



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:04 AM UTC

PDB ID : 3FRT / pdb_00003frt
Title : The structure of human CHMP3 (residues 8 - 222).
Authors : Schubert, H.L.; McCullough, J.; Hill, C.P.; Sundquist, W.I.
Deposited on : 2009-01-08
Resolution : 4.00 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

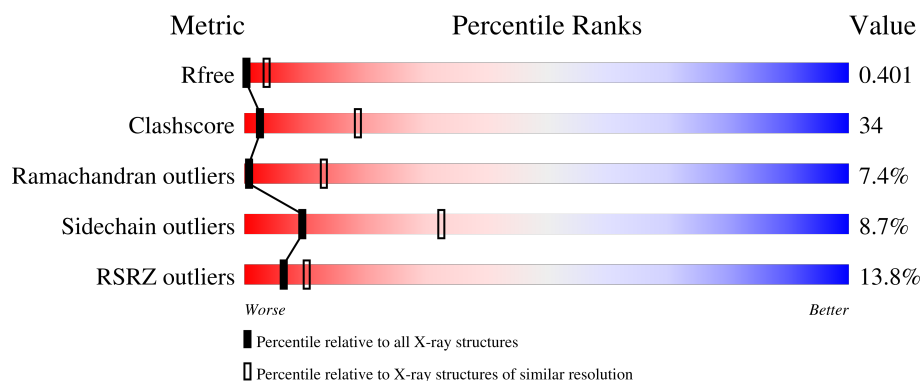
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	218	11% 27% 30% 6% 35%
1	B	218	7% 29% 28% 6% 35%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2270 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 Charged multivesicular body protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1133	709	203	208	13			
1	B	142	Total	C	N	O	S	0	0	0
			1137	711	204	209	13			

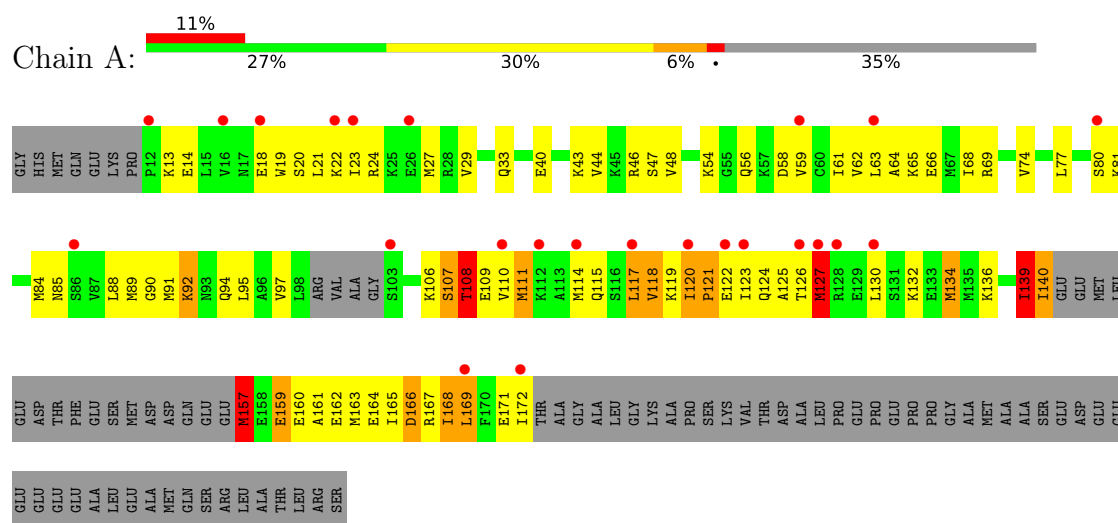
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	expression tag	UNP Q9Y3E7
A	6	HIS	-	expression tag	UNP Q9Y3E7
A	7	MET	-	expression tag	UNP Q9Y3E7
B	5	GLY	-	expression tag	UNP Q9Y3E7
B	6	HIS	-	expression tag	UNP Q9Y3E7
B	7	MET	-	expression tag	UNP Q9Y3E7

