



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:39 PM GMT

PDB ID : 4M8N
Title : Crystal Structure of PlexinC1/Rap1B Complex
Authors : Pascoe, H.G.; Wang, Y.; Brautigam, C.A.; He, H.; Zhang, X.
Deposited on : 2013-08-13
Resolution : 3.29 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

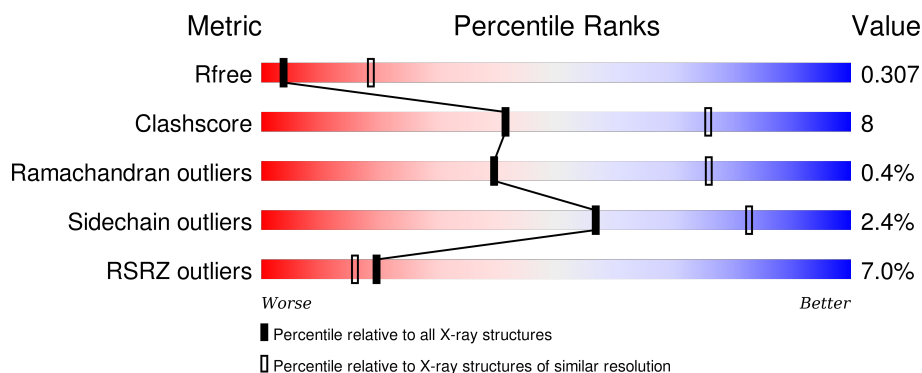
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 ≥ 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	599	<div> <div>4%</div> <div>78% 17% •</div> </div>
1	B	599	<div> <div>5%</div> <div>71% 22% • 5%</div> </div>
1	C	599	<div> <div>4%</div> <div>74% 18% • 7%</div> </div>
1	D	599	<div> <div>7%</div> <div>72% 20% • 7%</div> </div>
2	E	199	<div> <div>6%</div> <div>70% 14% • 16%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	199	
2	G	199	
2	H	199	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	AF3	E	202	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22228 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 PlexinC1 Intracellular Region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	574	Total	C	N	O	S	0	0	0
			4356	2818	717	801	20			
1	B	571	Total	C	N	O	S	0	0	0
			4262	2756	702	784	20			
1	C	560	Total	C	N	O	S	0	0	0
			4218	2719	699	780	20			
1	D	560	Total	C	N	O	S	0	0	0
			4230	2738	695	777	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	549	GLY	-	EXPRESSION TAG	UNP Q5RGW1
A	550	GLY	-	EXPRESSION TAG	UNP Q5RGW1
A	551	SER	-	EXPRESSION TAG	UNP Q5RGW1
B	549	GLY	-	EXPRESSION TAG	UNP Q5RGW1
B	550	GLY	-	EXPRESSION TAG	UNP Q5RGW1
B	551	SER	-	EXPRESSION TAG	UNP Q5RGW1
C	549	GLY	-	EXPRESSION TAG	UNP Q5RGW1
C	550	GLY	-	EXPRESSION TAG	UNP Q5RGW1
C	551	SER	-	EXPRESSION TAG	UNP Q5RGW1
D	549	GLY	-	EXPRESSION TAG	UNP Q5RGW1
D	550	GLY	-	EXPRESSION TAG	UNP Q5RGW1
D	551	SER	-	EXPRESSION TAG	UNP Q5RGW1

- Molecule 2 is a protein called Ras-related protein Rap-1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	168	Total	C	N	O	S	0	0	0
			1277	805	215	250	7			
2	F	166	Total	C	N	O	S	0	0	0
			1262	797	213	245	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	168	Total	C	N	O	S	0	0	0
			1258	793	211	247	7			
2	H	167	Total	C	N	O	S	0	0	0
			1223	779	206	232	6			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	EXPRESSION TAG	UNP P61224
E	-1	PRO	-	EXPRESSION TAG	UNP P61224
E	0	HIS	-	EXPRESSION TAG	UNP P61224
E	167	SER	-	EXPRESSION TAG	UNP P61224
E	168	GLY	-	EXPRESSION TAG	UNP P61224
E	169	GLY	-	EXPRESSION TAG	UNP P61224
E	170	SER	-	EXPRESSION TAG	UNP P61224
E	171	GLY	-	EXPRESSION TAG	UNP P61224
E	172	SER	-	EXPRESSION TAG	UNP P61224
E	173	GLY	-	EXPRESSION TAG	UNP P61224
E	174	SER	-	EXPRESSION TAG	UNP P61224
E	175	SER	-	EXPRESSION TAG	UNP P61224
E	176	GLY	-	EXPRESSION TAG	UNP P61224
E	177	GLY	-	EXPRESSION TAG	UNP P61224
E	178	SER	-	EXPRESSION TAG	UNP P61224
E	179	GLY	-	EXPRESSION TAG	UNP P61224
E	180	SER	-	EXPRESSION TAG	UNP P61224
E	181	GLY	-	EXPRESSION TAG	UNP P61224
E	182	GLY	-	EXPRESSION TAG	UNP P61224
E	183	GLY	-	EXPRESSION TAG	UNP P61224
E	184	SER	-	EXPRESSION TAG	UNP P61224
E	185	GLY	-	EXPRESSION TAG	UNP P61224
E	186	SER	-	EXPRESSION TAG	UNP P61224
E	187	GLY	-	EXPRESSION TAG	UNP P61224
E	188	SER	-	EXPRESSION TAG	UNP P61224
E	189	SER	-	EXPRESSION TAG	UNP P61224
E	190	GLY	-	EXPRESSION TAG	UNP P61224
E	191	LEU	-	EXPRESSION TAG	UNP P61224
E	192	PRO	-	EXPRESSION TAG	UNP P61224
E	193	GLU	-	EXPRESSION TAG	UNP P61224
E	194	THR	-	EXPRESSION TAG	UNP P61224
E	195	GLY	-	EXPRESSION TAG	UNP P61224
E	196	GLY	-	EXPRESSION TAG	UNP P61224
F	-2	GLY	-	EXPRESSION TAG	UNP P61224

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	PRO	-	EXPRESSION TAG	UNP P61224
F	0	HIS	-	EXPRESSION TAG	UNP P61224
F	167	SER	-	EXPRESSION TAG	UNP P61224
F	168	GLY	-	EXPRESSION TAG	UNP P61224
F	169	GLY	-	EXPRESSION TAG	UNP P61224
F	170	SER	-	EXPRESSION TAG	UNP P61224
F	171	GLY	-	EXPRESSION TAG	UNP P61224
F	172	SER	-	EXPRESSION TAG	UNP P61224
F	173	GLY	-	EXPRESSION TAG	UNP P61224
F	174	SER	-	EXPRESSION TAG	UNP P61224
F	175	SER	-	EXPRESSION TAG	UNP P61224
F	176	GLY	-	EXPRESSION TAG	UNP P61224
F	177	GLY	-	EXPRESSION TAG	UNP P61224
F	178	SER	-	EXPRESSION TAG	UNP P61224
F	179	GLY	-	EXPRESSION TAG	UNP P61224
F	180	SER	-	EXPRESSION TAG	UNP P61224
F	181	GLY	-	EXPRESSION TAG	UNP P61224
F	182	GLY	-	EXPRESSION TAG	UNP P61224
F	183	GLY	-	EXPRESSION TAG	UNP P61224
F	184	SER	-	EXPRESSION TAG	UNP P61224
F	185	GLY	-	EXPRESSION TAG	UNP P61224
F	186	SER	-	EXPRESSION TAG	UNP P61224
F	187	GLY	-	EXPRESSION TAG	UNP P61224
F	188	SER	-	EXPRESSION TAG	UNP P61224
F	189	SER	-	EXPRESSION TAG	UNP P61224
F	190	GLY	-	EXPRESSION TAG	UNP P61224
F	191	LEU	-	EXPRESSION TAG	UNP P61224
F	192	PRO	-	EXPRESSION TAG	UNP P61224
F	193	GLU	-	EXPRESSION TAG	UNP P61224
F	194	THR	-	EXPRESSION TAG	UNP P61224
F	195	GLY	-	EXPRESSION TAG	UNP P61224
F	196	GLY	-	EXPRESSION TAG	UNP P61224
G	-2	GLY	-	EXPRESSION TAG	UNP P61224
G	-1	PRO	-	EXPRESSION TAG	UNP P61224
G	0	HIS	-	EXPRESSION TAG	UNP P61224
G	167	SER	-	EXPRESSION TAG	UNP P61224
G	168	GLY	-	EXPRESSION TAG	UNP P61224
G	169	GLY	-	EXPRESSION TAG	UNP P61224
G	170	SER	-	EXPRESSION TAG	UNP P61224
G	171	GLY	-	EXPRESSION TAG	UNP P61224
G	172	SER	-	EXPRESSION TAG	UNP P61224
G	173	GLY	-	EXPRESSION TAG	UNP P61224

