



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:05 AM UTC

PDB ID : 2P1L / pdb_00002p1l
Title : Structure of the Bcl-XL:Beclin 1 complex
Authors : Jeffrey, P.D.; Shi, Y.; Oberstein, A.L.
Deposited on : 2007-03-05
Resolution : 2.50 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:

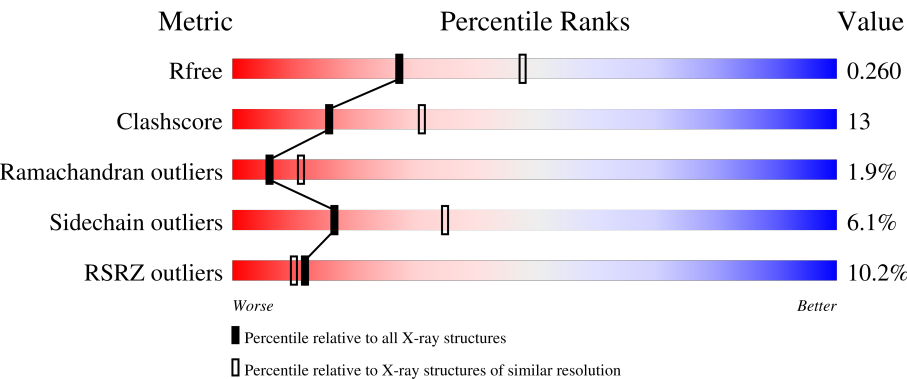
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



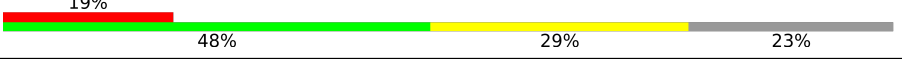
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	153	
1	C	153	
1	E	153	
1	G	153	
2	B	31	

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Mol	Chain	Length	Quality of chain
2	D	31	
2	F	31	
2	H	31	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5300 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 Apoptosis regulator Bcl-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1143	729	194	216	4			
1	C	141	Total	C	N	O	S	0	0	0
			1143	729	194	216	4			
1	E	141	Total	C	N	O	S	0	0	0
			1143	729	194	216	4			
1	G	141	Total	C	N	O	S	0	0	0
			1143	729	194	216	4			

- Molecule 2 is a protein called Beclin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	24	Total	C	N	O	S	0	0	0
			178	108	32	36	2			
2	D	24	Total	C	N	O	S	0	0	0
			178	108	32	36	2			
2	F	24	Total	C	N	O	S	0	0	0
			178	108	32	36	2			
2	H	24	Total	C	N	O	S	0	0	0
			178	108	32	36	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	105	GLY	-	cloning artifact	UNP Q14457
B	106	SER	-	cloning artifact	UNP Q14457
D	105	GLY	-	cloning artifact	UNP Q14457
D	106	SER	-	cloning artifact	UNP Q14457
F	105	GLY	-	cloning artifact	UNP Q14457
F	106	SER	-	cloning artifact	UNP Q14457
H	105	GLY	-	cloning artifact	UNP Q14457
H	106	SER	-	cloning artifact	UNP Q14457

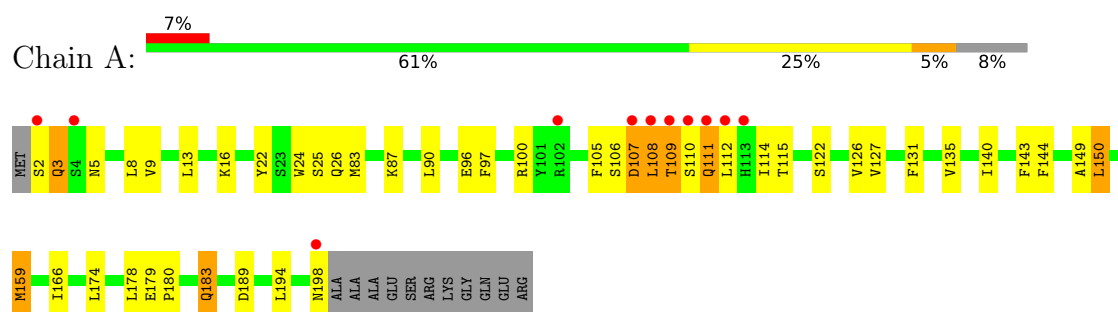
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	C	4	Total 4	O 4	0	0
3	E	5	Total 5	O 5	0	0
3	G	2	Total 2	O 2	0	0