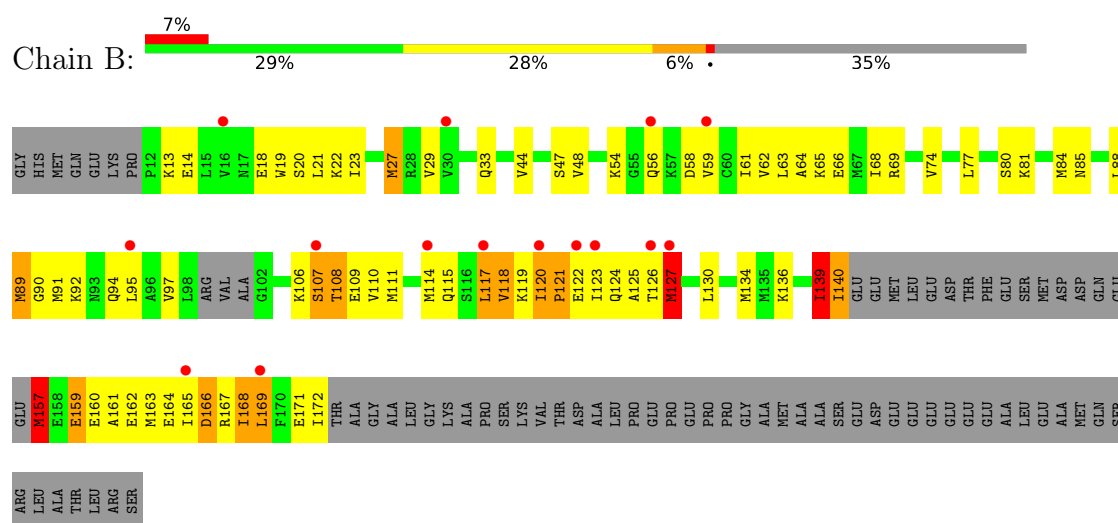
3 Residue-property plots

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: Charged multivesicular body protein 3



• Molecule 1: Charged multivesicular body protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.47Å 131.51Å 48.51Å 90.00° 108.06° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 30.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-4.00) 79.0 (30.00-4.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 3.99Å)	Xtriage
Refinement program		Depositor
R, R_{free}	0.383 , 0.436 0.402 , 0.401	Depositor DCC
R_{free} test set	126 reflections (3.35%)	wwPDB-VP
Wilson B-factor (Å ²)	135.4	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 12.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	2270	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.84% 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

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	0.93	5/1137 (0.4%)	1.05	6/1504 (0.4%)
1	B	0.95	5/1141 (0.4%)	1.05	6/1509 (0.4%)
All	All	0.94	10/2278 (0.4%)	1.05	12/3013 (0.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	MET	SD-CE	8.69	2.01	1.79
1	A	111	MET	SD-CE	8.51	2.00	1.79
1	B	27	MET	SD-CE	7.83	1.99	1.79
1	A	157	MET	SD-CE	7.10	1.97	1.79
1	B	157	MET	SD-CE	7.09	1.97	1.79
1	A	111	MET	CG-SD	6.03	1.95	1.80
1	B	157	MET	CG-SD	5.99	1.95	1.80
1	A	157	MET	CG-SD	5.98	1.95	1.80
1	A	134	MET	CG-SD	5.60	1.94	1.80
1	B	89	MET	CG-SD	5.34	1.94	1.80

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ILE	CA-C-N	6.72	128.25	119.84
1	A	120	ILE	C-N-CA	6.72	128.25	119.84
1	B	120	ILE	CA-C-N	6.72	128.24	119.84
1	B	120	ILE	C-N-CA	6.72	128.24	119.84
1	B	169	LEU	N-CA-C	-6.50	103.10	111.02
1	A	169	LEU	N-CA-C	-6.47	103.12	111.02
1	B	115	GLN	N-CA-C	-6.20	106.03	113.97
1	A	115	GLN	N-CA-C	-6.17	106.08	113.97
1	A	92	LYS	N-CA-C	-5.72	104.95	111.07
1	B	92	LYS	N-CA-C	-5.72	104.95	111.07
1	B	161	ALA	N-CA-C	-5.17	106.94	113.20
1	A	161	ALA	N-CA-C	-5.14	106.98	113.20

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	1133	0	1222	91	0
1	B	1137	0	1225	86	0
All	All	2270	0	2447	162	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 34.