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Chain	Residue	Modelled	Actual	Comment	Reference
G	174	SER	-	EXPRESSION TAG	UNP P61224
G	175	SER	-	EXPRESSION TAG	UNP P61224
G	176	GLY	-	EXPRESSION TAG	UNP P61224
G	177	GLY	-	EXPRESSION TAG	UNP P61224
G	178	SER	-	EXPRESSION TAG	UNP P61224
G	179	GLY	-	EXPRESSION TAG	UNP P61224
G	180	SER	-	EXPRESSION TAG	UNP P61224
G	181	GLY	-	EXPRESSION TAG	UNP P61224
G	182	GLY	-	EXPRESSION TAG	UNP P61224
G	183	GLY	-	EXPRESSION TAG	UNP P61224
G	184	SER	-	EXPRESSION TAG	UNP P61224
G	185	GLY	-	EXPRESSION TAG	UNP P61224
G	186	SER	-	EXPRESSION TAG	UNP P61224
G	187	GLY	-	EXPRESSION TAG	UNP P61224
G	188	SER	-	EXPRESSION TAG	UNP P61224
G	189	SER	-	EXPRESSION TAG	UNP P61224
G	190	GLY	-	EXPRESSION TAG	UNP P61224
G	191	LEU	-	EXPRESSION TAG	UNP P61224
G	192	PRO	-	EXPRESSION TAG	UNP P61224
G	193	GLU	-	EXPRESSION TAG	UNP P61224
G	194	THR	-	EXPRESSION TAG	UNP P61224
G	195	GLY	-	EXPRESSION TAG	UNP P61224
G	196	GLY	-	EXPRESSION TAG	UNP P61224
H	-2	GLY	-	EXPRESSION TAG	UNP P61224
H	-1	PRO	-	EXPRESSION TAG	UNP P61224
H	0	HIS	-	EXPRESSION TAG	UNP P61224
H	167	SER	-	EXPRESSION TAG	UNP P61224
H	168	GLY	-	EXPRESSION TAG	UNP P61224
H	169	GLY	-	EXPRESSION TAG	UNP P61224
H	170	SER	-	EXPRESSION TAG	UNP P61224
H	171	GLY	-	EXPRESSION TAG	UNP P61224
H	172	SER	-	EXPRESSION TAG	UNP P61224
H	173	GLY	-	EXPRESSION TAG	UNP P61224
H	174	SER	-	EXPRESSION TAG	UNP P61224
H	175	SER	-	EXPRESSION TAG	UNP P61224
H	176	GLY	-	EXPRESSION TAG	UNP P61224
H	177	GLY	-	EXPRESSION TAG	UNP P61224
H	178	SER	-	EXPRESSION TAG	UNP P61224
H	179	GLY	-	EXPRESSION TAG	UNP P61224
H	180	SER	-	EXPRESSION TAG	UNP P61224
H	181	GLY	-	EXPRESSION TAG	UNP P61224
H	182	GLY	-	EXPRESSION TAG	UNP P61224

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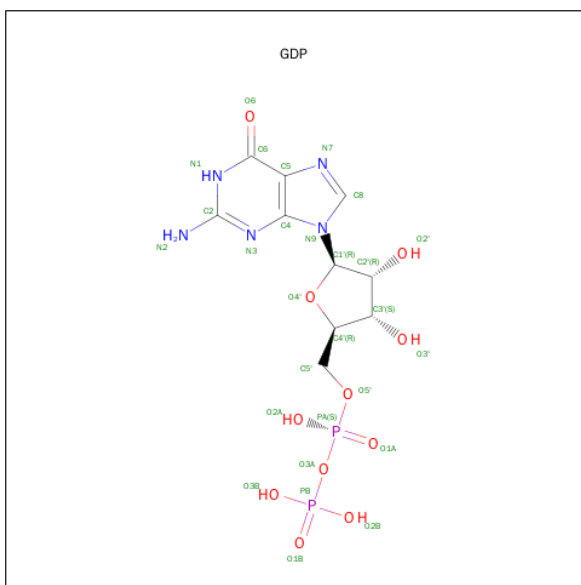
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Chain	Residue	Modelled	Actual	Comment	Reference
H	183	GLY	-	EXPRESSION TAG	UNP P61224
H	184	SER	-	EXPRESSION TAG	UNP P61224
H	185	GLY	-	EXPRESSION TAG	UNP P61224
H	186	SER	-	EXPRESSION TAG	UNP P61224
H	187	GLY	-	EXPRESSION TAG	UNP P61224
H	188	SER	-	EXPRESSION TAG	UNP P61224
H	189	SER	-	EXPRESSION TAG	UNP P61224
H	190	GLY	-	EXPRESSION TAG	UNP P61224
H	191	LEU	-	EXPRESSION TAG	UNP P61224
H	192	PRO	-	EXPRESSION TAG	UNP P61224
H	193	GLU	-	EXPRESSION TAG	UNP P61224
H	194	THR	-	EXPRESSION TAG	UNP P61224
H	195	GLY	-	EXPRESSION TAG	UNP P61224
H	196	GLY	-	EXPRESSION TAG	UNP P61224

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

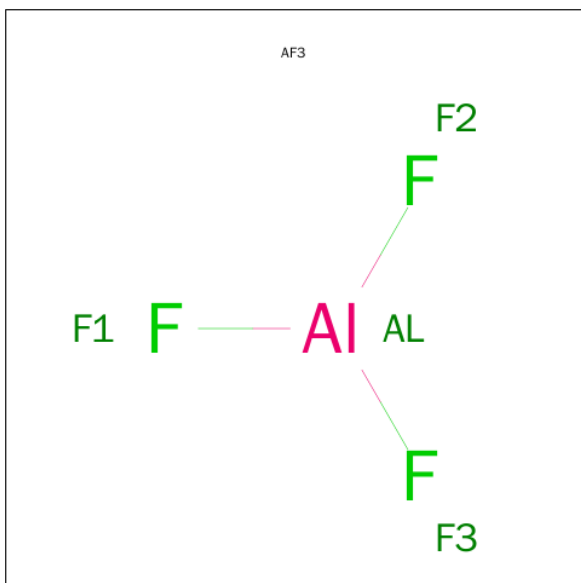
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	F	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	G	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	H	1	Total 28	C 10	N 5	O 11	P 2	0	0

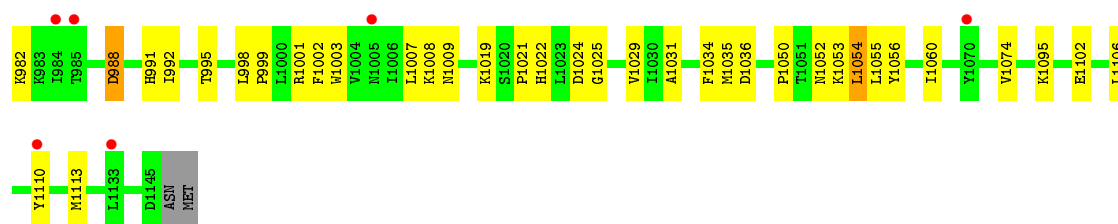
- Molecule 5 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



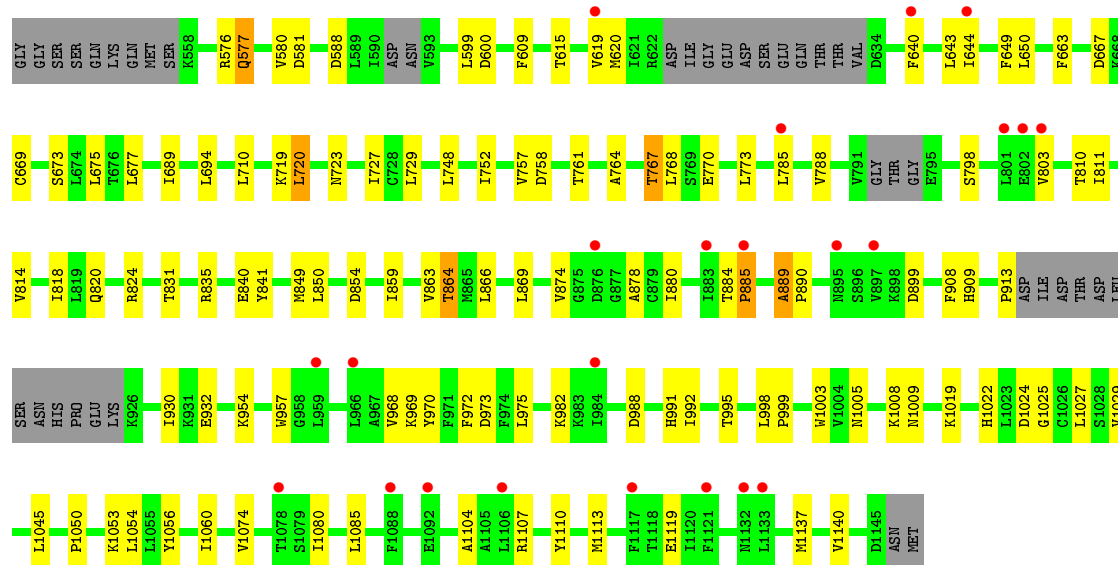
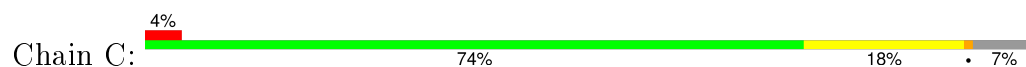
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total 4	Al 1	F 3	0	0
5	F	1	Total 4	Al 1	F 3	0	0
5	G	1	Total 4	Al 1	F 3	0	0
5	H	1	Total 4	Al 1	F 3	0	0

- Molecule 6 is water.

