



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 PM UTC

PDB ID : 7T7I / pdb_00007t7i
Title : EBV nuclear egress complex
Authors : Thorsen, M.K.; Heldwein, E.E.
Deposited on : 2021-12-15
Resolution : 3.97 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

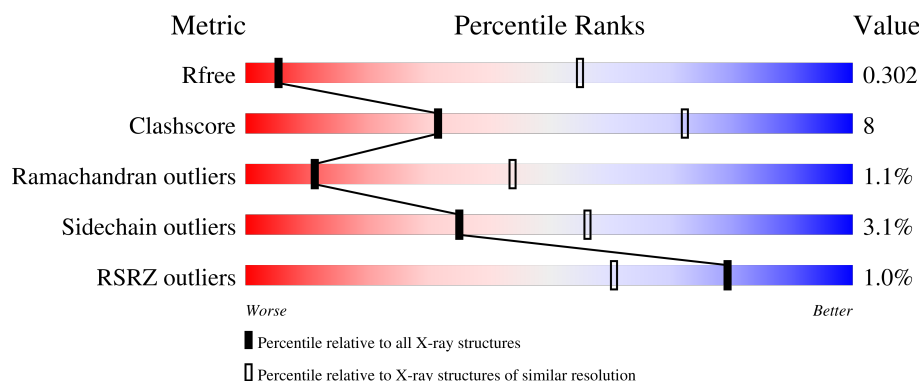
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.97 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	1016 (4.18-3.78)
Clashscore	190562	1007 (4.16-3.80)
Ramachandran outliers	187476	1000 (4.18-3.78)
Sidechain outliers	187428	1131 (4.20-3.76)
RSRZ outliers	180081	1016 (4.18-3.78)

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	200	2% 88% 8% .
1	C	200	% 82% 14% ..
1	E	200	90% 8% .
1	G	200	2% 84% 14% .
1	I	200	60% 16% 24%

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Mol	Chain	Length	Quality of chain
2	B	257	% 69% 23% • 7%
2	D	257	% 76% 16% • 6%
2	F	257	% 58% 21% • 19%
2	H	257	2% 63% 27% • 6%
2	J	257	61% 18% • 21%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 32335 atoms, of which 16193 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 Nuclear egress protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	194	Total	C	H	N	O	S	0	0	0
			3030	956	1519	260	281	14			
1	C	194	Total	C	H	N	O	S	0	0	0
			3030	956	1519	260	281	14			
1	E	194	Total	C	H	N	O	S	0	2	0
			3058	964	1536	261	282	15			
1	G	194	Total	C	H	N	O	S	0	1	0
			3044	960	1528	260	281	15			
1	I	153	Total	C	H	N	O	S	0	0	0
			2446	781	1228	205	221	11			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P03185
A	-3	PRO	-	expression tag	UNP P03185
A	-2	LEU	-	expression tag	UNP P03185
A	-1	GLY	-	expression tag	UNP P03185
A	0	SER	-	expression tag	UNP P03185
C	-4	GLY	-	expression tag	UNP P03185
C	-3	PRO	-	expression tag	UNP P03185
C	-2	LEU	-	expression tag	UNP P03185
C	-1	GLY	-	expression tag	UNP P03185
C	0	SER	-	expression tag	UNP P03185
E	-4	GLY	-	expression tag	UNP P03185
E	-3	PRO	-	expression tag	UNP P03185
E	-2	LEU	-	expression tag	UNP P03185
E	-1	GLY	-	expression tag	UNP P03185
E	0	SER	-	expression tag	UNP P03185
G	-4	GLY	-	expression tag	UNP P03185
G	-3	PRO	-	expression tag	UNP P03185
G	-2	LEU	-	expression tag	UNP P03185
G	-1	GLY	-	expression tag	UNP P03185

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	expression tag	UNP P03185
I	-4	GLY	-	expression tag	UNP P03185
I	-3	PRO	-	expression tag	UNP P03185
I	-2	LEU	-	expression tag	UNP P03185
I	-1	GLY	-	expression tag	UNP P03185
I	0	SER	-	expression tag	UNP P03185

- Molecule 2 is a protein called Nuclear egress protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	239	Total	C	H	N	O	S	0	0	0
			3736	1195	1867	314	348	12			
2	D	242	Total	C	H	N	O	S	0	0	0
			3791	1211	1897	319	352	12			
2	F	208	Total	C	H	N	O	S	0	0	0
			3227	1038	1611	269	298	11			
2	H	241	Total	C	H	N	O	S	0	0	0
			3775	1206	1888	318	351	12			
2	J	203	Total	C	H	N	O	S	0	0	0
			3190	1024	1600	263	291	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	62	GLY	-	expression tag	UNP P0CK47
B	63	PRO	-	expression tag	UNP P0CK47
B	64	GLY	-	expression tag	UNP P0CK47
B	65	SER	-	expression tag	UNP P0CK47
D	62	GLY	-	expression tag	UNP P0CK47
D	63	PRO	-	expression tag	UNP P0CK47
D	64	GLY	-	expression tag	UNP P0CK47
D	65	SER	-	expression tag	UNP P0CK47
F	62	GLY	-	expression tag	UNP P0CK47
F	63	PRO	-	expression tag	UNP P0CK47
F	64	GLY	-	expression tag	UNP P0CK47
F	65	SER	-	expression tag	UNP P0CK47
H	62	GLY	-	expression tag	UNP P0CK47
H	63	PRO	-	expression tag	UNP P0CK47
H	64	GLY	-	expression tag	UNP P0CK47
H	65	SER	-	expression tag	UNP P0CK47
J	62	GLY	-	expression tag	UNP P0CK47
J	63	PRO	-	expression tag	UNP P0CK47

