



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:56 PM UTC

PDB ID : 4BQ7 / pdb_00004bq7
Title : Crystal structure of the RGMB-Neo1 complex form 2
Authors : Bell, C.H.; Healey, E.; van Erp, S.; Bishop, B.; Tang, C.; Gilbert, R.J.C.; Aricescu, A.R.; Pasterkamp, R.J.; Siebold, C.
Deposited on : 2013-05-30
Resolution : 6.60 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:

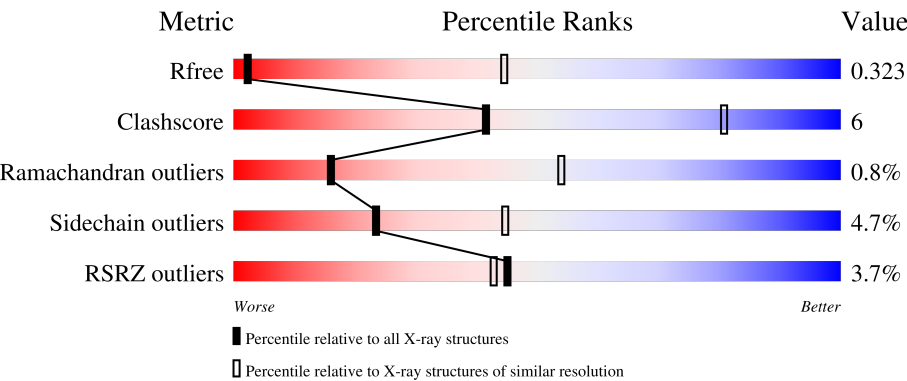
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 6.60 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	1162 (9.00-4.00)
Clashscore	190562	1000 (9.00-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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	264	3% 61% 13% 23%
1	B	264	3% 65% 9% 23%
2	C	122	% 10% 88%
2	E	122	% 10% 88%
3	D	251	% 49% 8% 41%

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Mol	Chain	Length	Quality of chain
3	F	251	3% 50% 7% 41%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5714 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 NEOGENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1591	1017	270	298	6			
1	B	202	Total	C	N	O	S	0	0	0
			1591	1017	270	298	6			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	880	GLU	-	expression tag	UNP P97798
A	881	THR	-	expression tag	UNP P97798
A	882	GLY	-	expression tag	UNP P97798
A	1134	ASN	-	expression tag	UNP P97798
A	1135	GLY	-	expression tag	UNP P97798
A	1136	THR	-	expression tag	UNP P97798
A	1137	LYS	-	expression tag	UNP P97798
A	1138	HIS	-	expression tag	UNP P97798
A	1139	HIS	-	expression tag	UNP P97798
A	1140	HIS	-	expression tag	UNP P97798
A	1141	HIS	-	expression tag	UNP P97798
A	1142	HIS	-	expression tag	UNP P97798
A	1143	HIS	-	expression tag	UNP P97798
B	880	GLU	-	expression tag	UNP P97798
B	881	THR	-	expression tag	UNP P97798
B	882	GLY	-	expression tag	UNP P97798
B	1134	ASN	-	expression tag	UNP P97798
B	1135	GLY	-	expression tag	UNP P97798
B	1136	THR	-	expression tag	UNP P97798
B	1137	LYS	-	expression tag	UNP P97798
B	1138	HIS	-	expression tag	UNP P97798
B	1139	HIS	-	expression tag	UNP P97798
B	1140	HIS	-	expression tag	UNP P97798
B	1141	HIS	-	expression tag	UNP P97798
B	1142	HIS	-	expression tag	UNP P97798

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1143	HIS	-	expression tag	UNP P97798

