



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:21 am GMT

PDB ID : 5B4W
Title : Crystal structure of Plexin inhibitor complex
Authors : Matsunaga, Y.; Kitago, Y.; Arimori, T.; Takagi, J.
Deposited on : 2016-04-19
Resolution : 2.60 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

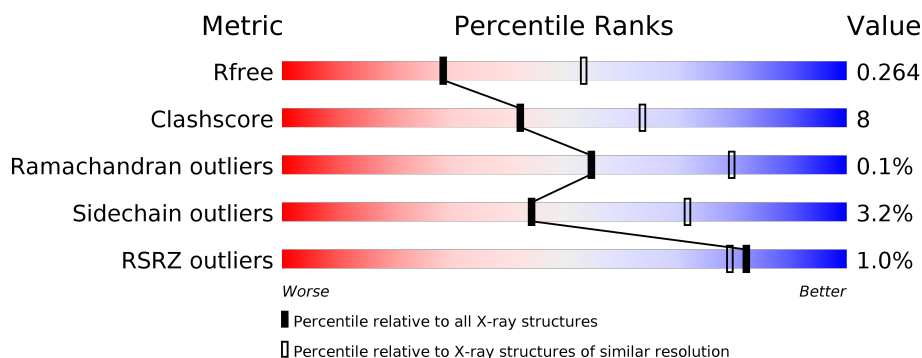
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	579	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>13%</div> <div>25%</div> </div> </div>
1	B	579	<div> <div></div> <div>63%</div> <div>12%</div> <div>25%</div> </div>
1	C	579	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>11%</div> <div>24%</div> </div> </div>
1	D	579	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>20%</div> <div>25%</div> </div> </div>
1	E	579	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>17%</div> <div>17%</div> </div> </div>
1	F	579	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>13%</div> <div>24%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	18	<div><div></div><div>72%17%11%</div></div>
2	H	18	<div><div></div><div>72%22%6%</div></div>
2	I	18	<div><div></div><div>83%17%</div></div>
2	J	18	<div><div></div><div>72%22%6%</div></div>
2	K	18	<div><div></div><div>44%50%6%</div></div>
2	L	18	<div><div></div><div>78%22%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21235 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 Plexin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3298	2075	571	638	14			
1	B	434	Total	C	N	O	S	0	0	0
			3298	2075	571	638	14			
1	C	442	Total	C	N	O	S	0	0	0
			3355	2109	585	647	14			
1	D	436	Total	C	N	O	S	0	0	0
			3304	2082	570	638	14			
1	E	478	Total	C	N	O	S	0	0	0
			3647	2289	640	697	21			
1	F	438	Total	C	N	O	S	0	0	0
			3323	2088	578	643	14			

There are 378 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	See Sequence details	UNP O43157
A	-11	ASP	-	See Sequence details	UNP O43157
A	-10	SER	-	See Sequence details	UNP O43157
A	-9	LYS	-	See Sequence details	UNP O43157
A	-8	GLY	-	See Sequence details	UNP O43157
A	-7	SER	-	See Sequence details	UNP O43157
A	-6	SER	-	See Sequence details	UNP O43157
A	-5	GLN	-	See Sequence details	UNP O43157
A	-4	LYS	-	See Sequence details	UNP O43157
A	-3	GLY	-	See Sequence details	UNP O43157
A	-2	SER	-	See Sequence details	UNP O43157
A	-1	ARG	-	See Sequence details	UNP O43157
A	0	LEU	-	See Sequence details	UNP O43157
A	1	LEU	-	See Sequence details	UNP O43157
A	2	LEU	-	See Sequence details	UNP O43157
A	3	LEU	-	See Sequence details	UNP O43157
A	4	LEU	-	See Sequence details	UNP O43157

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Chain	Residue	Modelled	Actual	Comment	Reference
A	5	VAL	-	See Sequence details	UNP O43157
A	6	VAL	-	See Sequence details	UNP O43157
A	7	SER	-	See Sequence details	UNP O43157
A	8	ASN	-	See Sequence details	UNP O43157
A	9	LEU	-	See Sequence details	UNP O43157
A	10	LEU	-	See Sequence details	UNP O43157
A	11	LEU	-	See Sequence details	UNP O43157
A	12	CYS	-	See Sequence details	UNP O43157
A	13	GLN	-	See Sequence details	UNP O43157
A	14	GLY	-	See Sequence details	UNP O43157
A	15	VAL	-	See Sequence details	UNP O43157
A	16	VAL	-	See Sequence details	UNP O43157
A	17	SER	-	See Sequence details	UNP O43157
A	18	GLY	-	See Sequence details	UNP O43157
A	19	SER	-	See Sequence details	UNP O43157
A	536	THR	-	expression tag	UNP O43157
A	537	ARG	-	expression tag	UNP O43157
A	538	GLU	-	expression tag	UNP O43157
A	539	ASN	-	expression tag	UNP O43157
A	540	LEU	-	expression tag	UNP O43157
A	541	TYR	-	expression tag	UNP O43157
A	542	PHE	-	expression tag	UNP O43157
A	543	GLN	-	expression tag	UNP O43157
A	544	GLY	-	expression tag	UNP O43157
A	545	LYS	-	expression tag	UNP O43157
A	546	ASP	-	expression tag	UNP O43157
A	547	GLY	-	expression tag	UNP O43157
A	548	GLY	-	expression tag	UNP O43157
A	549	GLY	-	expression tag	UNP O43157
A	550	GLY	-	expression tag	UNP O43157
A	551	GLY	-	expression tag	UNP O43157
A	552	SER	-	expression tag	UNP O43157
A	553	HIS	-	expression tag	UNP O43157
A	554	MET	-	expression tag	UNP O43157
A	555	GLY	-	expression tag	UNP O43157
A	556	VAL	-	expression tag	UNP O43157
A	557	ALA	-	expression tag	UNP O43157
A	558	MET	-	expression tag	UNP O43157
A	559	PRO	-	expression tag	UNP O43157
A	560	GLY	-	expression tag	UNP O43157
A	561	ALA	-	expression tag	UNP O43157
A	562	GLU	-	expression tag	UNP O43157

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Chain	Residue	Modelled	Actual	Comment	Reference
A	563	ASP	-	expression tag	UNP O43157
A	564	ASP	-	expression tag	UNP O43157
A	565	VAL	-	expression tag	UNP O43157
A	566	VAL	-	expression tag	UNP O43157
B	-12	MET	-	See Sequence details	UNP O43157
B	-11	ASP	-	See Sequence details	UNP O43157
B	-10	SER	-	See Sequence details	UNP O43157
B	-9	LYS	-	See Sequence details	UNP O43157
B	-8	GLY	-	See Sequence details	UNP O43157
B	-7	SER	-	See Sequence details	UNP O43157
B	-6	SER	-	See Sequence details	UNP O43157
B	-5	GLN	-	See Sequence details	UNP O43157
B	-4	LYS	-	See Sequence details	UNP O43157
B	-3	GLY	-	See Sequence details	UNP O43157
B	-2	SER	-	See Sequence details	UNP O43157
B	-1	ARG	-	See Sequence details	UNP O43157
B	0	LEU	-	See Sequence details	UNP O43157
B	1	LEU	-	See Sequence details	UNP O43157
B	2	LEU	-	See Sequence details	UNP O43157
B	3	LEU	-	See Sequence details	UNP O43157
B	4	LEU	-	See Sequence details	UNP O43157
B	5	VAL	-	See Sequence details	UNP O43157
B	6	VAL	-	See Sequence details	UNP O43157
B	7	SER	-	See Sequence details	UNP O43157
B	8	ASN	-	See Sequence details	UNP O43157
B	9	LEU	-	See Sequence details	UNP O43157
B	10	LEU	-	See Sequence details	UNP O43157
B	11	LEU	-	See Sequence details	UNP O43157
B	12	CYS	-	See Sequence details	UNP O43157
B	13	GLN	-	See Sequence details	UNP O43157
B	14	GLY	-	See Sequence details	UNP O43157
B	15	VAL	-	See Sequence details	UNP O43157
B	16	VAL	-	See Sequence details	UNP O43157
B	17	SER	-	See Sequence details	UNP O43157
B	18	GLY	-	See Sequence details	UNP O43157
B	19	SER	-	See Sequence details	UNP O43157
B	536	THR	-	expression tag	UNP O43157
B	537	ARG	-	expression tag	UNP O43157
B	538	GLU	-	expression tag	UNP O43157
B	539	ASN	-	expression tag	UNP O43157
B	540	LEU	-	expression tag	UNP O43157
B	541	TYR	-	expression tag	UNP O43157

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Chain	Residue	Modelled	Actual	Comment	Reference
B	542	PHE	-	expression tag	UNP O43157
B	543	GLN	-	expression tag	UNP O43157
B	544	GLY	-	expression tag	UNP O43157
B	545	LYS	-	expression tag	UNP O43157
B	546	ASP	-	expression tag	UNP O43157
B	547	GLY	-	expression tag	UNP O43157
B	548	GLY	-	expression tag	UNP O43157
B	549	GLY	-	expression tag	UNP O43157
B	550	GLY	-	expression tag	UNP O43157
B	551	GLY	-	expression tag	UNP O43157
B	552	SER	-	expression tag	UNP O43157
B	553	HIS	-	expression tag	UNP O43157
B	554	MET	-	expression tag	UNP O43157
B	555	GLY	-	expression tag	UNP O43157
B	556	VAL	-	expression tag	UNP O43157
B	557	ALA	-	expression tag	UNP O43157
B	558	MET	-	expression tag	UNP O43157
B	559	PRO	-	expression tag	UNP O43157
B	560	GLY	-	expression tag	UNP O43157
B	561	ALA	-	expression tag	UNP O43157
B	562	GLU	-	expression tag	UNP O43157
B	563	ASP	-	expression tag	UNP O43157
B	564	ASP	-	expression tag	UNP O43157
B	565	VAL	-	expression tag	UNP O43157
B	566	VAL	-	expression tag	UNP O43157
C	-12	MET	-	See Sequence details	UNP O43157
C	-11	ASP	-	See Sequence details	UNP O43157
C	-10	SER	-	See Sequence details	UNP O43157
C	-9	LYS	-	See Sequence details	UNP O43157
C	-8	GLY	-	See Sequence details	UNP O43157
C	-7	SER	-	See Sequence details	UNP O43157
C	-6	SER	-	See Sequence details	UNP O43157
C	-5	GLN	-	See Sequence details	UNP O43157
C	-4	LYS	-	See Sequence details	UNP O43157
C	-3	GLY	-	See Sequence details	UNP O43157
C	-2	SER	-	See Sequence details	UNP O43157
C	-1	ARG	-	See Sequence details	UNP O43157
C	0	LEU	-	See Sequence details	UNP O43157
C	1	LEU	-	See Sequence details	UNP O43157
C	2	LEU	-	See Sequence details	UNP O43157
C	3	LEU	-	See Sequence details	UNP O43157
C	4	LEU	-	See Sequence details	UNP O43157

