Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 11:06 PM GMT

PDB ID	:	5CVO
Title	:	WDR48:USP46 ubiquitin ternary complex
Authors	:	Harris, S.F.; Yin, J.
Deposited on	:	2015-07-27
Resolution	:	3.88 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

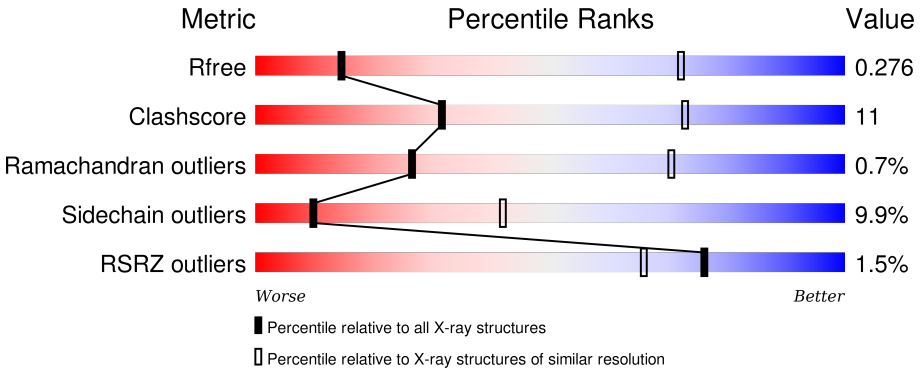
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.88 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	1005 (4.24-3.52)
Clashscore	102246	1026 (4.20-3.56)
Ramachandran outliers	100387	1003 (4.22-3.54)
Sidechain outliers	100360	1043 (4.24-3.52)
RSRZ outliers	91569	1009 (4.24-3.52)

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 <=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	677	% 65% 23% • 10%
1	D	677	% 65% 23% • 10%
2	B	358	% 62% 24% • • 10%
2	E	358	% 62% 23% • • 10%
3	C	96	% 56% 21% •• 21%

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Mol	Chain	Length	Quality of chain
3	F	96	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15554 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 WD repeat-containing protein 48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4528	2845	808	853	22			
1	D	612	Total	C	N	O	S	0	0	0
			4544	2855	811	856	22			