- Molecule 2 is a protein called RGM DOMAIN FAMILY MEMBER B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total 118	C 79	N 16	O 21	S 2	0	0	0
2	E	15	Total 118	C 79	N 16	O 21	S 2	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	47	GLU	-	expression tag	UNP Q6NW40
C	48	THR	-	expression tag	UNP Q6NW40
C	49	GLY	-	expression tag	UNP Q6NW40
E	47	GLU	-	expression tag	UNP Q6NW40
E	48	THR	-	expression tag	UNP Q6NW40
E	49	GLY	-	expression tag	UNP Q6NW40

- Molecule 3 is a protein called RGM DOMAIN FAMILY MEMBER B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	148	Total 1148	C 721	N 197	O 223	S 7	0	0	0
3	F	148	Total 1148	C 721	N 197	O 223	S 7	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	411	GLY	-	expression tag	UNP Q6NW40
D	412	THR	-	expression tag	UNP Q6NW40
D	413	LYS	-	expression tag	UNP Q6NW40
D	414	HIS	-	expression tag	UNP Q6NW40
D	415	HIS	-	expression tag	UNP Q6NW40
D	416	HIS	-	expression tag	UNP Q6NW40
D	417	HIS	-	expression tag	UNP Q6NW40
D	418	HIS	-	expression tag	UNP Q6NW40
D	419	HIS	-	expression tag	UNP Q6NW40
D	225	GLY	GLU	conflict	UNP Q6NW40
F	411	GLY	-	expression tag	UNP Q6NW40

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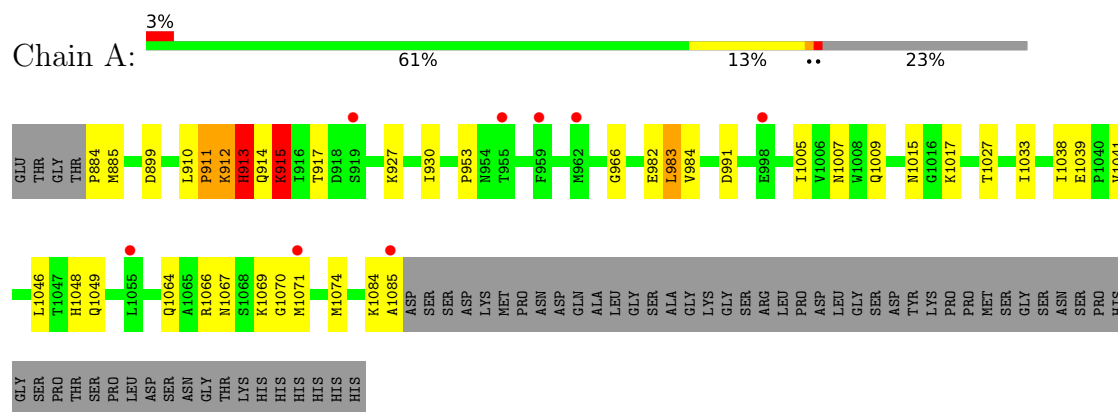
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Chain	Residue	Modelled	Actual	Comment	Reference
F	412	THR	-	expression tag	UNP Q6NW40
F	413	LYS	-	expression tag	UNP Q6NW40
F	414	HIS	-	expression tag	UNP Q6NW40
F	415	HIS	-	expression tag	UNP Q6NW40
F	416	HIS	-	expression tag	UNP Q6NW40
F	417	HIS	-	expression tag	UNP Q6NW40
F	418	HIS	-	expression tag	UNP Q6NW40
F	419	HIS	-	expression tag	UNP Q6NW40
F	225	GLY	GLU	conflict	UNP Q6NW40

