78
1:B:19:ALA:HB2	1:B:59:LEU:HD12	1.67	0.75
1:B:159:THR:O	1:B:160:PRO:C	2.29	0.75
1:B:153:ARG:NH2	1:C:57:GLN:O	2.20	0.72
1:D:105:HIS:O	1:D:113:ARG:NH1	2.21	0.72
1:D:131:VAL:HG23	1:D:203:VAL:HG23	1.72	0.71
1:C:74:ALA:HB2	1:C:212:ALA:HB1	1.75	0.69
1:C:20:THR:HG21	1:C:93:GLN:HA	1.75	0.67
1:C:58:ALA:O	1:C:61:HIS:ND1	2.25	0.67
1:A:134:GLU:HB3	1:A:208:PRO:HD3	1.77	0.67
1:C:71:VAL:O	1:C:75:CYS:HB2	1.95	0.66
1:D:134:GLU:HB3	1:D:208:PRO:HD3	1.75	0.66
1:D:203:VAL:O	1:D:207:GLY:N	2.26	0.65
1:A:68:ASN:ND2	1:A:183:MET:O	2.29	0.65
1:B:68:ASN:ND2	1:B:183:MET:O	2.20	0.65
1:A:52:ILE:HD12	1:A:168:VAL:HG11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:VAL:O	1:C:60:GLY:CA	2.33	0.64
1:D:199:ASP:N	1:D:199:ASP:OD1	2.30	0.63
1:D:126:THR:HG22	1:D:127:ALA:H	1.61	0.63
1:B:68:ASN:HB3	1:B:71:VAL:HG22	1.79	0.63
1:C:131:VAL:HG23	1:C:203:VAL:HG12	1.80	0.62
1:A:69:PRO:HD2	1:A:185:PRO:HD2	1.81	0.62
1:A:131:VAL:HG12	1:A:203:VAL:HG13	1.82	0.62
1:B:125:THR:HG21	1:C:109:PRO:HB3	1.83	0.61
1:D:204:PHE:O	1:D:208:PRO:HD2	1.99	0.61
1:C:48:PHE:HE2	1:C:187:ARG:HD3	1.64	0.61
1:C:148:SER:HB3	1:C:160:PRO:HB3	1.82	0.61
1:A:56:VAL:O	1:A:60:GLY:CA	2.44	0.61
1:D:218:LEU:HD12	1:D:222:VAL:HB	1.84	0.60
1:C:68:ASN:HB3	1:C:71:VAL:HG22	1.82	0.60
1:A:153:ARG:NH1	1:D:57:GLN:OE1	2.35	0.60
1:A:67:ILE:O	1:A:184:ASN:ND2	2.30	0.59
1:B:56:VAL:O	1:B:60:GLY:CA	2.33	0.59
1:A:156:ASN:N	1:A:156:ASN:OD1	2.35	0.58
1:D:68:ASN:ND2	1:D:183:MET:O	2.22	0.58
1:A:26:PHE:HB3	1:C:170:LEU:HD11	1.86	0.58
1:A:204:PHE:O	1:A:208:PRO:HD2	2.04	0.58
1:B:204:PHE:O	1:B:208:PRO:HD2	2.04	0.57
1:B:156:ASN:HB2	1:B:157:PRO:HD3	1.84	0.57
1:B:159:THR:O	1:B:161:ALA:N	2.38	0.57
1:A:138:THR:HG21	1:A:208:PRO:HB3	1.86	0.56
1:B:69:PRO:HD2	1:B:185:PRO:HD2	1.87	0.56
1:D:7:ILE:HG23	1:D:8:ALA:H	1.70	0.56
1:B:195:THR:O	1:B:197:LYS:N	2.38	0.56
1:B:191:PRO:HA	1:B:194:VAL:HG22	1.88	0.56
1:B:107:ILE:HD13	1:D:133:VAL:HG23	1.88	0.55
1:B:129:GLN:O	1:B:132:THR:OG1	2.14	0.55
1:D:119:ASN:HB3	1:D:204:PHE:CZ	2.42	0.55
1:B:118:VAL:HB	1:B:191:PRO:HB2	1.89	0.55
1:C:137:LEU:HB3	1:C:183:MET:HE3	1.88	0.55
1:B:107:ILE:HG12	1:D:129:GLN:HG3	1.88	0.55
1:B:159:THR:O	1:B:159:THR:HG22	2.07	0.55
1:C:206:ILE:O	1:C:210:VAL:HG23	2.07	0.54
1:A:184:ASN:HB3	1:A:187:ARG:HB3	1.89	0.54
1:B:22:LEU:HD23	1:D:140:GLN:HB3	1.89	0.54