There are 230 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	563	UNK	ASN	SEE REMARK 999	UNP Q8TAF3
A	564	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
A	565	UNK	ILE	SEE REMARK 999	UNP Q8TAF3
A	566	UNK	PRO	SEE REMARK 999	UNP Q8TAF3
A	567	UNK	PHE	SEE REMARK 999	UNP Q8TAF3
A	568	UNK	TYR	SEE REMARK 999	UNP Q8TAF3
A	569	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
A	570	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
A	571	UNK	PRO	SEE REMARK 999	UNP Q8TAF3
A	572	UNK	HIS	SEE REMARK 999	UNP Q8TAF3
A	573	UNK	ALA	SEE REMARK 999	UNP Q8TAF3
A	574	UNK	SER	SEE REMARK 999	UNP Q8TAF3
A	575	UNK	SER	SEE REMARK 999	UNP Q8TAF3
A	576	UNK	GLY	SEE REMARK 999	UNP Q8TAF3
A	577	UNK	ALA	SEE REMARK 999	UNP Q8TAF3
A	578	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
A	579	UNK	THR	SEE REMARK 999	UNP Q8TAF3
A	580	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
A	581	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
A	582	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
A	583	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
A	584	UNK	ARG	SEE REMARK 999	UNP Q8TAF3
A	585	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
A	586	UNK	SER	SEE REMARK 999	UNP Q8TAF3
A	587	UNK	ALA	SEE REMARK 999	UNP Q8TAF3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	588	UNK	SER	SEE REMARK 999	UNP Q8TAF3
A	589	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
A	590	UNK	MET	SEE REMARK 999	UNP Q8TAF3
A	591	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
A	592	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
A	593	UNK	VAL	SEE REMARK 999	UNP Q8TAF3
A	594	UNK	ARG	SEE REMARK 999	UNP Q8TAF3
A	595	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
A	596	UNK	VAL	SEE REMARK 999	UNP Q8TAF3
A	597	UNK	MET	SEE REMARK 999	UNP Q8TAF3
A	598	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
A	599	UNK	HIS	SEE REMARK 999	UNP Q8TAF3
A	600	UNK	VAL	SEE REMARK 999	UNP Q8TAF3
A	601	UNK	TYR	SEE REMARK 999	UNP Q8TAF3
A	602	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
A	603	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
A	604	UNK	ILE	SEE REMARK 999	UNP Q8TAF3
A	605	UNK	ILE	SEE REMARK 999	UNP Q8TAF3
A	606	UNK	ASN	SEE REMARK 999	UNP Q8TAF3
A	607	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
A	608	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
A	609	UNK	ASN	SEE REMARK 999	UNP Q8TAF3
A	610	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
A	611	UNK	SER	SEE REMARK 999	UNP Q8TAF3
A	612	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
A	613	UNK	THR	SEE REMARK 999	UNP Q8TAF3
A	614	UNK	THR	SEE REMARK 999	UNP Q8TAF3
A	615	UNK	SER	SEE REMARK 999	UNP Q8TAF3
A	616	UNK	SER	SEE REMARK 999	UNP Q8TAF3
A	617	UNK	SER	SEE REMARK 999	UNP Q8TAF3
A	618	UNK	ASN	SEE REMARK 999	UNP Q8TAF3
A	619	UNK	ASN	SEE REMARK 999	UNP Q8TAF3
A	620	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
A	621	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
A	622	UNK	PRO	SEE REMARK 999	UNP Q8TAF3
A	623	UNK	GLY	SEE REMARK 999	UNP Q8TAF3
A	624	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
A	625	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
A	626	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
A	627	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
A	628	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
A	629	UNK	GLU	SEE REMARK 999	UNP Q8TAF3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	630	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
A	631	UNK	ILE	SEE REMARK 999	UNP Q8TAF3
A	632	UNK	ALA	SEE REMARK 999	UNP Q8TAF3
A	633	UNK	VAL	SEE REMARK 999	UNP Q8TAF3
A	634	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
A	635	UNK	ALA	SEE REMARK 999	UNP Q8TAF3
A	636	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
A	637	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
A	638	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
A	639	UNK	ILE	SEE REMARK 999	UNP Q8TAF3
A	640	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
A	641	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
A	642	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
A	643	UNK	CYS	SEE REMARK 999	UNP Q8TAF3
A	644	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
A	645	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
A	646	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
A	647	UNK	VAL	SEE REMARK 999	UNP Q8TAF3
A	648	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
A	649	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
A	650	UNK	PRO	SEE REMARK 999	UNP Q8TAF3
A	651	UNK	ASN	SEE REMARK 999	UNP Q8TAF3
A	652	UNK	MET	SEE REMARK 999	UNP Q8TAF3
A	653	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
A	654	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
A	655	UNK	ARG	SEE REMARK 999	UNP Q8TAF3
A	656	UNK	THR	SEE REMARK 999	UNP Q8TAF3
A	657	UNK	VAL	SEE REMARK 999	UNP Q8TAF3
A	658	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
A	659	UNK	HIS	SEE REMARK 999	UNP Q8TAF3
A	660	UNK	PHE	SEE REMARK 999	UNP Q8TAF3
A	661	UNK	ILE	SEE REMARK 999	UNP Q8TAF3
A	662	UNK	TRP	SEE REMARK 999	UNP Q8TAF3
A	663	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
A	664	UNK	SER	SEE REMARK 999	UNP Q8TAF3
A	665	UNK	GLY	SEE REMARK 999	UNP Q8TAF3
A	666	UNK	GLY	SEE REMARK 999	UNP Q8TAF3
A	667	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
A	668	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
A	669	UNK	THR	SEE REMARK 999	UNP Q8TAF3
A	670	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
A	671	UNK	HIS	SEE REMARK 999	UNP Q8TAF3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	672	UNK	TYR	SEE REMARK 999	UNP Q8TAF3
A	673	UNK	ARG	SEE REMARK 999	UNP Q8TAF3
A	674	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
A	675	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
A	676	UNK	SER	SEE REMARK 999	UNP Q8TAF3
A	677	UNK	THR	SEE REMARK 999	UNP Q8TAF3
D	563	UNK	ASN	SEE REMARK 999	UNP Q8TAF3
D	564	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
D	565	UNK	ILE	SEE REMARK 999	UNP Q8TAF3
D	566	UNK	PRO	SEE REMARK 999	UNP Q8TAF3
D	567	UNK	PHE	SEE REMARK 999	UNP Q8TAF3
D	568	UNK	TYR	SEE REMARK 999	UNP Q8TAF3
D	569	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
D	570	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
D	571	UNK	PRO	SEE REMARK 999	UNP Q8TAF3
D	572	UNK	HIS	SEE REMARK 999	UNP Q8TAF3
D	573	UNK	ALA	SEE REMARK 999	UNP Q8TAF3
D	574	UNK	SER	SEE REMARK 999	UNP Q8TAF3
D	575	UNK	SER	SEE REMARK 999	UNP Q8TAF3
D	576	UNK	GLY	SEE REMARK 999	UNP Q8TAF3
D	577	UNK	ALA	SEE REMARK 999	UNP Q8TAF3
D	578	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
D	579	UNK	THR	SEE REMARK 999	UNP Q8TAF3
D	580	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
D	581	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
D	582	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
D	583	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
D	584	UNK	ARG	SEE REMARK 999	UNP Q8TAF3
D	585	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
D	586	UNK	SER	SEE REMARK 999	UNP Q8TAF3
D	587	UNK	ALA	SEE REMARK 999	UNP Q8TAF3
D	588	UNK	SER	SEE REMARK 999	UNP Q8TAF3
D	589	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
D	590	UNK	MET	SEE REMARK 999	UNP Q8TAF3
D	591	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
D	592	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
D	593	UNK	VAL	SEE REMARK 999	UNP Q8TAF3
D	594	UNK	ARG	SEE REMARK 999	UNP Q8TAF3
D	595	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
D	596	UNK	VAL	SEE REMARK 999	UNP Q8TAF3
D	597	UNK	MET	SEE REMARK 999	UNP Q8TAF3
D	598	UNK	GLU	SEE REMARK 999	UNP Q8TAF3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	599	UNK	HIS	SEE REMARK 999	UNP Q8TAF3
D	600	UNK	VAL	SEE REMARK 999	UNP Q8TAF3
D	601	UNK	TYR	SEE REMARK 999	UNP Q8TAF3
D	602	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
D	603	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
D	604	UNK	ILE	SEE REMARK 999	UNP Q8TAF3
D	605	UNK	ILE	SEE REMARK 999	UNP Q8TAF3
D	606	UNK	ASN	SEE REMARK 999	UNP Q8TAF3
D	607	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
D	608	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
D	609	UNK	ASN	SEE REMARK 999	UNP Q8TAF3
D	610	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
D	611	UNK	SER	SEE REMARK 999	UNP Q8TAF3
D	612	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
D	613	UNK	THR	SEE REMARK 999	UNP Q8TAF3
D	614	UNK	THR	SEE REMARK 999	UNP Q8TAF3
D	615	UNK	SER	SEE REMARK 999	UNP Q8TAF3
D	616	UNK	SER	SEE REMARK 999	UNP Q8TAF3
D	617	UNK	SER	SEE REMARK 999	UNP Q8TAF3
D	618	UNK	ASN	SEE REMARK 999	UNP Q8TAF3
D	619	UNK	ASN	SEE REMARK 999	UNP Q8TAF3
D	620	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
D	621	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
D	622	UNK	PRO	SEE REMARK 999	UNP Q8TAF3
D	623	UNK	GLY	SEE REMARK 999	UNP Q8TAF3
D	624	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
D	625	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
D	626	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
D	627	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
D	628	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
D	629	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
D	630	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
D	631	UNK	ILE	SEE REMARK 999	UNP Q8TAF3
D	632	UNK	ALA	SEE REMARK 999	UNP Q8TAF3
D	633	UNK	VAL	SEE REMARK 999	UNP Q8TAF3
D	634	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
D	635	UNK	ALA	SEE REMARK 999	UNP Q8TAF3
D	636	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
D	637	UNK	GLU	SEE REMARK 999	UNP Q8TAF3
D	638	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
D	639	UNK	ILE	SEE REMARK 999	UNP Q8TAF3
D	640	UNK	GLU	SEE REMARK 999	UNP Q8TAF3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	641	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
D	642	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
D	643	UNK	CYS	SEE REMARK 999	UNP Q8TAF3
D	644	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
D	645	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
D	646	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
D	647	UNK	VAL	SEE REMARK 999	UNP Q8TAF3
D	648	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
D	649	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
D	650	UNK	PRO	SEE REMARK 999	UNP Q8TAF3
D	651	UNK	ASN	SEE REMARK 999	UNP Q8TAF3
D	652	UNK	MET	SEE REMARK 999	UNP Q8TAF3
D	653	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
D	654	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
D	655	UNK	ARG	SEE REMARK 999	UNP Q8TAF3
D	656	UNK	THR	SEE REMARK 999	UNP Q8TAF3
D	657	UNK	VAL	SEE REMARK 999	UNP Q8TAF3
D	658	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
D	659	UNK	HIS	SEE REMARK 999	UNP Q8TAF3
D	660	UNK	PHE	SEE REMARK 999	UNP Q8TAF3
D	661	UNK	ILE	SEE REMARK 999	UNP Q8TAF3
D	662	UNK	TRP	SEE REMARK 999	UNP Q8TAF3
D	663	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
D	664	UNK	SER	SEE REMARK 999	UNP Q8TAF3
D	665	UNK	GLY	SEE REMARK 999	UNP Q8TAF3
D	666	UNK	GLY	SEE REMARK 999	UNP Q8TAF3
D	667	UNK	ASP	SEE REMARK 999	UNP Q8TAF3
D	668	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
D	669	UNK	THR	SEE REMARK 999	UNP Q8TAF3
D	670	UNK	LEU	SEE REMARK 999	UNP Q8TAF3
D	671	UNK	HIS	SEE REMARK 999	UNP Q8TAF3
D	672	UNK	TYR	SEE REMARK 999	UNP Q8TAF3
D	673	UNK	ARG	SEE REMARK 999	UNP Q8TAF3
D	674	UNK	GLN	SEE REMARK 999	UNP Q8TAF3
D	675	UNK	LYS	SEE REMARK 999	UNP Q8TAF3
D	676	UNK	SER	SEE REMARK 999	UNP Q8TAF3
D	677	UNK	THR	SEE REMARK 999	UNP Q8TAF3