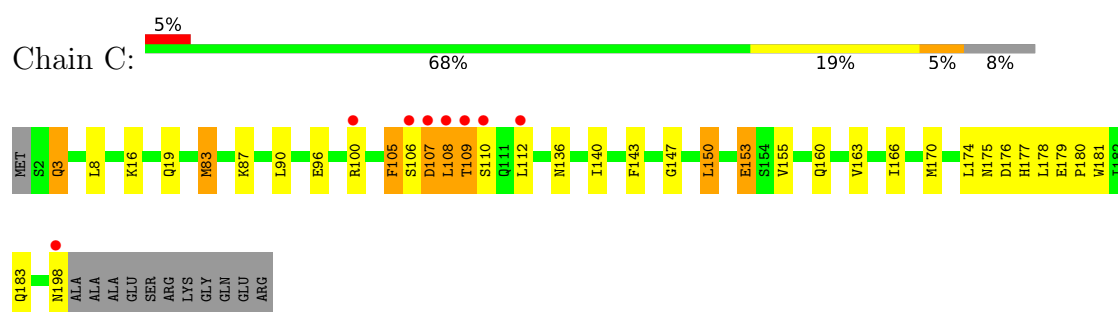
3 Residue-property plots [i](#)

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.

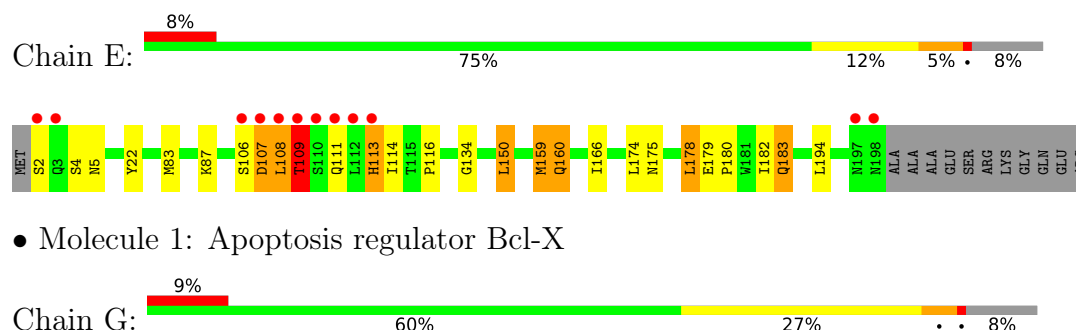
- Molecule 1: Apoptosis regulator Bcl-X



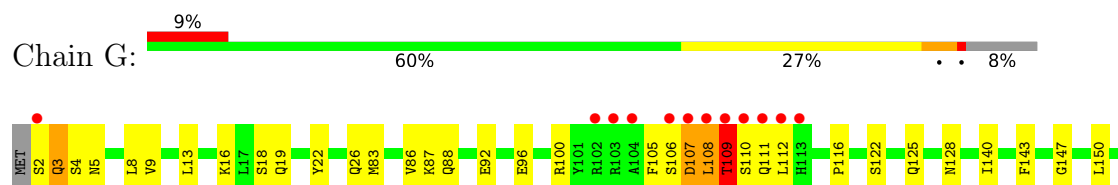
- Molecule 1: Apoptosis regulator Bcl-X



- Molecule 1: Apoptosis regulator Bcl-X

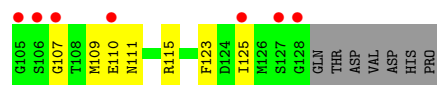


- Molecule 1: Apoptosis regulator Bcl-X

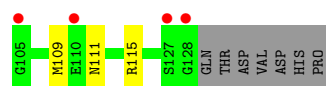




• Molecule 2: Beclin 1



• Molecule 2: Beclin 1



• Molecule 2: Beclin 1



• Molecule 2: Beclin 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.94Å 110.59Å 100.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.73 – 2.50 29.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.73-2.50) 97.5 (29.73-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.262 0.225 , 0.260	Depositor DCC
R_{free} test set	2115 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5300	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.42% 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	0.61	0/1171	0.93	4/1586 (0.3%)
1	C	0.58	0/1171	0.94	5/1586 (0.3%)
1	E	0.66	0/1171	0.98	4/1586 (0.3%)
1	G	0.60	0/1171	0.96	1/1586 (0.1%)
2	B	0.62	0/178	0.89	0/235
2	D	0.57	0/178	1.05	0/235
2	F	0.60	0/178	1.12	0/235
2	H	0.54	0/178	1.05	0/235
All	All	0.61	0/5396	0.96	14/7284 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	MET	N-CA-C	-6.44	102.64	110.88
1	E	134	GLY	N-CA-C	6.26	118.48	111.85
1	A	194	LEU	N-CA-C	6.07	118.86	111.82
1	E	159	MET	N-CA-C	-6.01	103.18	110.88
1	C	105	PHE	N-CA-C	5.85	116.00	108.34
1	A	127	VAL	N-CA-C	5.67	116.40	110.62
1	C	163	VAL	N-CA-C	5.66	116.11	110.23
1	C	177	HIS	N-CA-C	5.64	121.05	113.72
1	E	175	ASN	N-CA-C	5.45	116.90	111.07
1	G	194	LEU	N-CA-C	5.34	117.19	111.36
1	E	194	LEU	N-CA-C	5.23	117.06	111.36
1	C	176	ASP	N-CA-C	5.18	118.07	111.69
1	A	115	THR	N-CA-C	-5.15	102.28	108.25
1	C	3	GLN	N-CA-C	-5.05	106.62	112.89

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	1143	0	1083	37	0
1	C	1143	0	1083	24	0
1	E	1143	0	1083	30	0
1	G	1143	0	1083	44	0
2	B	178	0	179	5	0
2	D	178	0	179	3	0
2	F	178	0	179	7	0
2	H	178	0	179	8	0
3	A	5	0	0	0	0
3	C	4	0	0	0	0
3	E	5	0	0	1	0
3	G	2	0	0	0	0
All	All	5300	0	5048	136	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 13.