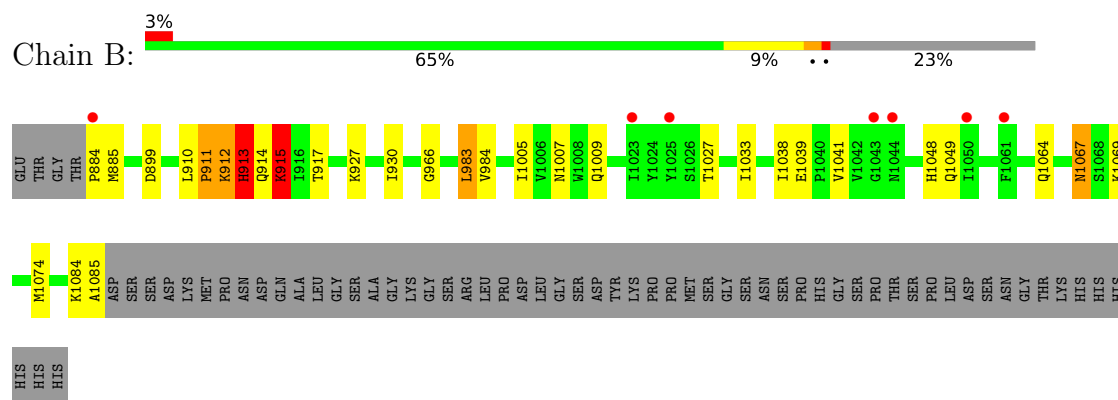
3 Residue-property plots [i](#)

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.

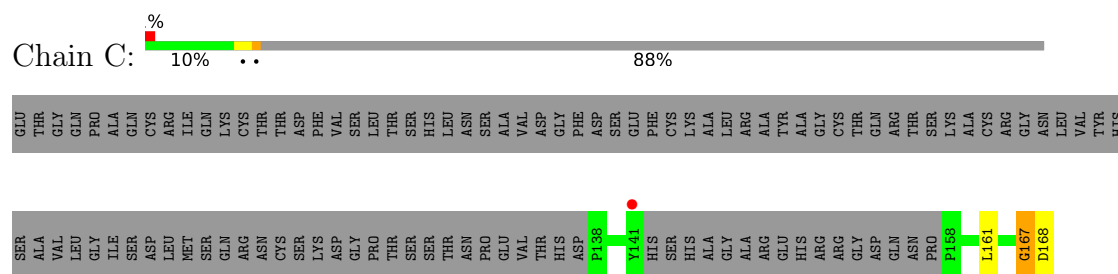
• Molecule 1: NEOGENIN



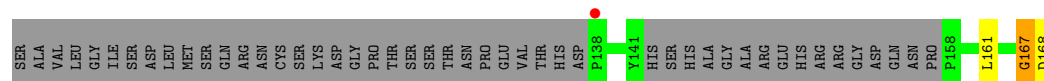
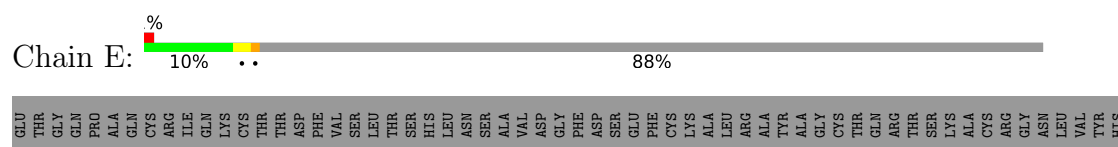
• Molecule 1: NEOGENIN



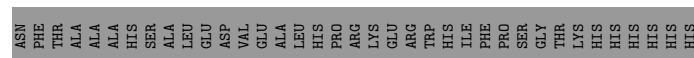
• Molecule 2: RGM DOMAIN FAMILY MEMBER B



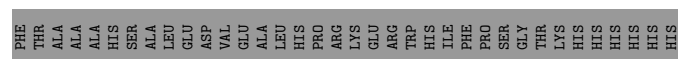
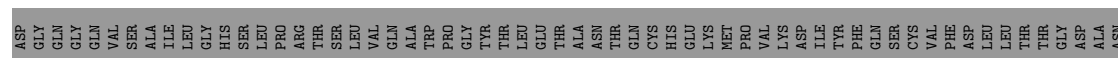
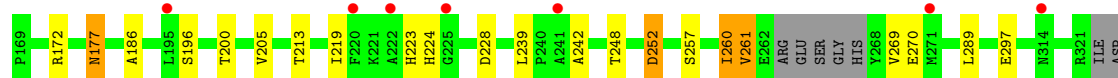
• Molecule 2: RGM DOMAIN FAMILY MEMBER B