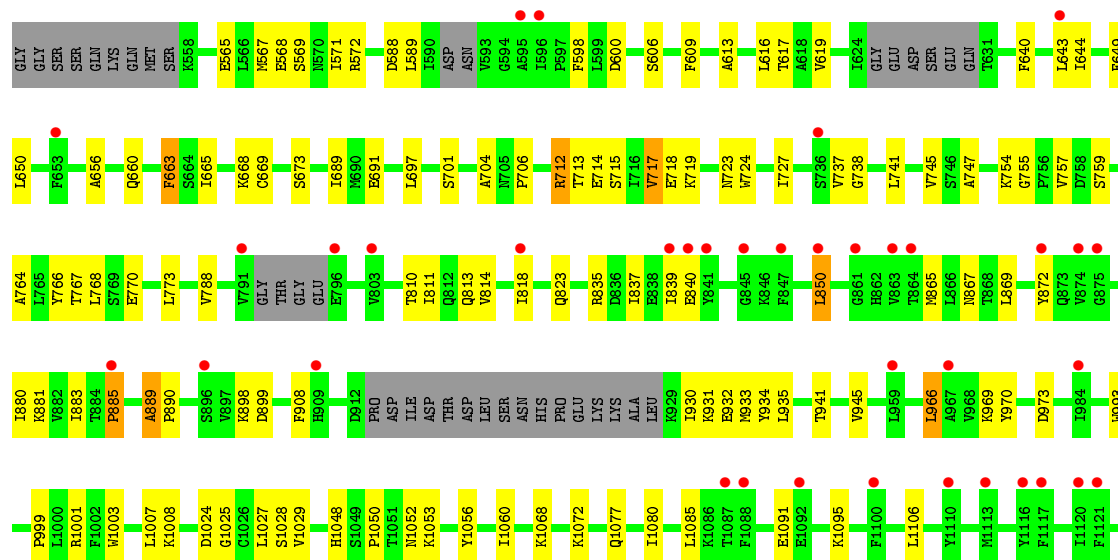
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total 4	O 4	0	0
6	B	1	Total 1	O 1	0	0
6	C	3	Total 3	O 3	0	0
6	D	1	Total 1	O 1	0	0
6	H	1	Total 1	O 1	0	0

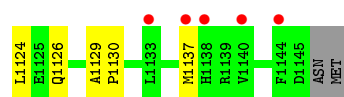


• Molecule 1: PlexinC1 Intracellular Region

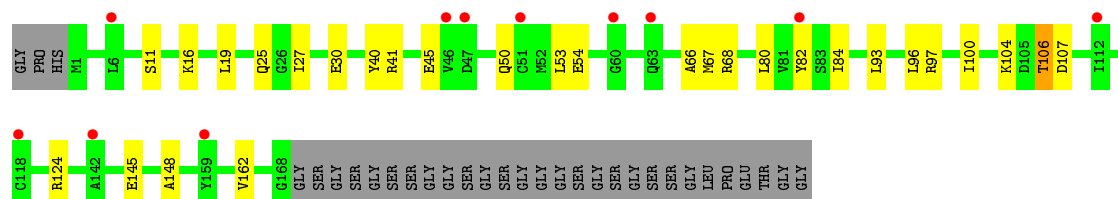


• Molecule 1: PlexinC1 Intracellular Region

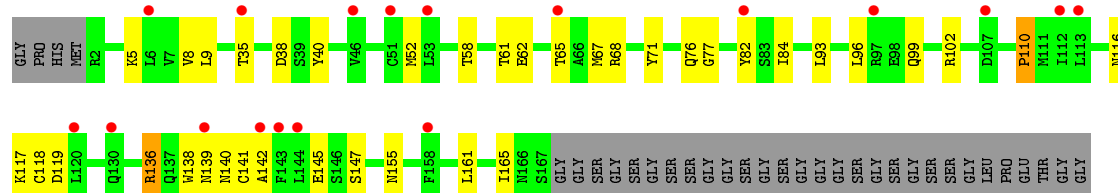




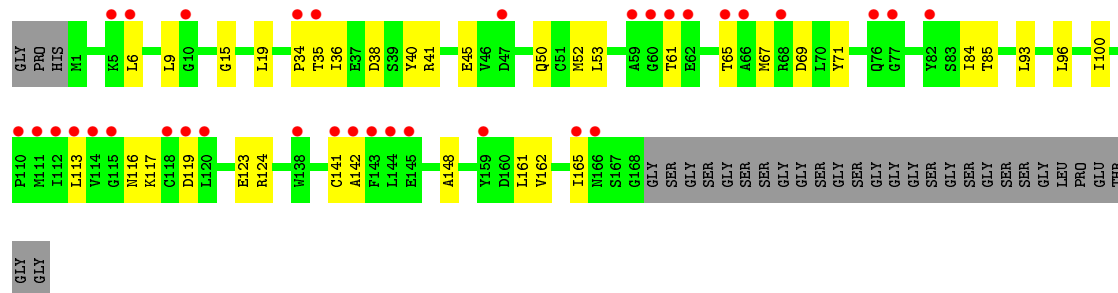
• Molecule 2: Ras-related protein Rap-1b



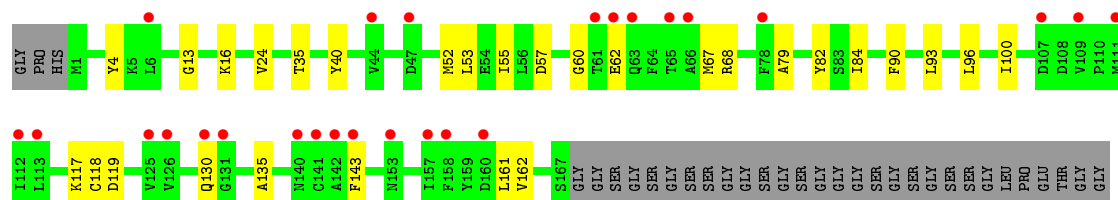
• Molecule 2: Ras-related protein Rap-1b



• Molecule 2: Ras-related protein Rap-1b



• Molecule 2: Ras-related protein Rap-1b



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.28Å 84.73Å 138.75Å 91.09° 95.15° 90.32°	Depositor
Resolution (Å)	41.05 – 3.29 42.36 – 3.29	Depositor EDS
% Data completeness (in resolution range)	90.2 (41.05-3.29) 89.9 (42.36-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.243 , 0.299 0.252 , 0.307	Depositor DCC
R_{free} test set	1804 reflections (3.97%)	DCC
Wilson B-factor (Å ²)	111.8	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 91.4	EDS
Estimated twinning fraction	0.033 for -h,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 47241 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22228	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.70% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, AF3

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	0.28	0/4437	0.45	4/6023 (0.1%)
1	B	0.28	0/4341	0.45	3/5905 (0.1%)
1	C	0.26	0/4298	0.43	3/5845 (0.1%)
1	D	0.26	0/4312	0.41	2/5861 (0.0%)
2	E	0.25	0/1293	0.40	0/1750
2	F	0.25	0/1278	0.41	0/1730
2	G	0.24	0/1274	0.39	0/1729
2	H	0.25	0/1239	0.41	0/1682
All	All	0.26	0/22472	0.43	12/30525 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	890	PRO	N-CA-CB	6.15	110.68	103.30
1	C	890	PRO	N-CA-CB	6.08	110.59	103.30
1	B	890	PRO	N-CA-CB	6.04	110.55	103.30
1	C	913	PRO	N-CA-CB	5.98	110.48	103.30
1	B	923	PRO	N-CA-CB	5.98	110.47	103.30
1	A	913	PRO	N-CA-CB	5.94	110.43	103.30
1	A	923	PRO	N-CA-CB	5.93	110.42	103.30
1	A	890	PRO	N-CA-CB	5.92	110.41	103.30
1	A	885	PRO	N-CA-CB	5.90	110.38	103.30
1	B	885	PRO	N-CA-CB	5.88	110.35	103.30
1	C	885	PRO	N-CA-CB	5.81	110.27	103.30
1	D	885	PRO	N-CA-CB	5.74	110.19	103.30

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	4356	0	4143	58	0
1	B	4262	0	3980	95	0
1	C	4218	0	3952	71	0
1	D	4230	0	3971	79	0
2	E	1277	0	1229	16	0
2	F	1262	0	1212	27	0
2	G	1258	0	1188	22	0
2	H	1223	0	1153	22	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	E	28	0	12	0	0
4	F	28	0	12	3	0
4	G	28	0	12	2	0
4	H	28	0	12	5	0
5	E	4	0	0	1	0
5	F	4	0	0	1	0
5	G	4	0	0	0	0
5	H	4	0	0	0	0
6	A	4	0	0	0	0
6	B	1	0	0	0	0
6	C	3	0	0	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
All	All	22228	0	20876	365	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 8.