All (162) 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:A:59:VAL:HG22	1:B:62:VAL:CG1	1.83	1.08
1:A:33:GLN:HE22	1:A:122:GLU:HG2	1.16	1.07
1:B:33:GLN:HE22	1:B:122:GLU:HG2	1.16	1.06
1:A:33:GLN:NE2	1:A:122:GLU:HG2	1.74	1.03
1:B:33:GLN:NE2	1:B:122:GLU:HG2	1.74	1.02
1:A:139:ILE:HD13	1:A:139:ILE:H	1.27	0.99
1:A:59:VAL:HG22	1:B:62:VAL:HG12	1.45	0.97
1:B:160:GLU:HB3	1:B:163:MET:HE2	1.47	0.97
1:B:139:ILE:H	1:B:139:ILE:HD13	1.27	0.97
1:A:58:ASP:O	1:A:62:VAL:HG23	1.67	0.95
1:A:40:GLU:CD	1:B:54:LYS:HE3	1.90	0.95
1:A:160:GLU:HB3	1:A:163:MET:HE2	1.47	0.94
1:B:165:ILE:HD12	1:B:166:ASP:N	1.82	0.94
1:A:165:ILE:HD12	1:A:166:ASP:N	1.82	0.93
1:B:165:ILE:HD12	1:B:166:ASP:H	1.34	0.93
1:B:58:ASP:O	1:B:62:VAL:HG23	1.67	0.92
1:B:27:MET:HG2	1:B:84:MET:SD	2.11	0.91
1:B:33:GLN:HE22	1:B:122:GLU:CG	1.84	0.91
1:A:33:GLN:HE22	1:A:122:GLU:CG	1.84	0.90
1:A:40:GLU:OE2	1:B:54:LYS:HE3	1.76	0.85
1:A:165:ILE:HD12	1:A:166:ASP:H	1.34	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:MET:CG	1:B:84:MET:SD	2.66	0.84
1:A:59:VAL:HG22	1:B:62:VAL:HG11	1.65	0.79
1:A:81:LYS:HA	1:A:84:MET:HE3	1.65	0.78
1:B:81:LYS:HA	1:B:84:MET:HE3	1.65	0.78
1:B:139:ILE:H	1:B:139:ILE:CD1	1.98	0.77
1:A:59:VAL:CG2	1:B:62:VAL:CG1	2.63	0.77
1:A:63:LEU:HD21	1:B:59:VAL:HG11	1.67	0.76
1:A:48:VAL:HG11	1:A:172:ILE:HD11	1.68	0.74
1:A:59:VAL:CG2	1:B:62:VAL:HG12	2.17	0.73
1:B:48:VAL:HG11	1:B:172:ILE:HD11	1.68	0.73
1:B:139:ILE:HD13	1:B:139:ILE:N	2.03	0.72
1:A:139:ILE:HD13	1:A:139:ILE:N	2.03	0.72
1:A:157:MET:HG3	1:A:159:GLU:HB2	1.71	0.71
1:B:29:VAL:O	1:B:33:GLN:HG3	1.90	0.71
1:A:29:VAL:O	1:A:33:GLN:HG3	1.90	0.71
1:B:157:MET:HG3	1:B:159:GLU:HB2	1.71	0.70
1:A:139:ILE:H	1:A:139:ILE:CD1	1.98	0.67
1:B:111:MET:SD	1:B:140:ILE:HB	2.35	0.66
1:A:23:ILE:HD11	1:A:114:MET:HE1	1.77	0.66
1:A:63:LEU:O	1:A:66:GLU:HB3	1.95	0.66
1:A:66:GLU:OE1	1:B:56:GLN:HG2	1.96	0.66
1:B:23:ILE:HD11	1:B:114:MET:HE1	1.77	0.66
1:B:63:LEU:O	1:B:66:GLU:HB3	1.95	0.65
1:B:157:MET:CG	1:B:159:GLU:HB2	2.27	0.65
1:A:157:MET:CG	1:A:159:GLU:HB2	2.26	0.65
1:B:27:MET:HG3	1:B:84:MET:SD	2.37	0.64
1:B:111:MET:SD	1:B:140:ILE:HD13	2.37	0.64
1:B:107:SER:H	1:B:139:ILE:HG22	1.63	0.64
1:A:107:SER:H	1:A:139:ILE:HG22	1.63	0.64
1:A:22:LYS:HD2	1:A:130:LEU:HD21	1.80	0.63
1:B:22:LYS:HD2	1:B:130:LEU:HD21	1.81	0.63
1:A:59:VAL:CG2	1:B:62:VAL:HG11	2.28	0.62
1:B:65:LYS:O	1:B:68:ILE:HG12	2.00	0.62