● Molecule 3: RGM DOMAIN FAMILY MEMBER B



● Molecule 3: RGM DOMAIN FAMILY MEMBER B



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	109.69Å 109.69Å 187.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.78 – 6.60 84.78 – 6.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (84.78-6.60) 97.2 (84.78-6.60)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 6.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.254 , 0.280 0.305 , 0.323	Depositor DCC
R_{free} test set	231 reflections (9.27%)	wwPDB-VP
Wilson B-factor (Å ²)	128.1	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 186.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.077 for -h,-k,l	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	5714	wwPDB-VP
Average B, all atoms (Å ²)	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.25	1/1635 (0.1%)	1.24	14/2234 (0.6%)
1	B	1.57	1/1635 (0.1%)	1.17	12/2234 (0.5%)
2	C	0.65	0/122	1.84	3/162 (1.9%)
2	E	0.66	0/122	1.84	3/162 (1.9%)
3	D	0.85	0/1170	1.26	5/1590 (0.3%)
3	F	0.85	0/1170	1.26	5/1590 (0.3%)
All	All	1.20	2/5854 (0.0%)	1.26	42/7972 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	E	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	983	LEU	C-N	53.90	1.94	1.33
1	A	983	LEU	C-N	-37.75	0.91	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	983	LEU	O-C-N	17.54	144.39	123.17
2	E	167	GLY	CA-C-N	12.05	143.40	121.70
2	E	167	GLY	C-N-CA	12.05	143.40	121.70
2	C	167	GLY	CA-C-N	11.99	143.28	121.70
2	C	167	GLY	C-N-CA	11.99	143.28	121.70
1	A	983	LEU	CA-C-N	-7.35	104.95	119.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	983	LEU	C-N-CA	-7.35	104.95	119.72
1	A	912	LYS	CA-C-N	7.27	135.43	121.54
1	A	912	LYS	C-N-CA	7.27	135.43	121.54
1	B	912	LYS	CA-C-N	7.27	135.42	121.54
1	B	912	LYS	C-N-CA	7.27	135.42	121.54
3	D	228	ASP	N-CA-C	-6.68	100.91	110.59
1	A	915	LYS	N-CA-C	6.62	119.39	109.25
1	B	915	LYS	N-CA-C	6.62	119.37	109.25
3	F	228	ASP	N-CA-C	-6.62	101.00	110.59
1	A	913	HIS	CA-C-N	6.13	132.74	121.70
1	A	913	HIS	C-N-CA	6.13	132.74	121.70
1	B	913	HIS	CA-C-N	6.13	132.73	121.70
1	B	913	HIS	C-N-CA	6.13	132.73	121.70
3	D	252	ASP	CA-CB-CG	6.08	118.68	112.60
3	F	252	ASP	CA-CB-CG	6.05	118.65	112.60
1	B	1027	THR	N-CA-C	-5.99	105.80	113.23
1	A	1027	THR	N-CA-C	-5.98	105.81	113.23
1	A	911	PRO	CA-C-N	5.79	132.60	121.54
1	A	911	PRO	C-N-CA	5.79	132.60	121.54
1	B	911	PRO	CA-C-N	5.78	132.58	121.54
1	B	911	PRO	C-N-CA	5.78	132.58	121.54
3	D	205	VAL	N-CA-C	-5.61	104.59	109.19
1	B	899	ASP	CA-CB-CG	5.60	118.20	112.60
3	F	205	VAL	N-CA-C	-5.57	104.62	109.19
1	A	899	ASP	CA-CB-CG	5.54	118.14	112.60
2	C	167	GLY	O-C-N	-5.41	115.70	122.84
1	B	1067	ASN	CA-CB-CG	5.40	118.00	112.60
1	A	1067	ASN	CA-CB-CG	5.40	118.00	112.60
1	A	1033	ILE	N-CA-C	5.37	116.74	110.62
2	E	167	GLY	O-C-N	-5.32	115.82	122.84
1	B	1033	ILE	N-CA-C	5.30	116.66	110.62
3	F	177	ASN	CA-CB-CG	5.10	117.70	112.60
3	D	177	ASN	CA-CB-CG	5.08	117.68	112.60
1	B	983	LEU	O-C-N	5.05	129.50	122.78
3	D	213	THR	N-CA-C	5.04	116.96	109.25
3	F	213	THR	N-CA-C	5.00	116.90	109.25