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Chain	Residue	Modelled	Actual	Comment	Reference
J	64	GLY	-	expression tag	UNP P0CK47
J	65	SER	-	expression tag	UNP P0CK47

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0
3	J	1	Total 1	Zn 1	0	0

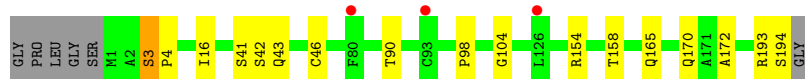
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total 1	O 1	0	0
4	G	1	Total 1	O 1	0	0
4	I	1	Total 1	O 1	0	0

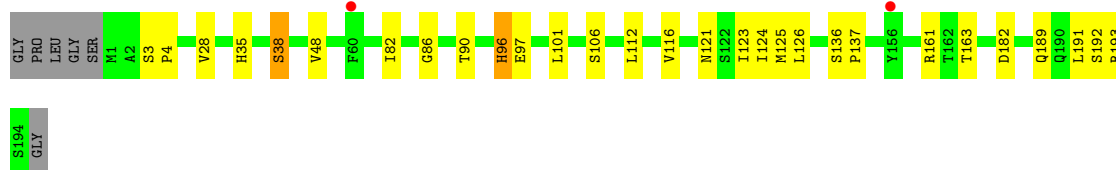
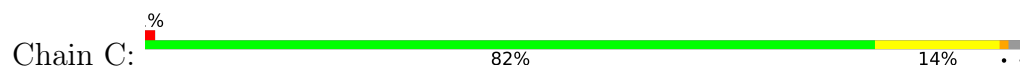
3 Residue-property plots [i](#)

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.

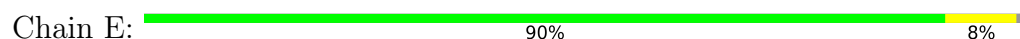
- Molecule 1: Nuclear egress protein 2



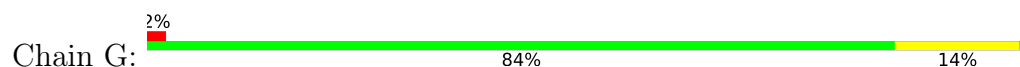
- Molecule 1: Nuclear egress protein 2



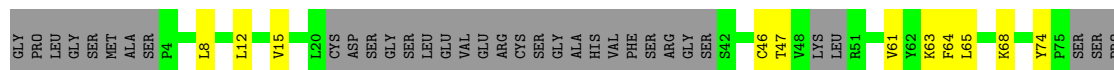
- Molecule 1: Nuclear egress protein 2

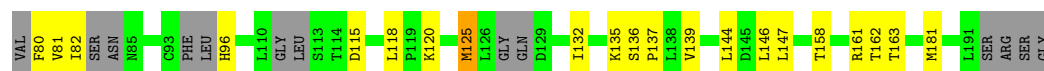


- Molecule 1: Nuclear egress protein 2

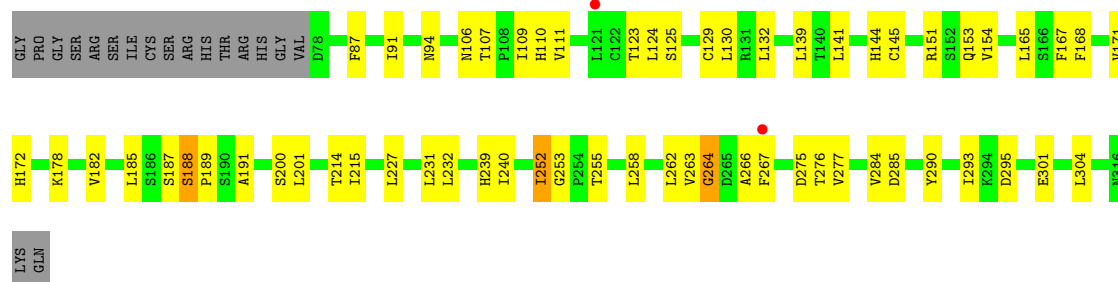


- Molecule 1: Nuclear egress protein 2

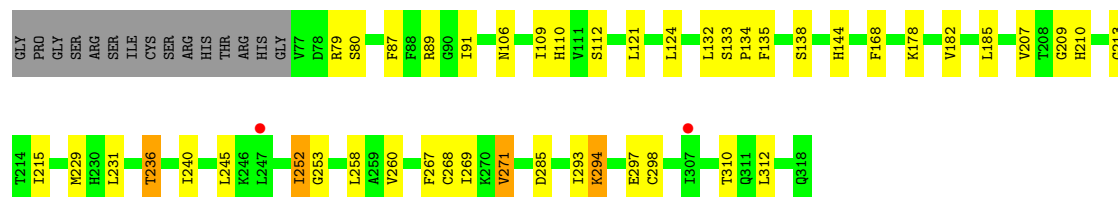
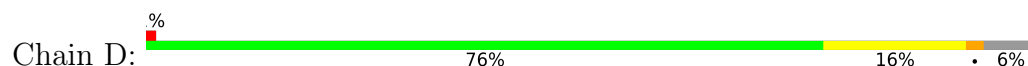