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Chain	Residue	Modelled	Actual	Comment	Reference
C	5	VAL	-	See Sequence details	UNP O43157
C	6	VAL	-	See Sequence details	UNP O43157
C	7	SER	-	See Sequence details	UNP O43157
C	8	ASN	-	See Sequence details	UNP O43157
C	9	LEU	-	See Sequence details	UNP O43157
C	10	LEU	-	See Sequence details	UNP O43157
C	11	LEU	-	See Sequence details	UNP O43157
C	12	CYS	-	See Sequence details	UNP O43157
C	13	GLN	-	See Sequence details	UNP O43157
C	14	GLY	-	See Sequence details	UNP O43157
C	15	VAL	-	See Sequence details	UNP O43157
C	16	VAL	-	See Sequence details	UNP O43157
C	17	SER	-	See Sequence details	UNP O43157
C	18	GLY	-	See Sequence details	UNP O43157
C	19	SER	-	See Sequence details	UNP O43157
C	536	THR	-	expression tag	UNP O43157
C	537	ARG	-	expression tag	UNP O43157
C	538	GLU	-	expression tag	UNP O43157
C	539	ASN	-	expression tag	UNP O43157
C	540	LEU	-	expression tag	UNP O43157
C	541	TYR	-	expression tag	UNP O43157
C	542	PHE	-	expression tag	UNP O43157
C	543	GLN	-	expression tag	UNP O43157
C	544	GLY	-	expression tag	UNP O43157
C	545	LYS	-	expression tag	UNP O43157
C	546	ASP	-	expression tag	UNP O43157
C	547	GLY	-	expression tag	UNP O43157
C	548	GLY	-	expression tag	UNP O43157
C	549	GLY	-	expression tag	UNP O43157
C	550	GLY	-	expression tag	UNP O43157
C	551	GLY	-	expression tag	UNP O43157
C	552	SER	-	expression tag	UNP O43157
C	553	HIS	-	expression tag	UNP O43157
C	554	MET	-	expression tag	UNP O43157
C	555	GLY	-	expression tag	UNP O43157
C	556	VAL	-	expression tag	UNP O43157
C	557	ALA	-	expression tag	UNP O43157
C	558	MET	-	expression tag	UNP O43157
C	559	PRO	-	expression tag	UNP O43157
C	560	GLY	-	expression tag	UNP O43157
C	561	ALA	-	expression tag	UNP O43157
C	562	GLU	-	expression tag	UNP O43157

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Chain	Residue	Modelled	Actual	Comment	Reference
C	563	ASP	-	expression tag	UNP O43157
C	564	ASP	-	expression tag	UNP O43157
C	565	VAL	-	expression tag	UNP O43157
C	566	VAL	-	expression tag	UNP O43157
D	-12	MET	-	See Sequence details	UNP O43157
D	-11	ASP	-	See Sequence details	UNP O43157
D	-10	SER	-	See Sequence details	UNP O43157
D	-9	LYS	-	See Sequence details	UNP O43157
D	-8	GLY	-	See Sequence details	UNP O43157
D	-7	SER	-	See Sequence details	UNP O43157
D	-6	SER	-	See Sequence details	UNP O43157
D	-5	GLN	-	See Sequence details	UNP O43157
D	-4	LYS	-	See Sequence details	UNP O43157
D	-3	GLY	-	See Sequence details	UNP O43157
D	-2	SER	-	See Sequence details	UNP O43157
D	-1	ARG	-	See Sequence details	UNP O43157
D	0	LEU	-	See Sequence details	UNP O43157
D	1	LEU	-	See Sequence details	UNP O43157
D	2	LEU	-	See Sequence details	UNP O43157
D	3	LEU	-	See Sequence details	UNP O43157
D	4	LEU	-	See Sequence details	UNP O43157
D	5	VAL	-	See Sequence details	UNP O43157
D	6	VAL	-	See Sequence details	UNP O43157
D	7	SER	-	See Sequence details	UNP O43157
D	8	ASN	-	See Sequence details	UNP O43157
D	9	LEU	-	See Sequence details	UNP O43157
D	10	LEU	-	See Sequence details	UNP O43157
D	11	LEU	-	See Sequence details	UNP O43157
D	12	CYS	-	See Sequence details	UNP O43157
D	13	GLN	-	See Sequence details	UNP O43157
D	14	GLY	-	See Sequence details	UNP O43157
D	15	VAL	-	See Sequence details	UNP O43157
D	16	VAL	-	See Sequence details	UNP O43157
D	17	SER	-	See Sequence details	UNP O43157
D	18	GLY	-	See Sequence details	UNP O43157
D	19	SER	-	See Sequence details	UNP O43157
D	536	THR	-	expression tag	UNP O43157
D	537	ARG	-	expression tag	UNP O43157
D	538	GLU	-	expression tag	UNP O43157
D	539	ASN	-	expression tag	UNP O43157
D	540	LEU	-	expression tag	UNP O43157
D	541	TYR	-	expression tag	UNP O43157

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Chain	Residue	Modelled	Actual	Comment	Reference
D	542	PHE	-	expression tag	UNP O43157
D	543	GLN	-	expression tag	UNP O43157
D	544	GLY	-	expression tag	UNP O43157
D	545	LYS	-	expression tag	UNP O43157
D	546	ASP	-	expression tag	UNP O43157
D	547	GLY	-	expression tag	UNP O43157
D	548	GLY	-	expression tag	UNP O43157
D	549	GLY	-	expression tag	UNP O43157
D	550	GLY	-	expression tag	UNP O43157
D	551	GLY	-	expression tag	UNP O43157
D	552	SER	-	expression tag	UNP O43157
D	553	HIS	-	expression tag	UNP O43157
D	554	MET	-	expression tag	UNP O43157
D	555	GLY	-	expression tag	UNP O43157
D	556	VAL	-	expression tag	UNP O43157
D	557	ALA	-	expression tag	UNP O43157
D	558	MET	-	expression tag	UNP O43157
D	559	PRO	-	expression tag	UNP O43157
D	560	GLY	-	expression tag	UNP O43157
D	561	ALA	-	expression tag	UNP O43157
D	562	GLU	-	expression tag	UNP O43157
D	563	ASP	-	expression tag	UNP O43157
D	564	ASP	-	expression tag	UNP O43157
D	565	VAL	-	expression tag	UNP O43157
D	566	VAL	-	expression tag	UNP O43157
E	-12	MET	-	See Sequence details	UNP O43157
E	-11	ASP	-	See Sequence details	UNP O43157
E	-10	SER	-	See Sequence details	UNP O43157
E	-9	LYS	-	See Sequence details	UNP O43157
E	-8	GLY	-	See Sequence details	UNP O43157
E	-7	SER	-	See Sequence details	UNP O43157
E	-6	SER	-	See Sequence details	UNP O43157
E	-5	GLN	-	See Sequence details	UNP O43157
E	-4	LYS	-	See Sequence details	UNP O43157
E	-3	GLY	-	See Sequence details	UNP O43157
E	-2	SER	-	See Sequence details	UNP O43157
E	-1	ARG	-	See Sequence details	UNP O43157
E	0	LEU	-	See Sequence details	UNP O43157
E	1	LEU	-	See Sequence details	UNP O43157
E	2	LEU	-	See Sequence details	UNP O43157
E	3	LEU	-	See Sequence details	UNP O43157
E	4	LEU	-	See Sequence details	UNP O43157

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Chain	Residue	Modelled	Actual	Comment	Reference
E	5	VAL	-	See Sequence details	UNP O43157
E	6	VAL	-	See Sequence details	UNP O43157
E	7	SER	-	See Sequence details	UNP O43157
E	8	ASN	-	See Sequence details	UNP O43157
E	9	LEU	-	See Sequence details	UNP O43157
E	10	LEU	-	See Sequence details	UNP O43157
E	11	LEU	-	See Sequence details	UNP O43157
E	12	CYS	-	See Sequence details	UNP O43157
E	13	GLN	-	See Sequence details	UNP O43157
E	14	GLY	-	See Sequence details	UNP O43157
E	15	VAL	-	See Sequence details	UNP O43157
E	16	VAL	-	See Sequence details	UNP O43157
E	17	SER	-	See Sequence details	UNP O43157
E	18	GLY	-	See Sequence details	UNP O43157
E	19	SER	-	See Sequence details	UNP O43157
E	536	THR	-	expression tag	UNP O43157
E	537	ARG	-	expression tag	UNP O43157
E	538	GLU	-	expression tag	UNP O43157
E	539	ASN	-	expression tag	UNP O43157
E	540	LEU	-	expression tag	UNP O43157
E	541	TYR	-	expression tag	UNP O43157
E	542	PHE	-	expression tag	UNP O43157
E	543	GLN	-	expression tag	UNP O43157
E	544	GLY	-	expression tag	UNP O43157
E	545	LYS	-	expression tag	UNP O43157
E	546	ASP	-	expression tag	UNP O43157
E	547	GLY	-	expression tag	UNP O43157
E	548	GLY	-	expression tag	UNP O43157
E	549	GLY	-	expression tag	UNP O43157
E	550	GLY	-	expression tag	UNP O43157
E	551	GLY	-	expression tag	UNP O43157
E	552	SER	-	expression tag	UNP O43157
E	553	HIS	-	expression tag	UNP O43157
E	554	MET	-	expression tag	UNP O43157
E	555	GLY	-	expression tag	UNP O43157
E	556	VAL	-	expression tag	UNP O43157
E	557	ALA	-	expression tag	UNP O43157
E	558	MET	-	expression tag	UNP O43157
E	559	PRO	-	expression tag	UNP O43157
E	560	GLY	-	expression tag	UNP O43157
E	561	ALA	-	expression tag	UNP O43157
E	562	GLU	-	expression tag	UNP O43157

