



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:52 PM UTC

PDB ID : 4DGI / pdb_00004dgi
Title : Structure of POM1 FAB fragment complexed with human PrPc Fragment 120-230
Authors : Baral, P.K.; Wieland, B.; Swayampakula, M.; James, M.N.
Deposited on : 2012-01-26
Resolution : 2.40 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

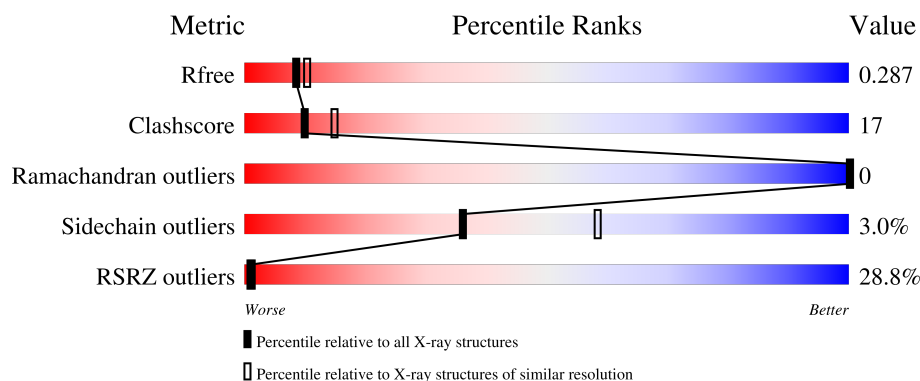
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	111	19% 54% 30% • • 13%
2	H	218	26% 78% 20% •
3	L	213	35% 72% 23% 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4276 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 Major prion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			811	501	141	160	9			

- Molecule 2 is a protein called POM1 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	4	0	0
			1642	1037	265	330	10			

- Molecule 3 is a protein called POM1 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1652	1022	280	345	5			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Na	0	0
			1	1		

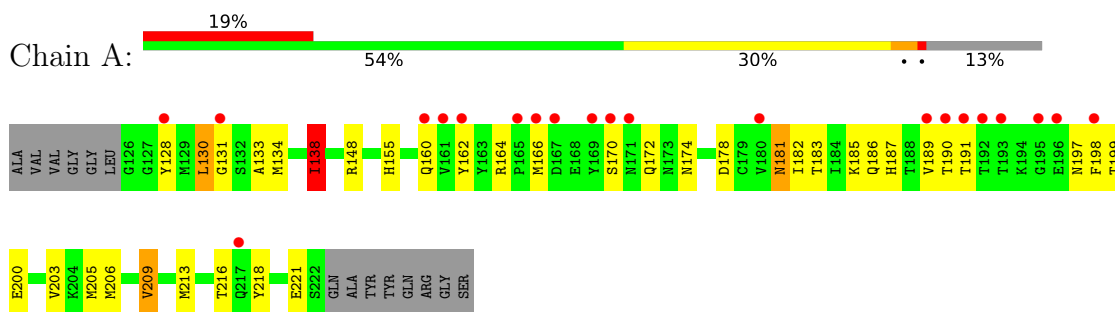
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	H	99	Total	O	0	0
			99	99		
5	L	50	Total	O	0	0
			50	50		