All (365) 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:C:577:GLN:NE2	1:C:581:ASP:OD2	2.21	0.74
1:C:811:ILE:HD12	1:C:850:LEU:HD13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:ARG:NH1	1:A:899:ASP:OD2	2.22	0.72
1:B:811:ILE:HD12	1:B:850:LEU:HD13	1.70	0.72
2:H:60:GLY:O	2:H:68:ARG:NH1	2.22	0.71
2:G:45:GLU:HA	2:G:50:GLN:HA	1.73	0.71
1:C:859:ILE:HG12	1:C:864:THR:HG23	1.72	0.71
1:A:691:GLU:OE2	1:A:970:TYR:OH	2.06	0.70
1:A:932:GLU:HA	1:A:935:LEU:HG	1.74	0.69
1:D:835:ARG:NH2	1:D:899:ASP:OD2	2.24	0.69
1:B:1110:TYR:HA	1:B:1113:MET:HB3	1.76	0.68
1:B:695:GLN:HG3	1:B:978:GLN:HE22	1.59	0.68
1:D:1091:GLU:HG2	1:D:1095:LYS:HD3	1.76	0.67
1:D:1008:LYS:NZ	1:D:1024:ASP:OD1	2.28	0.66
1:B:1095:LYS:HE3	1:D:1130:PRO:HG3	1.78	0.66
1:A:760:VAL:HG21	1:A:908:PHE:HA	1.75	0.66
1:B:576:ARG:NH2	1:C:770:GLU:OE2	2.28	0.66
1:A:811:ILE:HD12	1:A:850:LEU:HD13	1.78	0.66
1:B:841:TYR:HB2	1:B:850:LEU:HD23	1.78	0.65
2:H:82:TYR:HB3	2:H:93:LEU:HD11	1.79	0.65
1:D:932:GLU:HA	1:D:935:LEU:HD13	1.78	0.65
2:F:82:TYR:HB3	2:F:93:LEU:HD11	1.78	0.65
1:D:1050:PRO:HG2	1:D:1053:LYS:HB2	1.77	0.64
1:D:706:PRO:O	1:D:993:TRP:NE1	2.28	0.64
1:D:718:GLU:OE1	1:D:1001:ARG:NH1	2.31	0.64
1:A:803:VAL:HG11	1:A:818:ILE:HG22	1.80	0.64
1:C:885:PRO:HA	1:C:889:ALA:HB3	1.80	0.64
1:A:969:LYS:NZ	1:A:1074:VAL:O	2.24	0.64
1:B:809:ASP:OD2	1:B:817:LYS:NZ	2.22	0.64
1:D:650:LEU:HD23	1:D:689:ILE:HG12	1.79	0.64
1:B:570:ASN:OD1	1:B:573:ARG:NH2	2.30	0.63
2:E:106:THR:OG1	2:E:107:ASP:N	2.27	0.63
1:D:669:CYS:HA	1:D:719:LYS:HG2	1.80	0.63
1:A:811:ILE:HG22	1:A:815:LYS:HE3	1.81	0.63
1:B:885:PRO:HA	1:B:889:ALA:HB3	1.79	0.63
2:E:25:GLN:HB2	2:E:27:ILE:HG22	1.81	0.63
2:H:40:TYR:HB2	2:H:55:ILE:HB	1.79	0.63
1:C:640:PHE:HD1	1:C:1140:VAL:HG11	1.64	0.62
1:B:999:PRO:HA	1:B:1003:TRP:HB2	1.81	0.62
2:F:9:LEU:HB3	2:F:96:LEU:HD23	1.81	0.62
2:F:77:GLY:HA2	2:F:110:PRO:HB2	1.82	0.61
1:C:767:THR:OG1	1:C:768:LEU:N	2.33	0.61
1:A:966:LEU:HD12	1:A:1080:ILE:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:LEU:HD23	1:B:689:ILE:HG12	1.81	0.61
1:D:840:GLU:HB2	1:D:881:LYS:HB2	1.81	0.61
1:A:1056:TYR:O	1:A:1060:ILE:HG12	2.01	0.60
1:C:999:PRO:HA	1:C:1003:TRP:HB2	1.83	0.60
2:G:141:CYS:SG	2:G:142:ALA:N	2.75	0.60
1:B:606:SER:HB2	1:B:617:THR:HB	1.83	0.60
1:D:606:SER:HB2	1:D:617:THR:HB	1.83	0.60
1:D:1001:ARG:NH2	2:H:62:GLU:O	2.33	0.60
1:B:1054:LEU:HD21	1:C:580:VAL:HG22	1.84	0.60
1:B:640:PHE:HD2	1:B:1106:LEU:HD22	1.67	0.60
2:E:82:TYR:HB3	2:E:93:LEU:HD11	1.83	0.59
2:G:93:LEU:HD13	2:G:113:LEU:HD11	1.85	0.59
2:G:85:THR:HG23	2:G:123:GLU:HB3	1.84	0.59
1:D:770:GLU:HG2	1:D:931:LYS:HE2	1.84	0.58
1:D:613:ALA:HB1	1:D:616:LEU:HB2	1.85	0.58
1:D:588:ASP:OD1	1:D:754:LYS:NZ	2.30	0.58
1:B:810:THR:HG23	1:B:909:HIS:CE1	2.39	0.58
1:D:598:PHE:HE1	1:D:738:GLY:HA3	1.69	0.58
1:C:863:VAL:HG12	1:C:908:PHE:HD1	1.69	0.58
1:D:811:ILE:HD12	1:D:850:LEU:HD13	1.85	0.58
1:B:748:LEU:O	1:B:752:ILE:HG13	2.03	0.58
1:B:734:ARG:HH21	1:D:1126:GLN:HA	1.69	0.58
1:C:600:ASP:OD1	1:C:600:ASP:N	2.37	0.57
1:B:807:THR:HB	1:B:870:LYS:HG3	1.85	0.57
2:F:61:THR:O	2:F:68:ARG:NH2	2.37	0.57
1:A:590:ILE:HG23	1:A:593:VAL:HG23	1.87	0.57
1:D:759:SER:O	1:D:898:LYS:NZ	2.37	0.57
1:B:576:ARG:HB2	1:C:932:GLU:HG2	1.86	0.57
1:B:1036:ASP:OD2	1:B:1053:LYS:NZ	2.37	0.57
2:G:84:ILE:HD12	2:G:124:ARG:HE	1.68	0.56
1:D:1056:TYR:O	1:D:1060:ILE:HG12	2.05	0.56
1:A:576:ARG:HB2	1:D:932:GLU:HG2	1.86	0.56
1:C:988:ASP:O	1:C:992:ILE:HG12	2.06	0.56
1:B:707:LYS:HA	1:B:992:ILE:HG21	1.87	0.56
1:A:990:LEU:HD22	1:A:994:LYS:HE3	1.87	0.56
2:F:84:ILE:HD11	2:F:118:CYS:HA	1.88	0.56
1:C:1008:LYS:NZ	1:C:1024:ASP:OD1	2.39	0.56
1:B:644:ILE:O	1:B:685:TYR:OH	2.22	0.55
1:B:703:ASN:HD22	1:B:712:ARG:NH1	2.04	0.55
1:A:737:VAL:HG21	1:A:1003:TRP:HH2	1.70	0.55
1:C:1019:LYS:HE3	1:C:1024:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:966:LEU:HD23	1:D:1080:ILE:HD13	1.89	0.55
1:A:1129:ALA:HB3	1:A:1134:LYS:HE3	1.88	0.55
1:A:851:GLN:HE21	1:A:854:ASP:HB3	1.71	0.55
2:E:45:GLU:HA	2:E:50:GLN:HA	1.89	0.55
2:G:53:LEU:HD11	2:G:162:VAL:HG21	1.89	0.54
1:C:972:PHE:HD2	1:C:1074:VAL:HG11	1.72	0.54
2:H:117:LYS:HG2	4:H:201:GDP:C5	2.43	0.54
2:E:41:ARG:NH1	2:E:54:GLU:OE2	2.39	0.54
1:C:748:LEU:O	1:C:752:ILE:HG13	2.08	0.54
1:D:867:ASN:ND2	1:D:872:TYR:OH	2.40	0.54
2:E:11:SER:O	2:E:16:LYS:NZ	2.41	0.54
2:H:53:LEU:HD23	2:H:55:ILE:HD11	1.89	0.54
1:D:713:THR:HG21	2:H:62:GLU:HB3	1.90	0.53
2:F:35:THR:HB	5:F:202:AF3:F2	1.97	0.53
2:F:99:GLN:HG3	2:F:102:ARG:HH21	1.73	0.53
1:C:969:LYS:NZ	1:C:1074:VAL:O	2.27	0.53
1:B:605:ALA:HB1	1:B:609:PHE:CE2	2.43	0.53
2:E:19:LEU:HD23	2:E:148:ALA:HB2	1.90	0.53
2:F:118:CYS:HB3	2:F:145:GLU:HG2	1.91	0.53
1:D:885:PRO:HA	1:D:889:ALA:HB3	1.90	0.53
1:C:1009:ASN:HD21	2:F:65:THR:HB	1.74	0.53
1:D:609:PHE:HB3	1:D:673:SER:HB3	1.90	0.52
1:D:767:THR:OG1	1:D:768:LEU:N	2.42	0.52
2:H:119:ASP:OD1	2:H:119:ASP:N	2.43	0.52
1:B:900:ASP:OD1	1:B:901:LYS:N	2.43	0.52
1:B:942:LYS:HG3	1:B:1055:LEU:HD22	1.91	0.52
1:C:991:HIS:O	1:C:995:THR:HG23	2.09	0.52
1:D:643:LEU:HD11	1:D:1137:MET:HA	1.92	0.52
2:H:119:ASP:OD2	4:H:201:GDP:N2	2.40	0.52
1:A:645:ARG:NE	1:A:682:ASP:OD2	2.41	0.52
1:B:942:LYS:HE3	1:B:1056:TYR:CE2	2.45	0.51
1:B:1007:LEU:HD23	1:B:1031:ALA:HA	1.92	0.51
1:A:1050:PRO:HD3	2:E:40:TYR:CE2	2.45	0.51
1:C:620:MET:HB3	1:C:677:LEU:HD21	1.92	0.51
1:A:671:VAL:HG11	1:A:716:ILE:HD13	1.93	0.51
1:A:1124:LEU:HG	1:A:1129:ALA:HB2	1.92	0.51
1:A:706:PRO:O	1:A:993:TRP:NE1	2.42	0.51
1:C:810:THR:O	1:C:814:VAL:HG23	2.10	0.51
1:C:729:LEU:HD21	1:C:968:VAL:HG23	1.91	0.51
1:B:969:LYS:HE3	1:B:973:ASP:OD2	2.10	0.51
1:A:1008:LYS:O	1:A:1019:LYS:NZ	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:LYS:HB2	2:F:76:GLN:HG3	1.92	0.51
1:B:655:HIS:O	1:B:659:GLU:HG2	2.11	0.51
1:D:589:LEU:HD13	1:D:747:ALA:HB1	1.93	0.51
1:B:737:VAL:HG11	1:B:1003:TRP:CZ3	2.46	0.51
1:B:620:MET:HB3	1:B:677:LEU:HD21	1.91	0.50
1:D:837:ILE:HA	1:D:883:ILE:O	2.11	0.50
1:B:889:ALA:O	1:B:893:THR:OG1	2.28	0.50
1:B:884:THR:H	1:B:887:ILE:HD12	1.76	0.50
1:A:752:ILE:HD13	1:A:1022:HIS:CE1	2.46	0.50
1:D:668:LYS:HZ1	1:D:715:SER:HA	1.76	0.50
1:B:953:PHE:CZ	1:B:1034:PHE:HB2	2.47	0.50
1:B:1035:MET:HE2	2:G:36:ILE:HG13	1.92	0.50
1:A:748:LEU:O	1:A:752:ILE:HG13	2.11	0.50
1:B:770:GLU:OE2	1:C:576:ARG:NH2	2.44	0.50
1:B:760:VAL:HG21	1:B:908:PHE:HA	1.94	0.50
2:G:69:ASP:N	2:G:69:ASP:OD1	2.42	0.50
1:D:1048:HIS:HB3	2:H:24:VAL:HG12	1.94	0.50
1:A:884:THR:H	1:A:887:ILE:HD12	1.77	0.50
1:D:941:THR:O	1:D:945:VAL:HG22	2.12	0.50
1:A:1048:HIS:HB3	2:E:25:GLN:HG2	1.94	0.49
1:B:737:VAL:HG21	1:B:1003:TRP:HH2	1.76	0.49
1:D:715:SER:HB2	1:D:717:VAL:HG23	1.93	0.49
2:G:19:LEU:HD23	2:G:148:ALA:HB2	1.93	0.49
1:A:791:VAL:H	1:A:797:ILE:HB	1.76	0.49
2:F:118:CYS:SG	2:F:147:SER:HB2	2.52	0.49
1:C:841:TYR:HB2	1:C:850:LEU:HD23	1.95	0.49
1:C:835:ARG:NH1	1:C:899:ASP:OD2	2.33	0.49
1:C:1025:GLY:O	1:C:1029:VAL:HG23	2.13	0.49
1:C:954:LYS:HG2	1:C:957:TRP:HE1	1.77	0.49
1:B:752:ILE:HD13	1:B:1022:HIS:CE1	2.47	0.48
1:B:1056:TYR:O	1:B:1060:ILE:HG12	2.13	0.48
1:B:865:MET:HB2	1:B:908:PHE:CZ	2.48	0.48
1:D:1068:LYS:O	1:D:1072:LYS:HG2	2.13	0.48
2:E:124:ARG:NH1	2:E:145:GLU:OE2	2.41	0.48
1:A:602:LYS:HG3	1:A:603:HIS:CD2	2.49	0.48
1:C:969:LYS:HE3	1:C:973:ASP:OD2	2.13	0.48
1:C:650:LEU:HD23	1:C:689:ILE:HG12	1.96	0.48
2:G:15:GLY:HA3	2:G:116:ASN:HD22	1.77	0.48
1:B:854:ASP:OD1	1:B:867:ASN:ND2	2.36	0.48
2:G:9:LEU:HD21	2:G:71:TYR:CE1	2.49	0.48
1:D:704:ALA:HA	1:D:712:ARG:HH22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:LYS:HB3	1:B:834:ILE:HD11	1.96	0.48
1:B:952:LEU:HD21	1:B:1007:LEU:HD11	1.95	0.48
1:A:737:VAL:HG11	1:A:1003:TRP:CZ3	2.49	0.48
2:H:16:LYS:NZ	4:H:201:GDP:O1B	2.41	0.48
1:B:969:LYS:NZ	1:B:1074:VAL:O	2.34	0.48
1:A:711:ARG:NE	5:E:202:AF3:F3	2.37	0.48
1:D:600:ASP:OD1	1:D:600:ASP:N	2.46	0.48
1:C:1110:TYR:HA	1:C:1113:MET:HB3	1.95	0.48
1:B:758:ASP:OD1	1:B:909:HIS:HB3	2.13	0.47
1:C:752:ILE:HD13	1:C:1022:HIS:CE1	2.49	0.47
1:A:722:THR:O	1:A:726:SER:OG	2.32	0.47
2:F:8:VAL:O	2:F:58:THR:OG1	2.22	0.47
1:C:1104:ALA:HA	1:C:1107:ARG:HD2	1.97	0.47
1:B:687:THR:O	1:B:691:GLU:HG3	2.13	0.47
1:D:814:VAL:HG21	1:D:869:LEU:HD21	1.95	0.47
1:C:669:CYS:SG	2:F:62:GLU:HG2	2.55	0.47
1:B:839:ILE:HG23	1:B:880:ILE:HG23	1.96	0.47
2:F:119:ASP:OD1	2:F:119:ASP:N	2.47	0.47
1:D:1025:GLY:O	1:D:1028:SER:OG	2.25	0.47
1:D:660:GLN:HB2	1:D:663:PHE:HB2	1.97	0.47
1:B:613:ALA:O	1:B:617:THR:HG23	2.15	0.47