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Chain	Residue	Modelled	Actual	Comment	Reference
E	563	ASP	-	expression tag	UNP O43157
E	564	ASP	-	expression tag	UNP O43157
E	565	VAL	-	expression tag	UNP O43157
E	566	VAL	-	expression tag	UNP O43157
F	-12	MET	-	See Sequence details	UNP O43157
F	-11	ASP	-	See Sequence details	UNP O43157
F	-10	SER	-	See Sequence details	UNP O43157
F	-9	LYS	-	See Sequence details	UNP O43157
F	-8	GLY	-	See Sequence details	UNP O43157
F	-7	SER	-	See Sequence details	UNP O43157
F	-6	SER	-	See Sequence details	UNP O43157
F	-5	GLN	-	See Sequence details	UNP O43157
F	-4	LYS	-	See Sequence details	UNP O43157
F	-3	GLY	-	See Sequence details	UNP O43157
F	-2	SER	-	See Sequence details	UNP O43157
F	-1	ARG	-	See Sequence details	UNP O43157
F	0	LEU	-	See Sequence details	UNP O43157
F	1	LEU	-	See Sequence details	UNP O43157
F	2	LEU	-	See Sequence details	UNP O43157
F	3	LEU	-	See Sequence details	UNP O43157
F	4	LEU	-	See Sequence details	UNP O43157
F	5	VAL	-	See Sequence details	UNP O43157
F	6	VAL	-	See Sequence details	UNP O43157
F	7	SER	-	See Sequence details	UNP O43157
F	8	ASN	-	See Sequence details	UNP O43157
F	9	LEU	-	See Sequence details	UNP O43157
F	10	LEU	-	See Sequence details	UNP O43157
F	11	LEU	-	See Sequence details	UNP O43157
F	12	CYS	-	See Sequence details	UNP O43157
F	13	GLN	-	See Sequence details	UNP O43157
F	14	GLY	-	See Sequence details	UNP O43157
F	15	VAL	-	See Sequence details	UNP O43157
F	16	VAL	-	See Sequence details	UNP O43157
F	17	SER	-	See Sequence details	UNP O43157
F	18	GLY	-	See Sequence details	UNP O43157
F	19	SER	-	See Sequence details	UNP O43157
F	536	THR	-	expression tag	UNP O43157
F	537	ARG	-	expression tag	UNP O43157
F	538	GLU	-	expression tag	UNP O43157
F	539	ASN	-	expression tag	UNP O43157
F	540	LEU	-	expression tag	UNP O43157
F	541	TYR	-	expression tag	UNP O43157

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Chain	Residue	Modelled	Actual	Comment	Reference
F	542	PHE	-	expression tag	UNP O43157
F	543	GLN	-	expression tag	UNP O43157
F	544	GLY	-	expression tag	UNP O43157
F	545	LYS	-	expression tag	UNP O43157
F	546	ASP	-	expression tag	UNP O43157
F	547	GLY	-	expression tag	UNP O43157
F	548	GLY	-	expression tag	UNP O43157
F	549	GLY	-	expression tag	UNP O43157
F	550	GLY	-	expression tag	UNP O43157
F	551	GLY	-	expression tag	UNP O43157
F	552	SER	-	expression tag	UNP O43157
F	553	HIS	-	expression tag	UNP O43157
F	554	MET	-	expression tag	UNP O43157
F	555	GLY	-	expression tag	UNP O43157
F	556	VAL	-	expression tag	UNP O43157
F	557	ALA	-	expression tag	UNP O43157
F	558	MET	-	expression tag	UNP O43157
F	559	PRO	-	expression tag	UNP O43157
F	560	GLY	-	expression tag	UNP O43157
F	561	ALA	-	expression tag	UNP O43157
F	562	GLU	-	expression tag	UNP O43157
F	563	ASP	-	expression tag	UNP O43157
F	564	ASP	-	expression tag	UNP O43157
F	565	VAL	-	expression tag	UNP O43157
F	566	VAL	-	expression tag	UNP O43157

- Molecule 2 is a protein called Synthesized cyclic peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	18	Total	C	N	O	S	0	0	1
			144	93	29	21	1			
2	H	18	Total	C	N	O	S	0	0	1
			144	93	29	21	1			
2	I	18	Total	C	N	O	S	0	0	1
			144	93	29	21	1			
2	J	18	Total	C	N	O	S	0	0	1
			144	93	29	21	1			
2	K	18	Total	C	N	O	S	0	0	1
			144	93	29	21	1			
2	L	18	Total	C	N	O	S	0	0	1
			144	93	29	21	1			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	16	Total	O	0	0
			16	16		
4	C	8	Total	O	0	0
			8	8		
4	D	1	Total	O	0	0
			1	1		
4	E	7	Total	O	0	0
			7	7		

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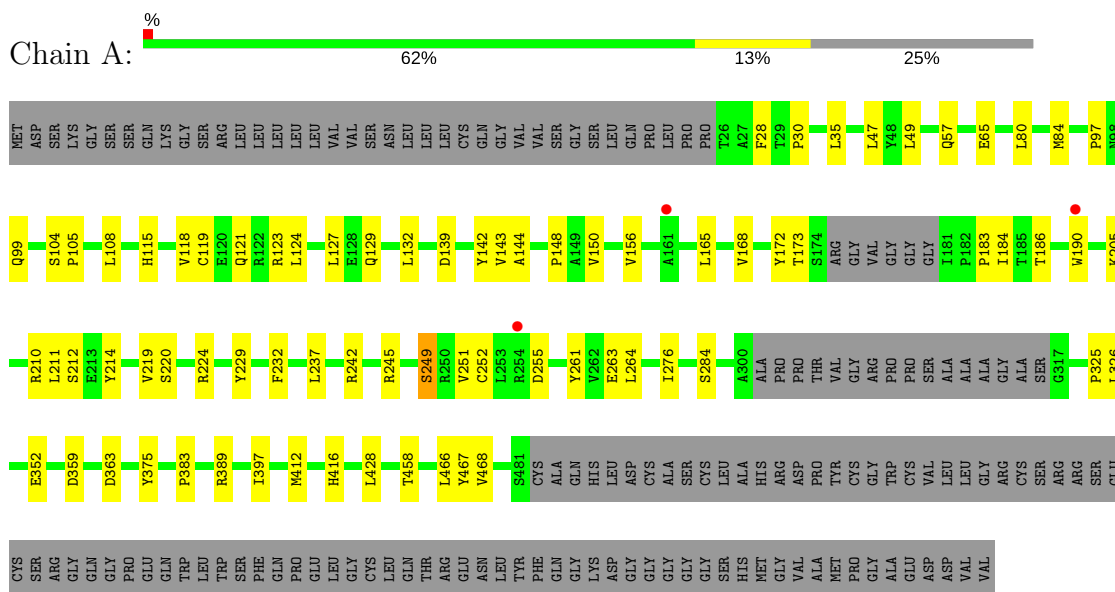
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	10	Total 10	O 10	0	0
4	H	1	Total 1	O 1	0	0
4	K	2	Total 2	O 2	0	0

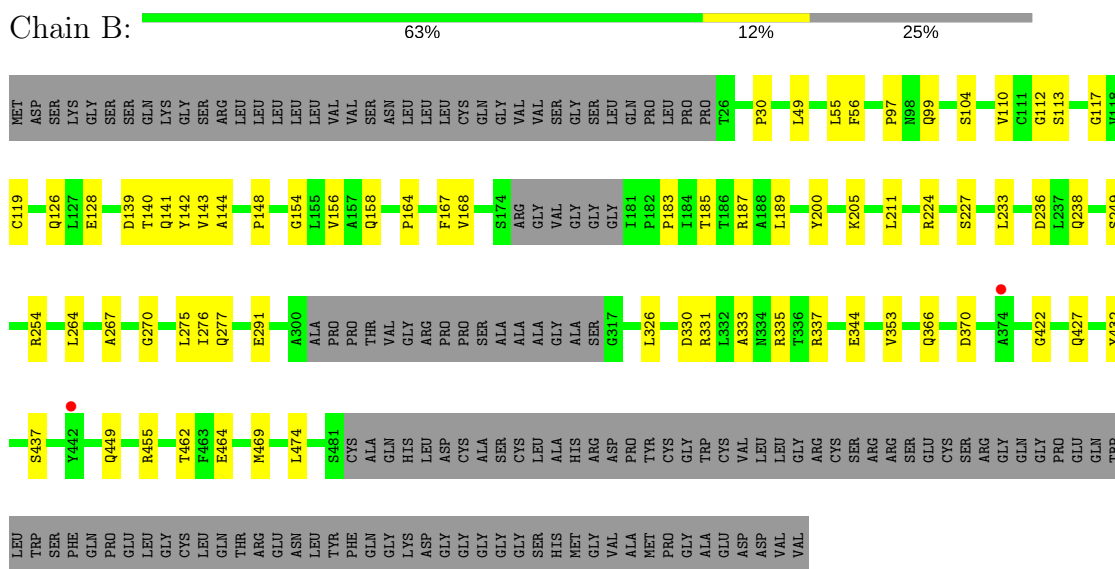
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