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	167	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	E	167	GLY	Peptide

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	1591	0	1585	48	0
1	B	1591	0	1585	15	0
2	C	118	0	101	1	0
2	E	118	0	101	1	0
3	D	1148	0	1122	35	1
3	F	1148	0	1122	14	0
All	All	5714	0	5616	73	1

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 6.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:983:LEU:C	1:B:984:VAL:N	1.94	1.25
1:A:1009:GLN:HG3	3:D:200:THR:OG1	1.68	0.94
1:A:991:ASP:OD2	3:D:200:THR:HG21	1.68	0.93
1:A:1009:GLN:HG3	3:D:200:THR:HG1	1.35	0.92
1:A:1009:GLN:HG2	3:D:186:ALA:HB2	1.55	0.86
1:A:1009:GLN:NE2	3:D:199:VAL:C	2.41	0.78
1:A:913:HIS:HA	1:A:914:GLN:HG2	1.67	0.77
1:B:913:HIS:HA	1:B:914:GLN:HG2	1.67	0.76
1:B:983:LEU:HG	1:B:984:VAL:N	2.03	0.74
1:A:991:ASP:OD2	3:D:200:THR:CG2	2.36	0.72
1:A:1046:LEU:HD13	3:D:198:GLN:HG2	1.71	0.72
1:A:1009:GLN:NE2	3:D:200:THR:OG1	2.23	0.71
1:A:984:VAL:HG21	3:F:224:HIS:CG	2.27	0.70
1:A:1046:LEU:HD12	3:D:198:GLN:HB2	1.74	0.69
3:F:261:VAL:HG23	3:F:270:GLU:HG3	1.74	0.69
3:D:261:VAL:HG23	3:D:270:GLU:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:GLN:HE22	3:D:199:VAL:C	2.02	0.67
1:B:930:ILE:HD11	3:F:242:ALA:HB3	1.77	0.66
1:A:1009:GLN:HG2	3:D:186:ALA:CB	2.25	0.66
1:A:1009:GLN:CG	3:D:200:THR:OG1	2.41	0.66
1:A:1046:LEU:HB2	3:D:198:GLN:CD	2.24	0.63
1:B:1009:GLN:NE2	3:F:200:THR:OG1	2.27	0.61
1:A:1084:LYS:HG2	1:A:1085:ALA:H	1.65	0.61
1:A:1046:LEU:HD12	3:D:198:GLN:CB	2.31	0.61
1:B:1084:LYS:HG2	1:B:1085:ALA:H	1.65	0.60
1:A:991:ASP:CG	3:D:200:THR:HG21	2.26	0.59
1:B:1039:GLU:HG2	1:B:1048:HIS:NE2	2.18	0.59
1:A:1039:GLU:HG2	1:A:1048:HIS:NE2	2.18	0.59
1:A:1066:ARG:NH2	3:F:223:HIS:NE2	2.49	0.58
1:A:1064:GLN:HB3	1:A:1074:MET:HG3	1.88	0.55
1:A:1017:LYS:HG3	3:D:229:GLN:NE2	2.20	0.55
1:A:982:GLU:C	1:A:1069:LYS:HG3	2.32	0.55