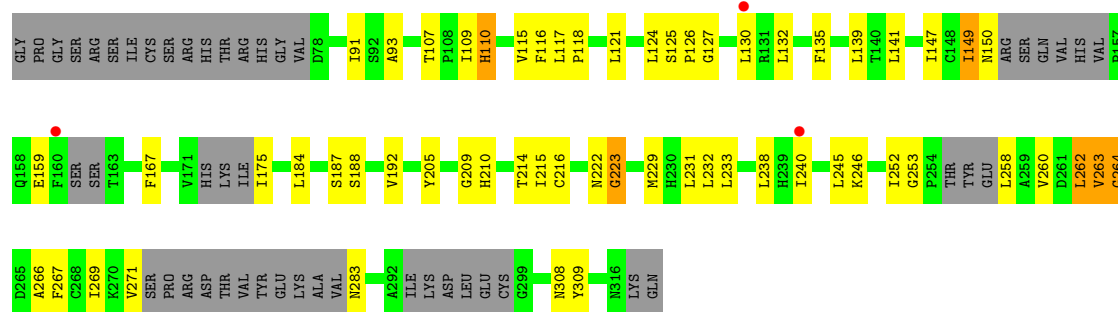
• Molecule 2: Nuclear egress protein 1



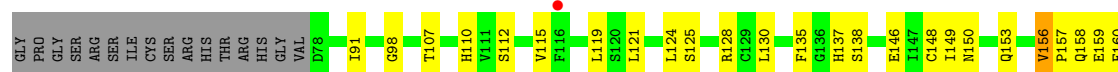
• Molecule 2: Nuclear egress protein 1

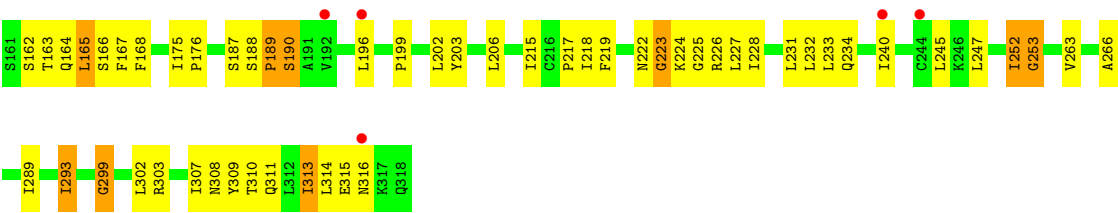


• Molecule 2: Nuclear egress protein 1

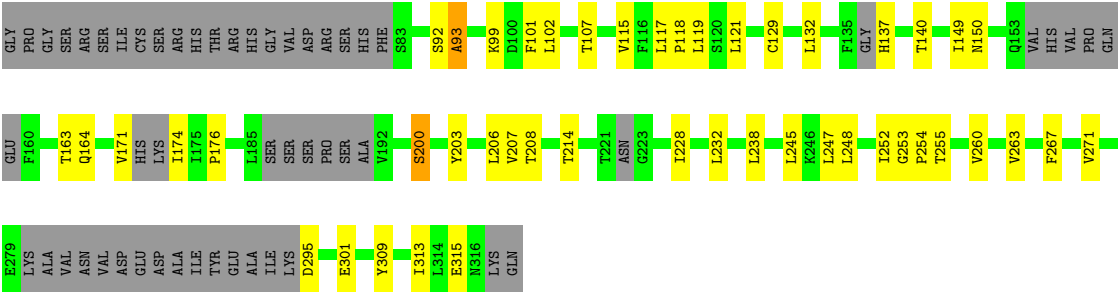


• Molecule 2: Nuclear egress protein 1





● Molecule 2: Nuclear egress protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	238.15Å 238.15Å 137.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.52 – 3.97 106.52 – 3.97	Depositor EDS
% Data completeness (in resolution range)	99.5 (106.52-3.97) 99.5 (106.52-3.97)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 4.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.270 , 0.308 0.268 , 0.302	Depositor DCC
R_{free} test set	2000 reflections (5.77%)	wwPDB-VP
Wilson B-factor (Å ²)	166.6	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 149.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32335	wwPDB-VP
Average B, all atoms (Å ²)	219.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: ZN

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	0.16	0/1540	0.40	0/2078
1	C	0.14	0/1540	0.38	0/2078
1	E	0.14	0/1557	0.33	0/2100
1	G	0.13	0/1548	0.38	0/2088
1	I	0.10	0/1236	0.25	0/1659
2	B	0.20	0/1910	0.52	0/2592
2	D	0.20	0/1935	0.51	0/2625
2	F	0.18	0/1646	0.51	0/2224
2	H	0.19	0/1928	0.52	0/2615
2	J	0.11	0/1618	0.29	0/2186
All	All	0.16	0/16458	0.43	0/22245

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

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	1511	1519	1521	8	0
1	C	1511	1519	1521	28	2
1	E	1522	1536	1538	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1516	1528	1530	20	0
1	I	1218	1228	1228	17	1
2	B	1869	1867	1867	34	2
2	D	1894	1897	1897	26	2
2	F	1616	1611	1611	52	1
2	H	1887	1888	1888	57	0
2	J	1590	1600	1600	31	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	16142	16193	16201	262	4

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 8.

