



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:10 PM GMT

PDB ID : 4BQ7  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

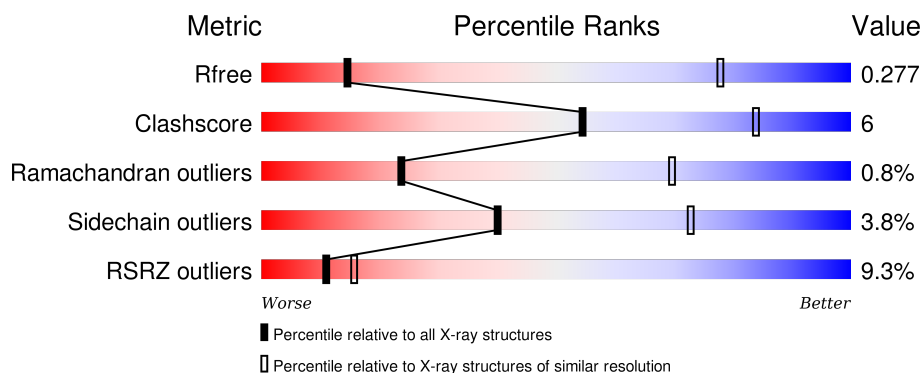
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1014 (9.50-3.66)
Clashscore	102246	1062 (9.50-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>11%</div> <div>23%</div> </div> </div>
1	B	264	<div> <div>7%</div> <div> <div></div> <div>67%</div> <div>8%</div> <div>23%</div> </div> </div>
2	C	122	<div> <div>2%</div> <div> <div></div> <div>10%</div> <div>88%</div> </div> </div>
2	E	122	<div> <div>5%</div> <div> <div></div> <div>10%</div> <div>88%</div> </div> </div>
3	D	251	<div> <div>3%</div> <div> <div></div> <div>50%</div> <div>8%</div> <div>41%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	251	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '7%', followed by a long green segment labeled '51%', a small yellow segment labeled '7%', and a long grey segment at the end labeled '41%'. The total length of the bar represents 100%.

## 2 Entry composition

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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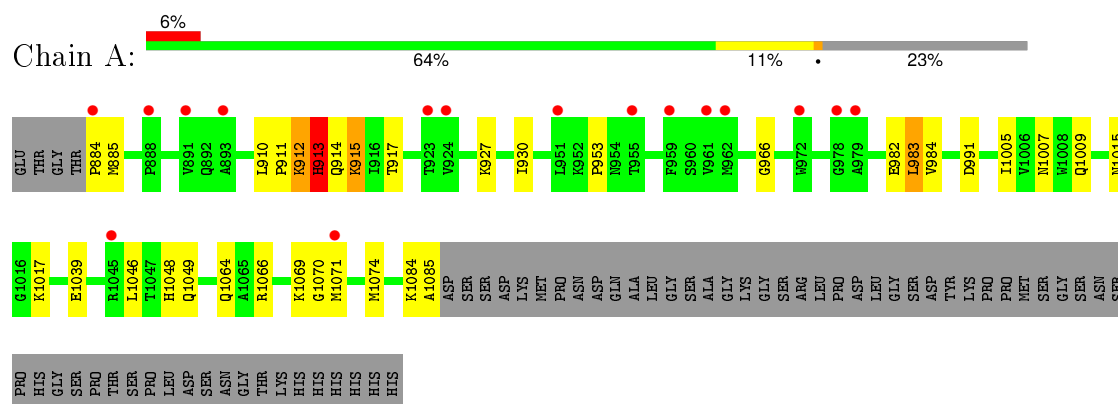
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Chain	Residue	Modelled	Actual	Comment	Reference
F	412	THR	-	EXPRESSION TAG	UNP Q6NW40
F	413	LYS	-	EXPRESSION TAG	UNP Q6NW40
F	414	HIS	-	EXPRESSION TAG	UNP Q6NW40
F	415	HIS	-	EXPRESSION TAG	UNP Q6NW40
F	416	HIS	-	EXPRESSION TAG	UNP Q6NW40
F	417	HIS	-	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