- Molecule 2 is a protein called Ubiquitin carboxyl-terminal hydrolase 46.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	321	Total	C	N	O	S	0	0	0
			2640	1677	449	497	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	321	Total	C	N	O	S	0	0	0
			2640	1677	449	497	17			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	expression tag	UNP P62068
B	10	HIS	-	expression tag	UNP P62068
B	11	HIS	-	expression tag	UNP P62068
B	12	HIS	-	expression tag	UNP P62068
B	13	HIS	-	expression tag	UNP P62068
B	14	HIS	-	expression tag	UNP P62068
B	15	HIS	-	expression tag	UNP P62068
B	16	GLY	-	expression tag	UNP P62068
B	17	GLU	-	expression tag	UNP P62068
B	18	ASN	-	expression tag	UNP P62068
B	19	LEU	-	expression tag	UNP P62068
B	20	TYR	-	expression tag	UNP P62068
B	21	PHE	-	expression tag	UNP P62068
B	22	GLN	-	expression tag	UNP P62068
B	23	GLY	-	expression tag	UNP P62068
B	24	SER	-	expression tag	UNP P62068
E	9	MET	-	expression tag	UNP P62068
E	10	HIS	-	expression tag	UNP P62068
E	11	HIS	-	expression tag	UNP P62068
E	12	HIS	-	expression tag	UNP P62068
E	13	HIS	-	expression tag	UNP P62068
E	14	HIS	-	expression tag	UNP P62068
E	15	HIS	-	expression tag	UNP P62068
E	16	GLY	-	expression tag	UNP P62068
E	17	GLU	-	expression tag	UNP P62068
E	18	ASN	-	expression tag	UNP P62068
E	19	LEU	-	expression tag	UNP P62068
E	20	TYR	-	expression tag	UNP P62068
E	21	PHE	-	expression tag	UNP P62068
E	22	GLN	-	expression tag	UNP P62068
E	23	GLY	-	expression tag	UNP P62068
E	24	SER	-	expression tag	UNP P62068

- Molecule 3 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	76	Total	C	N	O	S	0	0	0
			600	378	105	116	1			
3	F	76	Total	C	N	O	S	0	0	0
			600	378	105	116	1			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	expression tag	UNP P0CG47
C	-18	GLY	-	expression tag	UNP P0CG47
C	-17	SER	-	expression tag	UNP P0CG47
C	-16	SER	-	expression tag	UNP P0CG47
C	-15	HIS	-	expression tag	UNP P0CG47
C	-14	HIS	-	expression tag	UNP P0CG47
C	-13	HIS	-	expression tag	UNP P0CG47
C	-12	HIS	-	expression tag	UNP P0CG47
C	-11	HIS	-	expression tag	UNP P0CG47
C	-10	HIS	-	expression tag	UNP P0CG47
C	-9	SER	-	expression tag	UNP P0CG47
C	-8	SER	-	expression tag	UNP P0CG47
C	-7	GLY	-	expression tag	UNP P0CG47
C	-6	LEU	-	expression tag	UNP P0CG47
C	-5	VAL	-	expression tag	UNP P0CG47
C	-4	PRO	-	expression tag	UNP P0CG47
C	-3	ARG	-	expression tag	UNP P0CG47
C	-2	GLY	-	expression tag	UNP P0CG47
C	-1	SER	-	expression tag	UNP P0CG47
C	0	HIS	-	expression tag	UNP P0CG47
F	-19	MET	-	expression tag	UNP P0CG47
F	-18	GLY	-	expression tag	UNP P0CG47
F	-17	SER	-	expression tag	UNP P0CG47
F	-16	SER	-	expression tag	UNP P0CG47
F	-15	HIS	-	expression tag	UNP P0CG47
F	-14	HIS	-	expression tag	UNP P0CG47
F	-13	HIS	-	expression tag	UNP P0CG47
F	-12	HIS	-	expression tag	UNP P0CG47
F	-11	HIS	-	expression tag	UNP P0CG47
F	-10	HIS	-	expression tag	UNP P0CG47
F	-9	SER	-	expression tag	UNP P0CG47
F	-8	SER	-	expression tag	UNP P0CG47
F	-7	GLY	-	expression tag	UNP P0CG47
F	-6	LEU	-	expression tag	UNP P0CG47
F	-5	VAL	-	expression tag	UNP P0CG47

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	PRO	-	expression tag	UNP P0CG47
F	-3	ARG	-	expression tag	UNP P0CG47
F	-2	GLY	-	expression tag	UNP P0CG47
F	-1	SER	-	expression tag	UNP P0CG47
F	0	HIS	-	expression tag	UNP P0CG47