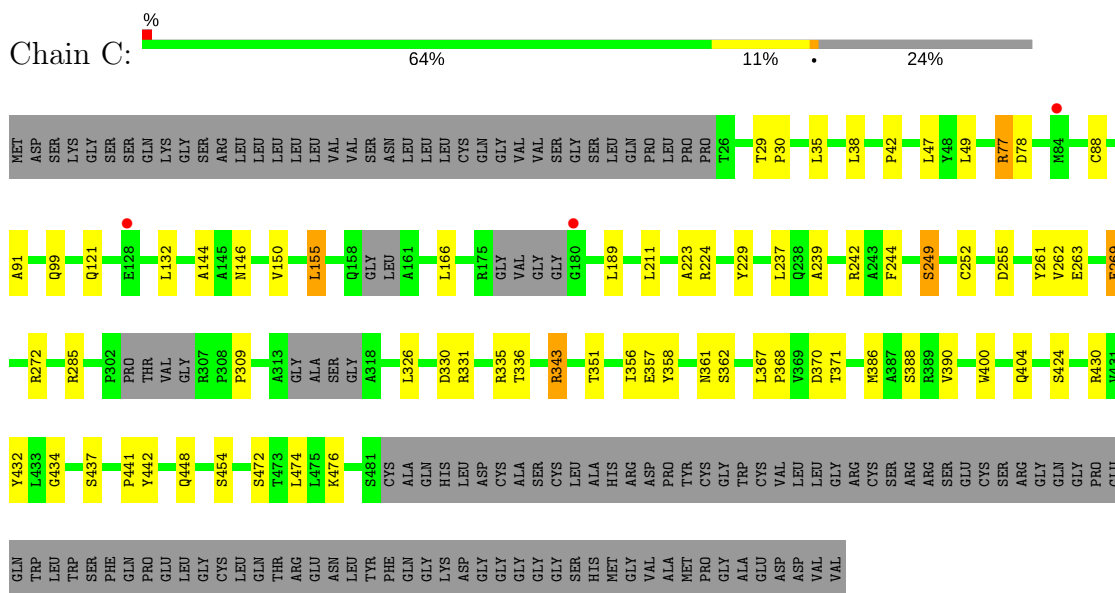
• Molecule 1: Plexin-B1



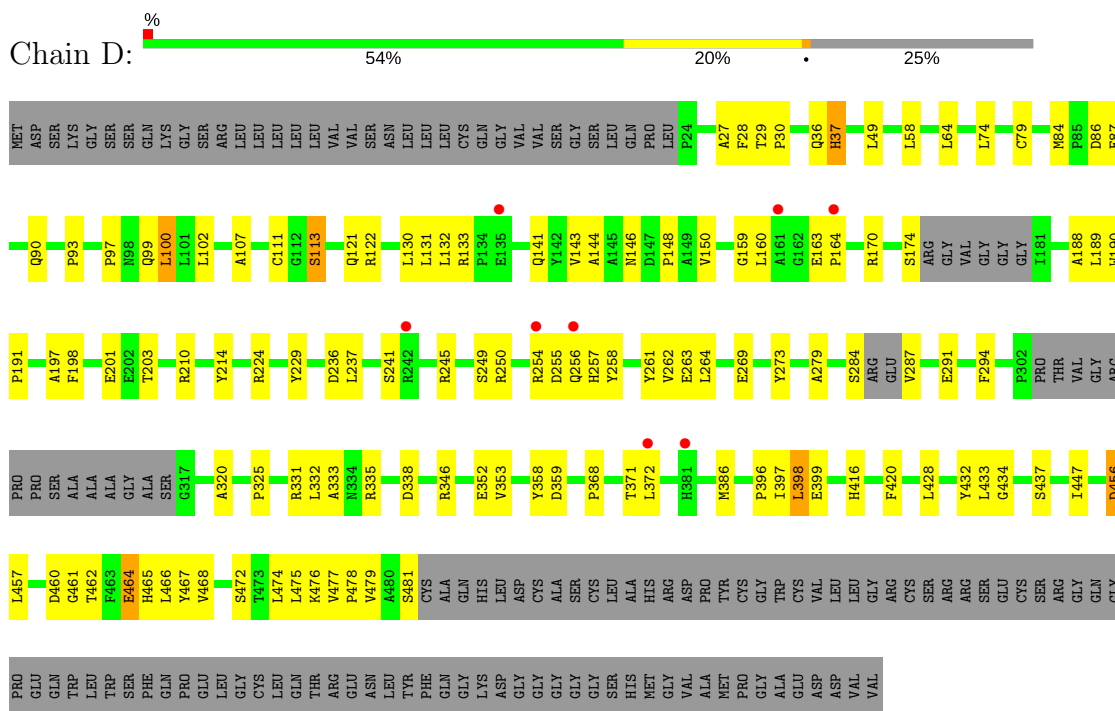
• Molecule 1: Plexin-B1



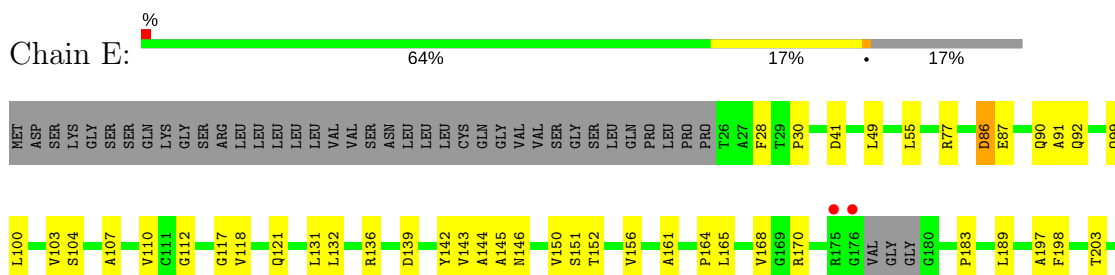
• Molecule 1: Plexin-B1

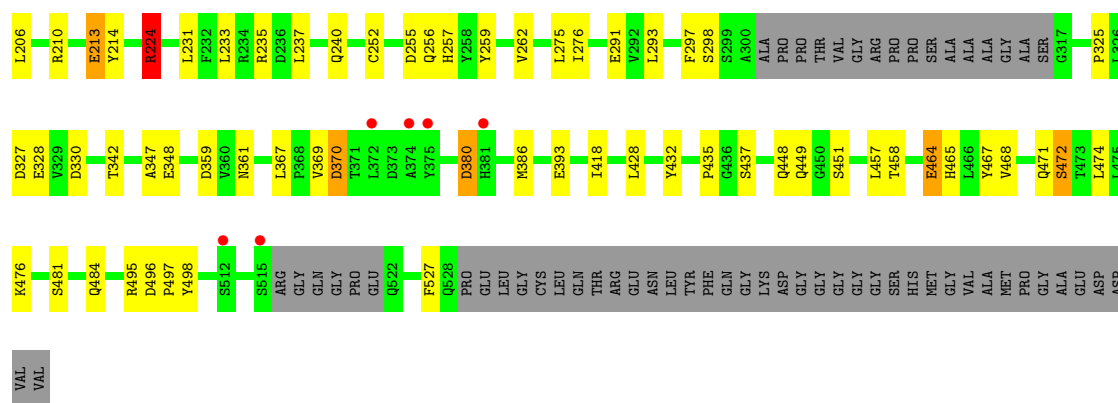


- Molecule 1: Plexin-B1

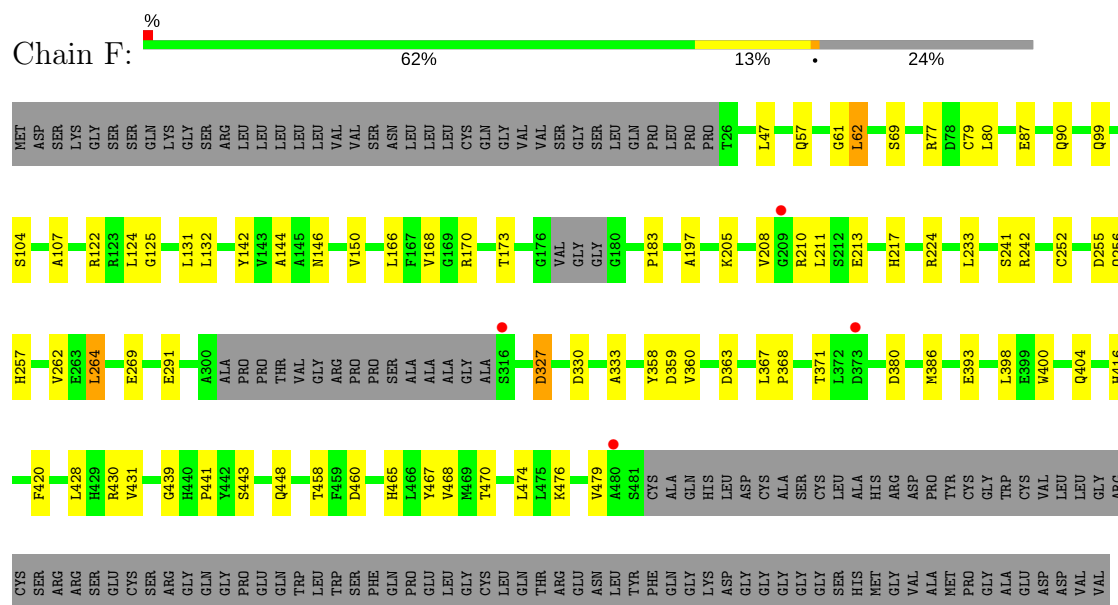


- Molecule 1: Plexin-B1

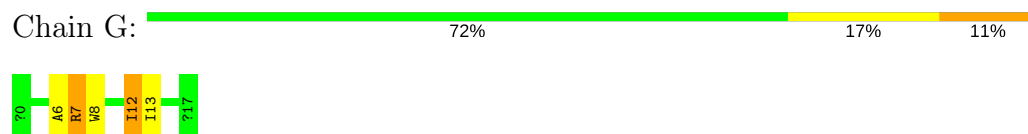




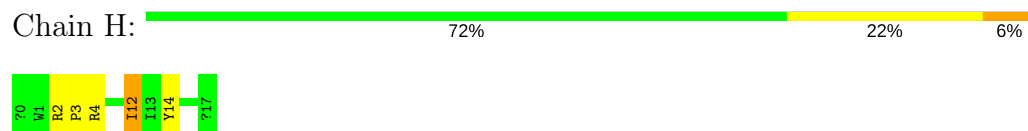
- Molecule 1: Plexin-B1



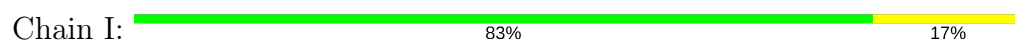
- Molecule 2: Synthesized cyclic peptide