1:C:609:PHE:HB3	1:C:673:SER:HB3	1.96	0.47
1:D:773:LEU:HD21	1:D:934:TYR:HB2	1.96	0.46
1:A:733:LEU:HD21	1:A:1006:ILE:HG12	1.97	0.46
1:B:733:LEU:HD12	1:B:737:VAL:HB	1.96	0.46
1:D:640:PHE:O	1:D:644:ILE:HG12	2.16	0.46
1:B:1050:PRO:HD3	2:G:40:TYR:CE2	2.51	0.46
1:B:998:LEU:O	1:B:1002:PHE:HB3	2.16	0.46
2:H:79:ALA:HB2	2:H:161:LEU:HD11	1.96	0.46
1:C:758:ASP:OD2	1:C:761:THR:OG1	2.23	0.46
1:D:613:ALA:O	1:D:617:THR:HG23	2.15	0.46
2:E:84:ILE:HD12	2:E:124:ARG:HG3	1.96	0.46
1:D:644:ILE:HG23	1:D:650:LEU:HD13	1.98	0.46
1:A:658:GLU:OE2	1:A:716:ILE:N	2.34	0.46
1:A:889:ALA:O	1:A:893:THR:OG1	2.34	0.46
2:H:117:LYS:HE2	4:H:201:GDP:C8	2.51	0.46
1:D:999:PRO:HA	1:D:1003:TRP:HB2	1.98	0.46
1:D:970:TYR:HB2	1:D:1080:ILE:HD12	1.98	0.46
1:A:665:ILE:HA	1:A:668:LYS:HD2	1.98	0.46
1:D:1124:LEU:HG	1:D:1129:ALA:HB2	1.97	0.45
1:C:1119:GLU:OE1	1:C:1119:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:ILE:HG21	1:B:679:LEU:HD21	1.98	0.45
2:H:135:ALA:HB2	2:H:143:PHE:HB2	1.97	0.45
1:B:663:PHE:CE1	1:B:667:ASP:HB3	2.52	0.45
1:D:788:VAL:N	1:D:880:ILE:O	2.40	0.45
1:D:930:ILE:HB	1:D:933:MET:HE3	1.99	0.45
1:A:650:LEU:HD23	1:A:689:ILE:HG12	1.99	0.45
2:F:136:ARG:HD3	2:F:140:ASN:HA	1.98	0.45
1:D:724:TRP:HA	1:D:727:ILE:HD12	1.99	0.45
2:F:119:ASP:OD2	4:F:201:GDP:N2	2.42	0.45
1:A:830:TYR:HD2	1:A:837:ILE:HD11	1.82	0.45
1:A:758:ASP:OD1	1:A:909:HIS:HB3	2.17	0.45
2:F:161:LEU:O	2:F:165:ILE:HG13	2.17	0.45
1:C:785:LEU:HD13	1:C:880:ILE:HD12	1.99	0.44
1:B:664:SER:O	1:B:668:LYS:HG3	2.16	0.44
1:D:713:THR:HA	1:D:718:GLU:OE1	2.16	0.44
1:C:1056:TYR:O	1:C:1060:ILE:HG12	2.17	0.44
1:C:840:GLU:HA	1:C:849:MET:HA	1.99	0.44
1:A:972:PHE:HD2	1:A:1074:VAL:HG11	1.82	0.44
2:F:116:ASN:OD1	2:F:117:LYS:N	2.48	0.44
1:B:694:LEU:HD22	1:B:974:PHE:HE2	1.83	0.44
2:E:96:LEU:O	2:E:100:ILE:HG12	2.17	0.44
1:A:613:ALA:O	1:A:617:THR:HG23	2.18	0.44
1:A:839:ILE:HG23	1:A:880:ILE:HG23	2.00	0.44
1:C:788:VAL:HG13	1:C:798:SER:HA	1.99	0.44
2:G:96:LEU:O	2:G:100:ILE:HG12	2.17	0.44
1:B:708:LEU:HD23	1:B:712:ARG:HH21	1.82	0.44
1:C:669:CYS:HA	1:C:719:LYS:HG2	2.00	0.44
1:B:869:LEU:HD23	1:B:869:LEU:HA	1.85	0.44
1:A:937:LYS:HA	1:A:937:LYS:HD3	1.66	0.44
1:C:675:LEU:HD23	1:C:720:LEU:HD11	1.99	0.44
1:A:930:ILE:HG23	1:D:572:ARG:HG2	1.99	0.44
1:B:571:ILE:O	1:B:575:ILE:HG13	2.18	0.44
2:E:104:LYS:HA	2:E:104:LYS:HD3	1.82	0.44
1:C:663:PHE:CE1	1:C:667:ASP:HB3	2.53	0.44
1:D:1050:PRO:HB2	1:D:1052:ASN:OD1	2.16	0.44
1:B:991:HIS:O	1:B:995:THR:HG23	2.17	0.44
1:D:865:MET:HB2	1:D:908:PHE:CZ	2.53	0.43
1:C:1050:PRO:HD3	2:F:40:TYR:CE1	2.53	0.43
1:B:814:VAL:O	1:B:818:ILE:HG13	2.18	0.43
2:F:139:ASN:O	2:F:139:ASN:ND2	2.51	0.43
1:D:723:ASN:O	1:D:727:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:952:LEU:O	1:B:956:ILE:HG13	2.19	0.43
1:C:820:GLN:O	1:C:824:ARG:HB2	2.19	0.43
1:B:1008:LYS:O	1:B:1019:LYS:NZ	2.30	0.43
1:D:567:MET:O	1:D:571:ILE:HG13	2.18	0.43
2:F:141:CYS:SG	2:F:142:ALA:N	2.91	0.43
1:A:991:HIS:O	1:A:995:THR:HG23	2.18	0.43
2:G:35:THR:HG23	2:G:38:ASP:OD2	2.18	0.43
2:H:96:LEU:O	2:H:100:ILE:HG12	2.19	0.43
1:B:988:ASP:O	1:B:992:ILE:HG12	2.18	0.43
2:F:117:LYS:HG2	4:F:201:GDP:C6	2.53	0.43
1:C:1045:LEU:HD13	1:C:1054:LEU:HD12	2.01	0.43
1:C:803:VAL:HG11	1:C:818:ILE:HG12	2.00	0.43
1:C:970:TYR:CE1	1:C:1085:LEU:HD11	2.54	0.43
2:G:6:LEU:HD22	2:G:161:LEU:HD13	2.01	0.43
1:C:1027:LEU:HD23	1:C:1027:LEU:HA	1.85	0.43
1:B:1025:GLY:O	1:B:1029:VAL:HG23	2.19	0.43
1:B:734:ARG:NH2	1:D:1126:GLN:HA	2.33	0.43
1:D:668:LYS:HZ3	1:D:714:GLU:C	2.22	0.43
2:H:40:TYR:N	2:H:55:ILE:O	2.48	0.42
1:D:691:GLU:OE2	1:D:970:TYR:OH	2.28	0.42
1:B:1009:ASN:HD21	2:G:65:THR:HB	1.84	0.42
1:C:841:TYR:HE1	1:C:878:ALA:HB1	1.84	0.42
2:F:9:LEU:HD21	2:F:71:TYR:HE1	1.83	0.42
1:D:656:ALA:O	1:D:660:GLN:NE2	2.30	0.42
1:D:697:LEU:O	1:D:701:SER:HB3	2.19	0.42
1:A:869:LEU:HD22	1:A:874:VAL:HG21	2.01	0.42
1:D:757:VAL:HG22	1:D:764:ALA:HB2	2.00	0.42
2:F:9:LEU:HD21	2:F:71:TYR:CE1	2.54	0.42
1:B:1050:PRO:HB2	1:B:1052:ASN:OD1	2.20	0.42
1:B:1008:LYS:HB3	1:B:1008:LYS:HE3	1.91	0.42
2:F:138:TRP:HB2	2:F:141:CYS:HB2	2.01	0.42
2:H:4:TYR:CE2	2:H:162:VAL:HG13	2.55	0.42
1:C:694:LEU:HD11	1:C:710:LEU:HD21	2.01	0.42
1:C:640:PHE:O	1:C:644:ILE:HG12	2.20	0.42
2:E:80:LEU:HB3	2:E:93:LEU:HD22	2.00	0.42
1:B:703:ASN:O	1:B:712:ARG:NH1	2.53	0.42
2:F:117:LYS:HG2	4:F:201:GDP:C5	2.54	0.42
1:A:598:PHE:HZ	1:A:738:GLY:HA3	1.84	0.42
2:G:117:LYS:HE2	4:G:201:GDP:C4	2.54	0.42
1:B:613:ALA:HB1	1:B:616:LEU:HB2	2.02	0.42
1:D:588:ASP:N	1:D:588:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:758:ASP:OD1	1:C:909:HIS:HB3	2.20	0.42
1:C:643:LEU:HD11	1:C:1137:MET:HA	2.01	0.42
1:B:711:ARG:HH21	2:G:34:PRO:HA	1.85	0.42
1:C:599:LEU:HD23	1:C:599:LEU:HA	1.91	0.42
1:B:930:ILE:HB	1:B:933:MET:HE3	2.00	0.42
1:A:959:LEU:HD22	1:A:964:ALA:HA	2.02	0.42
1:B:1102:GLU:OE1	1:B:1102:GLU:N	2.52	0.42
1:A:787:VAL:HB	1:A:801:LEU:HB3	2.01	0.42
1:A:695:GLN:HG3	1:A:978:GLN:HE22	1.84	0.42
1:D:766:TYR:HB3	1:D:941:THR:OG1	2.20	0.42
2:G:161:LEU:O	2:G:165:ILE:HG13	2.20	0.42
1:A:858:GLU:HG2	1:A:865:MET:HE2	2.01	0.42
1:A:1141:LYS:HE2	1:A:1141:LYS:HB3	1.79	0.42
1:B:932:GLU:HA	1:B:935:LEU:HG	2.01	0.42
1:B:640:PHE:CE2	1:B:644:ILE:HD11	2.55	0.42
1:C:869:LEU:HD22	1:C:874:VAL:HG21	2.01	0.42
1:C:854:ASP:OD1	1:C:854:ASP:N	2.52	0.42
2:H:84:ILE:HD11	2:H:118:CYS:HA	2.02	0.42
1:A:966:LEU:HD11	1:A:1080:ILE:HG21	2.01	0.42
1:B:572:ARG:HG2	1:C:930:ILE:HG23	2.00	0.42
1:D:741:LEU:O	1:D:745:VAL:HG23	2.19	0.42
1:A:769:SER:HB3	1:A:772:TRP:HB2	2.02	0.42
1:D:640:PHE:HD2	1:D:1106:LEU:HD22	1.85	0.41
1:D:755:GLY:HA3	1:D:766:TYR:CD1	2.54	0.41
1:B:694:LEU:O	1:B:698:MET:HG2	2.20	0.41
2:H:90:PHE:HE2	2:H:130:GLN:HE21	1.66	0.41
1:C:850:LEU:HD12	1:C:850:LEU:O	2.20	0.41
1:A:966:LEU:CD1	1:A:1080:ILE:HD13	2.48	0.41
1:D:810:THR:O	1:D:814:VAL:HG23	2.20	0.41
1:D:565:GLU:O	1:D:569:SER:OG	2.22	0.41
1:C:972:PHE:HD1	1:C:975:LEU:HD12	1.86	0.41
1:B:788:VAL:HA	1:B:799:GLU:O	2.21	0.41
1:A:719:LYS:HD2	1:A:719:LYS:HA	1.84	0.41
1:D:1007:LEU:O	1:D:1027:LEU:HD13	2.21	0.41
2:G:117:LYS:HG2	4:G:201:GDP:C6	2.56	0.41
1:C:1053:LYS:NZ	2:F:38:ASP:OD1	2.53	0.41
2:H:35:THR:HG21	2:H:57:ASP:OD2	2.21	0.41
1:C:757:VAL:HG22	1:C:764:ALA:HB2	2.02	0.41
1:B:776:GLN:HG2	1:B:778:GLN:HE21	1.86	0.41
1:D:1024:ASP:OD2	2:H:67:MET:HB3	2.20	0.41
1:B:645:ARG:HA	1:B:685:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:GLY:HA2	4:H:201:GDP:O3A	2.21	0.41
1:C:588:ASP:OD1	1:C:588:ASP:N	2.53	0.41
1:A:742:PHE:HB2	1:A:1014:PHE:CZ	2.55	0.41
1:D:814:VAL:O	1:D:818:ILE:HG13	2.21	0.41
1:C:970:TYR:HB2	1:C:1080:ILE:HG13	2.03	0.41
1:A:569:SER:HA	1:A:572:ARG:HD2	2.03	0.41
1:B:665:ILE:HD12	2:G:61:THR:HG21	2.03	0.41
1:B:766:TYR:HB3	1:B:941:THR:OG1	2.21	0.41
1:D:1008:LYS:HE3	1:D:1008:LYS:HB3	1.89	0.41
1:A:737:VAL:HG21	1:A:1003:TRP:CH2	2.53	0.41
1:C:810:THR:HG21	1:C:866:LEU:HD12	2.02	0.41
1:B:1021:PRO:O	1:B:1024:ASP:HB3	2.21	0.41
1:D:969:LYS:HD3	1:D:1077:GLN:HB3	2.03	0.41
1:B:610:PHE:HB2	1:B:617:THR:HG22	2.03	0.41
2:E:53:LEU:HD11	2:E:162:VAL:HG21	2.03	0.41
1:C:723:ASN:O	1:C:727:ILE:HG13	2.21	0.41
1:B:982:LYS:HE3	1:B:982:LYS:HB3	1.85	0.41
1:B:1003:TRP:O	1:B:1007:LEU:HB2	2.21	0.40
1:B:599:LEU:HD23	1:B:599:LEU:HA	1.93	0.40
1:B:1055:LEU:HA	1:B:1055:LEU:HD23	1.86	0.40
1:C:677:LEU:HA	1:C:677:LEU:HD12	1.95	0.40
1:D:737:VAL:HG11	1:D:1003:TRP:CZ3	2.55	0.40
2:E:66:ALA:HB3	2:E:68:ARG:CZ	2.51	0.40
1:D:1027:LEU:HA	1:D:1027:LEU:HD23	1.89	0.40
1:B:840:GLU:HB2	1:B:881:LYS:HB3	2.04	0.40
2:G:119:ASP:N	2:G:119:ASP:OD1	2.52	0.40
1:B:616:LEU:HA	1:B:616:LEU:HD23	1.96	0.40
1:D:839:ILE:HG23	1:D:880:ILE:HG23	2.03	0.40
1:C:643:LEU:HB3	1:C:649:PHE:CE2	2.57	0.40
1:C:982:LYS:HB3	1:C:982:LYS:HE2	1.81	0.40
1:C:767:THR:HG22	1:C:773:LEU:HD13	2.04	0.40
1:D:643:LEU:HD13	1:D:649:PHE:CZ	2.56	0.40
1:B:755:GLY:HA3	1:B:766:TYR:CE1	2.56	0.40
1:B:718:GLU:HB3	1:B:1001:ARG:CZ	2.51	0.40
1:B:939:LEU:O	1:B:943:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	564/599 (94%)	522 (93%)	40 (7%)	2 (0%)	39	76
1	B	561/599 (94%)	527 (94%)	31 (6%)	3 (0%)	34	71
1	C	550/599 (92%)	514 (94%)	34 (6%)	2 (0%)	39	76
1	D	550/599 (92%)	505 (92%)	43 (8%)	2 (0%)	39	76
2	E	166/199 (83%)	152 (92%)	13 (8%)	1 (1%)	30	68
2	F	164/199 (82%)	153 (93%)	10 (6%)	1 (1%)	30	68
2	G	166/199 (83%)	157 (95%)	9 (5%)	0	100	100
2	H	165/199 (83%)	151 (92%)	14 (8%)	0	100	100
All	All	2886/3192 (90%)	2681 (93%)	194 (7%)	11 (0%)	39	76