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

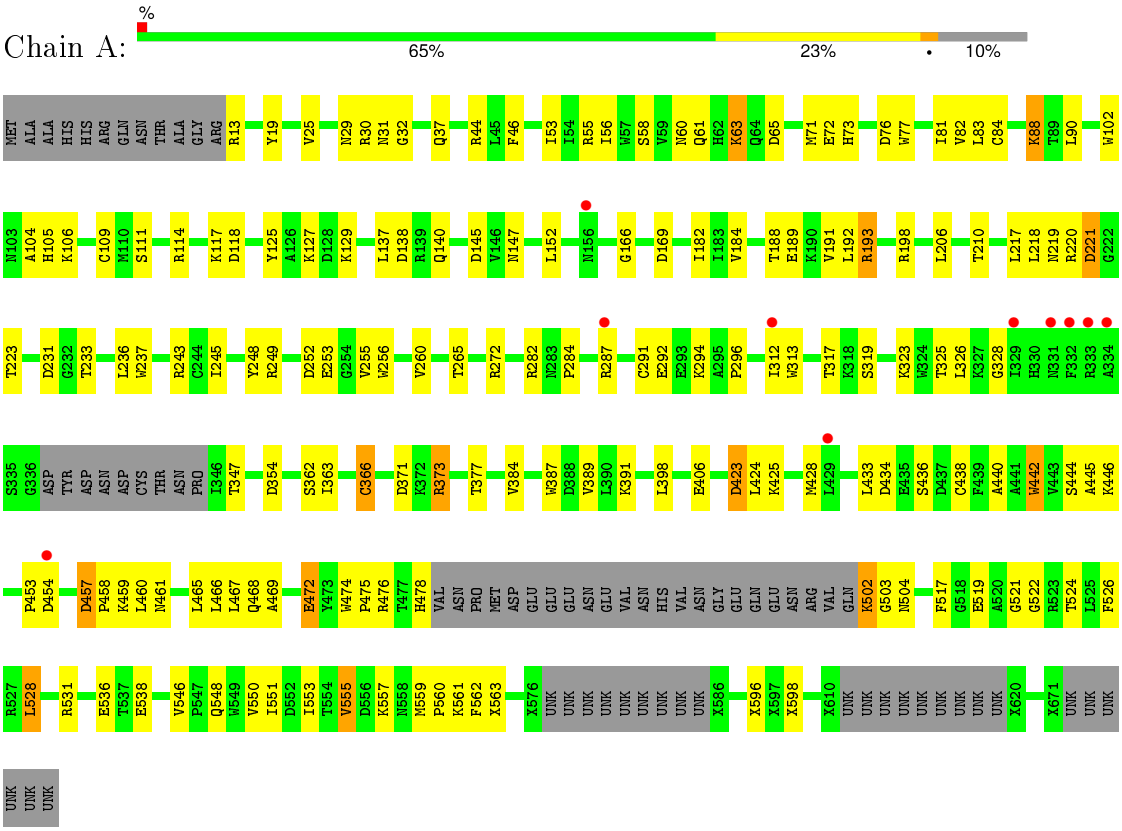
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	E	1	Total Zn 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

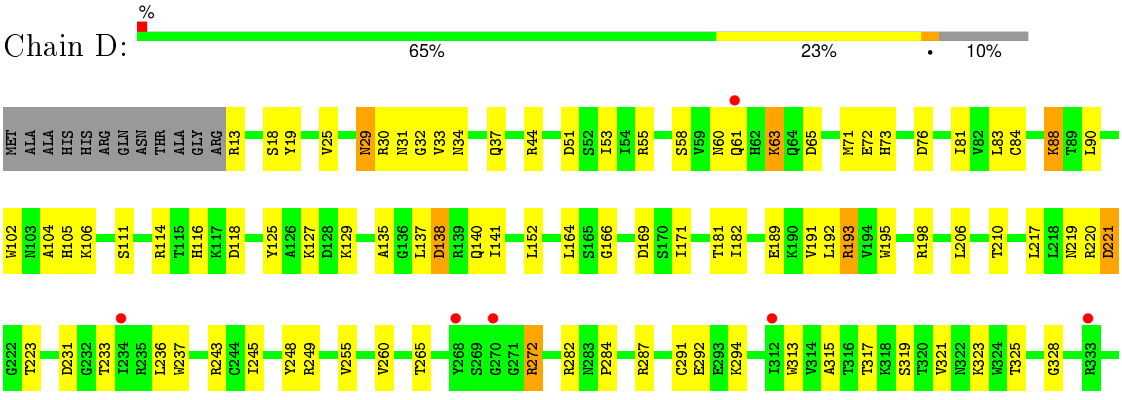
- Molecule 1: WD repeat-containing protein 48

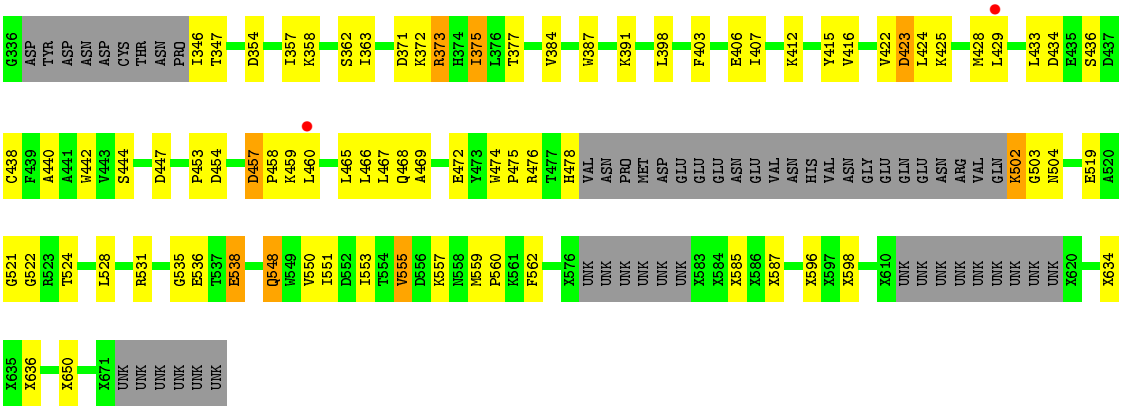
Chain A:



- Molecule 1: WD repeat-containing protein 48

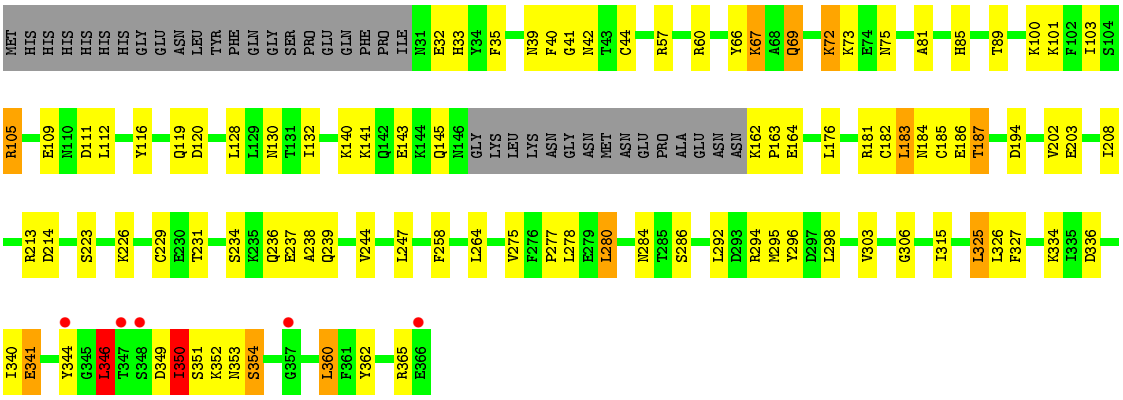
Chain D:





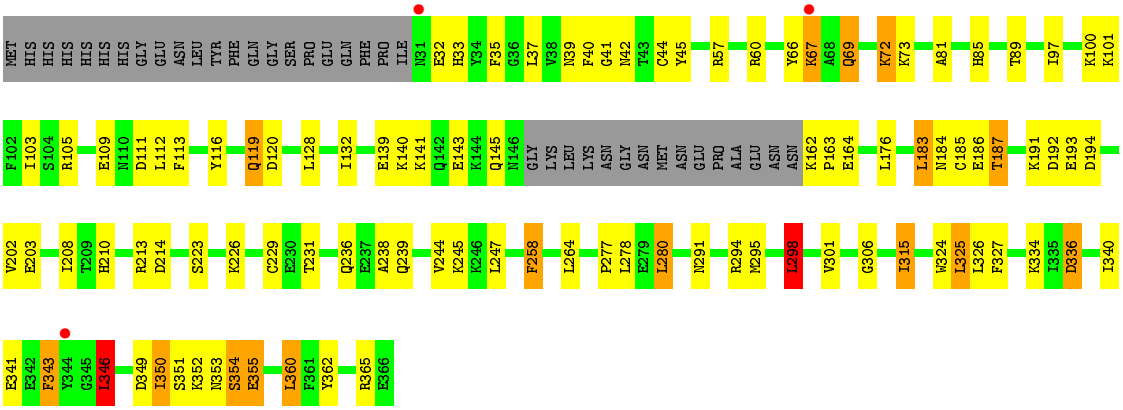
• Molecule 2: Ubiquitin carboxyl-terminal hydrolase 46

Chain B:



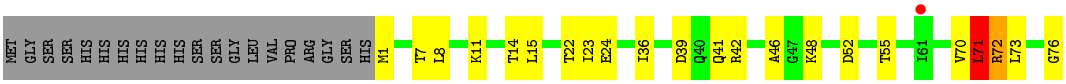
• Molecule 2: Ubiquitin carboxyl-terminal hydrolase 46

Chain E:



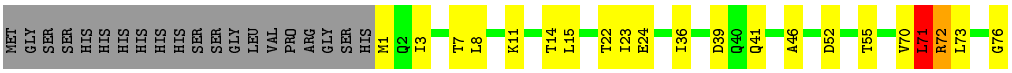
• Molecule 3: Polyubiquitin-B

Chain C:



- Molecule 3: Polyubiquitin-B

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	211.34Å 103.76Å 190.95Å 90.00° 119.03° 90.00°	Depositor
Resolution (Å)	47.70 – 3.88 49.55 – 3.88	Depositor EDS
% Data completeness (in resolution range)	68.2 (47.70-3.88) 68.4 (49.55-3.88)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.222 , 0.275 0.214 , 0.276	Depositor DCC
R_{free} test set	1189 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	78.8	Xtriage
Anisotropy	0.811	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	2 of 22979 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	15554	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.31	1/4158 (0.0%)	0.66	1/5642 (0.0%)
1	D	0.29	0/4158	0.64	1/5642 (0.0%)
2	B	0.32	0/2693	0.64	1/3631 (0.0%)
2	E	0.31	0/2693	0.64	2/3631 (0.1%)
3	C	0.30	0/606	0.62	1/815 (0.1%)
3	F	0.30	0/606	0.62	1/815 (0.1%)
All	All	0.31	1/14914 (0.0%)	0.64	7/20176 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	472	GLU	CD-OE2	5.21	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	71	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	371	ASP	N-CA-C	-5.50	96.14	111.00
2	E	298	LEU	CA-CB-CG	5.42	127.78	115.30
3	C	71	LEU	CA-CB-CG	5.39	127.69	115.30
2	E	346	LEU	CA-CB-CG	5.21	127.29	115.30
1	D	371	ASP	N-CA-C	-5.16	97.08	111.00
2	B	346	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4528	0	4180	109	0
1	D	4544	0	4187	89	0
2	B	2640	0	2591	66	0
2	E	2640	0	2591	60	0
3	C	600	0	629	14	0
3	F	600	0	629	13	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
All	All	15554	0	14807	324	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 11.