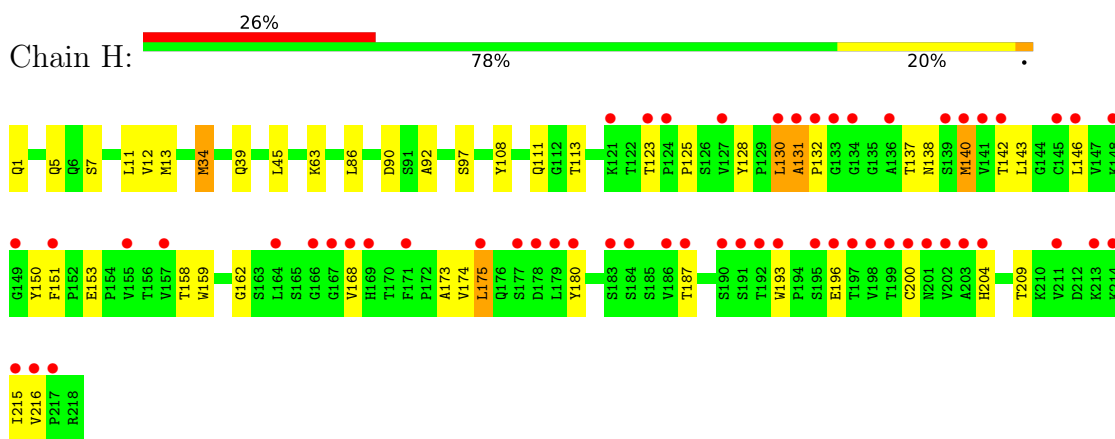
3 Residue-property plots

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.

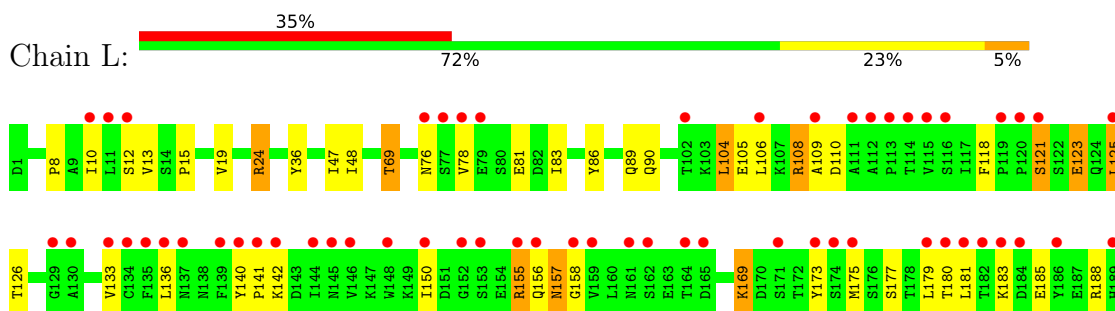
- Molecule 1: Major prion protein



- Molecule 2: POM1 Fab Heavy chain



- Molecule 3: POM1 Fab Light chain



H190	T191	Y192	T193	C194	E195	A196	T197	H198	K199	T200	S201	T202	S203	P204	T205	V206	F207	S208	F209	N210	R211	N212	E213
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.53Å 105.92Å 76.23Å 90.00° 95.08° 90.00°	Depositor
Resolution (Å)	35.19 – 2.40 35.19 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.19-2.40) 99.2 (35.19-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.258 , 0.289 0.251 , 0.287	Depositor DCC
R_{free} test set	1331 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4276	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.09	1/829 (0.1%)	1.47	7/1118 (0.6%)
2	H	1.22	0/1688	1.38	11/2306 (0.5%)
3	L	0.94	1/1687 (0.1%)	1.28	4/2291 (0.2%)
All	All	1.09	2/4204 (0.0%)	1.36	22/5715 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	157	ASN	CA-C	6.20	1.60	1.52
1	A	198	PHE	CA-C	-5.95	1.45	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	131	ALA	CA-C-N	-9.45	108.03	119.84
2	H	131	ALA	C-N-CA	-9.45	108.03	119.84
1	A	197	ASN	N-CA-C	8.23	122.50	109.50
2	H	216	VAL	CA-C-N	8.19	128.25	119.89
2	H	216	VAL	C-N-CA	8.19	128.25	119.89
2	H	123	THR	CA-C-N	-7.64	114.16	119.66
2	H	123	THR	C-N-CA	-7.64	114.16	119.66
1	A	181	ASN	N-CA-C	7.08	118.64	111.07
1	A	209	VAL	N-CA-C	6.53	117.31	110.72
1	A	138	ILE	N-CA-C	-6.44	101.23	109.80
2	H	196	GLU	N-CA-C	6.18	118.59	109.69
3	L	69	THR	N-CA-C	-5.89	107.08	114.56
2	H	140	MET	N-CA-C	5.67	118.79	109.72
2	H	204	HIS	CA-C-N	5.59	125.69	119.32
2	H	204	HIS	C-N-CA	5.59	125.69	119.32
3	L	155	ARG	CA-CB-CG	-5.43	103.24	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	LEU	CA-C-N	5.39	126.63	120.53
1	A	130	LEU	C-N-CA	5.39	126.63	120.53
1	A	216	THR	N-CA-C	-5.29	105.59	111.36
3	L	125	LEU	N-CA-C	-5.22	105.71	111.71
3	L	155	ARG	N-CA-CB	5.11	118.95	110.52
2	H	168	VAL	N-CA-C	5.09	115.64	108.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	811	0	750	33	1
2	H	1642	0	1578	54	0
3	L	1652	0	1573	53	1
4	L	1	0	0	0	0
5	A	21	0	0	3	1
5	H	99	0	0	10	1
5	L	50	0	0	4	1
All	All	4276	0	3901	139	3