All (262) 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:101:LEU:HD22	1:E:125:MET:HE2	1.61	0.83
2:H:289:ILE:O	2:H:293:ILE:HG23	1.80	0.82
2:F:238:LEU:HD12	2:F:267:PHE:CZ	2.17	0.79
2:H:175:ILE:HG22	2:H:176:PRO:HD3	1.64	0.78
2:F:127:GLY:O	2:F:141:LEU:HD12	1.84	0.77
1:A:90:THR:HG21	2:H:135:PHE:O	1.85	0.77
1:C:121:ASN:OD1	2:F:117:LEU:HD23	1.87	0.75
2:F:132:LEU:HD11	2:F:267:PHE:CZ	2.23	0.74
1:A:154:ARG:NH2	1:A:165:GLN:OE1	2.20	0.74
1:C:101:LEU:HD21	2:F:116:PHE:CZ	2.24	0.72
1:C:116:VAL:HG11	1:C:124:ILE:HD11	1.71	0.72
2:J:174:ILE:HG22	2:J:176:PRO:HD2	1.72	0.71
2:F:132:LEU:HD11	2:F:267:PHE:CE1	2.27	0.69
2:J:132:LEU:HD13	2:J:267:PHE:CD1	2.29	0.68
2:F:245:LEU:HD12	2:F:246:LYS:N	2.10	0.67
1:C:86:GLY:HA3	2:F:262:LEU:HD11	1.77	0.66
2:B:145:CYS:SG	2:B:239:HIS:CE1	2.88	0.65
1:G:50:LEU:HD12	1:G:89:THR:HG22	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:121:LEU:HD13	2:J:245:LEU:HD22	1.77	0.65
2:F:124:LEU:HD23	2:F:125:SER:O	1.98	0.63
1:I:144:LEU:HD23	1:I:144:LEU:O	1.98	0.63
1:C:38:SER:HB3	2:F:109:ILE:HD11	1.80	0.62
2:D:252:ILE:HD12	2:D:252:ILE:C	2.24	0.62
2:H:218:ILE:HD13	2:H:232:LEU:HD13	1.81	0.62
2:F:308:ASN:OD1	2:F:309:TYR:N	2.32	0.61
1:C:101:LEU:HD21	2:F:116:PHE:CE1	2.35	0.61
2:D:293:ILE:HD12	2:D:294:LYS:N	2.15	0.61
2:H:314:LEU:HD23	2:H:314:LEU:O	2.01	0.61
1:G:105:GLN:HB2	2:J:149:ILE:HD13	1.83	0.60
2:B:293:ILE:HD12	2:B:295:ASP:H	1.68	0.59
2:H:146:GLU:O	2:H:150:ASN:N	2.35	0.59
1:E:154:ARG:HH22	2:F:141:LEU:HD11	1.67	0.59
1:G:21:CYS:CB	1:G:26:LEU:HD11	2.33	0.58
2:F:238:LEU:HD12	2:F:267:PHE:HZ	1.63	0.58
1:I:132:ILE:HB	1:I:144:LEU:HD21	1.85	0.58
2:D:106:ASN:O	2:D:144:HIS:NE2	2.37	0.57
2:J:115:VAL:CG1	2:J:119:LEU:HD22	2.35	0.57
2:J:115:VAL:HG11	2:J:119:LEU:HD22	1.85	0.57
1:C:101:LEU:HD22	1:C:123:ILE:CD1	2.34	0.56
1:G:161:ARG:NH1	1:G:163:THR:OG1	2.39	0.56
2:B:106:ASN:OD1	2:B:107:THR:HG23	2.06	0.56
1:C:101:LEU:HD13	1:C:125:MET:HE1	1.87	0.56
2:B:284:VAL:HG23	2:B:284:VAL:O	2.06	0.56
2:H:175:ILE:CG2	2:H:176:PRO:HD3	2.35	0.55
2:H:156:VAL:N	2:H:157:PRO:CD	2.70	0.55
2:H:162:SER:HB3	2:H:165:LEU:HD23	1.89	0.55
2:B:215:ILE:HG21	2:B:231:LEU:HB3	1.89	0.55
2:D:252:ILE:HD12	2:D:253:GLY:N	2.22	0.55
2:J:132:LEU:HD12	2:J:132:LEU:O	2.07	0.54
2:B:290:TYR:O	2:B:293:ILE:HG13	2.06	0.54
2:J:301:GLU:OE1	2:J:301:GLU:N	2.40	0.54
2:D:240:ILE:HD12	2:D:240:ILE:H	1.72	0.54
2:D:121:LEU:HD13	2:D:258:LEU:CD2	2.38	0.54
2:H:232:LEU:HD12	2:H:232:LEU:N	2.23	0.54
2:H:202:LEU:O	2:H:206:LEU:HD23	2.08	0.53
2:B:111:VAL:HG11	2:B:144:HIS:HB2	1.89	0.53
2:H:203:TYR:CE2	2:H:247:LEU:HD21	2.43	0.53
2:B:167:PHE:O	2:B:171:VAL:HG13	2.09	0.53
2:H:188:SER:N	2:H:189:PRO:HD2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:222:ASN:O	2:H:223:GLY:C	2.50	0.53
2:H:247:LEU:C	2:H:247:LEU:HD23	2.34	0.53
2:D:121:LEU:HD13	2:D:258:LEU:HD23	1.91	0.53
1:I:147:LEU:HD11	1:I:181:MET:HG2	1.91	0.53
1:E:101:LEU:HD22	1:E:125:MET:CE	2.37	0.53
2:H:165:LEU:HD12	2:H:166:SER:N	2.23	0.53
2:J:203:TYR:O	2:J:207:VAL:HG12	2.07	0.53
1:C:86:GLY:CA	2:F:262:LEU:HD11	2.40	0.52
1:E:191:LEU:HD11	2:F:93:ALA:HB2	1.91	0.52
2:F:258:LEU:CD1	2:F:271:VAL:HG22	2.39	0.52
1:G:21:CYS:HB3	1:G:26:LEU:HD11	1.91	0.52
2:H:115:VAL:HG12	2:H:137:HIS:O	2.10	0.52
2:H:218:ILE:CD1	2:H:232:LEU:HD13	2.39	0.52
1:C:28:VAL:HG22	1:C:48:VAL:HG22	1.92	0.51
2:J:92:SER:O	2:J:93:ALA:CB	2.58	0.51
2:J:295:ASP:OD1	2:J:295:ASP:N	2.42	0.51
2:B:94:ASN:ND2	1:E:136:SER:OG	2.43	0.51
2:D:178:LYS:O	2:D:182:VAL:HG23	2.11	0.51
2:H:156:VAL:N	2:H:157:PRO:HD3	2.26	0.51
1:E:184:ILE:CD1	2:F:91:ILE:HD11	2.40	0.51
2:B:87:PHE:CZ	2:B:91:ILE:HD11	2.46	0.51
2:D:240:ILE:HD12	2:D:240:ILE:N	2.26	0.51
2:B:129:CYS:O	2:B:139:LEU:HD23	2.11	0.51
2:F:205:TYR:CD1	2:F:215:ILE:HD11	2.45	0.51
1:G:74:TYR:CD1	1:G:75:PRO:HD2	2.46	0.51
1:G:83:SER:HB3	1:G:123:ILE:HG22	1.93	0.51
2:H:310:THR:O	2:H:313:ILE:HG13	2.11	0.51
2:H:315:GLU:O	2:H:316:ASN:HB2	2.11	0.50
1:C:3:SER:N	1:C:4:PRO:HD2	2.26	0.50
2:H:91:ILE:HD12	2:H:98:GLY:CA	2.42	0.50
1:C:101:LEU:HD22	1:C:123:ILE:HD11	1.92	0.50
1:I:118:LEU:HD23	1:I:162:THR:HB	1.94	0.50
2:H:263:VAL:HG23	2:H:263:VAL:O	2.12	0.50
2:H:299:GLY:HA3	2:H:302:LEU:HD12	1.93	0.50
1:G:116:VAL:HG11	1:G:124:ILE:HD11	1.93	0.50
2:D:121:LEU:HD23	2:D:245:LEU:HD22	1.94	0.50
2:J:149:ILE:HD12	2:J:149:ILE:C	2.37	0.49
2:B:185:LEU:HD22	2:B:293:ILE:HD13	1.94	0.49
1:G:83:SER:CB	1:G:123:ILE:HG22	2.42	0.49
2:F:258:LEU:HD13	2:F:271:VAL:HG22	1.94	0.49
2:B:132:LEU:C	2:B:132:LEU:HD12	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:260:VAL:HG23	2:F:269:ILE:HG22	1.93	0.49
1:I:12:LEU:HD22	1:I:65:LEU:HD22	1.94	0.49
2:D:121:LEU:HD11	2:D:260:VAL:HG23	1.94	0.49
2:H:233:LEU:HD12	2:H:234:GLN:H	1.78	0.49
1:G:21:CYS:HB2	1:G:26:LEU:HD11	1.94	0.49
1:I:135:LYS:O	1:I:139:VAL:HG12	2.13	0.49
2:J:92:SER:O	2:J:93:ALA:HB3	2.12	0.49
2:J:99:LYS:HA	2:J:102:LEU:HD23	1.95	0.49
2:D:168:PHE:O	2:D:168:PHE:CG	2.66	0.49
2:B:189:PRO:HG2	2:B:191:ALA:HB3	1.95	0.48
2:H:121:LEU:HD22	2:H:245:LEU:HD22	1.95	0.48
2:D:133:SER:OG	2:D:134:PRO:HD2	2.13	0.48
1:G:99:SER:O	2:J:150:ASN:ND2	2.46	0.48
1:G:172:ALA:HB2	2:H:107:THR:HG21	1.95	0.48
1:A:172:ALA:HB2	2:B:107:THR:HG21	1.96	0.48
2:B:188:SER:N	2:B:189:PRO:HD3	2.29	0.48
1:G:37:PHE:O	1:G:96:HIS:CE1	2.66	0.48
2:F:107:THR:O	2:F:107:THR:HG23	2.14	0.48
2:H:125:SER:OG	2:H:128:ARG:NH1	2.47	0.48
2:H:130:LEU:HD12	2:H:138:SER:O	2.14	0.48
2:J:107:THR:HG23	2:J:107:THR:O	2.14	0.48
2:H:219:PHE:HB3	2:H:227:LEU:HD21	1.95	0.47
1:I:46:CYS:SG	1:I:47:THR:N	2.87	0.47
2:F:233:LEU:HD22	2:F:267:PHE:CE2	2.49	0.47
2:F:187:SER:O	2:F:188:SER:C	2.57	0.47
1:G:192:SER:O	1:G:193:ARG:HB2	2.13	0.47
2:B:262:LEU:HA	2:B:267:PHE:HA	1.97	0.47
1:G:10:ASP:OD1	1:G:30:ARG:NH1	2.48	0.47
2:H:159:GLU:OE1	2:H:159:GLU:HA	2.15	0.47