1:A:27:MET:HG2	1:A:84:MET:SD	2.40	0.62
1:B:134:MET:HB3	1:B:139:ILE:HG12	1.80	0.62
1:A:65:LYS:O	1:A:68:ILE:HG12	2.00	0.62
1:B:106:LYS:HA	1:B:139:ILE:HA	1.83	0.61
1:B:33:GLN:HE22	1:B:122:GLU:CD	2.09	0.60
1:A:106:LYS:HA	1:A:139:ILE:HA	1.83	0.60
1:A:33:GLN:HE22	1:A:122:GLU:CD	2.09	0.60
1:A:68:ILE:HG13	1:A:69:ARG:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:GLN:NE2	1:B:94:GLN:HA	2.17	0.59
1:A:56:GLN:HB3	1:A:59:VAL:HG23	1.84	0.59
1:A:169:LEU:O	1:A:172:ILE:HG12	2.03	0.59
1:A:164:GLU:HG3	1:A:167:ARG:NH1	2.18	0.59
1:B:169:LEU:O	1:B:172:ILE:HG12	2.03	0.59
1:A:94:GLN:NE2	1:A:94:GLN:HA	2.17	0.58
1:B:61:ILE:O	1:B:64:ALA:HB3	2.04	0.58
1:B:68:ILE:HG13	1:B:69:ARG:N	2.17	0.58
1:B:56:GLN:HB3	1:B:59:VAL:HG23	1.84	0.58
1:B:164:GLU:HG3	1:B:167:ARG:NH1	2.18	0.58
1:A:111:MET:SD	1:A:140:ILE:HB	2.43	0.58
1:B:126:THR:O	1:B:127:MET:C	2.46	0.58
1:A:126:THR:O	1:A:127:MET:C	2.46	0.57
1:A:61:ILE:O	1:A:64:ALA:HB3	2.04	0.57
1:A:111:MET:SD	1:A:140:ILE:HD13	2.45	0.57
1:A:157:MET:HA	1:A:157:MET:HE3	1.87	0.56
1:A:24:ARG:O	1:A:27:MET:HB2	2.04	0.56
1:B:74:VAL:O	1:B:77:LEU:HB2	2.06	0.55
1:B:157:MET:HE3	1:B:157:MET:HA	1.87	0.55
1:A:74:VAL:O	1:A:77:LEU:HB2	2.06	0.54
1:A:134:MET:HB3	1:A:139:ILE:HG12	1.90	0.54
1:A:157:MET:HA	1:A:157:MET:CE	2.38	0.53
1:B:157:MET:HA	1:B:157:MET:CE	2.38	0.53
1:B:106:LYS:O	1:B:106:LYS:HG3	2.09	0.53
1:A:106:LYS:O	1:A:106:LYS:HG3	2.09	0.52
1:B:90:GLY:HA3	1:B:110:VAL:HG11	1.92	0.52
1:A:120:ILE:HD13	1:A:123:ILE:HD11	1.92	0.52
1:B:140:ILE:HD12	1:B:140:ILE:H	1.75	0.52
1:A:62:VAL:HG11	1:B:58:ASP:HB2	1.91	0.52
1:B:120:ILE:O	1:B:124:GLN:N	2.38	0.51
1:A:66:GLU:OE1	1:B:56:GLN:CG	2.58	0.51
1:A:90:GLY:HA3	1:A:110:VAL:HG11	1.92	0.51
1:A:120:ILE:O	1:A:124:GLN:N	2.38	0.51
1:A:54:LYS:HE2	1:A:56:GLN:NE2	2.25	0.51
1:A:80:SER:OG	1:A:120:ILE:HG12	2.11	0.51
1:B:80:SER:OG	1:B:120:ILE:HG12	2.11	0.51
1:B:120:ILE:HD13	1:B:123:ILE:HD11	1.92	0.51
1:B:68:ILE:CG1	1:B:69:ARG:N	2.74	0.50
1:A:40:GLU:OE2	1:B:54:LYS:CE	2.54	0.50
1:A:140:ILE:HD12	1:A:140:ILE:H	1.75	0.50
1:A:90:GLY:HA3	1:A:110:VAL:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:GLY:HA3	1:B:110:VAL:CG1	2.42	0.50
1:A:68:ILE:CG1	1:A:69:ARG:N	2.74	0.49
1:B:157:MET:HG3	1:B:159:GLU:H	1.77	0.49
1:A:44:VAL:O	1:A:48:VAL:HG23	2.13	0.48
1:B:44:VAL:O	1:B:48:VAL:HG23	2.13	0.48
1:A:157:MET:HG3	1:A:159:GLU:H	1.77	0.48
1:A:159:GLU:O	1:A:162:GLU:HG2	2.13	0.48