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 17.

All (139) 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)
2:H:153:GLU:OE1	5:H:361:HOH:O	1.93	0.85
3:L:13:VAL:HG11	3:L:19:VAL:HG11	1.57	0.85
1:A:181:ASN:O	1:A:185:LYS:HG3	1.79	0.83
1:A:130:LEU:HB2	1:A:162:TYR:HE1	1.44	0.82
1:A:130:LEU:HB2	1:A:162:TYR:CE1	2.15	0.81
2:H:137:THR:HG22	2:H:140:MET:O	1.79	0.81
2:H:12:VAL:HG21	2:H:86:LEU:HD12	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLU:O	1:A:203:VAL:HG22	1.82	0.78
3:L:155:ARG:HE	3:L:157:ASN:HB3	1.48	0.78
1:A:200:GLU:HA	1:A:203:VAL:HG22	1.66	0.74
3:L:83:ILE:HG23	3:L:104:LEU:O	1.88	0.73
3:L:118:PHE:HB2	3:L:133:VAL:CG1	2.18	0.73
1:A:178:ASP:O	1:A:182:ILE:HG12	1.90	0.72
3:L:142:LYS:HD3	3:L:173:TYR:CG	2.26	0.70
1:A:199:THR:O	1:A:203:VAL:HG13	1.93	0.69
2:H:12:VAL:CG2	2:H:86:LEU:HD12	2.24	0.67
3:L:142:LYS:HD3	3:L:173:TYR:CD1	2.31	0.65
3:L:108:ARG:CG	3:L:108:ARG:HH11	2.11	0.64
2:H:125:PRO:HB3	2:H:150:TYR:HB3	1.80	0.64
2:H:138:ASN:C	2:H:140:MET:H	2.06	0.64
2:H:1:GLN:CD	2:H:1:GLN:N	2.55	0.63
1:A:186:GLN:O	1:A:189:VAL:HG12	1.99	0.63
2:H:1:GLN:CD	2:H:1:GLN:H1	2.09	0.61
2:H:39:GLN:O	2:H:92:ALA:HB1	2.01	0.61
2:H:137:THR:CG2	2:H:140:MET:O	2.48	0.60
1:A:134:MET:HE1	1:A:213:MET:HB3	1.84	0.60
2:H:12:VAL:HG11	2:H:86:LEU:CD1	2.32	0.60
3:L:155:ARG:HG3	3:L:156:GLN:N	2.17	0.59
1:A:205:MET:O	1:A:209:VAL:HG12	2.02	0.59
3:L:123:GLU:O	3:L:126:THR:HB	2.02	0.59
3:L:155:ARG:HD2	3:L:156:GLN:H	1.69	0.58
3:L:8:PRO:HD3	5:L:424:HOH:O	2.03	0.58
2:H:45:LEU:N	5:H:303:HOH:O	2.37	0.58
2:H:158:THR:HG22	2:H:159:TRP:N	2.17	0.57
3:L:118:PHE:HB2	3:L:133:VAL:HG13	1.85	0.57
1:A:130:LEU:CB	1:A:162:TYR:CE1	2.88	0.57
1:A:138:ILE:O	1:A:138:ILE:HG12	2.03	0.57
3:L:155:ARG:NE	3:L:157:ASN:HB3	2.17	0.57
3:L:121:SER:HB3	3:L:123:GLU:HG2	1.86	0.57
3:L:155:ARG:HE	3:L:157:ASN:CB	2.18	0.57
1:A:200:GLU:CA	1:A:203:VAL:HG22	2.36	0.55
2:H:11:LEU:CD2	2:H:151:PHE:HZ	2.19	0.54
1:A:200:GLU:O	1:A:203:VAL:CG2	2.54	0.54
2:H:153:GLU:OE1	2:H:173:ALA:HB3	2.08	0.54
1:A:200:GLU:HA	1:A:203:VAL:CG2	2.36	0.54