All (136) 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:109:THR:HG23	1:A:110:SER:H	1.39	0.88
1:C:109:THR:HG23	1:C:110:SER:H	1.39	0.87
1:E:83:MET:CE	1:E:87:LYS:HE3	2.05	0.86
1:E:83:MET:HE3	1:E:87:LYS:HE3	1.58	0.84
1:E:2:SER:HB2	1:G:86:VAL:HG21	1.62	0.81
1:E:2:SER:CB	1:G:86:VAL:HG21	2.13	0.78
1:E:107:ASP:OD2	1:E:109:THR:HG23	1.85	0.76
2:F:111:ASN:HD21	2:F:115:ARG:CZ	2.01	0.73
1:G:83:MET:HE3	1:G:87:LYS:HE3	1.69	0.73
1:G:107:ASP:HB2	1:G:109:THR:HG22	1.71	0.72
1:C:107:ASP:HB2	1:C:109:THR:HG22	1.70	0.72
1:A:8:LEU:HD22	1:C:90:LEU:HD23	1.73	0.71
1:G:107:ASP:HB2	1:G:109:THR:CG2	2.20	0.71
2:D:111:ASN:O	2:D:115:ARG:HG3	1.90	0.70
1:A:108:LEU:H	1:A:108:LEU:HD23	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASP:HB2	1:A:109:THR:HG22	1.73	0.69
1:E:174:LEU:HD12	1:E:178:LEU:HD23	1.77	0.66
1:E:160:GLN:H	1:E:160:GLN:CD	2.04	0.65
1:E:183:GLN:HE21	1:E:183:GLN:CA	2.10	0.64
1:A:150:LEU:HB3	1:A:166:ILE:HD13	1.78	0.64
1:E:179:GLU:HB3	1:E:180:PRO:HD3	1.81	0.63
1:G:116:PRO:HA	1:G:162:LEU:HD21	1.81	0.63
1:E:114:ILE:O	1:E:159:MET:HE1	1.99	0.62
1:G:179:GLU:HA	1:G:179:GLU:OE1	2.00	0.62
1:E:174:LEU:HD23	1:G:5:ASN:HB3	1.80	0.62
1:E:183:GLN:HE21	1:E:183:GLN:HA	1.64	0.62
1:A:96:GLU:OE2	1:A:100:ARG:HD2	2.00	0.61
1:A:2:SER:HB3	1:C:175:ASN:OD1	2.01	0.61
1:E:150:LEU:HB3	1:E:166:ILE:HD13	1.84	0.60
2:H:107:GLY:HA2	2:H:110:GLU:OE1	2.02	0.60
1:G:109:THR:OG1	1:G:153:GLU:HG2	2.02	0.59
1:G:16:LYS:HD3	1:G:19:GLN:OE1	2.03	0.59
1:E:113:HIS:NE2	2:F:105:GLY:HA2	2.18	0.59
1:E:178:LEU:O	1:E:182:ILE:HG13	2.02	0.59
1:E:183:GLN:HA	1:E:183:GLN:NE2	2.17	0.58
1:E:87:LYS:NZ	3:E:214:HOH:O	2.33	0.58
2:B:111:ASN:O	2:B:115:ARG:HG3	2.04	0.58
1:C:150:LEU:HB3	1:C:166:ILE:HD13	1.86	0.58
2:F:114:ARG:O	2:F:118:VAL:HG23	2.04	0.58
1:E:160:GLN:CD	1:E:160:GLN:N	2.62	0.58
1:C:109:THR:HG23	1:C:110:SER:N	2.16	0.57
1:G:150:LEU:HB3	1:G:166:ILE:HD13	1.84	0.57
1:C:179:GLU:HB3	1:C:180:PRO:HD3	1.87	0.56
1:A:109:THR:HG23	1:A:110:SER:N	2.16	0.56