1:B:1064:GLN:HB3	1:B:1074:MET:HG3	1.88	0.54
1:A:1071:MET:HG2	3:F:224:HIS:O	2.08	0.54
1:A:984:VAL:HG21	3:F:224:HIS:CD2	2.42	0.54
1:A:1009:GLN:NE2	3:D:200:THR:N	2.57	0.53
1:A:1007:ASN:HB3	3:D:186:ALA:O	2.09	0.52
3:F:196:SER:HB2	3:F:219:ILE:HB	1.92	0.52
1:A:1046:LEU:HB3	3:D:198:GLN:NE2	2.26	0.51
3:D:196:SER:HB2	3:D:219:ILE:HB	1.92	0.51
1:B:911:PRO:HB2	1:B:915:LYS:NZ	2.28	0.49
1:A:911:PRO:HB2	1:A:915:LYS:NZ	2.28	0.49
1:A:911:PRO:HB2	1:A:915:LYS:HZ3	1.77	0.48
1:A:1046:LEU:CB	3:D:198:GLN:CD	2.87	0.48
3:D:248:THR:HA	3:D:260:ILE:HD12	1.96	0.48
1:A:983:LEU:O	1:A:984:VAL:C	2.48	0.47
3:F:248:THR:HA	3:F:260:ILE:HD12	1.96	0.47
1:A:1046:LEU:CD1	3:D:198:GLN:CB	2.93	0.47
1:A:953:PRO:HB2	1:A:1015:ASN:HB3	1.96	0.47
1:A:1009:GLN:HE21	3:D:199:VAL:C	2.23	0.46
1:A:983:LEU:HG	1:A:984:VAL:HG12	1.97	0.46
1:B:1005:ILE:HG12	1:B:1049:GLN:HG2	1.98	0.45
1:A:1005:ILE:HG12	1:A:1049:GLN:HG2	1.98	0.44
1:B:983:LEU:O	1:B:1067:ASN:ND2	2.48	0.44
1:A:1009:GLN:CD	3:D:200:THR:OG1	2.61	0.43
1:B:983:LEU:CA	1:B:1069:LYS:HG3	2.48	0.43
1:A:1005:ILE:HG21	3:D:309:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:LEU:HD13	3:D:198:GLN:CG	2.45	0.42
1:A:1046:LEU:CD1	3:D:198:GLN:HG2	2.46	0.42
1:A:1070:GLY:HA3	3:F:224:HIS:HB3	2.01	0.42
1:B:1007:ASN:CB	3:F:186:ALA:O	2.67	0.42
3:F:239:LEU:HD11	3:F:289:LEU:HD22	2.01	0.42
1:A:1070:GLY:HA3	3:F:224:HIS:CB	2.49	0.42
1:B:884:PRO:HB2	1:B:885:MET:H	1.75	0.42
1:A:1046:LEU:CB	3:D:198:GLN:NE2	2.82	0.42
1:B:983:LEU:CA	1:B:984:VAL:N	2.80	0.42
3:D:239:LEU:HD11	3:D:289:LEU:HD22	2.01	0.42
1:A:1009:GLN:HE21	3:D:200:THR:N	2.18	0.41
1:A:1007:ASN:CB	3:D:186:ALA:O	2.69	0.41
2:E:161:LEU:HD11	3:F:297:GLU:HG3	2.03	0.41
1:A:884:PRO:HB2	1:A:885:MET:H	1.75	0.40
1:A:930:ILE:HD13	3:D:240:PRO:HB3	2.02	0.40
2:C:161:LEU:HD11	3:D:297:GLU:HG3	2.03	0.40

All (1) 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)
3:D:305:GLU:OE1	3:D:305:GLU:OE1[4_445]	1.91	0.29