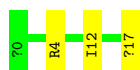


- Molecule 2: Synthesized cyclic peptide



- Molecule 2: Synthesized cyclic peptide





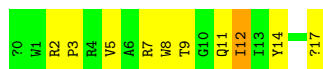
- Molecule 2: Synthesized cyclic peptide

Chain J: 72% 22% 6%



- Molecule 2: Synthesized cyclic peptide

Chain K: 44% 50% 6%



- Molecule 2: Synthesized cyclic peptide

Chain L: 78% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.43Å 217.92Å 106.47Å 90.00° 115.30° 90.00°	Depositor
Resolution (Å)	40.80 – 2.60 45.64 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.1 (40.80-2.60) 94.6 (45.64-2.55)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.54Å)	Xtriage
Refinement program	PHENIX (dev_2341: ???)	Depositor
R, R_{free}	0.225 , 0.265 0.219 , 0.264	Depositor DCC
R_{free} test set	5691 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21235	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTR, NAG, ACE, NH2

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	0.41	0/3377	0.60	0/4614
1	B	0.41	0/3377	0.62	0/4614
1	C	0.41	0/3435	0.62	0/4692
1	D	0.38	0/3385	0.61	1/4627 (0.0%)
1	E	0.42	0/3736	0.61	1/5098 (0.0%)
1	F	0.41	0/3402	0.61	0/4646
2	G	0.39	0/129	0.59	0/174
2	H	0.34	0/129	0.56	0/174
2	I	0.47	0/129	0.57	0/174
2	J	0.38	0/129	0.60	0/174
2	K	0.49	0/129	0.65	0/174
2	L	0.44	0/129	0.53	0/174
All	All	0.41	0/21486	0.61	2/29335 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	398	LEU	CA-CB-CG	5.08	126.98	115.30
1	E	224	ARG	NE-CZ-NH2	-5.05	117.78	120.30

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	3298	0	3180	42	0
1	B	3298	0	3179	43	0
1	C	3355	0	3236	44	0
1	D	3304	0	3187	82	0
1	E	3647	0	3496	64	1
1	F	3323	0	3204	45	1
2	G	144	0	140	5	0
2	H	144	0	140	7	0
2	I	144	0	140	2	0
2	J	144	0	140	4	0
2	K	144	0	140	9	0
2	L	144	0	140	2	0
3	A	14	0	13	0	0
3	B	28	0	26	3	0
3	C	14	0	13	1	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
3	F	14	0	13	1	0
4	A	3	0	0	0	0
4	B	16	0	0	2	0
4	C	8	0	0	1	0
4	D	1	0	0	0	0
4	E	7	0	0	0	0
4	F	10	0	0	0	0
4	H	1	0	0	0	0
4	K	2	0	0	0	0
All	All	21235	0	20413	329	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 8.