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	889	ALA
1	D	889	ALA
1	A	889	ALA
1	A	884	THR
1	B	585	GLU
1	D	663	PHE
1	C	889	ALA
2	E	30	GLU
1	B	884	THR
1	C	998	LEU
2	F	110	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	439/552 (80%)	431 (98%)	8 (2%)	66	85
1	B	418/552 (76%)	406 (97%)	12 (3%)	50	80
1	C	420/552 (76%)	411 (98%)	9 (2%)	61	84
1	D	421/552 (76%)	409 (97%)	12 (3%)	50	80
2	E	133/163 (82%)	130 (98%)	3 (2%)	58	83
2	F	131/163 (80%)	127 (97%)	4 (3%)	47	79
2	G	128/163 (78%)	125 (98%)	3 (2%)	58	83
2	H	118/163 (72%)	117 (99%)	1 (1%)	86	93
All	All	2208/2860 (77%)	2156 (98%)	52 (2%)	57	83

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	661	LYS
1	A	850	LEU
1	A	884	THR
1	A	950	GLU
1	A	957	TRP
1	A	1028	SER
1	A	1041	THR
1	A	1137	MET
1	B	577	GLN
1	B	709	LEU
1	B	712	ARG
1	B	717	VAL
1	B	720	LEU
1	B	748	LEU
1	B	850	LEU
1	B	884	THR
1	B	942	LYS
1	B	957	TRP
1	B	988	ASP
1	B	1054	LEU
1	C	577	GLN
1	C	615	THR
1	C	619	VAL
1	C	720	LEU