1:B:156:ASN:CB	1:B:157:PRO:HD3	2.38	0.54
1:C:119:ASN:OD1	1:C:187:ARG:NH2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:PRO:O	1:C:157:PRO:HB3	2.09	0.53
1:C:73:VAL:HA	1:C:76:LEU:HB2	1.91	0.53
1:D:195:THR:O	1:D:197:LYS:N	2.35	0.53
1:A:133:VAL:HG23	1:D:107:ILE:HG21	1.89	0.53
1:C:116:LEU:HD23	1:C:191:PRO:HA	1.90	0.53
1:A:170:LEU:HD22	1:D:51:GLY:HA2	1.91	0.53
1:C:109:PRO:HB2	1:C:112:ILE:HD12	1.91	0.53
1:D:85:ARG:NH1	1:D:89:TYR:OH	2.42	0.52
1:C:76:LEU:HD11	1:C:86:ALA:HB2	1.91	0.52
1:A:225:PRO:HG3	1:D:11:ARG:HH12	1.75	0.52
1:B:127:ALA:O	1:B:130:ALA:HB3	2.10	0.52
1:B:43:GLN:HG2	1:D:42:LEU:HB2	1.91	0.52
1:B:176:ILE:HA	1:B:180:GLY:HA2	1.91	0.52
1:A:32:LEU:HD21	1:A:117:ALA:N	2.25	0.51
1:A:34:TRP:H	1:A:112:ILE:HG21	1.76	0.51
1:A:42:LEU:O	1:A:46:MET:HB2	2.10	0.51
1:B:182:SER:C	1:B:184:ASN:H	2.19	0.51
1:B:189:LEU:HD22	1:B:205:TRP:HZ2	1.75	0.51
1:B:107:ILE:O	1:B:108:THR:OG1	2.26	0.51
1:A:39:PRO:HB2	1:A:44:ILE:HD11	1.93	0.50
1:D:219:TYR:HA	1:D:223:LEU:HB2	1.94	0.50
1:C:219:TYR:HA	1:C:223:LEU:HB2	1.93	0.50
1:A:43:GLN:HA	1:C:42:LEU:HD13	1.94	0.50
1:B:153:ARG:CZ	1:C:61:HIS:HB3	2.42	0.50
1:B:128:GLY:O	1:B:131:VAL:N	2.46	0.49
1:C:137:LEU:O	1:C:140:GLN:HG3	2.12	0.49
1:A:155:GLU:N	1:A:155:GLU:OE1	2.46	0.49
1:D:137:LEU:O	1:D:140:GLN:HG3	2.13	0.49
1:B:50:LEU:HD22	1:D:166:PHE:HB3	1.94	0.49
1:B:128:GLY:HA2	1:B:131:VAL:HG23	1.95	0.49
1:C:19:ALA:HB2	1:C:59:LEU:HD12	1.95	0.48
1:B:125:THR:HG22	1:B:126:THR:OG1	2.14	0.48
1:A:118:VAL:HG21	1:A:197:LYS:HB3	1.94	0.48
1:B:151:GLU:CD	1:B:151:GLU:H	2.21	0.48
1:A:203:VAL:O	1:A:207:GLY:N	2.39	0.48
1:A:219:TYR:HA	1:A:223:LEU:HB2	1.96	0.47
1:B:26:PHE:HA	1:D:174:LEU:HD22	1.95	0.47
1:B:156:ASN:HB2	1:B:157:PRO:CD	2.44	0.47
1:A:153:ARG:CZ	1:D:61:HIS:HB2	2.44	0.47
1:C:204:PHE:O	1:C:208:PRO:HD2	2.13	0.47
1:D:52:ILE:HG21	1:D:168:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LEU:HA	1:B:221:TYR:HD2	1.80	0.47
1:A:80:HIS:CG	1:A:83:VAL:HG21	2.50	0.46
1:B:121:LEU:HD12	1:B:123:ASN:H	1.80	0.46
1:C:192:ALA:O	1:C:196:GLY:N	2.43	0.46
1:C:32:LEU:HD21	1:C:117:ALA:N	2.31	0.46
1:D:131:VAL:O	1:D:135:LEU:HB2	2.16	0.46
1:D:13:VAL:HG11	1:D:88:PHE:HB3	1.98	0.46
1:D:182:SER:C	1:D:184:ASN:H	2.25	0.45
1:A:51:GLY:HA2	1:C:170:LEU:HD22	1.97	0.45
1:A:28:LEU:HD22	1:A:117:ALA:HB3	1.98	0.45
1:B:175:GLY:HA3	1:B:181:CYS:HB2	1.97	0.45