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	200/264 (76%)	187 (94%)	10 (5%)	3 (2%)	8	40
1	B	200/264 (76%)	187 (94%)	10 (5%)	3 (2%)	8	40
2	C	11/122 (9%)	11 (100%)	0	0	100	100
2	E	11/122 (9%)	11 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	144/251 (57%)	134 (93%)	10 (7%)	0	100	100
3	F	144/251 (57%)	133 (92%)	11 (8%)	0	100	100
All	All	710/1274 (56%)	663 (93%)	41 (6%)	6 (1%)	16	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	912	LYS
1	A	913	HIS
1	B	912	LYS
1	B	913	HIS
1	B	966	GLY
1	A	966	GLY

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	178/232 (77%)	171 (96%)	7 (4%)	28	49
1	B	178/232 (77%)	171 (96%)	7 (4%)	28	49
2	C	13/103 (13%)	12 (92%)	1 (8%)	12	32
2	E	13/103 (13%)	12 (92%)	1 (8%)	12	32
3	D	128/215 (60%)	121 (94%)	7 (6%)	19	41
3	F	128/215 (60%)	121 (94%)	7 (6%)	19	41
All	All	638/1100 (58%)	608 (95%)	30 (5%)	23	45

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	910	LEU
1	A	913	HIS
1	A	915	LYS
1	A	917	THR

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Mol	Chain	Res	Type
1	A	927	LYS
1	A	1038	ILE
1	A	1041	VAL
1	B	910	LEU
1	B	913	HIS
1	B	915	LYS
1	B	917	THR
1	B	927	LYS
1	B	1038	ILE
1	B	1041	VAL
2	C	168	ASP
3	D	172	ARG
3	D	177	ASN
3	D	252	ASP
3	D	257	SER
3	D	260	ILE
3	D	261	VAL
3	D	269	VAL
2	E	168	ASP
3	F	172	ARG
3	F	177	ASN
3	F	252	ASP
3	F	257	SER
3	F	260	ILE
3	F	261	VAL
3	F	269	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	938	ASN
1	A	1009	GLN
1	B	908	ASN
1	B	954	ASN
1	B	1009	GLN
3	D	214	ASN
3	F	214	ASN
3	F	224	HIS
3	F	233	GLN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	983:LEU	C	984:VAL	N	1.94
1	A	983:LEU	C	984:VAL	N	0.91

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	202/264 (76%)	0.36	8 (3%)	42	41	132, 150, 189, 225	0
1	B	202/264 (76%)	0.30	7 (3%)	47	43	132, 177, 214, 238	0
2	C	15/122 (12%)	0.53	1 (6%)	24	29	140, 153, 176, 188	0
2	E	15/122 (12%)	0.51	1 (6%)	24	29	157, 164, 172, 174	0
3	D	148/251 (58%)	0.32	3 (2%)	65	56	134, 150, 174, 203	0
3	F	148/251 (58%)	0.46	7 (4%)	36	37	154, 167, 182, 209	0
All	All	730/1274 (57%)	0.36	27 (3%)	45	43	132, 164, 203, 238	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	138	PRO	3.8
1	A	919	SER	3.4
1	B	1061	PHE	3.3
1	A	1085	ALA	3.2
1	B	1025	TYR	3.1
1	A	1071	MET	3.0
3	F	225	GLY	3.0
1	A	998	GLU	3.0
3	F	195	LEU	2.9
3	D	314	ASN	2.9
2	C	141	TYR	2.8
1	B	1050	ILE	2.6
1	B	1043	GLY	2.6
3	D	301	MET	2.6
3	D	319	SER	2.6
3	F	271	MET	2.5
3	F	220	PHE	2.5
3	F	241	ALA	2.4
1	B	1023	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	884	PRO	2.3
1	A	959	PHE	2.2
3	F	222	ALA	2.1
3	F	314	ASN	2.1
1	A	962	MET	2.1
1	A	1055	LEU	2.0
1	A	955	THR	2.0
1	B	1044	ASN	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.