All (329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:393:GLU:HG2	1:F:393:GLU:HG2	1.53	0.90
1:F:252:CYS:HB2	1:F:255:ASP:HB2	1.55	0.87
1:C:224:ARG:NH2	1:C:330:ASP:OD2	2.13	0.82
1:F:224:ARG:NH2	1:F:330:ASP:OD2	2.12	0.82
1:C:38:LEU:HD11	1:C:47:LEU:HD22	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ARG:NH2	1:D:359:ASP:OD2	2.15	0.79
1:C:99:GLN:HG2	1:C:144:ALA:HB1	1.66	0.78
1:A:252:CYS:HB2	1:A:255:ASP:HB2	1.65	0.78
1:D:203:THR:HG1	1:D:257:HIS:HD1	1.30	0.77
1:D:130:LEU:HD22	1:D:133:ARG:HH11	1.50	0.77
1:E:233:LEU:HD21	1:E:275:LEU:HA	1.66	0.76
1:D:465:HIS:HA	1:D:478:PRO:HA	1.66	0.75
2:H:3:PRO:HB3	2:H:12:ILE:HD12	1.68	0.74
1:B:99:GLN:HG2	1:B:144:ALA:HB1	1.70	0.73
2:K:7:ARG:HG2	2:K:8:TRP:CD1	2.25	0.71
1:E:449:GLN:OE1	1:E:449:GLN:N	2.26	0.68
1:E:210:ARG:HB3	1:E:213:GLU:HG3	1.75	0.68
1:B:254:ARG:HD3	1:F:368:PRO:HG3	1.76	0.67
1:D:99:GLN:NE2	1:D:150:VAL:O	2.28	0.67
1:C:49:LEU:HD11	1:C:474:LEU:HD22	1.76	0.67
1:D:428:LEU:HD22	1:D:468:VAL:HG21	1.76	0.67
2:H:2:ARG:HH11	2:H:2:ARG:HG2	1.60	0.67
1:D:99:GLN:HG2	1:D:144:ALA:HB1	1.78	0.66
1:D:284:SER:HG	1:D:287:VAL:N	1.94	0.66
1:B:277:GLN:O	1:B:455:ARG:NH1	2.29	0.66
1:B:126:GLN:NE2	1:B:128:GLU:OE1	2.29	0.66
1:D:130:LEU:CD2	1:D:133:ARG:HH11	2.10	0.65
1:E:231:LEU:HD11	1:E:293:LEU:HD21	1.79	0.65
1:A:416:HIS:CE1	2:G:7:ARG:NH1	2.65	0.64
1:A:123:ARG:NH2	1:A:129:GLN:HG2	2.13	0.64
1:C:476:LYS:NZ	4:C:701:HOH:O	2.29	0.64
1:E:348:GLU:OE2	3:F:601:NAG:O3	2.16	0.64
1:E:224:ARG:NH2	1:E:330:ASP:OD2	2.31	0.64
1:F:398:LEU:HD21	1:F:431:VAL:HG11	1.79	0.64
1:D:236:ASP:OD2	1:D:245:ARG:NH1	2.31	0.64
1:E:77:ARG:NH1	1:E:146:ASN:O	2.31	0.64
1:F:183:PRO:HD3	1:F:211:LEU:HD21	1.79	0.64
1:D:255:ASP:OD1	1:D:258:TYR:N	2.29	0.63
1:D:210:ARG:HH11	1:D:237:LEU:HD13	1.62	0.63
1:D:79:CYS:SG	1:D:90:GLN:NE2	2.71	0.63
1:D:462:THR:OG1	1:D:464:GLU:OE1	2.18	0.62
1:C:237:LEU:HD22	1:C:242:ARG:HD2	1.81	0.62
1:D:456:ASP:N	1:D:456:ASP:OD2	2.32	0.62
1:C:99:GLN:NE2	1:C:150:VAL:O	2.33	0.62
1:D:141:GLN:NE2	1:D:197:ALA:O	2.31	0.62
1:D:420:PHE:HZ	1:D:479:VAL:HG23	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:GLU:HB2	1:D:164:PRO:HA	1.80	0.62
1:D:28:PHE:CD2	1:D:58:LEU:HD11	2.35	0.62
1:A:224:ARG:HD3	1:A:326:LEU:HD13	1.82	0.61
1:A:97:PRO:HG2	1:A:148:PRO:HB3	1.81	0.61
1:E:99:GLN:HG2	1:E:144:ALA:HB1	1.82	0.61
1:E:164:PRO:HB2	1:E:189:LEU:HB2	1.83	0.61
1:A:363:ASP:O	1:A:383:PRO:HB3	2.00	0.61
1:F:107:ALA:HA	1:F:124:LEU:HG	1.84	0.60
1:F:224:ARG:HD2	1:F:291:GLU:OE1	2.02	0.60
1:A:232:PHE:HE1	1:A:249:SER:HB3	1.67	0.60
1:B:140:THR:HG22	1:B:200:TYR:H	1.68	0.59
1:C:269:GLU:HG3	1:C:269:GLU:O	2.02	0.59
1:A:428:LEU:HD22	1:A:468:VAL:HG21	1.86	0.58
1:E:224:ARG:NH1	1:E:291:GLU:OE1	2.27	0.58
1:F:99:GLN:HG2	1:F:144:ALA:HB1	1.85	0.58
1:A:57:GLN:HG2	1:A:65:GLU:HB2	1.85	0.57
1:B:141:GLN:O	4:B:701:HOH:O	2.17	0.57
1:D:432:TYR:CD2	1:D:437:SER:HB2	2.38	0.57
1:F:107:ALA:HB2	1:F:131:LEU:HD12	1.86	0.57
1:E:107:ALA:HB2	1:E:131:LEU:HD12	1.85	0.57
1:E:393:GLU:HG2	1:F:393:GLU:CG	2.32	0.57
1:E:49:LEU:HD11	1:E:474:LEU:HD22	1.85	0.57
1:B:462:THR:OG1	1:B:464:GLU:OE1	2.19	0.57
1:C:262:VAL:HA	1:C:386:MET:O	2.05	0.57
1:F:420:PHE:CE1	1:F:430:ARG:HG2	2.39	0.56
1:E:467:TYR:CE1	1:E:476:LYS:HG3	2.40	0.56
1:F:460:ASP:HB2	1:F:465:HIS:HB2	1.86	0.56
1:F:430:ARG:HD2	1:F:443:SER:HB3	1.88	0.56
1:B:164:PRO:HB2	1:B:189:LEU:HB2	1.88	0.56
1:B:233:LEU:HD21	1:B:275:LEU:HA	1.86	0.56
1:F:252:CYS:HB2	1:F:255:ASP:CB	2.32	0.56
1:A:115:HIS:O	1:A:118:VAL:HG23	2.06	0.56
1:C:155:LEU:HD11	1:C:223:ALA:HB2	1.87	0.56
1:D:49:LEU:HD21	1:D:474:LEU:HD22	1.89	0.55
1:A:210:ARG:NH2	1:A:359:ASP:OD1	2.40	0.55
1:B:344:GLU:HG3	1:B:366:GLN:HG3	1.88	0.55
1:C:351:THR:HA	2:J:11:GLN:NE2	2.21	0.55
1:D:131:LEU:O	1:D:132:LEU:HD23	2.06	0.55
1:D:320:ALA:HB1	1:D:396:PRO:HB3	1.89	0.55
2:K:12:ILE:HD11	2:K:14:TYR:CD2	2.41	0.55
1:D:264:LEU:HD22	1:D:332:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:ASP:N	1:E:380:ASP:OD2	2.28	0.55
1:D:273:TYR:OH	1:D:399:GLU:OE2	2.21	0.55
1:E:90:GLN:OE1	1:E:90:GLN:N	2.37	0.55
1:D:28:PHE:CZ	1:D:30:PRO:HG3	2.42	0.55
1:F:80:LEU:HD22	1:F:142:TYR:HE2	1.71	0.55
2:K:9:THR:HB	2:K:11:GLN:HE21	1.71	0.55
1:D:397:ILE:HG21	1:D:433:LEU:HD22	1.89	0.55
1:F:256:GLN:HG3	1:F:257:HIS:CD2	2.42	0.55
1:C:434:GLY:O	2:I:4:ARG:HD2	2.06	0.54
1:A:150:VAL:HG21	1:A:173:THR:HG22	1.89	0.54
1:D:28:PHE:CE1	1:D:64:LEU:HD11	2.42	0.54
1:C:331:ARG:HG3	3:C:601:NAG:H81	1.90	0.54
1:E:203:THR:HG21	1:E:257:HIS:HD1	1.72	0.54
1:D:97:PRO:O	1:D:113:SER:OG	2.22	0.54
1:C:252:CYS:HB2	1:C:255:ASP:HB2	1.91	0.53
1:D:107:ALA:HB1	1:D:122:ARG:O	2.08	0.53
1:F:47:LEU:HD11	1:F:467:TYR:CE1	2.42	0.53
1:A:183:PRO:HD3	1:A:211:LEU:HD21	1.91	0.53
1:D:28:PHE:HD2	1:D:58:LEU:HD11	1.74	0.53
1:B:233:LEU:HD21	1:B:276:ILE:H	1.74	0.52
1:D:224:ARG:HB3	1:D:229:TYR:CE1	2.45	0.52
1:E:210:ARG:HH21	1:E:359:ASP:CG	2.13	0.52
1:D:467:TYR:CE1	1:D:476:LYS:HD2	2.44	0.52
1:F:416:HIS:NE2	2:L:7:ARG:NH1	2.56	0.52
1:A:35:LEU:HD22	1:A:49:LEU:HD13	1.90	0.52
1:D:143:VAL:O	1:D:170:ARG:HD2	2.10	0.52
1:C:448:GLN:OE1	1:C:472:SER:HB2	2.09	0.52
1:F:80:LEU:HD22	1:F:142:TYR:CE2	2.44	0.52
1:A:172:TYR:CZ	1:A:212:SER:HB3	2.45	0.52
1:D:160:LEU:HD22	1:D:254:ARG:HG3	1.92	0.52
2:H:3:PRO:O	2:H:4:ARG:NH1	2.43	0.52
1:D:368:PRO:O	1:D:371:THR:OG1	2.22	0.52
1:A:325:PRO:HG3	2:G:12:ILE:HG21	1.93	0.51
2:K:3:PRO:HB3	2:K:12:ILE:HD13	1.91	0.51
1:D:465:HIS:CG	1:D:476:LYS:HE3	2.45	0.51
1:E:262:VAL:HA	1:E:386:MET:O	2.11	0.51
1:D:447:ILE:HG23	1:D:475:LEU:HD12	1.93	0.51
1:D:263:GLU:OE2	1:D:358:TYR:OH	2.19	0.51
1:D:86:ASP:OD1	1:D:87:GLU:N	2.44	0.51
1:A:99:GLN:HG2	1:A:144:ALA:HB1	1.92	0.51
1:D:261:TYR:OH	1:D:263:GLU:OE2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:SER:HB2	1:E:156:VAL:HG11	1.91	0.51
1:D:36:GLN:C	1:D:37:HIS:HD1	2.13	0.51
1:D:122:ARG:HG2	1:D:130:LEU:HD12	1.92	0.50
1:E:342:THR:HG22	1:E:367:LEU:O	2.11	0.50
1:C:272:ARG:HD2	2:J:1:DTR:CE2	2.41	0.50
1:A:123:ARG:HH21	1:A:129:GLN:HG2	1.76	0.50
1:C:357:GLU:HG3	1:C:358:TYR:N	2.26	0.50
1:C:368:PRO:HB2	1:C:370:ASP:OD1	2.11	0.50
1:B:224:ARG:NH1	1:B:291:GLU:OE1	2.45	0.50
1:E:448:GLN:NE2	1:E:472:SER:HB2	2.26	0.50
1:A:165:LEU:HD22	1:A:186:THR:HG22	1.94	0.50
1:B:185:THR:HG22	1:B:205:LYS:HB3	1.94	0.50
1:A:251:VAL:CG2	1:A:261:TYR:HD1	2.25	0.50
1:E:252:CYS:HB2	1:E:255:ASP:HB2	1.94	0.50
1:D:241:SER:H	2:I:17:NH2:N	2.10	0.50
1:B:224:ARG:HD3	1:B:326:LEU:HD13	1.93	0.50
1:F:170:ARG:NH1	1:F:173:THR:OG1	2.31	0.50
1:C:404:GLN:HB3	1:C:424:SER:HB3	1.94	0.49
1:E:481:SER:O	1:E:484:GLN:HG2	2.12	0.49
1:B:224:ARG:NH2	1:B:330:ASP:OD2	2.46	0.49
1:E:240:GLN:OE1	1:E:240:GLN:HA	2.12	0.49
2:K:3:PRO:HB3	2:K:12:ILE:CD1	2.42	0.49
1:A:375:TYR:CZ	1:E:161:ALA:HB2	2.47	0.49
1:E:28:PHE:CE2	1:E:30:PRO:HG3	2.48	0.49
1:F:430:ARG:NH1	1:F:479:VAL:O	2.46	0.49
1:C:121:GLN:HE21	1:C:132:LEU:HD23	1.78	0.49
1:F:99:GLN:NE2	1:F:150:VAL:O	2.43	0.49
1:B:99:GLN:CG	1:B:144:ALA:HB1	2.39	0.49
1:D:224:ARG:NH1	1:D:291:GLU:OE2	2.45	0.49
1:F:416:HIS:N	1:F:416:HIS:CD2	2.81	0.49
1:B:432:TYR:CD2	1:B:437:SER:HB2	2.47	0.49
1:F:428:LEU:HD22	1:F:468:VAL:HG21	1.95	0.49
1:D:146:ASN:H	1:D:170:ARG:HH21	1.61	0.48
1:E:276:ILE:HB	1:E:297:PHE:CE1	2.48	0.48
1:A:352:GLU:CD	1:A:389:ARG:HE	2.17	0.48
1:D:465:HIS:HD2	1:D:478:PRO:HG3	1.78	0.48
1:B:183:PRO:HD3	1:B:211:LEU:HD11	1.95	0.48