1:C:112:LEU:HD21	2:D:109:MET:HG2	1.88	0.56
1:G:160:GLN:H	1:G:160:GLN:CD	2.13	0.55
1:G:112:LEU:HD23	2:H:108:THR:HB	1.88	0.54
1:G:160:GLN:CD	1:G:160:GLN:N	2.66	0.54
1:A:183:GLN:HE21	1:A:183:GLN:CA	2.20	0.54
1:G:107:ASP:OD2	1:G:109:THR:HG23	2.08	0.53
1:E:107:ASP:HB2	1:E:109:THR:CG2	2.38	0.53
1:A:8:LEU:HD22	1:C:90:LEU:CD2	2.39	0.53
2:F:111:ASN:HD21	2:F:115:ARG:NE	2.07	0.53
1:A:114:ILE:HG22	1:A:159:MET:HE1	1.91	0.52
1:E:2:SER:HB3	1:G:86:VAL:HG21	1.91	0.52
2:F:106:SER:HA	2:F:109:MET:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:MET:CE	1:A:87:LYS:HE3	2.40	0.51
1:A:140:ILE:O	1:A:143:PHE:HB3	2.11	0.51
1:G:116:PRO:HD3	1:G:159:MET:SD	2.51	0.51
1:E:108:LEU:H	1:E:108:LEU:HD23	1.75	0.51
1:G:157:LYS:HB2	1:G:159:MET:HE2	1.93	0.51
1:A:105:PHE:CD2	2:B:115:ARG:HD3	2.46	0.51
1:A:108:LEU:HA	1:A:111:GLN:HE21	1.77	0.50
2:F:111:ASN:HD21	2:F:115:ARG:NH2	2.11	0.49
1:A:106:SER:O	1:A:107:ASP:C	2.56	0.49
1:C:83:MET:HE3	1:C:87:LYS:HE3	1.94	0.49
1:E:106:SER:O	1:E:107:ASP:C	2.56	0.49
1:E:183:GLN:CA	1:E:183:GLN:NE2	2.76	0.48
1:A:22:TYR:CG	1:C:155:VAL:HG11	2.49	0.48
1:A:26:GLN:NE2	1:A:189:ASP:OD1	2.47	0.48
1:C:108:LEU:HD23	1:C:108:LEU:H	1.78	0.48
1:A:179:GLU:HB3	1:A:180:PRO:HD3	1.95	0.48
1:C:96:GLU:OE2	1:C:100:ARG:HD2	2.14	0.48
1:A:97:PHE:CD1	1:A:97:PHE:C	2.92	0.48
1:A:112:LEU:HD21	2:B:109:MET:HG2	1.96	0.48
1:G:88:GLN:HE21	1:G:92:GLU:CD	2.21	0.47
1:G:105:PHE:CE1	2:H:115:ARG:HB3	2.49	0.47
1:A:83:MET:HE1	1:A:87:LYS:HE3	1.97	0.47
1:G:2:SER:HB2	1:G:3:GLN:NE2	2.29	0.47
1:G:18:SER:HA	1:G:22:TYR:O	2.14	0.47
1:G:96:GLU:OE2	1:G:100:ARG:HD2	2.14	0.47
1:G:153:GLU:OE2	1:G:157:LYS:HE2	2.15	0.46
1:G:96:GLU:HG3	2:H:123:PHE:HE1	1.78	0.46
1:G:109:THR:HG23	1:G:110:SER:H	1.80	0.46
1:A:90:LEU:HD21	1:A:144:PHE:CE1	2.50	0.46
1:E:5:ASN:HB3	1:G:174:LEU:HD23	1.96	0.46
1:A:131:PHE:CD1	1:A:135:VAL:HG22	2.50	0.46
1:E:174:LEU:CD1	1:E:178:LEU:HD23	2.45	0.46
1:G:140:ILE:O	1:G:143:PHE:HB3	2.16	0.46
1:A:96:GLU:HG3	2:B:123:PHE:HE1	1.81	0.46