2:J:253:GLY:N	2:J:254:PRO:HD2	2.29	0.47
2:F:222:ASN:O	2:F:223:GLY:C	2.58	0.47
2:D:87:PHE:CZ	2:D:91:ILE:HD11	2.50	0.47
1:E:82:ILE:HD13	1:E:164:MET:HE3	1.96	0.47
1:G:35:HIS:HB2	1:G:43:GLN:CD	2.39	0.47
2:H:224:LYS:O	2:H:226:ARG:N	2.48	0.46
1:E:139:VAL:HG12	2:F:109:ILE:HD13	1.97	0.46
2:J:248:LEU:O	2:J:253:GLY:N	2.49	0.46
2:B:124:LEU:HD23	2:B:125:SER:O	2.14	0.46
1:C:182:ASP:OD2	2:D:79:ARG:NH2	2.47	0.46
1:C:192:SER:O	1:C:193:ARG:HG3	2.15	0.46
2:B:111:VAL:HG13	2:B:141:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:209:GLY:O	2:D:210:HIS:C	2.59	0.46
2:B:214:THR:HG23	2:B:214:THR:O	2.16	0.46
2:D:121:LEU:N	2:D:121:LEU:HD12	2.31	0.46
2:B:263:VAL:O	2:B:264:GLY:C	2.59	0.46
2:H:308:ASN:HA	2:H:311:GLN:OE1	2.16	0.46
1:E:184:ILE:HD13	2:F:91:ILE:HD11	1.97	0.46
2:F:216:CYS:HB2	2:F:232:LEU:HD21	1.98	0.46
2:F:231:LEU:HG	2:F:269:ILE:HG13	1.98	0.45
2:J:117:LEU:CB	2:J:118:PRO:HD3	2.46	0.45
2:H:314:LEU:HD23	2:H:314:LEU:C	2.41	0.45
2:J:117:LEU:HB2	2:J:118:PRO:HD3	1.97	0.45
2:J:263:VAL:HG21	2:J:313:ILE:HD13	1.97	0.45
1:C:191:LEU:HD12	1:C:193:ARG:HH21	1.81	0.45
2:J:121:LEU:HD13	2:J:245:LEU:CD2	2.45	0.45
2:D:297:GLU:HG2	2:D:298:CYS:H	1.81	0.45
2:F:229:MET:HE2	2:F:231:LEU:HB3	1.98	0.45
2:B:168:PHE:O	2:B:168:PHE:CG	2.69	0.45
1:C:3:SER:O	1:C:4:PRO:C	2.59	0.45
2:F:231:LEU:HD11	2:F:269:ILE:HD11	1.98	0.45
2:B:153:GLN:HE21	2:B:154:VAL:HG23	1.81	0.45
1:I:8:LEU:HD11	1:I:68:LYS:O	2.17	0.45
2:D:132:LEU:HD23	2:D:267:PHE:CD2	2.52	0.45
2:H:233:LEU:HD12	2:H:234:GLN:N	2.31	0.45
1:C:112:LEU:HD21	1:C:126:LEU:HD21	1.98	0.45
2:H:165:LEU:HD12	2:H:165:LEU:C	2.41	0.45
1:I:74:TYR:HH	1:I:96:HIS:N	2.15	0.45
2:H:121:LEU:HD23	2:H:124:LEU:HD21	1.97	0.44
2:H:187:SER:O	2:H:188:SER:C	2.60	0.44
1:I:147:LEU:HD12	2:J:101:PHE:CE1	2.52	0.44
2:D:293:ILE:HD12	2:D:293:ILE:C	2.41	0.44
2:F:263:VAL:O	2:F:266:ALA:O	2.35	0.44
2:D:185:LEU:HD21	2:D:293:ILE:HD13	1.99	0.44
1:E:154:ARG:NH2	1:E:165:GLN:OE1	2.49	0.44
2:H:222:ASN:HB2	2:H:228:ILE:HG13	2.00	0.44
1:C:161:ARG:NH1	1:C:163:THR:OG1	2.51	0.44
1:C:116:VAL:CG1	1:C:124:ILE:HD11	2.44	0.44
1:A:193:ARG:O	1:A:194:SER:C	2.61	0.44
1:I:61:VAL:O	1:I:65:LEU:HG	2.17	0.44
1:I:63:LYS:HG3	1:I:146:LEU:HD22	2.00	0.44
2:J:309:TYR:O	2:J:313:ILE:HG12	2.18	0.44
2:D:231:LEU:O	2:D:269:ILE:HD12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:LEU:HD13	1:E:125:MET:HE1	1.99	0.44
2:H:158:GLN:HB2	2:H:160:PHE:CE2	2.53	0.44
2:F:209:GLY:O	2:F:210:HIS:CG	2.71	0.43
1:G:9:LEU:HD21	1:G:36:VAL:HG11	2.00	0.43
1:I:81:VAL:HG13	1:I:125:MET:HG3	2.00	0.43
1:E:35:HIS:O	1:E:36:VAL:C	2.59	0.43
1:A:170:GLN:CD	2:B:109:ILE:HD13	2.43	0.43
2:F:132:LEU:C	2:F:132:LEU:HD12	2.43	0.43
2:B:232:LEU:HD21	2:B:266:ALA:HB3	1.98	0.43
2:H:130:LEU:HB3	2:H:240:ILE:CG2	2.49	0.43
2:H:310:THR:HA	2:H:313:ILE:HG23	2.01	0.43
2:H:196:LEU:HD11	2:H:289:ILE:HD11	2.00	0.43
1:A:3:SER:N	1:A:4:PRO:CD	2.82	0.43
2:B:145:CYS:SG	2:B:239:HIS:HE1	2.36	0.43
1:C:82:ILE:CG1	1:C:124:ILE:HB	2.49	0.43
1:A:41:SER:HA	2:H:110:HIS:CE1	2.54	0.43
2:H:252:ILE:O	2:H:253:GLY:C	2.61	0.43
2:F:209:GLY:C	2:F:210:HIS:CG	2.97	0.42
2:H:163:THR:HG23	2:H:164:GLN:N	2.34	0.42
1:C:191:LEU:HD23	2:D:89:ARG:HD3	2.00	0.42
2:D:121:LEU:HD12	2:D:121:LEU:H	1.84	0.42
1:C:116:VAL:HG11	1:C:124:ILE:CD1	2.45	0.42
1:G:116:VAL:CG1	1:G:124:ILE:HD11	2.49	0.42
2:F:132:LEU:HD21	2:F:267:PHE:CE2	2.54	0.42
2:F:214:THR:O	2:F:214:THR:HG23	2.20	0.42
2:F:283:ASN:CG	2:F:283:ASN:O	2.63	0.42
1:A:16:ILE:HD13	1:A:46:CYS:SG	2.60	0.42
2:B:301:GLU:O	2:B:304:LEU:HG	2.19	0.42
1:C:90:THR:HG21	2:F:135:PHE:HA	2.01	0.42
2:H:303:ARG:O	2:H:307:ILE:HG12	2.18	0.42
1:I:158:THR:OG1	1:I:161:ARG:O	2.27	0.42
2:J:207:VAL:HG13	2:J:208:THR:N	2.34	0.42
1:C:121:ASN:HB3	2:F:118:PRO:HG3	2.02	0.42
2:D:229:MET:HB3	2:D:271:VAL:HG22	2.01	0.42
2:F:149:ILE:HG22	2:F:150:ASN:N	2.33	0.42
2:H:168:PHE:O	2:H:168:PHE:CG	2.73	0.42
1:E:126:LEU:HD12	1:E:126:LEU:N	2.35	0.42
2:H:115:VAL:HG21	2:H:119:LEU:HD22	2.01	0.42
2:H:188:SER:O	2:H:189:PRO:C	2.63	0.42
2:J:232:LEU:HD13	2:J:309:TYR:CD2	2.55	0.42
2:B:178:LYS:O	2:B:182:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:252:ILE:O	2:F:253:GLY:C	2.63	0.42
2:J:253:GLY:N	2:J:254:PRO:CD	2.83	0.42
1:G:39:ARG:CG	1:G:96:HIS:ND1	2.83	0.41
1:E:41:SER:O	1:E:96:HIS:HE1	2.04	0.41
2:F:130:LEU:CD1	2:F:139:LEU:HD13	2.51	0.41
2:H:203:TYR:CZ	2:H:247:LEU:HD21	2.54	0.41
2:B:276:THR:O	2:B:276:THR:HG23	2.21	0.41
1:C:136:SER:HB3	1:C:137:PRO:HD3	2.03	0.41
1:I:15:VAL:HG21	1:I:64:PHE:CE1	2.55	0.41
2:B:130:LEU:HB3	2:B:240:ILE:HB	2.02	0.41
2:D:109:ILE:HG23	2:D:110:HIS:N	2.36	0.41
2:F:184:LEU:C	2:F:192:VAL:HG22	2.44	0.41
1:I:136:SER:HB2	1:I:137:PRO:HD3	2.03	0.41
2:B:252:ILE:CG2	2:B:258:LEU:HD21	2.51	0.41
1:C:106:SER:HB2	2:F:116:PHE:HB2	2.03	0.41
2:F:109:ILE:O	2:F:110:HIS:C	2.64	0.41
2:F:231:LEU:HG	2:F:269:ILE:CG1	2.50	0.41
1:I:115:ASP:OD1	1:I:115:ASP:N	2.54	0.41
1:C:96:HIS:O	1:C:97:GLU:C	2.64	0.41
2:F:240:ILE:O	2:F:240:ILE:HG13	2.19	0.41
1:G:35:HIS:O	1:G:36:VAL:C	2.64	0.41
2:H:232:LEU:HD22	2:H:309:TYR:CD1	2.56	0.41
2:J:119:LEU:HB3	2:J:260:VAL:HG12	2.02	0.41
2:J:228:ILE:HG13	2:J:271:VAL:O	2.21	0.41
2:F:121:LEU:H	2:F:121:LEU:HD22	1.86	0.41
2:F:130:LEU:HD11	2:F:139:LEU:HD13	2.01	0.40
2:F:263:VAL:O	2:F:264:GLY:C	2.62	0.40
2:H:167:PHE:CD1	2:H:199:PRO:HB3	2.56	0.40
2:B:200:SER:HA	2:B:252:ILE:HD11	2.03	0.40
2:F:233:LEU:HD22	2:F:267:PHE:HE2	1.87	0.40
2:J:163:THR:HG23	2:J:164:GLN:N	2.36	0.40
2:B:109:ILE:HG23	2:B:110:HIS:N	2.36	0.40
2:B:201:LEU:HD11	2:B:227:LEU:HD21	2.03	0.40
2:H:217:PRO:HB3	2:H:231:LEU:HD23	2.03	0.40
2:H:310:THR:O	2:H:313:ILE:CG1	2.69	0.40
2:J:200:SER:HB3	2:J:252:ILE:HB	2.03	0.40
1:C:191:LEU:HD12	1:C:193:ARG:NH2	2.36	0.40
2:H:188:SER:O	2:H:190:SER:N	2.54	0.40
2:H:233:LEU:O	2:H:266:ALA:HB1	2.22	0.40