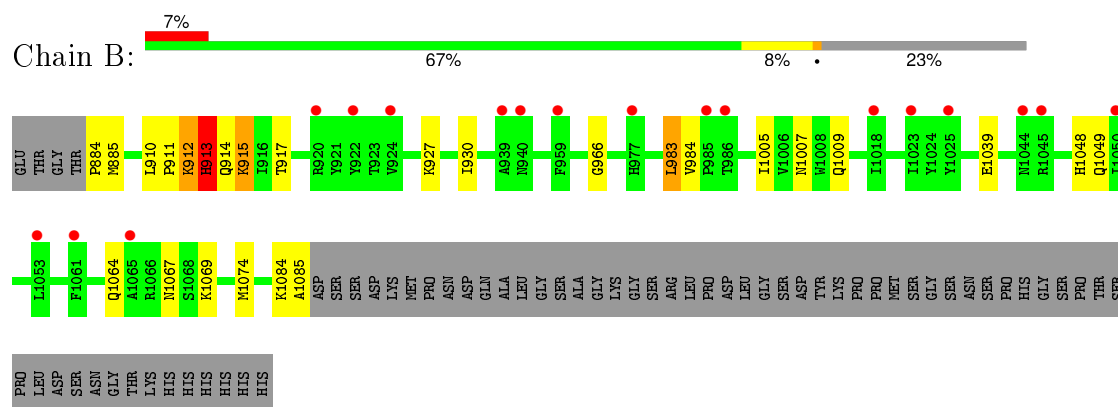
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

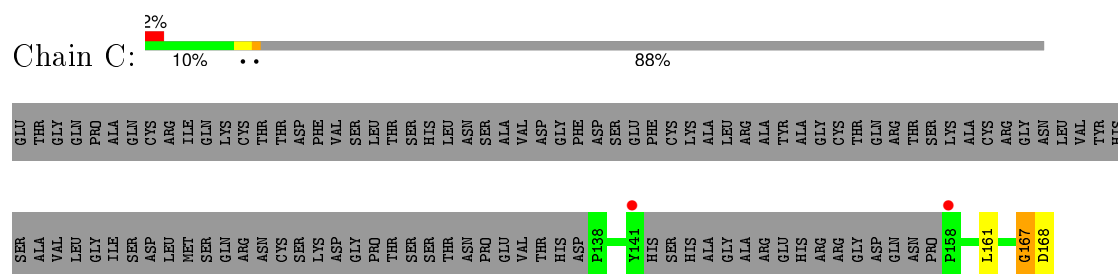
#### • Molecule 1: NEOGENIN



#### • Molecule 1: NEOGENIN



#### • Molecule 2: RGM DOMAIN FAMILY MEMBER B



#### • Molecule 2: RGM DOMAIN FAMILY MEMBER B



GLU	THR	ALA	GLY	PRO	GLN	ALA	CYS	ARG	ILE	GLN	LYS	THR	THR	ASP	THR	ASP	PHE	VAL	SER	LEU	THR	THR	SER	HIS	LEU	ASN	SER	VAL	ALA	THR	ASP	GLY	ASP	PHE	SER	GLU	HIS	GLY	LYS	ALA	LEU	ALA	ARG	TYR	ALA	GLY	CYS	THR	GLN	ARG	THR	SER	LYS	ALA	ARG	CYS	GLY	ASN	LEU	VAL	TYR	HIS
SER	ALA	VAL	LEU	GLY	ILE	SER	ASP	LEU	MET	SER	GLN	ARG	ASN	CYS	SER	ASP	LYS	GLY	PRO	THR	THR	SER	SER	THR	ASN	PRO	GLU	VAL	THR	HIS	ASP	P138	Y141	HIS	SER	GLY	HIS	ALA	GLY	ALA	ARG	GLU	HIS	ARG	ARG	GLY	THR	GLN	ASN	PRO	P158	L161	G164	L165	F166	G167	D168					

• Molecule 3: RGM DOMAIN FAMILY MEMBER B



P169	R172	M177	A186	S196	V197	Q198	V199	T200	I219	Q229	L239	P240	A241	T248	D252	S257	I258	R259	I260	V261	E262	ARG	GLU	SER	GLY	HIS	V268	V269	E270	P271	V275	I276	L289	E297	V301	E305	L309	R321	ILE	ASP	ASP	GLY					
GLN	GLY	GLN	VAL	SER	ALA	ILE	LEU	GLY	HIS	SER	GLN	ALA	TRP	PRO	THR	CYS	HIS	GLU	LYS	THR	GLN	GLN	HIS	GLU	LYS	THR	VAL	LYS	ASP	ILE	TYR	PHE	GLN	SER	CYS	VAL	PHE	ASP	LEU	LEU	THR	THR	GLY	ALA	ASN	PHE	THR