1:C:172:HIS:O	1:C:176:ILE:CB	2.46	0.45
1:B:8:ALA:HA	1:B:11:ARG:HG3	1.98	0.45
1:A:214:LEU:HD23	1:A:218:LEU:HG	1.97	0.45
1:B:131:VAL:HG22	1:B:203:VAL:CG1	2.41	0.45
1:B:31:ALA:HA	1:B:44:ILE:HD12	1.98	0.44
1:A:218:LEU:HD22	1:A:222:VAL:HG21	1.99	0.44
1:C:115:ASP:OD1	1:C:115:ASP:N	2.35	0.44
1:D:97:ALA:HB2	1:D:186:ALA:HB1	1.99	0.44
1:A:119:ASN:N	1:A:119:ASN:OD1	2.50	0.44
1:B:42:LEU:O	1:B:46:MET:HB2	2.17	0.44
1:A:80:HIS:CD2	1:A:83:VAL:HG21	2.53	0.44
1:B:160:PRO:C	1:B:163:SER:H	2.07	0.44
1:B:191:PRO:O	1:B:195:THR:HB	2.17	0.44
1:B:160:PRO:HG3	1:C:158:GLY:HA3	1.99	0.44
1:C:218:LEU:HG	1:C:223:LEU:HG	1.99	0.44
1:A:54:THR:O	1:A:57:GLN:HB3	2.18	0.43
1:A:134:GLU:CB	1:A:208:PRO:HD3	2.48	0.43
1:B:135:LEU:HD23	1:B:211:GLY:HA2	2.00	0.43
1:C:109:PRO:HB2	1:C:112:ILE:CD1	2.47	0.43
1:C:111:ASP:OD1	1:C:111:ASP:N	2.51	0.43
1:C:34:TRP:CD1	1:C:34:TRP:H	2.36	0.43
1:A:137:LEU:O	1:A:140:GLN:HG3	2.17	0.43
1:B:142:VAL:HG21	1:B:212:ALA:HA	2.00	0.43
1:C:204:PHE:O	1:C:208:PRO:CD	2.66	0.43
1:C:182:SER:HA	1:C:187:ARG:NH2	2.33	0.43
1:A:61:HIS:CE1	1:C:153:ARG:HG2	2.53	0.43
1:A:128:GLY:O	1:A:131:VAL:HG22	2.19	0.43
1:C:46:MET:O	1:C:50:LEU:HB2	2.19	0.43
1:C:28:LEU:HD22	1:C:117:ALA:HB3	2.01	0.43
1:C:182:SER:HA	1:C:187:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ASN:HB3	1:C:187:ARG:HB2	2.01	0.42
1:D:76:LEU:HA	1:D:81:VAL:HG23	2.01	0.42
1:A:135:LEU:HG	1:A:211:GLY:HA2	2.02	0.42
1:D:52:ILE:HD13	1:D:168:VAL:HG21	2.01	0.42
1:B:9:PHE:HE1	1:B:88:PHE:HD2	1.67	0.42
1:B:223:LEU:HB3	1:C:62:ILE:HD13	2.01	0.42
1:C:135:LEU:O	1:C:139:LEU:HB2	2.19	0.42
1:D:10:SER:HA	1:D:13:VAL:HG22	2.01	0.42
1:C:32:LEU:HD11	1:C:116:LEU:HA	2.00	0.42
1:B:41:VAL:HG13	1:B:176:ILE:HG21	2.01	0.42
1:B:135:LEU:HD21	1:B:210:VAL:HG12	2.01	0.42
1:A:19:ALA:HB2	1:A:59:LEU:HD22	2.01	0.41
1:B:20:THR:HG21	1:B:93:GLN:HA	2.03	0.41
1:C:20:THR:HG23	1:C:96:GLY:HA3	2.02	0.41
1:B:219:TYR:HA	1:B:223:LEU:HB2	2.01	0.41
1:D:50:LEU:O	1:D:54:THR:HG22	2.19	0.41
1:D:192:ALA:O	1:D:198:PHE:HE1	2.04	0.41
1:A:133:VAL:O	1:A:137:LEU:HG	2.21	0.41
1:B:160:PRO:C	1:B:162:LEU:N	2.76	0.41
1:A:26:PHE:CZ	1:C:140:GLN:HG2	2.56	0.41
1:B:209:LEU:O	1:B:210:VAL:C	2.64	0.41
1:C:122:SER:HB3	1:C:178:TYR:O	2.21	0.41
1:D:32:LEU:HA	1:D:32:LEU:HD12	1.87	0.41
1:D:69:PRO:HB3	1:D:90:VAL:HG13	2.03	0.41