1:B:159:GLU:O	1:B:162:GLU:HG2	2.13	0.48
1:B:88:LEU:O	1:B:91:MET:HB2	2.13	0.48
1:A:43:LYS:HG2	1:A:46:ARG:HH22	1.78	0.47
1:A:48:VAL:HG11	1:A:172:ILE:CD1	2.42	0.47
1:A:88:LEU:O	1:A:91:MET:HB2	2.13	0.47
1:A:43:LYS:HG2	1:A:46:ARG:NH2	2.30	0.47
1:A:85:ASN:O	1:A:89:MET:HG2	2.14	0.47
1:A:63:LEU:CD2	1:B:59:VAL:HG11	2.43	0.47
1:A:19:TRP:O	1:A:20:SER:C	2.59	0.46
1:A:107:SER:O	1:A:109:GLU:N	2.49	0.46
1:A:117:LEU:O	1:A:120:ILE:HD12	2.16	0.46
1:B:117:LEU:O	1:B:120:ILE:HD12	2.16	0.46
1:B:107:SER:O	1:B:109:GLU:N	2.49	0.46
1:A:89:MET:O	1:A:92:LYS:N	2.49	0.45
1:B:109:GLU:HA	1:B:109:GLU:OE2	2.16	0.45
1:B:19:TRP:O	1:B:20:SER:C	2.59	0.45
1:A:27:MET:CG	1:A:84:MET:SD	3.04	0.45
1:B:48:VAL:HG11	1:B:172:ILE:CD1	2.42	0.45
1:B:107:SER:N	1:B:139:ILE:HG22	2.30	0.45
1:B:117:LEU:HD12	1:B:117:LEU:HA	1.79	0.45
1:A:165:ILE:CD1	1:A:166:ASP:H	2.17	0.45
1:A:168:ILE:O	1:A:169:LEU:C	2.60	0.45
1:B:13:LYS:HZ3	1:B:95:LEU:HD21	1.82	0.45
1:A:107:SER:N	1:A:139:ILE:HG22	2.30	0.44
1:B:33:GLN:NE2	1:B:122:GLU:OE2	2.50	0.44
1:A:62:VAL:CG1	1:B:58:ASP:HB2	2.48	0.44
1:A:132:LYS:HE3	1:A:132:LYS:HB2	1.84	0.44
1:B:168:ILE:O	1:B:169:LEU:C	2.59	0.43
1:A:33:GLN:NE2	1:A:122:GLU:OE2	2.49	0.43
1:B:18:GLU:O	1:B:21:LEU:HB2	2.19	0.43
1:B:109:GLU:C	1:B:111:MET:H	2.26	0.43
1:A:77:LEU:O	1:A:80:SER:HB2	2.19	0.43
1:B:122:GLU:OE1	1:B:122:GLU:N	2.27	0.43
1:B:107:SER:C	1:B:109:GLU:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:O	1:B:80:SER:HB2	2.19	0.42
1:B:117:LEU:C	1:B:119:LYS:H	2.27	0.42
1:A:13:LYS:HZ3	1:A:95:LEU:HD21	1.83	0.42
1:A:94:GLN:NE2	1:A:94:GLN:CA	2.81	0.42
1:A:109:GLU:C	1:A:111:MET:H	2.26	0.42
1:A:18:GLU:O	1:A:21:LEU:HB2	2.19	0.42
1:B:165:ILE:CD1	1:B:166:ASP:H	2.18	0.42
1:A:117:LEU:C	1:A:119:LYS:H	2.27	0.42
1:A:107:SER:C	1:A:109:GLU:N	2.77	0.42
1:A:121:PRO:HA	1:A:124:GLN:OE1	2.20	0.42
1:B:85:ASN:O	1:B:89:MET:HG2	2.20	0.41
1:B:118:VAL:HG12	1:B:127:MET:HB3	2.03	0.41
1:A:88:LEU:HD12	1:A:88:LEU:HA	1.88	0.41
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.86	0.41
1:B:68:ILE:CG1	1:B:69:ARG:H	2.35	0.40
1:B:121:PRO:HA	1:B:124:GLN:OE1	2.20	0.40
1:A:106:LYS:O	1:A:108:THR:N	2.55	0.40
1:A:118:VAL:HG12	1:A:127:MET:HB3	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	135/218 (62%)	112 (83%)	13 (10%)	10 (7%)	1	13
1	B	136/218 (62%)	113 (83%)	13 (10%)	10 (7%)	1	13
All	All	271/436 (62%)	225 (83%)	26 (10%)	20 (7%)	1	13