ALA	ALA	ALA	HIS	SER	ALA	ALA	LEU	GLU	ASP	VAL	GLU	VAL	ALA	ALA	LEU	HIS	PRO	ARG	SER	ARG	LYS	GLU	THR	TRP	ARG	HIS	ILE	PHE	PRO	SER	GLY	THR	LYS	HIS	HIS	HIS	HIS	HIS
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• Molecule 3: RGM DOMAIN FAMILY MEMBER B



P169	H170	L171	R172	M177	A186	N193	Y194	L195	S196	T200	A212	I219	F220	H223	G225	C226	T227	Y232	L239	P240	A241	A242	T248	D252	S257	I260	V261	E262	ARG	GLU	SER	GLY	HIS	V268	V269	E270	P271	H272	I276	L289	E297																	
R321	ILE	ASP	ASP	GLY	GLN	GLN	VAL	SER	ALA	ILE	LEU	GLY	HIS	SER	LEU	PRO	ARG	THR	SER	LEU	VAL	GLN	ALA	TRP	PRO	GLY	TYR	THR	LEU	GLU	THR	ALA	ASN	THR	GLN	CYS	HIS	GLU	LYS	MET	PRO	VAL	LYS	ASP	ILE	TYR	PHE	GLN	SER	CYS	VAL	PHE	ASP	LEU	LEU	THR	THR	GLY

ASP	ALA	ASN	PHE	THR	ALA	ALA	HIS	SER	LEU	LEU	GLU	ASP	VAL	GLU	ALA	HIS	PRO	ARG	ARG	LYS	GLU	TRP	HIS	ILE	PHE	PRO	SER	GLY	THR	LYS	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.69Å 109.69Å 187.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.78 – 6.60 94.99 – 6.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (84.78-6.60) 97.3 (94.99-6.60)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 6.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.254 , 0.280 0.248 , 0.277	Depositor DCC
$R_{free}$ test set	229 reflections (9.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	128.1	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 152.7	EDS
Estimated twinning fraction	0.077 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 2491 reflections	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	5714	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.68	1/1635 (0.1%)	0.80	4/2234 (0.2%)
1	B	0.82	1/1635 (0.1%)	0.71	1/2234 (0.0%)
2	C	0.46	0/122	1.01	1/162 (0.6%)
2	E	0.46	0/122	1.01	1/162 (0.6%)
3	D	0.51	0/1170	0.73	0/1590
3	F	0.51	0/1170	0.74	0/1590
All	All	0.65	2/5854 (0.0%)	0.76	7/7972 (0.1%)

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	26.18	1.94	1.34
1	A	983	LEU	C-N	-18.64	0.91	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	983	LEU	O-C-N	13.56	144.39	122.70
1	A	983	LEU	CA-C-N	-9.95	95.31	117.20
2	E	167	GLY	C-N-CA	8.68	143.40	121.70
2	C	167	GLY	C-N-CA	8.63	143.28	121.70
1	A	983	LEU	C-N-CA	-6.70	104.95	121.70
1	A	912	LYS	C-N-CA	5.49	135.43	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	912	LYS	C-N-CA	5.49	135.42	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	167	GLY	Peptide
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	46	0
1	B	1591	0	1585	16	0
2	C	118	0	101	1	0
2	E	118	0	101	1	0
3	D	1148	0	1122	33	1
3	F	1148	0	1122	14	0
All	All	5714	0	5616	72	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 (72) 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	1.21
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:GLN:NE2	3:D:199:VAL:C	2.41	0.73
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
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:1009:GLN:HE22	3:D:199:VAL:C	2.02	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: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:1046:LEU:HB2	3:D:198:GLN:CD	2.24	0.58
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:991:ASP:CG	3:D:200:THR:HG21	2.26	0.54
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:A:982:GLU:C	1:A:1069:LYS:HG3	2.32	0.50
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
3:D:248:THR:HA	3:D:260:ILE:HD12	1.96	0.48
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: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:B:983:LEU:O	1:B:1067:ASN:ND2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:ILE:HG12	1:A:1049:GLN:HG2	1.98	0.44
1:A:911:PRO:HB2	1:A:915:LYS:HZ3	1.82	0.43
1:B:911:PRO:HB2	1:B:915:LYS:HZ3	1.83	0.43
1:B:983:LEU:CA	1:B:1069:LYS:HG3	2.48	0.43
1:A:1046:LEU:CB	3:D:198:GLN:CD	2.87	0.43
1:A:1005:ILE:HG21	3:D:309:LEU:HD22	2.01	0.43
1:A:983:LEU:O	1:A:984:VAL:C	2.48	0.43
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:B:983:LEU:CA	1:B:984:VAL:N	2.80	0.42
1:A:1046:LEU:CB	3:D:198:GLN:NE2	2.82	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%)	13	57
1	B	200/264 (76%)	187 (94%)	10 (5%)	3 (2%)	13	57
2	C	11/122 (9%)	11 (100%)	0	0	100	100
2	E	11/122 (9%)	11 (100%)	0	0	100	100
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%)	24	69