All (324) 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)
2:E:44:CYS:SG	3:F:76:GLY:C	2.26	1.15
2:B:44:CYS:SG	3:C:76:GLY:C	2.26	1.12
1:A:76:ASP:OD2	1:A:425:LYS:NZ	1.91	1.03
1:A:13:ARG:HH11	1:A:521:GLY:HA3	1.23	1.00
1:D:13:ARG:HH11	1:D:521:GLY:HA3	1.28	0.97
1:D:29:ASN:HA	1:D:55:ARG:HH11	1.29	0.97
1:A:272:ARG:NH1	2:B:186:GLU:HB2	1.83	0.93
1:D:116:HIS:ND1	1:D:138:ASP:OD2	2.01	0.92
1:A:29:ASN:HA	1:A:55:ARG:HH11	1.33	0.91
2:B:120:ASP:HB2	3:C:72:ARG:HG3	1.53	0.91
1:A:13:ARG:NH1	1:A:521:GLY:HA3	1.87	0.89
1:D:44:ARG:HH21	1:D:88:LYS:HZ1	0.95	0.89
1:A:561:LYS:HG3	1:A:562:PHE:H	1.36	0.88
2:B:352:LYS:HG3	2:E:352:LYS:HG3	1.56	0.87
2:E:120:ASP:HB2	3:F:72:ARG:HG3	1.55	0.87
2:E:185:CYS:SG	2:E:187:THR:OG1	2.34	0.85
1:D:44:ARG:HH21	1:D:88:LYS:NZ	1.74	0.85
1:D:13:ARG:NH1	1:D:521:GLY:HA3	1.91	0.84
1:D:44:ARG:NH2	1:D:88:LYS:HZ1	1.75	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:ASP:OD2	2:E:245:LYS:NZ	2.13	0.81
1:A:272:ARG:HH12	2:B:186:GLU:CD	1.84	0.80
1:A:44:ARG:HH21	1:A:88:LYS:NZ	1.80	0.79
1:D:29:ASN:ND2	1:D:51:ASP:OD2	2.16	0.79
1:A:444:SER:OG	1:A:457:ASP:OD2	2.00	0.78
2:B:185:CYS:SG	2:B:187:THR:OG1	2.41	0.78
1:A:553:ILE:HD12	1:A:560:PRO:HD3	1.66	0.78
1:A:256:TRP:HZ2	1:A:272:ARG:NH1	1.82	0.77
1:D:377:THR:HG1	1:D:387:TRP:HE1	1.29	0.77
1:A:377:THR:HG1	1:A:387:TRP:HE1	1.32	0.76
2:B:183:LEU:HD11	2:B:239:GLN:HG3	1.69	0.75
1:A:44:ARG:HH21	1:A:88:LYS:HZ2	1.37	0.73
2:E:67:LYS:HB2	2:E:81:ALA:HB1	1.71	0.73
2:B:346:LEU:HD12	2:B:351:SER:HB3	1.72	0.72
1:A:366:CYS:HB2	1:A:377:THR:HG22	1.72	0.71
2:E:298:LEU:HD22	2:E:324:TRP:HH2	1.56	0.71
2:B:306:GLY:O	2:B:354:SER:OG	2.09	0.70
1:A:561:LYS:HG3	1:A:562:PHE:N	2.05	0.70
1:A:272:ARG:NH1	2:B:185:CYS:O	2.25	0.69
2:E:184:ASN:HB2	2:E:236:GLN:HG2	1.74	0.69
1:A:433:LEU:HD21	1:A:466:LEU:HD23	1.73	0.69
1:D:138:ASP:N	1:D:138:ASP:OD1	2.18	0.69
2:B:67:LYS:HB2	2:B:81:ALA:HB1	1.74	0.68
2:B:247:LEU:HD13	2:B:294:ARG:HG2	1.75	0.67
1:D:363:ILE:HG22	1:D:424:LEU:HD13	1.78	0.66
1:D:81:ILE:HB	1:D:90:LEU:HD11	1.77	0.66
1:D:433:LEU:HD21	1:D:466:LEU:HD23	1.78	0.65
1:D:248:TYR:HE2	1:D:284:PRO:HG3	1.60	0.65
3:F:8:LEU:HD21	3:F:71:LEU:HD13	1.79	0.64
2:B:42:ASN:ND2	2:B:116:TYR:O	2.28	0.64
1:A:219:ASN:OD1	1:A:220:ARG:N	2.31	0.64
1:D:478:HIS:CD2	1:D:502:LYS:HA	2.33	0.63
1:D:219:ASN:OD1	1:D:220:ARG:N	2.31	0.63
1:A:478:HIS:CD2	1:A:502:LYS:HA	2.34	0.63
1:A:88:LYS:HG2	1:A:104:ALA:HB1	1.80	0.63
1:A:81:ILE:HB	1:A:90:LEU:HD11	1.79	0.63
2:E:42:ASN:ND2	2:E:116:TYR:O	2.30	0.63
1:D:291:CYS:SG	1:D:292:GLU:N	2.71	0.63
2:E:229:CYS:SG	2:E:231:THR:OG1	2.57	0.62
1:D:71:MET:HB3	1:D:102:TRP:CZ3	2.34	0.62
1:D:323:LYS:HE3	1:D:354:ASP:OD2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:183:LEU:HD11	2:E:239:GLN:HG3	1.80	0.62
1:A:248:TYR:HE2	1:A:284:PRO:HG3	1.65	0.62
1:A:291:CYS:SG	1:A:292:GLU:N	2.73	0.61
1:A:313:TRP:CE2	1:A:323:LYS:HD3	2.35	0.61
2:E:306:GLY:O	2:E:354:SER:OG	2.19	0.61
1:D:265:THR:HB	1:D:282:ARG:HE	1.66	0.61
1:A:37:GLN:HE21	1:A:83:LEU:H	1.47	0.61
1:D:553:ILE:HD12	1:D:560:PRO:HD3	1.82	0.61
2:B:130:ASN:OD1	3:C:48:LYS:NZ	2.19	0.61
1:D:13:ARG:HD3	1:D:521:GLY:H	1.65	0.61
1:D:233:THR:HG22	1:D:249:ARG:HG2	1.83	0.60
1:D:313:TRP:CE2	1:D:323:LYS:HD3	2.37	0.60
1:A:272:ARG:HH11	2:B:185:CYS:C	2.05	0.60
2:B:184:ASN:HB2	2:B:236:GLN:HG2	1.83	0.60
1:A:445:ALA:N	1:A:457:ASP:OD2	2.34	0.60
1:A:323:LYS:HE3	1:A:354:ASP:OD2	2.01	0.59
2:B:315:ILE:HD13	2:B:326:LEU:HD11	1.85	0.59
3:F:3:ILE:HD11	3:F:15:LEU:HD12	1.84	0.59
1:A:233:THR:HG22	1:A:249:ARG:HG2	1.85	0.59
2:E:346:LEU:HD12	2:E:351:SER:HB3	1.83	0.59
1:A:363:ILE:HG22	1:A:424:LEU:HD13	1.84	0.59
1:D:88:LYS:HG2	1:D:104:ALA:HB1	1.84	0.58
2:E:194:ASP:O	3:F:46:ALA:HA	2.04	0.57
2:B:194:ASP:O	3:C:46:ALA:HA	2.04	0.57
1:A:13:ARG:HD2	1:A:519:GLU:HB3	1.87	0.57