1:B:223:LEU:HB3	1:C:62:ILE:CD1	2.51	0.40
1:D:191:PRO:O	1:D:195:THR:HG22	2.21	0.40
1:B:140:GLN:HG2	1:C:26:PHE:CZ	2.56	0.40
1:B:107:ILE:HG23	1:D:129:GLN:CG	2.51	0.40
1:C:204:PHE:O	1:C:206:ILE:N	2.54	0.40
1:C:41:VAL:HG13	1:C:176:ILE:HG21	2.03	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	226/242 (93%)	189 (84%)	32 (14%)	5 (2%)	5	31
1	B	226/242 (93%)	186 (82%)	33 (15%)	7 (3%)	3	26
1	C	220/242 (91%)	190 (86%)	27 (12%)	3 (1%)	9	37
1	D	218/242 (90%)	193 (88%)	20 (9%)	5 (2%)	5	30
All	All	890/968 (92%)	758 (85%)	112 (13%)	20 (2%)	5	31

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	ASN
1	B	159	THR
1	D	157	PRO
1	A	119	ASN
1	B	58	ALA
1	B	196	GLY
1	D	125	THR
1	A	35	PRO
1	C	35	PRO
1	A	181	CYS
1	A	209	LEU
1	B	160	PRO
1	B	183	MET
1	C	181	CYS
1	D	67	ILE
1	D	181	CYS
1	D	196	GLY
1	A	57	GLN
1	B	181	CYS
1	C	58	ALA

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	173/184 (94%)	160 (92%)	13 (8%)	12	39
1	B	173/184 (94%)	151 (87%)	22 (13%)	4	21
1	C	167/184 (91%)	144 (86%)	23 (14%)	3	19
1	D	165/184 (90%)	150 (91%)	15 (9%)	9	33
All	All	678/736 (92%)	605 (89%)	73 (11%)	6	27

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	75	CYS
1	A	80	HIS
1	A	83	VAL
1	A	131	VAL
1	A	139	LEU
1	A	156	ASN
1	A	176	ILE
1	A	198	PHE
1	A	199	ASP
1	A	220	ASN
1	A	222	VAL
1	A	228	LYS
1	B	7	ILE
1	B	46	MET
1	B	61	HIS
1	B	79	CYS
1	B	83	VAL
1	B	84	LEU
1	B	121	LEU
1	B	126	THR
1	B	129	GLN
1	B	135	LEU
1	B	143	LEU
1	B	151	GLU
1	B	152	ARG
1	B	155	GLU
1	B	156	ASN
1	B	159	THR
1	B	163	SER
1	B	170	LEU
1	B	172	HIS
1	B	173	LEU

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Mol	Chain	Res	Type
1	B	187	ARG
1	B	236	VAL
1	C	34	TRP
1	C	38	LEU
1	C	42	LEU
1	C	56	VAL
1	C	57	GLN
1	C	61	HIS
1	C	75	CYS
1	C	76	LEU
1	C	84	LEU
1	C	111	ASP
1	C	112	ILE
1	C	121	LEU
1	C	131	VAL
1	C	151	GLU
1	C	170	LEU
1	C	172	HIS
1	C	176	ILE
1	C	187	ARG
1	C	195	THR
1	C	200	ASP
1	C	201	HIS
1	C	206	ILE
1	C	209	LEU
1	D	7	ILE
1	D	18	LEU
1	D	20	THR
1	D	21	LEU
1	D	81	VAL
1	D	84	LEU
1	D	103	LEU
1	D	121	LEU
1	D	122	SER
1	D	124	SER
1	D	131	VAL
1	D	176	ILE
1	D	200	ASP
1	D	203	VAL
1	D	209	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	129	GLN
1	B	93	GLN
1	B	119	ASN
1	B	123	ASN
1	C	36	GLN
1	D	105	HIS
1	D	156	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	228/242 (94%)	0.93	31 (13%) 7 8	35, 104, 157, 232	0