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%)	173 (97%)	5 (3%)	51	78
1	B	178/232 (77%)	173 (97%)	5 (3%)	51	78
2	C	13/103 (13%)	12 (92%)	1 (8%)	16	52
2	E	13/103 (13%)	12 (92%)	1 (8%)	16	52
3	D	128/215 (60%)	122 (95%)	6 (5%)	32	68
3	F	128/215 (60%)	122 (95%)	6 (5%)	32	68
All	All	638/1100 (58%)	614 (96%)	24 (4%)	40	73

All (24) 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
1	A	927	LYS
1	B	910	LEU
1	B	913	HIS
1	B	915	LYS
1	B	917	THR
1	B	927	LYS
2	C	168	ASP
3	D	172	ARG
3	D	177	ASN
3	D	252	ASP
3	D	257	SER
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	261	VAL
3	F	269	VAL

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

Mol	Chain	Res	Type
1	A	1009	GLN
3	D	229	GLN
3	F	224	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 [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	202/264 (76%)	0.68	16 (7%)	15 19	132, 150, 189, 225	0
1	B	202/264 (76%)	0.73	18 (8%)	12 16	132, 177, 214, 238	0
2	C	15/122 (12%)	1.07	2 (13%)	4 10	140, 153, 176, 188	0
2	E	15/122 (12%)	1.70	6 (40%)	0 4	157, 164, 172, 174	0
3	D	148/251 (58%)	0.79	8 (5%)	29 30	134, 150, 174, 203	0
3	F	148/251 (58%)	0.89	18 (12%)	5 11	154, 167, 182, 209	0
All	All	730/1274 (57%)	0.79	68 (9%)	11 16	132, 164, 203, 238	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1044	ASN	4.9
2	E	168	ASP	4.7
3	F	241	ALA	4.1
2	E	158	PRO	3.9
1	A	891	VAL	3.9
1	A	1071	MET	3.7
2	C	158	PRO	3.7
1	A	893	ALA	3.6
3	D	301	MET	3.5
3	F	271	MET	3.3
3	D	271	MET	3.2
3	D	241	ALA	2.9
1	A	978	GLY	2.8
1	B	1061	PHE	2.8
3	F	262	GLU	2.8
1	A	884	PRO	2.8
1	A	979	ALA	2.8
3	F	226	CYS	2.8
1	A	888	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	962	MET	2.8
3	F	169	PRO	2.8
3	F	225	GLY	2.7
1	B	924	VAL	2.7
1	B	922	TYR	2.7
1	A	961	VAL	2.7
3	F	272	HIS	2.6
1	B	920	ARG	2.6
3	F	276	ILE	2.6
1	B	1065	ALA	2.6
2	E	165	LEU	2.6
1	B	959	PHE	2.6
3	F	220	PHE	2.5
3	F	194	TYR	2.5
1	B	939	ALA	2.5
2	C	141	TYR	2.5
1	B	977	HIS	2.4
3	D	268	TYR	2.4
3	F	171	LEU	2.4
1	B	1025	TYR	2.4
1	A	951	LEU	2.4
3	F	232	TYR	2.4
1	A	959	PHE	2.4
3	D	276	ILE	2.4
2	E	141	TYR	2.4
1	B	1023	ILE	2.4
1	B	1050	ILE	2.4
3	D	309	LEU	2.3
1	A	924	VAL	2.3
3	F	240	PRO	2.3
1	B	1045	ARG	2.3
1	B	1053	LEU	2.3
1	B	940	ASN	2.3
2	E	164	GLY	2.3
2	E	167	GLY	2.3
3	F	170	HIS	2.3
1	A	955	THR	2.2
1	A	923	THR	2.2
1	B	1018	ILE	2.2
3	F	193	ASN	2.2
1	A	1045	ARG	2.1
3	D	275	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	257	SER	2.1
1	B	986	THR	2.1
1	B	985	PRO	2.1
3	D	258	LEU	2.0
1	A	972	TRP	2.0
3	F	212	ALA	2.0
3	F	227	THR	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 carbohydrates 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.