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Mol	Chain	Res	Type
1	C	767	THR
1	C	831	THR
1	C	864	THR
1	C	884	THR
1	C	1005	ASN
1	D	568	GLU
1	D	619	VAL
1	D	665	ILE
1	D	712	ARG
1	D	717	VAL
1	D	813	GLN
1	D	823	GLN
1	D	850	LEU
1	D	966	LEU
1	D	973	ASP
1	D	1029	VAL
1	D	1085	LEU
2	E	67	MET
2	E	97	ARG
2	E	106	THR
2	F	52	MET
2	F	67	MET
2	F	136	ARG
2	F	155	ASN
2	G	41	ARG
2	G	52	MET
2	G	67	MET
2	H	52	MET

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

Mol	Chain	Res	Type
1	A	603	HIS
1	A	813	GLN
1	A	823	GLN
1	A	867	ASN
1	A	946	HIS
1	A	978	GLN
1	A	1009	ASN
1	A	1136	ASN
1	B	703	ASN
1	B	894	GLN

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Mol	Chain	Res	Type
1	B	978	GLN
1	C	577	GLN
1	C	695	GLN
1	C	1005	ASN
1	C	1009	ASN
1	C	1090	GLN
1	C	1101	ASN
1	D	867	ASN
1	D	946	HIS
1	D	978	GLN
2	F	91	ASN
2	F	94	GLN
2	G	49	GLN
2	H	22	GLN
2	H	153	ASN
2	H	164	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GDP	E	201	3	23,30,30	1.15	2 (8%)	30,47,47	1.76	7 (23%)
5	AF3	E	202	-	0,3,3	0.00	-	0,3,3	0.00	-
4	GDP	F	201	3	23,30,30	1.17	2 (8%)	30,47,47	1.87	7 (23%)
5	AF3	F	202	-	0,3,3	0.00	-	0,3,3	0.00	-
4	GDP	G	201	3	23,30,30	1.16	2 (8%)	30,47,47	1.85	7 (23%)
5	AF3	G	202	-	0,3,3	0.00	-	0,3,3	0.00	-
4	GDP	H	201	3	23,30,30	1.16	2 (8%)	30,47,47	1.82	7 (23%)
5	AF3	H	202	-	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	E	201	3	-	0/12/32/32	0/3/3/3
5	AF3	E	202	-	-	0/0/0/0	0/0/0/0
4	GDP	F	201	3	-	0/12/32/32	0/3/3/3
5	AF3	F	202	-	-	0/0/0/0	0/0/0/0
4	GDP	G	201	3	-	0/12/32/32	0/3/3/3
5	AF3	G	202	-	-	0/0/0/0	0/0/0/0
4	GDP	H	201	3	-	0/12/32/32	0/3/3/3
5	AF3	H	202	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	201	GDP	C5-C4	2.99	1.47	1.40
4	H	201	GDP	C5-C4	3.01	1.47	1.40
4	G	201	GDP	C5-C4	3.03	1.47	1.40
4	F	201	GDP	C5-C4	3.04	1.47	1.40
4	E	201	GDP	C6-C5	3.55	1.48	1.41
4	H	201	GDP	C6-C5	3.56	1.48	1.41
4	G	201	GDP	C6-C5	3.58	1.48	1.41
4	F	201	GDP	C6-C5	3.68	1.48	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	201	GDP	C5-C6-N1	-4.16	117.91	123.59
4	H	201	GDP	C5-C6-N1	-4.06	118.03	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	201	GDP	C5-C6-N1	-4.06	118.04	123.59
4	F	201	GDP	C5-C6-N1	-3.94	118.20	123.59
4	H	201	GDP	C2'-C1'-N9	-3.90	108.33	114.29
4	F	201	GDP	C2'-C1'-N9	-3.72	108.61	114.29
4	G	201	GDP	PA-O3A-PB	-3.45	121.09	132.67
4	G	201	GDP	C2'-C1'-N9	-3.26	109.31	114.29
4	G	201	GDP	C6-C5-C4	-3.13	117.16	120.90
4	F	201	GDP	C6-C5-C4	-3.10	117.19	120.90
4	E	201	GDP	C2'-C1'-N9	-3.10	109.56	114.29
4	F	201	GDP	N3-C2-N1	-3.08	122.76	127.44
4	F	201	GDP	C4-C5-N7	-3.05	106.67	109.48
4	H	201	GDP	N3-C2-N1	-3.02	122.85	127.44
4	G	201	GDP	N3-C2-N1	-2.98	122.90	127.44
4	E	201	GDP	C6-C5-C4	-2.97	117.35	120.90
4	H	201	GDP	C4-C5-N7	-2.97	106.75	109.48
4	F	201	GDP	PA-O3A-PB	-2.96	122.73	132.67
4	G	201	GDP	C4-C5-N7	-2.96	106.75	109.48
4	H	201	GDP	PA-O3A-PB	-2.96	122.74	132.67
4	E	201	GDP	N3-C2-N1	-2.92	122.99	127.44
4	E	201	GDP	PA-O3A-PB	-2.88	123.02	132.67
4	H	201	GDP	C6-C5-C4	-2.81	117.54	120.90
4	E	201	GDP	C4-C5-N7	-2.79	106.92	109.48
4	H	201	GDP	C6-N1-C2	4.41	122.06	115.94
4	F	201	GDP	C6-N1-C2	4.51	122.19	115.94
4	E	201	GDP	C6-N1-C2	4.53	122.23	115.94
4	G	201	GDP	C6-N1-C2	4.67	122.42	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	202	AF3	1	0
4	F	201	GDP	3	0
5	F	202	AF3	1	0
4	G	201	GDP	2	0
4	H	201	GDP	5	0