1:F:465:HIS:CG	1:F:476:LYS:HE2	2.49	0.48
1:B:254:ARG:HD2	1:B:254:ARG:N	2.29	0.48
1:D:432:TYR:CZ	1:D:434:GLY:HA3	2.49	0.48
1:D:432:TYR:HD2	1:D:437:SER:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:LEU:HD21	1:E:197:ALA:HB2	1.95	0.48
1:A:108:LEU:HB2	1:A:124:LEU:HD23	1.95	0.48
1:D:121:GLN:HG3	1:D:198:PHE:HZ	1.79	0.48
1:D:338:ASP:OD1	1:D:372:LEU:HD11	2.14	0.48
1:F:264:LEU:HD21	1:F:333:ALA:HA	1.95	0.48
1:B:337:ARG:NH1	3:B:602:NAG:O6	2.47	0.47
1:C:244:PHE:CZ	1:C:309:PRO:HG3	2.48	0.47
1:D:159:GLY:H	1:D:163:GLU:HA	1.79	0.47
1:A:139:ASP:HA	1:A:142:TYR:CE2	2.50	0.47
1:E:55:LEU:HD11	1:E:110:VAL:HG11	1.95	0.47
1:C:432:TYR:CD2	1:C:437:SER:HB2	2.49	0.47
1:A:219:VAL:HG21	1:A:276:ILE:HG23	1.96	0.47
1:C:336:THR:OG1	1:C:388:SER:HB2	2.15	0.47
1:E:210:ARG:NH2	1:E:359:ASP:OD1	2.48	0.47
1:F:241:SER:H	2:K:17:NH2:N	2.12	0.47
1:B:104:SER:HB2	1:B:156:VAL:HG11	1.96	0.47
1:B:139:ASP:HA	1:B:142:TYR:CE2	2.49	0.47
2:H:3:PRO:HB3	2:H:12:ILE:CD1	2.42	0.47
1:A:214:TYR:CZ	1:A:237:LEU:HD12	2.49	0.47
1:D:416:HIS:HB3	1:D:432:TYR:HE1	1.79	0.47
1:D:464:GLU:O	1:D:479:VAL:HG12	2.15	0.47
1:A:263:GLU:O	1:A:264:LEU:HD23	2.15	0.47
1:E:451:SER:OG	1:E:471:GLN:HG2	2.15	0.47
1:D:262:VAL:HA	1:D:386:MET:O	2.14	0.46
1:E:481:SER:HB2	1:E:484:GLN:NE2	2.30	0.46
1:F:61:GLY:O	1:F:62:LEU:HB2	2.16	0.46
1:C:224:ARG:HD3	1:C:326:LEU:HD13	1.96	0.46
1:A:119:CYS:SG	1:A:143:VAL:HB	2.55	0.46
1:B:49:LEU:HD21	1:B:474:LEU:HD22	1.96	0.46
1:E:256:GLN:HG3	1:E:257:HIS:HD2	1.81	0.46
1:E:121:GLN:HG3	1:E:198:PHE:HZ	1.81	0.46
1:F:208:VAL:HG22	1:F:358:TYR:CG	2.51	0.46
1:C:367:LEU:HD13	1:C:371:THR:HG21	1.98	0.46
1:C:335:ARG:HH22	1:C:390:VAL:HG21	1.80	0.45
1:D:264:LEU:HD21	1:D:333:ALA:HA	1.96	0.45
1:C:166:LEU:HB2	1:C:189:LEU:HD13	1.99	0.45
1:C:357:GLU:HG3	1:C:358:TYR:H	1.82	0.45
1:E:112:GLY:O	1:E:117:GLY:HA2	2.15	0.45
1:D:203:THR:O	1:D:257:HIS:HA	2.17	0.45
1:F:213:GLU:OE1	1:F:242:ARG:NH1	2.49	0.45
1:B:112:GLY:O	1:B:117:GLY:HA2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ARG:NE	1:D:353:VAL:HG11	2.32	0.45
2:G:6:ALA:HA	2:G:13:ILE:HD11	1.98	0.45
1:A:416:HIS:CE1	2:G:7:ARG:HH11	2.32	0.45
1:D:457:LEU:HB3	1:D:466:LEU:HD11	1.98	0.45
1:B:49:LEU:HB2	1:B:56:PHE:HB2	1.99	0.45
1:E:41:ASP:HA	1:E:103:VAL:HG11	1.98	0.45
1:B:449:GLN:HG3	1:C:42:PRO:O	2.17	0.44
1:D:74:LEU:HD23	1:D:93:PRO:HA	1.99	0.44
2:H:2:ARG:NH1	2:H:2:ARG:HG2	2.31	0.44
1:D:107:ALA:HB2	1:D:131:LEU:HD12	1.97	0.44
1:E:203:THR:HG21	1:E:257:HIS:ND1	2.33	0.44
1:D:100:LEU:HB2	1:D:111:CYS:HB2	1.97	0.44
1:D:97:PRO:HG2	1:D:148:PRO:HB3	2.00	0.44
1:F:398:LEU:HD23	1:F:439:GLY:O	2.17	0.44
1:D:250:ARG:O	1:D:261:TYR:HA	2.18	0.44
1:E:369:VAL:O	1:E:370:ASP:CB	2.66	0.44
1:E:432:TYR:CD2	1:E:437:SER:HB3	2.52	0.44
1:E:435:PRO:HD3	2:K:5:VAL:O	2.17	0.44
1:F:367:LEU:HD13	1:F:371:THR:HG21	1.99	0.44
1:D:346:ARG:NH1	1:D:352:GLU:OE2	2.50	0.44
1:F:217:HIS:HB2	1:F:233:LEU:HB3	2.00	0.44
1:B:422:GLY:HA2	1:B:427:GLN:O	2.18	0.44
1:D:201:GLU:C	1:D:203:THR:H	2.21	0.44
1:E:418:ILE:HD11	1:E:497:PRO:HB2	1.99	0.44
1:E:213:GLU:O	1:E:235:ARG:NH1	2.49	0.44
1:F:467:TYR:HB3	1:F:474:LEU:HD11	2.00	0.44
1:B:158:GLN:NE2	4:B:703:HOH:O	2.37	0.43
1:F:166:LEU:HG	1:F:168:VAL:HG23	2.00	0.43
1:C:343:ARG:HE	1:C:343:ARG:HB2	1.49	0.43
1:E:255:ASP:OD2	1:E:259:TYR:N	2.51	0.43
1:C:356:ILE:HG21	1:C:362:SER:HB3	1.98	0.43
1:E:256:GLN:HG3	1:E:257:HIS:CD2	2.53	0.43
1:F:448:GLN:HB2	1:F:470:THR:HG21	2.01	0.43
1:A:458:THR:O	1:A:466:LEU:HD12	2.18	0.43
1:B:264:LEU:HD21	1:B:333:ALA:HA	2.00	0.43
1:C:400:TRP:CZ2	1:C:441:PRO:HD3	2.54	0.43
1:E:99:GLN:O	1:E:152:THR:HB	2.18	0.43
1:B:143:VAL:HG22	1:B:187:ARG:NE	2.34	0.43
1:C:88:CYS:SG	1:C:91:ALA:HB2	2.58	0.43
1:D:164:PRO:HB2	1:D:189:LEU:HD12	2.01	0.43
1:E:464:GLU:HB3	1:E:465:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:THR:HG23	1:D:256:GLN:O	2.18	0.43
1:B:119:CYS:SG	1:B:143:VAL:HB	2.58	0.43
1:B:331:ARG:HG3	3:B:602:NAG:H81	2.01	0.43
1:E:214:TYR:CZ	1:E:237:LEU:HD12	2.54	0.43
1:A:229:TYR:HA	1:A:249:SER:O	2.19	0.43
1:A:237:LEU:HD22	1:A:242:ARG:CZ	2.48	0.43
1:E:91:ALA:O	1:E:92:GLN:HG3	2.19	0.43
1:D:214:TYR:OH	1:D:358:TYR:HA	2.19	0.43
1:B:55:LEU:HD11	1:B:110:VAL:HG11	2.01	0.42
1:B:211:LEU:HA	1:B:211:LEU:HD23	1.82	0.42
1:A:132:LEU:HD22	1:A:190:TRP:CE3	2.55	0.42
1:B:97:PRO:HG2	1:B:148:PRO:HB3	2.01	0.42
1:C:252:CYS:HB2	1:C:255:ASP:CB	2.49	0.42
1:E:342:THR:HG21	1:E:369:VAL:HG12	2.00	0.42
1:C:331:ARG:NH2	1:D:335:ARG:HG3	2.34	0.42
1:F:262:VAL:HA	1:F:386:MET:O	2.19	0.42
1:A:47:LEU:HD11	1:A:467:TYR:CE1	2.53	0.42
1:C:239:ALA:HB1	2:J:17:NH2:N	2.34	0.42
1:B:143:VAL:HG13	1:B:168:VAL:HG21	2.02	0.42
1:D:188:ALA:HB3	1:D:191:PRO:HG3	2.01	0.42
1:D:210:ARG:NH1	1:D:237:LEU:HD13	2.31	0.42
1:B:183:PRO:HG3	1:B:211:LEU:HD21	2.01	0.42
1:A:284:SER:OG	1:A:412:MET:N	2.53	0.42
1:A:80:LEU:HD22	1:A:142:TYR:OH	2.19	0.42
1:C:261:TYR:CE2	1:C:263:GLU:HG3	2.55	0.42
1:C:30:PRO:HG3	1:C:35:LEU:HD21	2.02	0.42
1:E:325:PRO:HB2	1:E:328:GLU:HG2	2.01	0.42
1:E:457:LEU:HD23	1:E:457:LEU:HA	1.92	0.42
1:A:245:ARG:HD3	1:A:245:ARG:HH11	1.70	0.42
1:E:99:GLN:NE2	1:E:150:VAL:O	2.53	0.42
1:F:90:GLN:CD	1:F:90:GLN:H	2.23	0.42
2:L:7:ARG:HG2	2:L:8:TRP:CE3	2.55	0.41
1:A:412:MET:HA	1:A:416:HIS:O	2.19	0.41
1:B:30:PRO:HA	3:B:601:NAG:H82	2.02	0.41
1:C:249:SER:OG	1:C:261:TYR:OH	2.35	0.41
2:H:12:ILE:HD11	2:H:14:TYR:CD2	2.56	0.41
2:K:9:THR:HB	2:K:11:GLN:NE2	2.34	0.41
1:A:168:VAL:O	1:A:184:ILE:HA	2.21	0.41
1:D:420:PHE:CZ	1:D:479:VAL:HG23	2.50	0.41
1:E:100:LEU:HD13	1:E:152:THR:HG22	2.01	0.41
1:B:267:ALA:HB1	1:B:270:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:496:ASP:OD1	1:E:498:TYR:HB2	2.20	0.41
1:B:236:ASP:OD1	1:B:238:GLN:HB2	2.21	0.41
1:D:249:SER:OG	1:D:263:GLU:HG2	2.21	0.41
1:E:464:GLU:HB3	1:E:465:HIS:CE1	2.55	0.41
1:F:77:ARG:HD3	1:F:146:ASN:HD22	1.85	0.41
1:A:105:PRO:HD3	1:A:156:VAL:HG11	2.03	0.41
1:C:229:TYR:HA	1:C:249:SER:O	2.21	0.41
1:E:165:LEU:HD23	1:E:165:LEU:HA	1.85	0.41
1:F:79:CYS:SG	1:F:90:GLN:NE2	2.94	0.41
1:A:28:PHE:CD2	1:A:30:PRO:HD3	2.56	0.41
1:D:27:ALA:HB2	1:D:475:LEU:HD23	2.02	0.41
1:F:132:LEU:HD21	1:F:197:ALA:HB2	2.03	0.41
1:A:121:GLN:NE2	1:A:132:LEU:HD23	2.36	0.41
1:C:430:ARG:HB3	1:C:442:TYR:CZ	2.56	0.41
1:D:29:THR:HG23	1:D:472:SER:O	2.20	0.41
1:D:460:ASP:OD1	1:D:461:GLY:N	2.54	0.41
1:E:143:VAL:HG13	1:E:168:VAL:HG21	2.02	0.41
1:E:145:ALA:HA	1:E:170:ARG:CZ	2.51	0.41
2:K:2:ARG:HA	2:K:3:PRO:HD3	1.92	0.41
1:B:335:ARG:NE	1:B:353:VAL:HG11	2.35	0.41
1:B:469:MET:HB2	1:B:474:LEU:HD13	2.02	0.41
1:C:432:TYR:CZ	1:C:434:GLY:HA3	2.55	0.41
1:F:400:TRP:CZ2	1:F:441:PRO:HD3	2.55	0.41
1:B:154:GLY:HA2	1:B:167:PHE:O	2.20	0.40
1:E:347:ALA:HB1	1:F:327:ASP:OD2	2.21	0.40
1:E:428:LEU:HD22	1:E:468:VAL:HG21	2.03	0.40
2:G:7:ARG:HG2	2:G:8:TRP:CE3	2.56	0.40
1:C:335:ARG:HD3	1:D:331:ARG:CD	2.51	0.40
1:D:100:LEU:CD2	1:D:102:LEU:HG	2.51	0.40
1:D:132:LEU:HD11	1:D:190:TRP:CE3	2.57	0.40
1:D:279:ALA:HA	1:D:294:PHE:O	2.21	0.40
1:E:183:PRO:HG2	1:E:206:LEU:HD23	2.02	0.40
1:F:57:GLN:NE2	1:F:125:GLY:O	2.43	0.40
1:D:325:PRO:HG3	2:J:12:ILE:HG21	2.04	0.40
1:C:77:ARG:HD3	1:C:146:ASN:O	2.22	0.40
1:E:139:ASP:HA	1:E:142:TYR:CE2	2.56	0.40
2:H:12:ILE:HG12	2:H:14:TYR:CE1	2.57	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)
1:E:86:ASP:OD1	1:F:122:ARG:NH2[1_656]	2.01	0.19