1:G:183:GLN:HE21	1:G:183:GLN:CA	2.29	0.45
1:A:183:GLN:HE21	1:A:183:GLN:HA	1.82	0.45
1:A:16:LYS:HD3	1:A:16:LYS:HA	1.78	0.45
1:E:106:SER:O	1:E:107:ASP:O	2.35	0.45
1:G:9:VAL:O	1:G:13:LEU:HG	2.17	0.45
1:G:183:GLN:NE2	1:G:183:GLN:HA	2.32	0.45
1:C:106:SER:O	1:C:107:ASP:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:ASN:HD22	1:G:128:ASN:HA	1.68	0.44
1:G:108:LEU:HD23	1:G:108:LEU:H	1.82	0.44
1:A:106:SER:O	1:A:107:ASP:O	2.35	0.44
1:C:106:SER:O	1:C:107:ASP:C	2.60	0.44
1:A:9:VAL:O	1:A:13:LEU:HG	2.18	0.44
1:E:107:ASP:HB2	1:E:109:THR:HG22	2.00	0.43
1:A:109:THR:HA	1:A:149:ALA:HB1	1.99	0.43
2:F:121:ASP:O	2:F:125:ILE:HG13	2.19	0.43
1:A:5:ASN:O	1:A:9:VAL:HG23	2.19	0.43
1:G:26:GLN:NE2	1:G:189:ASP:OD1	2.52	0.43
1:G:112:LEU:HD13	1:G:122:SER:HB3	2.01	0.42
1:E:116:PRO:HD3	1:E:159:MET:SD	2.60	0.42
1:C:105:PHE:CD2	2:D:115:ARG:HD3	2.54	0.42
2:B:107:GLY:HA2	2:B:110:GLU:OE2	2.20	0.42
1:C:109:THR:OG1	1:C:153:GLU:HG2	2.20	0.42
1:A:108:LEU:HA	1:A:111:GLN:NE2	2.34	0.42
1:A:107:ASP:OD2	1:A:109:THR:HG23	2.20	0.41
1:A:122:SER:O	1:A:126:VAL:HG23	2.20	0.41
1:C:8:LEU:HD23	1:C:8:LEU:HA	1.89	0.41
1:C:136:ASN:HA	1:C:181:TRP:CZ2	2.55	0.41
1:G:150:LEU:HD12	1:G:150:LEU:HA	1.92	0.41
1:A:3:GLN:OE1	1:A:3:GLN:HA	2.20	0.41
1:A:183:GLN:HA	1:A:183:GLN:NE2	2.35	0.41
1:G:183:GLN:CA	1:G:183:GLN:NE2	2.82	0.41
1:E:22:TYR:OH	1:G:156:ASP:OD1	2.32	0.41
1:C:16:LYS:HD3	1:C:19:GLN:OE1	2.21	0.41
1:C:83:MET:O	1:C:87:LYS:HG3	2.21	0.41
1:C:140:ILE:O	1:C:143:PHE:HB3	2.20	0.41
1:C:147:GLY:HA3	1:C:170:MET:SD	2.61	0.41
1:C:166:ILE:O	1:C:170:MET:HG3	2.21	0.41
1:E:2:SER:HB2	1:G:86:VAL:CG2	2.39	0.41
2:H:106:SER:HA	2:H:109:MET:HE3	2.03	0.41
1:G:125:GLN:OE1	2:H:109:MET:SD	2.79	0.40
1:G:147:GLY:HA3	1:G:170:MET:SD	2.61	0.40
1:G:112:LEU:HD21	2:H:109:MET:HG3	2.04	0.40
2:H:121:ASP:O	2:H:125:ILE:HG13	2.21	0.40
1:A:24:TRP:CD1	1:A:25:SER:HB3	2.56	0.40
1:G:106:SER:O	1:G:107:ASP:C	2.64	0.40
1:G:106:SER:O	1:G:107:ASP:O	2.40	0.40