1:A:200:GLU:C	1:A:203:VAL:HG22	2.33	0.53
1:A:166:MET:SD	1:A:166:MET:N	2.80	0.52
2:H:132:PRO:HD2	2:H:193:TRP:CH2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:GLN:CG	5:H:377:HOH:O	2.57	0.52
3:L:169:LYS:HB2	3:L:169:LYS:NZ	2.26	0.51
1:A:130:LEU:CG	1:A:162:TYR:CE1	2.94	0.51
3:L:136:LEU:HD21	3:L:196:ALA:HB2	1.94	0.50
3:L:180:THR:O	3:L:181:LEU:HD12	2.12	0.50
1:A:130:LEU:HG	1:A:162:TYR:CE1	2.47	0.49
2:H:130:LEU:HD11	2:H:146:LEU:HB2	1.95	0.49
3:L:110:ASP:HB3	3:L:200:THR:HG22	1.94	0.49
2:H:97:SER:HA	2:H:108:TYR:O	2.14	0.48
2:H:138:ASN:C	2:H:140:MET:N	2.70	0.48
3:L:24:ARG:NH1	5:L:438:HOH:O	2.46	0.48
3:L:13:VAL:CG1	3:L:19:VAL:HG11	2.36	0.48
1:A:148:ARG:HD3	5:A:321:HOH:O	2.13	0.48
3:L:15:PRO:HA	3:L:78:VAL:HG13	1.95	0.48
3:L:121:SER:OG	3:L:123:GLU:OE2	2.24	0.48
2:H:111:GLN:CG	5:H:342:HOH:O	2.61	0.48
2:H:111:GLN:HG3	5:H:342:HOH:O	2.14	0.48
3:L:89:GLN:HG2	3:L:90:GLN:N	2.29	0.48
3:L:108:ARG:HH11	3:L:108:ARG:HG2	1.79	0.47
2:H:175:LEU:HD13	2:H:175:LEU:HA	1.66	0.47
3:L:158:GLY:O	3:L:179:LEU:HD12	2.14	0.47
2:H:63:LYS:HD2	5:H:392:HOH:O	2.13	0.47
1:A:187:HIS:O	1:A:191:THR:HG23	2.14	0.47
2:H:5:GLN:NE2	5:H:377:HOH:O	2.36	0.47
3:L:47:ILE:C	3:L:48:ILE:HG12	2.39	0.47
3:L:108:ARG:HG3	3:L:109:ALA:N	2.29	0.47
1:A:170:SER:HB3	1:A:174:ASN:ND2	2.30	0.47
3:L:83:ILE:HG13	3:L:106:LEU:HG	1.96	0.47
3:L:175:MET:HE2	3:L:177:SER:HB2	1.97	0.47
2:H:138:ASN:O	2:H:140:MET:N	2.48	0.46
2:H:158:THR:CG2	2:H:162:GLY:HA2	2.45	0.46
2:H:143:LEU:HD11	2:H:193:TRP:CE2	2.50	0.46
3:L:140:TYR:CG	3:L:141:PRO:HA	2.51	0.46
3:L:190:ASN:HD21	3:L:212:ASN:ND2	2.14	0.46
3:L:193:THR:OG1	3:L:208:SER:HB3	2.16	0.46
2:H:137:THR:HG23	2:H:138:ASN:N	2.31	0.46
3:L:125:LEU:O	3:L:183:LYS:HD2	2.16	0.46
2:H:63:LYS:CD	5:H:392:HOH:O	2.63	0.46
2:H:131:ALA:HB2	2:H:215:ILE:CG2	2.45	0.46
1:A:182:ILE:HG13	1:A:183:THR:N	2.32	0.45
3:L:191:THR:HG22	3:L:210:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLN:O	1:A:190:THR:HG23	2.16	0.45
2:H:131:ALA:HB2	2:H:215:ILE:HG22	1.97	0.45