1:A:71:MET:HB3	1:A:102:TRP:CZ3	2.40	0.56
1:D:13:ARG:HD2	1:D:519:GLU:HB3	1.87	0.56
1:A:272:ARG:HH12	2:B:186:GLU:HB2	1.70	0.56
1:A:272:ARG:CZ	2:B:186:GLU:HB2	2.35	0.56
2:B:229:CYS:SG	2:B:231:THR:OG1	2.59	0.56
1:A:30:ARG:HH11	1:A:428:MET:HG2	1.69	0.56
1:D:423:ASP:OD2	1:D:425:LYS:HG2	2.05	0.56
2:E:183:LEU:HD13	2:E:238:ALA:HA	1.88	0.56
1:D:415:TYR:HB3	1:D:650:UNK:HA	1.87	0.56
1:A:265:THR:HB	1:A:282:ARG:HE	1.71	0.56
1:A:129:LYS:NZ	1:A:198:ARG:HD2	2.22	0.55
1:D:236:LEU:HG	1:D:245:ILE:HD11	1.87	0.55
1:A:60:ASN:O	1:A:61:GLN:HB2	2.06	0.55
2:E:298:LEU:HD21	2:E:301:VAL:HG23	1.88	0.54
2:E:40:PHE:HD2	2:E:103:ILE:HD12	1.72	0.54
1:D:472:GLU:HG3	1:D:503:GLY:HA2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LYS:NZ	1:D:198:ARG:HD2	2.22	0.54
1:A:517:PHE:CE2	1:A:546:VAL:HG22	2.42	0.54
3:C:8:LEU:HD21	3:C:71:LEU:HD13	1.90	0.54
1:D:585:UNK:O	1:D:587:UNK:N	2.40	0.54
2:B:183:LEU:HD13	2:B:238:ALA:HA	1.90	0.54
1:D:32:GLY:HA2	1:D:319:SER:HA	1.90	0.54
1:A:272:ARG:NH1	2:B:186:GLU:CB	2.63	0.53
1:D:444:SER:HB3	1:D:447:ASP:OD2	2.09	0.53
1:A:423:ASP:OD2	1:A:425:LYS:HG2	2.09	0.53
1:A:377:THR:O	1:A:384:VAL:HA	2.09	0.53
1:D:60:ASN:O	1:D:61:GLN:HB2	2.07	0.52
1:D:30:ARG:HH11	1:D:428:MET:HG2	1.75	0.52
1:A:13:ARG:HD3	1:A:521:GLY:H	1.74	0.52
1:A:125:TYR:CZ	1:A:127:LYS:HA	2.45	0.52
1:A:44:ARG:NH2	1:A:88:LYS:NZ	2.54	0.51
1:A:460:LEU:HD23	1:A:465:LEU:HD21	1.92	0.51
1:A:236:LEU:HG	1:A:245:ILE:HD11	1.92	0.51
2:B:40:PHE:HD2	2:B:103:ILE:HD12	1.74	0.51
2:E:44:CYS:SG	3:F:76:GLY:CA	2.99	0.51
2:E:140:LYS:HD3	2:E:164:GLU:OE2	2.10	0.51
1:A:88:LYS:HG2	1:A:104:ALA:CB	2.41	0.51
2:B:66:TYR:O	2:B:69:GLN:HG3	2.10	0.51
1:D:469:ALA:HB2	1:D:504:ASN:ND2	2.26	0.51
1:D:460:LEU:HD23	1:D:465:LEU:HD21	1.92	0.51
1:D:63:LYS:NZ	1:D:65:ASP:O	2.44	0.51
1:D:206:LEU:HB3	1:D:237:TRP:CZ3	2.46	0.51
1:D:373:ARG:HH12	1:D:391:LYS:HE3	1.76	0.50
1:A:32:GLY:HA2	1:A:319:SER:HA	1.92	0.50
1:D:29:ASN:HA	1:D:55:ARG:NH1	2.12	0.50
1:A:37:GLN:NE2	1:A:82:VAL:HA	2.26	0.50
1:D:468:GLN:HB2	1:D:504:ASN:HB3	1.92	0.50
2:E:277:PRO:HG2	2:E:280:LEU:HD12	1.94	0.50
1:A:76:ASP:OD1	1:A:77:TRP:N	2.38	0.50
2:B:295:MET:HG2	2:B:365:ARG:HE	1.77	0.50
2:E:66:TYR:O	2:E:69:GLN:HG3	2.12	0.49
1:D:535:GLY:HA3	1:D:538:GLU:OE2	2.12	0.49
1:D:53:ILE:HG12	1:D:72:GLU:HG2	1.94	0.49
2:E:340:ILE:HG13	2:E:341:GLU:H	1.78	0.49
2:B:277:PRO:HG2	2:B:280:LEU:HD12	1.95	0.49
1:A:117:LYS:N	1:A:138:ASP:OD2	2.24	0.49
1:A:434:ASP:O	1:A:438:CYS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:TYR:CZ	1:D:127:LYS:HA	2.48	0.49
2:B:353:ASN:O	2:B:353:ASN:ND2	2.46	0.49
1:A:206:LEU:HB3	1:A:237:TRP:CZ3	2.47	0.49
1:D:76:ASP:OD1	1:D:425:LYS:HE2	2.13	0.49
1:A:138:ASP:HB3	1:A:140:GLN:HG2	1.95	0.49
1:A:272:ARG:HH12	2:B:186:GLU:CG	2.25	0.49
3:F:23:ILE:HB	3:F:52:ASP:HA	1.94	0.49
1:D:114:ARG:NH1	1:D:524:THR:O	2.46	0.49
2:B:128:LEU:O	2:B:132:ILE:HG12	2.13	0.49
1:A:252:ASP:O	1:A:253:GLU:HG2	2.13	0.48
1:A:44:ARG:HH21	1:A:88:LYS:HZ1	1.59	0.48
1:A:475:PRO:HA	1:A:478:HIS:ND1	2.28	0.48
1:A:468:GLN:HB2	1:A:504:ASN:HB3	1.94	0.48
2:E:343:PHE:N	2:E:343:PHE:HD1	2.11	0.48
2:B:140:LYS:HD3	2:B:164:GLU:OE2	2.14	0.48
2:B:185:CYS:SG	2:B:231:THR:OG1	2.71	0.48
2:E:85:HIS:CE1	2:E:89:THR:HG21	2.49	0.48
2:E:336:ASP:N	2:E:336:ASP:OD1	2.47	0.48
3:C:7:THR:HG22	3:C:11:LYS:O	2.13	0.48
1:D:467:LEU:HD13	1:D:550:VAL:HG13	1.95	0.48
1:D:118:ASP:HB3	1:D:137:LEU:HB2	1.96	0.48
1:D:90:LEU:H	1:D:104:ALA:HB2	1.78	0.48
2:E:298:LEU:HB2	2:E:362:TYR:CE1	2.49	0.48
1:A:596:UNK:O	1:A:598:UNK:N	2.47	0.48
1:A:373:ARG:HH12	1:A:391:LYS:HE3	1.79	0.48
1:A:189:GLU:C	1:A:191:VAL:H	2.17	0.48
2:E:325:LEU:HD12	2:E:327:PHE:CE1	2.49	0.48
2:E:40:PHE:CD2	2:E:103:ILE:HD12	2.49	0.48
2:E:343:PHE:N	2:E:343:PHE:CD1	2.82	0.48
2:B:140:LYS:O	2:B:143:GLU:HG3	2.14	0.48
1:A:373:ARG:O	1:A:389:VAL:HG23	2.14	0.48