There are no symmetry-related clashes.

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	139/153 (91%)	135 (97%)	1 (1%)	3 (2%)	5	9
1	C	139/153 (91%)	134 (96%)	3 (2%)	2 (1%)	9	17
1	E	139/153 (91%)	131 (94%)	4 (3%)	4 (3%)	3	5
1	G	139/153 (91%)	132 (95%)	4 (3%)	3 (2%)	5	9
2	B	22/31 (71%)	22 (100%)	0	0	100	100
2	D	22/31 (71%)	22 (100%)	0	0	100	100
2	F	22/31 (71%)	22 (100%)	0	0	100	100
2	H	22/31 (71%)	22 (100%)	0	0	100	100
All	All	644/736 (88%)	620 (96%)	12 (2%)	12 (2%)	6	11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ASP
1	A	109	THR
1	C	107	ASP
1	C	109	THR
1	E	107	ASP
1	E	109	THR
1	G	107	ASP
1	G	109	THR
1	E	4	SER
1	A	111	GLN
1	G	111	GLN
1	E	111	GLN

5.3.2 Protein sidechains [i](#)

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	120/128 (94%)	113 (94%)	7 (6%)	18	38
1	C	120/128 (94%)	110 (92%)	10 (8%)	10	22
1	E	120/128 (94%)	113 (94%)	7 (6%)	18	38
1	G	120/128 (94%)	111 (92%)	9 (8%)	12	26
2	B	20/27 (74%)	19 (95%)	1 (5%)	22	44
2	D	20/27 (74%)	20 (100%)	0	100	100
2	F	20/27 (74%)	20 (100%)	0	100	100
2	H	20/27 (74%)	20 (100%)	0	100	100
All	All	560/620 (90%)	526 (94%)	34 (6%)	17	35

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	108	LEU
1	A	150	LEU
1	A	174	LEU
1	A	178	LEU
1	A	183	GLN
1	A	198	ASN
2	B	125	ILE
1	C	3	GLN
1	C	83	MET
1	C	108	LEU
1	C	150	LEU
1	C	153	GLU
1	C	160	GLN
1	C	174	LEU
1	C	178	LEU
1	C	183	GLN
1	C	198	ASN
1	E	108	LEU
1	E	109	THR
1	E	113	HIS
1	E	150	LEU
1	E	160	GLN