3:L:193:THR:CG2	3:L:206:VAL:HG13	2.45	0.45
3:L:157:ASN:ND2	5:L:425:HOH:O	2.50	0.45
2:H:12:VAL:HG11	2:H:86:LEU:HD12	1.99	0.44
3:L:108:ARG:CG	3:L:108:ARG:NH1	2.76	0.44
1:A:133:ALA:HA	1:A:160:GLN:HB3	1.99	0.44
2:H:140:MET:HE3	2:H:187:THR:HG22	1.99	0.44
2:H:11:LEU:HD21	2:H:151:PHE:HZ	1.81	0.44
1:A:128:TYR:CE1	1:A:164:ARG:HG3	2.52	0.44
2:H:159:TRP:CZ3	2:H:200:CYS:HB3	2.53	0.44
2:H:11:LEU:HD23	2:H:151:PHE:HZ	1.82	0.44
1:A:206:MET:HA	1:A:209:VAL:HG12	1.99	0.43
3:L:36:TYR:O	3:L:86:TYR:HA	2.18	0.43
2:H:13:MET:HE3	2:H:13:MET:HB3	1.89	0.43
3:L:8:PRO:CD	5:L:424:HOH:O	2.65	0.43
3:L:155:ARG:CG	3:L:156:GLN:N	2.81	0.43
3:L:195:GLU:O	3:L:195:GLU:HG2	2.12	0.43
1:A:130:LEU:HD23	1:A:131:GLY:O	2.19	0.43
1:A:166:MET:HE2	1:A:221:GLU:OE1	2.18	0.43
2:H:12:VAL:HG21	2:H:86:LEU:CD1	2.41	0.43
2:H:11:LEU:HD21	2:H:151:PHE:CZ	2.54	0.42
1:A:155:HIS:CE1	5:A:313:HOH:O	2.72	0.42
2:H:5:GLN:HG2	5:H:377:HOH:O	2.20	0.42
3:L:185:GLU:HA	3:L:188:ARG:HD3	2.01	0.42
2:H:34:MET:HE2	2:H:34:MET:HB3	1.52	0.42
2:H:173:ALA:HB3	5:H:361:HOH:O	2.19	0.42
2:H:174:VAL:O	2:H:180:TYR:HA	2.20	0.42
2:H:11:LEU:CD2	2:H:151:PHE:CZ	3.01	0.42
2:H:130:LEU:HD11	2:H:146:LEU:CB	2.50	0.41
1:A:185:LYS:HA	5:A:315:HOH:O	2.20	0.41
3:L:136:LEU:HD12	3:L:136:LEU:N	2.34	0.41
3:L:150:ILE:O	3:L:150:ILE:HG23	2.18	0.41
3:L:150:ILE:HD13	3:L:192:TYR:CE2	2.55	0.41
2:H:158:THR:CG2	2:H:159:TRP:N	2.82	0.41
3:L:169:LYS:NZ	3:L:169:LYS:CB	2.83	0.41
2:H:86:LEU:HA	2:H:90:ASP:OD2	2.19	0.41
1:A:128:TYR:CD1	1:A:164:ARG:HG3	2.56	0.41
3:L:125:LEU:HA	3:L:125:LEU:HD23	1.87	0.41
2:H:125:PRO:CB	2:H:150:TYR:HB3	2.48	0.41
3:L:105:GLU:HG2	3:L:106:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:179:LEU:HG	3:L:181:LEU:HD13	2.03	0.41
1:A:172:GLN:HB2	1:A:218:TYR:CE2	2.55	0.41
2:H:7:SER:O	2:H:113:THR:HA	2.20	0.41
2:H:128:TYR:O	2:H:130:LEU:HD13	2.20	0.41
2:H:12:VAL:CG1	2:H:86:LEU:HD12	2.51	0.41
3:L:169:LYS:HB2	3:L:169:LYS:HZ2	1.86	0.40
2:H:11:LEU:HD13	2:H:11:LEU:C	2.46	0.40
3:L:24:ARG:HA	3:L:69:THR:O	2.22	0.40
2:H:142:THR:HG22	3:L:118:PHE:HZ	1.86	0.40