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/579 (74%)	413 (96%)	15 (4%)	0	100	100
1	B	428/579 (74%)	414 (97%)	14 (3%)	0	100	100
1	C	432/579 (75%)	418 (97%)	14 (3%)	0	100	100
1	D	428/579 (74%)	408 (95%)	20 (5%)	0	100	100
1	E	470/579 (81%)	448 (95%)	21 (4%)	1 (0%)	51	76
1	F	432/579 (75%)	416 (96%)	15 (4%)	1 (0%)	51	76
2	G	15/18 (83%)	13 (87%)	2 (13%)	0	100	100
2	H	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
2	I	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
2	J	15/18 (83%)	13 (87%)	1 (7%)	1 (7%)	1	1
2	K	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
2	L	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
All	All	2708/3582 (76%)	2599 (96%)	106 (4%)	3 (0%)	55	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	370	ASP
2	J	16	SER
1	F	380	ASP

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	352/464 (76%)	345 (98%)	7 (2%)	60	83
1	B	352/464 (76%)	348 (99%)	4 (1%)	78	92
1	C	357/464 (77%)	346 (97%)	11 (3%)	45	73
1	D	353/464 (76%)	342 (97%)	11 (3%)	45	73
1	E	389/464 (84%)	373 (96%)	16 (4%)	35	63
1	F	354/464 (76%)	340 (96%)	14 (4%)	36	64
2	G	13/13 (100%)	11 (85%)	2 (15%)	3	5
2	H	13/13 (100%)	12 (92%)	1 (8%)	15	29
2	I	13/13 (100%)	12 (92%)	1 (8%)	15	29
2	J	13/13 (100%)	12 (92%)	1 (8%)	15	29
2	K	13/13 (100%)	12 (92%)	1 (8%)	15	29
2	L	13/13 (100%)	11 (85%)	2 (15%)	3	5
All	All	2235/2862 (78%)	2164 (97%)	71 (3%)	44	72

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	MET
1	A	104	SER
1	A	127	LEU
1	A	205	LYS
1	A	220	SER
1	A	249	SER
1	A	397	ILE
1	B	113	SER
1	B	227	SER
1	B	249	SER
1	B	370	ASP
1	C	29	THR
1	C	77	ARG
1	C	78	ASP

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Mol	Chain	Res	Type
1	C	155	LEU
1	C	211	LEU
1	C	249	SER
1	C	269	GLU
1	C	285	ARG
1	C	343	ARG
1	C	361	ASN
1	C	454	SER
1	D	37	HIS
1	D	84	MET
1	D	100	LEU
1	D	113	SER
1	D	174	SER
1	D	269	GLU
1	D	398	LEU
1	D	456	ASP
1	D	464	GLU
1	D	477	VAL
1	D	481	SER
1	E	86	ASP
1	E	87	GLU
1	E	118	VAL
1	E	136	ARG
1	E	151	SER
1	E	213	GLU
1	E	224	ARG
1	E	298	SER
1	E	327	ASP
1	E	361	ASN
1	E	380	ASP
1	E	458	THR
1	E	464	GLU
1	E	472	SER
1	E	495	ARG
1	E	527	PHE
1	F	62	LEU
1	F	69	SER
1	F	87	GLU
1	F	104	SER
1	F	205	LYS
1	F	210	ARG
1	F	264	LEU

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Mol	Chain	Res	Type
1	F	269	GLU
1	F	327	ASP
1	F	359	ASP
1	F	360	VAL
1	F	363	ASP
1	F	404	GLN
1	F	458	THR
2	G	7	ARG
2	G	12	ILE
2	H	12	ILE
2	I	12	ILE
2	J	12	ILE
2	K	12	ILE
2	L	9	THR
2	L	12	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
2	DTR	G	1	2	14,15,16	1.07	1 (7%)	13,20,22	0.98	0
2	DTR	H	1	2	14,15,16	0.93	1 (7%)	13,20,22	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DTR	I	1	2	14,15,16	0.87	0	13,20,22	0.99	0
2	DTR	J	1	2	14,15,16	0.98	1 (7%)	13,20,22	0.97	0
2	DTR	K	1	2	14,15,16	1.12	1 (7%)	13,20,22	0.91	0
2	DTR	L	1	2	14,15,16	1.02	1 (7%)	13,20,22	0.93	0

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
2	DTR	G	1	2	-	0/3/6/8	0/2/2/2
2	DTR	H	1	2	-	0/3/6/8	0/2/2/2
2	DTR	I	1	2	-	0/3/6/8	0/2/2/2
2	DTR	J	1	2	-	0/3/6/8	0/2/2/2
2	DTR	K	1	2	-	0/3/6/8	0/2/2/2
2	DTR	L	1	2	-	0/3/6/8	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	DTR	CA-C	2.19	1.53	1.50
2	J	1	DTR	CA-C	2.62	1.53	1.50
2	L	1	DTR	CA-C	2.62	1.53	1.50
2	G	1	DTR	CA-C	2.88	1.54	1.50
2	K	1	DTR	CA-C	3.26	1.54	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	DTR	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

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$
3	NAG	A	601	1	14,14,15	0.79	1 (7%)	15,19,21	0.76	1 (6%)
3	NAG	B	601	1	14,14,15	0.49	0	15,19,21	0.70	1 (6%)
3	NAG	B	602	1	14,14,15	0.49	0	15,19,21	0.85	1 (6%)
3	NAG	C	601	1	14,14,15	0.41	0	15,19,21	0.92	1 (6%)
3	NAG	D	601	1	14,14,15	0.43	0	15,19,21	0.58	0
3	NAG	E	601	1	14,14,15	0.32	0	15,19,21	0.84	1 (6%)
3	NAG	F	601	1	14,14,15	0.31	0	15,19,21	0.79	1 (6%)

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
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
3	NAG	B	601	1	-	0/6/23/26	0/1/1/1
3	NAG	B	602	1	-	0/6/23/26	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	D	601	1	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1	-	0/6/23/26	0/1/1/1
3	NAG	F	601	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NAG	O5-C1	-2.85	1.39	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	601	NAG	C1-O5-C5	2.01	114.94	112.17
3	B	602	NAG	C1-O5-C5	2.38	115.45	112.17
3	A	601	NAG	C1-O5-C5	2.41	115.49	112.17
3	F	601	NAG	C1-O5-C5	2.62	115.77	112.17
3	E	601	NAG	C1-O5-C5	2.67	115.85	112.17
3	C	601	NAG	C1-O5-C5	3.01	116.31	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NAG	1	0
3	B	602	NAG	2	0
3	C	601	NAG	1	0
3	F	601	NAG	1	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	434/579 (74%)	-0.26	3 (0%) 87 85	31, 50, 73, 118	0
1	B	434/579 (74%)	-0.29	2 (0%) 90 89	28, 46, 71, 88	0
1	C	442/579 (76%)	-0.23	3 (0%) 87 85	30, 51, 76, 90	0
1	D	436/579 (75%)	0.07	8 (1%) 69 63	38, 65, 97, 124	0
1	E	478/579 (82%)	-0.13	8 (1%) 70 65	31, 51, 79, 133	0
1	F	438/579 (75%)	-0.13	4 (0%) 84 81	31, 57, 84, 109	0
2	G	15/18 (83%)	-0.66	0 100 100	40, 46, 56, 56	0
2	H	15/18 (83%)	-0.54	0 100 100	37, 40, 50, 51	0
2	I	15/18 (83%)	-0.51	0 100 100	33, 42, 50, 52	0
2	J	15/18 (83%)	-0.19	0 100 100	51, 59, 79, 96	0
2	K	15/18 (83%)	-0.44	0 100 100	29, 31, 43, 60	0
2	L	15/18 (83%)	-0.14	0 100 100	45, 50, 68, 79	0
All	All	2752/3582 (76%)	-0.17	28 (1%) 82 79	28, 52, 82, 133	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	316	SER	5.4
1	D	161	ALA	5.3
1	A	254	ARG	4.3
1	E	176	GLY	3.6
1	E	372	LEU	3.6
1	D	164	PRO	3.5
1	E	374	ALA	3.3
1	C	84	MET	3.3
1	F	373	ASP	2.9
1	F	480	ALA	2.8
1	E	381	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	381	HIS	2.6
1	D	256	GLN	2.5
1	B	374	ALA	2.5
1	D	254	ARG	2.5
1	A	161	ALA	2.4
1	D	372	LEU	2.4
1	C	128	GLU	2.4
1	F	209	GLY	2.4
1	E	175	ARG	2.3
1	D	135	GLU	2.3
1	A	190	TRP	2.3
1	E	515	SER	2.2
1	E	512	SER	2.2
1	B	442	TYR	2.2
1	D	242	ARG	2.1
1	C	180	GLY	2.1
1	E	375	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	DTR	H	1	14/15	0.96	0.13	-	44,47,49,49	0
2	DTR	L	1	14/15	0.97	0.22	-	51,57,60,60	0
2	DTR	G	1	14/15	0.93	0.14	-	55,59,60,60	0
2	DTR	K	1	14/15	0.97	0.12	-	43,47,49,49	0
2	DTR	I	1	14/15	0.96	0.15	-	43,48,50,50	0
2	DTR	J	1	14/15	0.93	0.15	-	59,62,64,66	0

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
3	NAG	B	601	14/15	0.78	0.18	1.32	68,71,73,74	0
3	NAG	A	601	14/15	0.94	0.16	0.12	53,67,72,72	0
3	NAG	C	601	14/15	0.92	0.15	-0.18	54,56,58,58	0
3	NAG	F	601	14/15	0.94	0.15	-0.50	61,62,65,68	0
3	NAG	E	601	14/15	0.96	0.14	-0.55	47,51,54,55	0
3	NAG	D	601	14/15	0.89	0.13	-0.67	72,80,82,82	0
3	NAG	B	602	14/15	0.96	0.12	-1.15	50,58,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.