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Mol	Chain	Res	Type
1	E	178	LEU
1	E	183	GLN
1	G	3	GLN
1	G	4	SER
1	G	8	LEU
1	G	108	LEU
1	G	109	THR
1	G	153	GLU
1	G	160	GLN
1	G	183	GLN
1	G	198	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	113	HIS
1	A	125	GLN
1	A	128	ASN
1	A	183	GLN
1	A	197	ASN
1	A	198	ASN
1	C	111	GLN
1	C	121	GLN
1	C	128	ASN
1	C	160	GLN
1	C	183	GLN
1	C	185	ASN
1	C	198	ASN
2	D	111	ASN
1	E	26	GLN
1	E	121	GLN
1	E	125	GLN
1	E	128	ASN
1	E	183	GLN
1	E	197	ASN
1	E	198	ASN
2	F	111	ASN
1	G	3	GLN
1	G	128	ASN
1	G	177	HIS
1	G	183	GLN

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Mol	Chain	Res	Type
1	G	185	ASN
1	G	198	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](#)

There are no ligands in this entry.

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	141/153 (92%)	0.20	11 (7%) 19 17	36, 51, 93, 127	0
1	C	141/153 (92%)	0.35	8 (5%) 29 26	36, 54, 99, 131	0
1	E	141/153 (92%)	0.09	12 (8%) 16 14	34, 48, 100, 127	0
1	G	141/153 (92%)	0.28	14 (9%) 13 11	36, 54, 103, 130	0
2	B	24/31 (77%)	1.32	7 (29%) 1 1	51, 68, 107, 115	0
2	D	24/31 (77%)	0.99	4 (16%) 4 3	49, 66, 106, 112	0
2	F	24/31 (77%)	1.23	5 (20%) 2 2	45, 65, 108, 117	0
2	H	24/31 (77%)	1.28	6 (25%) 2 1	55, 72, 112, 117	0
All	All	660/736 (89%)	0.37	67 (10%) 12 10	34, 54, 109, 131	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	108	LEU	12.1
1	G	108	LEU	9.2
1	C	109	THR	7.9
2	B	105	GLY	7.7
2	B	128	GLY	7.6
2	F	128	GLY	7.3
1	A	108	LEU	7.0
1	E	108	LEU	6.8
1	G	109	THR	6.7
2	F	105	GLY	6.1
1	G	107	ASP	5.9
2	H	128	GLY	5.4
1	E	109	THR	5.1
2	D	105	GLY	5.0
1	G	198	ASN	5.0
1	E	113	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
2	D	128	GLY	4.5
2	H	105	GLY	4.5
1	A	107	ASP	4.5
1	E	198	ASN	4.2
1	A	109	THR	4.2
1	E	112	LEU	4.1
1	C	198	ASN	4.1
1	A	110	SER	4.0
1	A	198	ASN	4.0
1	E	107	ASP	3.9
1	C	107	ASP	3.9
1	C	110	SER	3.6
1	A	112	LEU	3.6
1	E	110	SER	3.6
1	G	111	GLN	3.5
2	B	107	GLY	3.3
1	G	112	LEU	3.2
1	E	111	GLN	3.1
1	G	106	SER	3.1
1	G	113	HIS	3.1
1	E	2	SER	3.1
1	A	111	GLN	3.1
1	G	110	SER	3.0
1	E	106	SER	2.9
1	E	197	ASN	2.9
2	F	109	MET	2.8
2	H	106	SER	2.8
1	G	197	ASN	2.7
1	C	112	LEU	2.7
1	G	104	ALA	2.5
2	B	125	ILE	2.5
2	H	111	ASN	2.5
2	H	109	MET	2.4
1	G	2	SER	2.4
2	F	106	SER	2.3
1	E	3	GLN	2.2
1	C	106	SER	2.2
1	G	103	ARG	2.2
1	A	113	HIS	2.2
2	D	127	SER	2.2
2	D	110	GLU	2.2
1	G	102	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	107	GLY	2.1
2	F	127	SER	2.1
1	A	102	ARG	2.1
2	B	110	GLU	2.1
1	A	2	SER	2.1
1	A	4	SER	2.1
2	B	106	SER	2.1
1	C	100	ARG	2.0
2	B	127	SER	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.