All (3) 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:A:164:ARG:NH1	3:L:76:ASN:OD1[3_455]	2.05	0.15
5:A:317:HOH:O	5:H:390:HOH:O[2_554]	2.13	0.07
5:L:425:HOH:O	5:L:443:HOH:O[2_555]	2.13	0.07

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	95/111 (86%)	92 (97%)	3 (3%)	0	100	100
2	H	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
3	L	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
All	All	522/542 (96%)	505 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	91/100 (91%)	90 (99%)	1 (1%)	65	82
2	H	187/187 (100%)	183 (98%)	4 (2%)	47	69
3	L	191/191 (100%)	182 (95%)	9 (5%)	23	41
All	All	469/478 (98%)	455 (97%)	14 (3%)	36	58

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	ILE
2	H	34	MET
2	H	130	LEU
2	H	175	LEU
2	H	209	THR
3	L	10	ILE
3	L	12	SER
3	L	24	ARG
3	L	81	GLU
3	L	104	LEU
3	L	108	ARG
3	L	121	SER
3	L	123	GLU
3	L	169	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	39	GLN
2	H	60	HIS
2	H	176	GLN
3	L	38	GLN
3	L	76	ASN
3	L	145	ASN
3	L	190	ASN

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 1 ligands modelled in this entry, 1 is 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 [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	97/111 (87%)	1.12	21 (21%)	2 2	26, 64, 99, 106	0
2	H	217/218 (99%)	0.97	56 (25%)	1 1	22, 44, 105, 127	0
3	L	213/213 (100%)	1.48	75 (35%)	1 1	26, 77, 113, 124	0
All	All	527/542 (97%)	1.20	152 (28%)	1 1	22, 67, 110, 127	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	SER	6.7
3	L	186	TYR	5.2
2	H	141	VAL	4.9
3	L	144	ILE	4.8
2	H	191	SER	4.7
3	L	197	THR	4.5
3	L	206	VAL	4.4
2	H	196	GLU	4.3
2	H	195	SER	4.2
3	L	106	LEU	4.1
2	H	215	ILE	4.1
2	H	155	VAL	4.1
2	H	167	GLY	4.0
3	L	112	ALA	4.0
2	H	198	VAL	3.9
3	L	209	PHE	3.9
2	H	133	GLY	3.8
3	L	141	PRO	3.7
2	H	202	VAL	3.7
2	H	134	GLY	3.6
2	H	204	HIS	3.6
2	H	187	THR	3.6
3	L	193	THR	3.6