All (4) 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)
2:B:172:HIS:HA	2:D:135:PHE:HE1[7_555]	1.35	0.25
2:B:151:ARG:NH2	1:C:189:GLN:O[8_554]	2.09	0.11
1:C:136:SER:OG	2:D:80:SER:OG[8_554]	2.12	0.08
2:F:159:GLU:OE2	1:I:120:LYS:NZ[4_444]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	192/200 (96%)	179 (93%)	11 (6%)	2 (1%)	12	45
1	C	192/200 (96%)	186 (97%)	6 (3%)	0	100	100
1	E	194/200 (97%)	188 (97%)	6 (3%)	0	100	100
1	G	193/200 (96%)	186 (96%)	7 (4%)	0	100	100
1	I	137/200 (68%)	124 (90%)	13 (10%)	0	100	100
2	B	237/257 (92%)	211 (89%)	21 (9%)	5 (2%)	5	32
2	D	240/257 (93%)	218 (91%)	20 (8%)	2 (1%)	16	51
2	F	194/257 (76%)	179 (92%)	11 (6%)	4 (2%)	5	32
2	H	239/257 (93%)	214 (90%)	17 (7%)	8 (3%)	3	25
2	J	189/257 (74%)	174 (92%)	14 (7%)	1 (0%)	24	60
All	All	2007/2285 (88%)	1859 (93%)	126 (6%)	22 (1%)	11	44