1	B	230/242 (95%)	0.88	26 (11%) 10 11	42, 97, 158, 199	1 (0%)
1	C	222/242 (91%)	0.81	18 (8%) 18 14	35, 96, 156, 190	0
1	D	220/242 (90%)	0.96	26 (11%) 9 10	49, 112, 170, 227	1 (0%)
All	All	900/968 (92%)	0.90	101 (11%) 10 11	35, 102, 161, 232	2 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	176	ILE	6.2
1	C	120	ALA	5.1
1	C	121	LEU	4.5
1	A	118	VAL	4.4
1	C	6	SER	4.4
1	C	115	ASP	4.3
1	D	8	ALA	4.3
1	A	103	LEU	4.3
1	A	66	HIS	4.2
1	D	117	ALA	4.1
1	B	117	ALA	3.9
1	A	219	TYR	3.8
1	A	154	GLY	3.7
1	B	132	THR	3.7
1	A	60	GLY	3.6
1	B	178	TYR	3.4
1	D	119	ASN	3.3
1	B	65	ALA	3.2
1	D	142	VAL	3.2
1	B	177	HIS	3.2
1	A	64	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	80	HIS	3.1
1	B	163	SER	3.0
1	C	197	LYS	3.0
1	D	116	LEU	3.0
1	A	200	ASP	3.0
1	A	177	HIS	3.0
1	D	81	VAL	3.0
1	D	212	ALA	2.9
1	D	59	LEU	2.9
1	B	116	LEU	2.9
1	B	174	LEU	2.9
1	B	173	LEU	2.9
1	C	7	ILE	2.8
1	C	30	SER	2.8
1	A	157	PRO	2.8
1	A	149	THR	2.8
1	A	175	GLY	2.8
1	D	61	HIS	2.7
1	A	178	TYR	2.7
1	B	31	ALA	2.7
1	D	62	ILE	2.7
1	C	128	GLY	2.7
1	B	66	HIS	2.6
1	A	81	VAL	2.6
1	D	121	LEU	2.6
1	C	105	HIS	2.6
1	A	31	ALA	2.6
1	A	127	ALA	2.6
1	C	208	PRO	2.6
1	C	33	ASN	2.5
1	A	65	ALA	2.5
1	D	30	SER	2.5
1	D	201	HIS	2.5
1	A	181	CYS	2.5
1	B	110	ALA	2.4
1	B	158	GLY	2.4
1	A	63	SER	2.4
1	B	229	SER	2.4
1	A	107	ILE	2.4
1	B	154	GLY	2.4
1	A	196	GLY	2.4
1	B	236	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	33	ASN	2.4
1	B	119	ASN	2.4
1	D	208	PRO	2.4
1	A	155	GLU	2.4
1	B	200	ASP	2.4
1	C	210	VAL	2.3
1	C	205	TRP	2.3
1	A	173	LEU	2.3
1	B	118	VAL	2.3
1	A	62	ILE	2.3
1	C	14	PHE	2.3
1	D	15	ALA	2.3
1	D	33	ASN	2.2
1	D	156	ASN	2.2
1	B	115	ASP	2.2
1	B	159	THR	2.2
1	A	190	ALA	2.2
1	B	175	GLY	2.2
1	C	201	HIS	2.1
1	A	176	ILE	2.1
1	D	28	LEU	2.1
1	C	114	GLY	2.1
1	C	28	LEU	2.1
1	A	79	CYS	2.1
1	A	193	VAL	2.1
1	D	34	TRP	2.1
1	D	129	GLN	2.1
1	B	185	PRO	2.1
1	A	145	ILE	2.1
1	B	135	LEU	2.1
1	D	200	ASP	2.0
1	C	133	VAL	2.0
1	D	71	VAL	2.0
1	D	128	GLY	2.0
1	B	126	THR	2.0
1	D	136	PHE	2.0
1	A	82	SER	2.0
1	D	118	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	B	301[A]	1/1	0.72	0.11	136,136,136,136	1
2	CD	B	301[B]	1/1	0.72	0.11	119,119,119,119	1
2	CD	D	301	1/1	0.92	0.06	135,135,135,135	0
2	CD	C	301	1/1	0.99	0.12	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.