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	SER
1	A	136	LYS
1	B	107	SER
1	B	136	LYS
1	A	118	VAL
1	A	125	ALA
1	A	171	GLU
1	B	118	VAL
1	B	125	ALA
1	B	171	GLU
1	A	108	THR
1	B	108	THR
1	A	127	MET
1	B	127	MET
1	A	121	PRO
1	A	139	ILE
1	B	121	PRO
1	B	139	ILE
1	A	97	VAL
1	B	97	VAL

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	127/188 (68%)	116 (91%)	11 (9%)	9	32
1	B	127/188 (68%)	116 (91%)	11 (9%)	9	32
All	All	254/376 (68%)	232 (91%)	22 (9%)	9	32

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	47	SER
1	A	108	THR
1	A	117	LEU

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Mol	Chain	Res	Type
1	A	127	MET
1	A	139	ILE
1	A	140	ILE
1	A	157	MET
1	A	159	GLU
1	A	166	ASP
1	A	168	ILE
1	B	14	GLU
1	B	47	SER
1	B	108	THR
1	B	117	LEU
1	B	127	MET
1	B	139	ILE
1	B	140	ILE
1	B	157	MET
1	B	159	GLU
1	B	166	ASP
1	B	168	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	94	GLN
1	B	94	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	141/218 (64%)	1.05	24 (17%) 4 7	34, 58, 81, 89	0
1	B	142/218 (65%)	0.67	15 (10%) 11 13	34, 59, 82, 90	0
All	All	283/436 (64%)	0.86	39 (13%) 6 10	34, 59, 82, 90	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	ILE	8.9
1	B	123	ILE	8.2
1	A	120	ILE	7.4
1	B	120	ILE	6.8
1	B	127	MET	4.6
1	B	169	LEU	4.6
1	A	169	LEU	4.5
1	A	172	ILE	4.2
1	A	117	LEU	3.9
1	A	59	VAL	3.8
1	A	127	MET	3.7
1	A	22	LYS	3.4
1	A	80	SER	3.3
1	B	122	GLU	3.2
1	B	117	LEU	3.1
1	B	114	MET	3.1
1	B	16	VAL	3.1
1	B	56	GLN	3.0
1	A	86	SER	2.9
1	B	95	LEU	2.8
1	A	130	LEU	2.7
1	B	59	VAL	2.7
1	A	23	ILE	2.5
1	A	16	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	18	GLU	2.3
1	A	103	SER	2.3
1	A	128	ARG	2.3
1	A	26	GLU	2.3
1	A	12	PRO	2.3
1	A	126	THR	2.3
1	A	63	LEU	2.3
1	B	107	SER	2.3
1	A	112	LYS	2.2
1	A	114	MET	2.2
1	A	110	VAL	2.1
1	B	126	THR	2.1
1	A	122	GLU	2.1
1	B	30	VAL	2.1
1	B	165	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.