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	574/599 (95%)	0.15	21 (3%)	45	38	66, 132, 194, 219	0
1	B	571/599 (95%)	0.26	29 (5%)	32	25	62, 135, 220, 277	0
1	C	560/599 (93%)	0.09	23 (4%)	41	34	70, 134, 189, 214	0
1	D	560/599 (93%)	0.37	42 (7%)	17	14	83, 153, 223, 253	0
2	E	168/199 (84%)	0.47	11 (6%)	22	18	91, 139, 179, 208	0
2	F	166/199 (83%)	0.72	18 (10%)	8	6	94, 147, 186, 205	0
2	G	168/199 (84%)	1.00	34 (20%)	1	1	95, 166, 214, 234	0
2	H	167/199 (83%)	0.85	26 (15%)	3	2	110, 168, 222, 243	0
All	All	2934/3192 (91%)	0.34	204 (6%)	19	16	62, 143, 207, 277	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	76	GLN	8.8
2	H	113	LEU	5.8
1	D	847	PHE	5.6
2	H	141	CYS	5.3
2	G	142	ALA	5.3
1	D	1140	VAL	5.2
1	D	1121	PHE	5.2
1	B	652	CYS	4.9
2	H	142	ALA	4.8
2	G	118	CYS	4.8
1	B	985	THR	4.6
2	G	59	ALA	4.5
2	G	144	LEU	4.5
1	D	1117	PHE	4.5
2	H	112	ILE	4.4
1	D	1087	THR	4.4

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Mol	Chain	Res	Type	RSRZ
2	G	112	ILE	4.3
1	B	1110	TYR	4.3
1	B	587	SER	4.2
1	D	791	VAL	4.0
2	G	60	GLY	3.9
1	B	789	PHE	3.9
1	A	700	GLN	3.9
1	B	593	VAL	3.9
1	C	1121	PHE	3.8
1	A	794	GLY	3.8
2	F	143	PHE	3.7
1	A	783	LEU	3.7
2	F	6	LEU	3.7
2	G	65	THR	3.7
1	B	632	THR	3.6
1	D	796	GLU	3.6
1	D	1120	ILE	3.6
1	A	818	ILE	3.6
1	B	874	VAL	3.6
1	D	1110	TYR	3.5
1	A	1110	TYR	3.4
2	E	118	CYS	3.4
2	F	142	ALA	3.4
1	C	895	ASN	3.3
1	A	911	VAL	3.3
1	D	885	PRO	3.3
2	G	66	ALA	3.3
1	B	783	LEU	3.3
2	G	145	GLU	3.3
2	E	6	LEU	3.3
1	B	556	MET	3.3
2	F	113	LEU	3.2
1	D	874	VAL	3.2
2	G	119	ASP	3.2
1	B	1133	LEU	3.2
2	G	138	TRP	3.2
2	H	158	PHE	3.2
2	F	144	LEU	3.2
2	G	113	LEU	3.2
2	E	47	ASP	3.1
2	H	125	VAL	3.1
1	A	652	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	909	HIS	3.1
2	G	6	LEU	3.1
1	D	653	PHE	3.0
2	G	34	PRO	3.0
2	H	131	GLY	3.0
1	D	1137	MET	3.0
1	A	633	VAL	3.0
1	C	1092	GLU	3.0
1	A	789	PHE	3.0
1	D	872	TYR	2.9
1	C	802	GLU	2.9
2	F	53	LEU	2.9
1	D	1144	PHE	2.9
1	D	1116	TYR	2.9
2	H	78	PHE	2.9
2	G	110	PRO	2.9
1	A	632	THR	2.8
1	D	596	ILE	2.8
2	E	112	ILE	2.8
1	B	557	SER	2.8
2	G	62	GLU	2.8
2	H	126	VAL	2.8
2	G	47	ASP	2.8
2	G	159	TYR	2.8
2	F	107	ASP	2.8
1	A	557	SER	2.8
2	G	115	GLY	2.7
2	G	35	THR	2.7
2	G	77	GLY	2.7
1	D	863	VAL	2.7
2	H	47	ASP	2.7
1	D	864	THR	2.7
2	G	61	THR	2.7
1	D	840	GLU	2.7
2	H	109	VAL	2.7
2	H	157	ILE	2.7
1	B	594	GLY	2.6
2	G	141	CYS	2.6
2	G	120	LEU	2.6
1	B	984	ILE	2.6
1	B	869	LEU	2.6
1	C	619	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1113	MET	2.6
1	C	966	LEU	2.6
2	E	60	GLY	2.6
2	G	165	ILE	2.6
1	A	1124	LEU	2.5
1	D	1088	PHE	2.6
1	D	959	LEU	2.5
1	B	649	PHE	2.5
1	B	850	LEU	2.5
1	C	1117	PHE	2.5
1	D	896	SER	2.5
1	A	612	GLU	2.5
1	C	959	LEU	2.5
2	F	35	THR	2.5
1	B	1005	ASN	2.5
1	C	1078	THR	2.5
2	H	66	ALA	2.5
1	B	653	PHE	2.5
2	E	51	CYS	2.5
2	F	158	PHE	2.5
1	D	1138	HIS	2.5
2	H	61	THR	2.5
2	F	51	CYS	2.4
1	C	885	PRO	2.4
2	H	160	ASP	2.4
2	F	82	TYR	2.4
2	F	46	VAL	2.4
1	A	909	HIS	2.4
2	H	107	ASP	2.4
1	D	1092	GLU	2.4
1	A	1063	TYR	2.4
1	D	839	ILE	2.4
1	C	1088	PHE	2.4
1	B	561	ASN	2.4
1	D	984	ILE	2.4
2	H	62	GLU	2.4
1	D	875	GLY	2.3
2	H	65	THR	2.3
2	E	82	TYR	2.3
1	C	984	ILE	2.3
1	D	841	TYR	2.3
2	F	139	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	555	GLN	2.3
1	D	850	LEU	2.3
2	H	63	GLN	2.3
2	F	130	GLN	2.3
2	H	140	ASN	2.3
1	D	861	GLY	2.3
1	B	713	THR	2.3
1	B	839	ILE	2.3
2	E	46	VAL	2.3
1	A	801	LEU	2.2
1	D	845	GLY	2.2
2	H	44	VAL	2.2
1	A	841	TYR	2.2
2	F	65	THR	2.2
1	B	1070	TYR	2.2
2	G	10	GLY	2.2
2	G	143	PHE	2.2
1	D	967	ALA	2.2
1	C	801	LEU	2.2
1	B	795	GLU	2.2
2	G	111	MET	2.2
1	D	1100	PHE	2.2
1	D	818	ILE	2.2
2	H	143	PHE	2.2
1	C	876	ASP	2.2
1	C	1132	ASN	2.2
2	G	166	ASN	2.2
1	C	803	VAL	2.2
2	E	63	GLN	2.1
2	E	159	TYR	2.1
1	D	1113	MET	2.1
2	G	114	VAL	2.1
1	C	1133	LEU	2.1
2	F	97	ARG	2.1
1	B	782	PRO	2.1
1	C	897	VAL	2.1
1	D	803	VAL	2.1
1	B	677	LEU	2.1
2	H	111	MET	2.1
1	B	596	ILE	2.1
1	D	643	LEU	2.1
2	F	120	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	142	ALA	2.1
2	F	112	ILE	2.1
1	B	611	PRO	2.1
1	C	785	LEU	2.1
2	G	5	LYS	2.1
1	A	850	LEU	2.1
1	C	1106	LEU	2.1
2	G	68	ARG	2.1
2	H	130	GLN	2.1
1	C	640	PHE	2.1
1	C	883	ILE	2.1
1	A	782	PRO	2.1
1	C	644	ILE	2.0
2	H	6	LEU	2.0
1	D	736	SER	2.0
1	D	1133	LEU	2.0
1	A	839	ILE	2.0
1	D	595	ALA	2.0
2	H	153	ASN	2.0
2	G	82	TYR	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	AF3	E	202	4/4	0.98	0.42	1.13	89,128,128,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	AF3	H	202	4/4	0.98	0.35	0.78	115,121,159,159	0
5	AF3	F	202	4/4	0.99	0.33	0.45	91,103,128,169	0
5	AF3	G	202	4/4	0.98	0.39	-0.15	87,91,97,125	0
4	GDP	E	201	28/28	0.89	0.23	-0.40	91,127,141,183	0
4	GDP	H	201	28/28	0.91	0.25	-0.49	123,139,162,166	0
4	GDP	F	201	28/28	0.91	0.24	-0.64	97,120,134,138	0
3	MG	E	200	1/1	0.89	0.22	-0.80	88,88,88,88	0
4	GDP	G	201	28/28	0.86	0.21	-0.86	107,139,151,162	0
3	MG	F	200	1/1	0.97	0.28	-	88,88,88,88	0
3	MG	H	200	1/1	0.89	0.29	-	113,113,113,113	0
3	MG	G	200	1/1	0.93	0.24	-	108,108,108,108	0

6.5 Other polymers ⓘ

There are no such residues in this entry.