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	188	SER
2	H	225	GLY
2	J	93	ALA
1	A	104	GLY
2	B	123	THR
2	F	223	GLY

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Mol	Chain	Res	Type
2	H	189	PRO
2	H	223	GLY
2	H	253	GLY
2	D	236	THR
2	F	110	HIS
2	F	126	PRO
2	B	253	GLY
2	B	275	ASP
2	F	264	GLY
2	H	149	ILE
2	D	213	GLY
2	H	190	SER
2	B	264	GLY
2	H	299	GLY
2	H	156	VAL
1	A	98	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	174/177 (98%)	170 (98%)	4 (2%)	44	64
1	C	174/177 (98%)	171 (98%)	3 (2%)	53	68
1	E	176/177 (99%)	176 (100%)	0	100	100
1	G	175/177 (99%)	174 (99%)	1 (1%)	78	81
1	I	140/177 (79%)	136 (97%)	4 (3%)	37	58
2	B	215/230 (94%)	209 (97%)	6 (3%)	38	59
2	D	218/230 (95%)	205 (94%)	13 (6%)	17	41
2	F	185/230 (80%)	178 (96%)	7 (4%)	29	51
2	H	217/230 (94%)	209 (96%)	8 (4%)	30	52
2	J	184/230 (80%)	173 (94%)	11 (6%)	17	41
All	All	1858/2035 (91%)	1801 (97%)	57 (3%)	35	56