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Mol	Chain	Res	Type	RSRZ
3	L	111	ALA	3.6
1	A	166	MET	3.6
3	L	120	PRO	3.6
2	H	184	SER	3.5
3	L	162	SER	3.5
3	L	198	HIS	3.5
2	H	164	LEU	3.5
3	L	146	VAL	3.4
3	L	134	CYS	3.4
3	L	174	SER	3.4
2	H	139	SER	3.4
3	L	115	VAL	3.4
2	H	193	TRP	3.3
3	L	145	ASN	3.3
3	L	200	THR	3.3
3	L	189	HIS	3.3
2	H	123	THR	3.3
3	L	142	LYS	3.3
3	L	196	ALA	3.3
1	A	189	VAL	3.2
3	L	171	SER	3.2
3	L	158	GLY	3.2
3	L	130	ALA	3.2
3	L	109	ALA	3.1
2	H	199	THR	3.1
3	L	136	LEU	3.1
1	A	193	THR	3.1
3	L	140	TYR	3.0
1	A	169	TYR	3.0
2	H	179	LEU	3.0
3	L	207	LYS	3.0
1	A	191	THR	3.0
3	L	12	SER	2.9
1	A	161	VAL	2.9
3	L	179	LEU	2.9
1	A	128	TYR	2.9
1	A	195	GLY	2.9
1	A	167	ASP	2.9
2	H	127	VAL	2.9
2	H	192	THR	2.9
3	L	135	PHE	2.9
3	L	159	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	190	SER	2.8
3	L	173	TYR	2.8
1	A	192	THR	2.8
3	L	208	SER	2.8
3	L	148	TRP	2.7
2	H	136	ALA	2.7
3	L	180	THR	2.7
3	L	129	GLY	2.7
3	L	10	ILE	2.7
3	L	212	ASN	2.7
3	L	202	THR	2.7
3	L	113	PRO	2.7
3	L	78	VAL	2.7
3	L	213	GLU	2.7
3	L	150	ILE	2.7
2	H	216	VAL	2.6
3	L	121	SER	2.6
3	L	156	GLN	2.6
3	L	164	THR	2.6
3	L	76	ASN	2.6
2	H	140	MET	2.5
1	A	190	THR	2.5
3	L	204	PRO	2.5
3	L	79	GLU	2.5
2	H	175	LEU	2.5
3	L	139	PHE	2.5
1	A	171	ASN	2.5
3	L	119	PRO	2.4
2	H	151	PHE	2.4
2	H	203	ALA	2.4
3	L	77	SER	2.4
2	H	145	CYS	2.4
3	L	194	CYS	2.4
3	L	205	ILE	2.4
1	A	162	TYR	2.4
2	H	197	THR	2.4
1	A	160	GLN	2.3
1	A	198	PHE	2.3
2	H	180	TYR	2.3
1	A	165	PRO	2.3
3	L	116	SER	2.3
3	L	183	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	201	ASN	2.3
2	H	132	PRO	2.3
3	L	114	THR	2.3
3	L	181	LEU	2.3
2	H	211	VAL	2.3
2	H	217	PRO	2.3
2	H	166	GLY	2.3
3	L	165	ASP	2.3
2	H	124	PRO	2.3
3	L	155	ARG	2.3
3	L	182	THR	2.2
3	L	152	GLY	2.2
2	H	200	CYS	2.2
1	A	180	VAL	2.2
2	H	121	LYS	2.2
2	H	214	LYS	2.2
1	A	131	GLY	2.2
3	L	175	MET	2.2
3	L	184	ASP	2.2
2	H	157	VAL	2.2
3	L	137	ASN	2.2
3	L	190	ASN	2.2
3	L	125	LEU	2.2
3	L	192	TYR	2.2
2	H	148	LYS	2.2
2	H	168	VAL	2.1
2	H	131	ALA	2.1
1	A	217	GLN	2.1
3	L	161	ASN	2.1
2	H	142	THR	2.1
3	L	102	THR	2.1
2	H	186	VAL	2.1
2	H	130	LEU	2.1
2	H	178	ASP	2.1
2	H	183	SER	2.1
2	H	171	PHE	2.1
3	L	133	VAL	2.1
3	L	11	LEU	2.1
1	A	196	GLU	2.1
2	H	213	LYS	2.1
2	H	177	SER	2.1
3	L	153	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	169	HIS	2.0
2	H	146	LEU	2.0
2	H	149	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 [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
4	NA	L	300	1/1	0.97	0.37	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.