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	42	SER
1	A	43	GLN
1	A	158	THR
2	B	165	LEU
2	B	187	SER
2	B	252	ILE
2	B	255	THR
2	B	277	VAL
2	B	285	ASP
1	C	35	HIS
1	C	38	SER
1	C	96	HIS
2	D	112	SER
2	D	124	LEU
2	D	138	SER
2	D	207	VAL
2	D	215	ILE
2	D	236	THR
2	D	252	ILE
2	D	268	CYS
2	D	271	VAL
2	D	285	ASP
2	D	294	LYS
2	D	310	THR
2	D	312	LEU
2	F	115	VAL
2	F	147	ILE
2	F	149	ILE
2	F	167	PHE
2	F	175	ILE
2	F	262	LEU
2	F	263	VAL
1	G	97	GLU
2	H	112	SER
2	H	148	CYS
2	H	153	GLN
2	H	165	LEU
2	H	215	ILE
2	H	252	ILE
2	H	293	ILE
2	H	313	ILE

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Mol	Chain	Res	Type
1	I	80	PHE
1	I	82	ILE
1	I	125	MET
1	I	163	THR
2	J	129	CYS
2	J	137	HIS
2	J	140	THR
2	J	171	VAL
2	J	200	SER
2	J	206	LEU
2	J	214	THR
2	J	238	LEU
2	J	247	LEU
2	J	255	THR
2	J	315	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
2	B	153	GLN
2	B	210	HIS
2	B	283	ASN
1	C	71	ASN
2	D	81	HIS
2	D	210	HIS
2	D	251	ASN
2	D	283	ASN
1	E	13	ASN
1	E	85	ASN
1	E	96	HIS
2	F	198	GLN
2	F	316	ASN
1	G	43	GLN
1	G	54	GLN
1	G	71	ASN
1	G	105	GLN
2	H	81	HIS
2	H	153	GLN
2	H	234	GLN
2	H	251	ASN
2	H	308	ASN

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Mol	Chain	Res	Type
2	H	316	ASN
2	H	318	GLN
1	I	96	HIS

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 5 ligands modelled in this entry, 5 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	194/200 (97%)	-0.13	3 (1%) 72 52	137, 165, 231, 301	0
1	C	194/200 (97%)	-0.21	2 (1%) 79 61	142, 173, 227, 283	0
1	E	194/200 (97%)	-0.45	0 100 100	106, 202, 251, 309	2 (1%)
1	G	194/200 (97%)	-0.15	3 (1%) 72 52	117, 194, 238, 303	1 (0%)
1	I	153/200 (76%)	-0.24	0 100 100	219, 262, 311, 341	0
2	B	239/257 (92%)	-0.15	2 (0%) 82 65	143, 208, 250, 276	0
2	D	242/257 (94%)	-0.16	2 (0%) 82 65	151, 223, 267, 294	0
2	F	208/257 (80%)	-0.11	3 (1%) 73 54	186, 262, 309, 348	0
2	H	241/257 (93%)	0.08	6 (2%) 58 43	162, 207, 257, 335	0
2	J	203/257 (78%)	-0.30	0 100 100	226, 280, 320, 346	0
All	All	2062/2285 (90%)	-0.17	21 (1%) 79 61	106, 214, 294, 348	3 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	165	GLN	4.7
2	B	267	PHE	4.5
2	F	240	ILE	3.4
1	A	126	LEU	3.4
1	C	60	PHE	3.3
2	H	192	VAL	3.2
2	D	247	LEU	3.1
2	H	316	ASN	3.0
2	H	244	CYS	3.0
2	F	130	LEU	3.0
1	G	60	PHE	2.9
2	B	121	LEU	2.7
2	H	196	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	307	ILE	2.6
1	G	37	PHE	2.5
1	A	80	PHE	2.4
2	H	240	ILE	2.4
2	H	116	PHE	2.2
1	A	93	CYS	2.1
1	C	156	TYR	2.1
2	F	160	PHE	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
3	ZN	J	401	1/1	0.95	0.08	205,205,205,205	0
3	ZN	H	401	1/1	0.98	0.05	145,145,145,145	0
3	ZN	B	401	1/1	0.99	0.03	125,125,125,125	0
3	ZN	F	401	1/1	0.99	0.06	166,166,166,166	0
3	ZN	D	401	1/1	1.00	0.08	140,140,140,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.