1:A:502:LYS:NZ	1:A:502:LYS:HB3	2.29	0.48
2:E:66:TYR:OH	2:E:139:GLU:OE1	2.29	0.48
2:E:128:LEU:O	2:E:132:ILE:HG12	2.14	0.47
1:D:166:GLY:O	1:D:193:ARG:NH2	2.47	0.47
3:C:42:ARG:HD2	3:C:72:ARG:NH1	2.30	0.47
2:B:284:ASN:HB2	2:B:292:LEU:HB2	1.96	0.47
1:D:475:PRO:HA	1:D:478:HIS:ND1	2.29	0.47
2:E:340:ILE:HG13	2:E:341:GLU:N	2.30	0.47
1:A:469:ALA:HB2	1:A:504:ASN:ND2	2.30	0.47
2:B:39:ASN:O	2:E:41:GLY:HA2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:LYS:HB2	1:D:105:HIS:CE1	2.50	0.47
1:A:446:LYS:H	1:A:457:ASP:CG	2.18	0.47
1:D:457:ASP:HA	1:D:458:PRO:HD2	1.77	0.47
2:B:72:LYS:HA	2:B:72:LYS:HD3	1.50	0.47
1:A:166:GLY:O	1:A:193:ARG:NH2	2.48	0.47
1:A:442:TRP:CE2	1:A:461:ASN:HB2	2.50	0.47
1:D:210:THR:HB	1:D:231:ASP:HB3	1.98	0.46
3:F:7:THR:HG22	3:F:11:LYS:O	2.15	0.46
1:D:88:LYS:HG2	1:D:104:ALA:CB	2.45	0.46
1:D:377:THR:O	1:D:384:VAL:HA	2.15	0.46
1:A:19:TYR:CE1	1:A:466:LEU:HD21	2.49	0.46
2:B:202:VAL:HG12	2:B:203:GLU:N	2.30	0.46
1:D:551:ILE:O	1:D:555:VAL:HG13	2.16	0.46
1:D:248:TYR:CE2	1:D:284:PRO:HG3	2.46	0.46
1:D:596:UNK:O	1:D:598:UNK:N	2.48	0.46
3:C:23:ILE:HB	3:C:52:ASP:HA	1.96	0.46
3:F:22:THR:HG22	3:F:55:THR:HG22	1.97	0.46
2:E:72:LYS:HA	2:E:72:LYS:HD3	1.50	0.46
2:B:176:LEU:HD23	2:B:244:VAL:HA	1.98	0.46
1:A:562:PHE:CG	1:A:563:UNK:N	2.84	0.46
2:B:349:ASP:O	2:B:351:SER:N	2.47	0.46
1:D:555:VAL:O	1:D:557:LYS:HG2	2.16	0.46
1:D:321:VAL:HB	1:D:357:ILE:HB	1.97	0.46
2:B:275:VAL:HB	2:B:341:GLU:OE2	2.16	0.46
1:A:145:ASP:OD2	1:A:147:ASN:HB2	2.16	0.46
1:A:88:LYS:HB2	1:A:105:HIS:CE1	2.51	0.46
1:A:453:PRO:HA	1:A:454:ASP:HA	1.53	0.46
1:D:189:GLU:C	1:D:191:VAL:H	2.20	0.46
1:A:114:ARG:NH1	1:A:524:THR:O	2.49	0.46
1:D:30:ARG:NH1	1:D:428:MET:HG2	2.31	0.45
2:E:202:VAL:HG12	2:E:203:GLU:N	2.31	0.45
1:D:434:ASP:O	1:D:438:CYS:HB2	2.16	0.45
2:E:191:LYS:HD3	2:E:193:GLU:OE2	2.17	0.45
1:D:141:ILE:HB	1:D:164:LEU:HB2	1.98	0.45
2:B:182:CYS:O	2:B:186:GLU:HA	2.16	0.45
2:E:208:ILE:HD13	2:E:360:LEU:HD22	1.99	0.45
1:A:44:ARG:NH2	1:A:88:LYS:HZ1	2.14	0.45
1:A:474:TRP:HD1	1:A:475:PRO:HD2	1.81	0.45
3:C:22:THR:HG22	3:C:55:THR:HG22	1.98	0.45
2:E:315:ILE:HD13	2:E:326:LEU:HD11	1.98	0.45
1:D:458:PRO:HG2	1:D:460:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:ARG:HB3	2:E:57:ARG:CZ	2.46	0.45
2:E:140:LYS:O	2:E:143:GLU:HG3	2.17	0.45
2:B:303:VAL:HG21	2:B:344:TYR:CE1	2.52	0.45
1:D:272:ARG:NH2	2:E:185:CYS:O	2.46	0.45
1:A:555:VAL:O	1:A:557:LYS:HG2	2.17	0.45
2:E:223:SER:O	2:E:226:LYS:HG3	2.17	0.45
2:E:73:LYS:HA	2:E:73:LYS:HD2	1.64	0.45
2:B:67:LYS:HE3	2:B:67:LYS:HB3	1.76	0.44
2:E:67:LYS:HE3	2:E:67:LYS:HB3	1.84	0.44
1:A:210:THR:HB	1:A:231:ASP:HB3	1.98	0.44
1:D:138:ASP:HB2	1:D:140:GLN:HG2	1.99	0.44
1:D:474:TRP:HD1	1:D:475:PRO:HD2	1.83	0.44
1:A:53:ILE:HG12	1:A:72:GLU:HG2	1.99	0.44
2:B:40:PHE:CD2	2:B:103:ILE:HD12	2.52	0.44
1:A:118:ASP:HB3	1:A:137:LEU:HB2	1.98	0.44
1:A:467:LEU:HD13	1:A:550:VAL:HG13	2.00	0.44
1:D:31:ASN:HA	1:D:362:SER:OG	2.17	0.44
2:E:162:LYS:HB3	2:E:163:PRO:HD3	2.00	0.44
1:A:425:LYS:HB3	2:B:234:SER:HB3	2.00	0.44
1:A:551:ILE:O	1:A:555:VAL:HG13	2.17	0.44
1:D:221:ASP:HB2	1:D:223:THR:HG23	1.98	0.43
1:A:272:ARG:HH12	2:B:186:GLU:CB	2.29	0.43
3:C:36:ILE:O	3:C:41:GLN:NE2	2.49	0.43
1:A:272:ARG:HA	1:A:296:PRO:HB3	2.00	0.43
2:B:223:SER:O	2:B:226:LYS:HG3	2.18	0.43
3:F:14:THR:O	3:F:15:LEU:HD23	2.19	0.43
1:A:472:GLU:HG3	1:A:503:GLY:HA2	2.00	0.43
2:B:120:ASP:HB2	3:C:72:ARG:CG	2.35	0.43
3:C:14:THR:O	3:C:15:LEU:HD23	2.19	0.43
2:B:181:ARG:NH1	2:B:186:GLU:HB3	2.33	0.43
2:E:280:LEU:HD13	2:E:362:TYR:CZ	2.53	0.43
2:B:181:ARG:NH1	2:B:186:GLU:HG2	2.34	0.43
1:D:453:PRO:HA	1:D:454:ASP:HA	1.49	0.43
1:A:559:MET:SD	1:A:560:PRO:HD2	2.59	0.43
1:D:19:TYR:CE1	1:D:466:LEU:HD21	2.53	0.43
1:A:31:ASN:HA	1:A:362:SER:OG	2.19	0.43
1:D:403:PHE:CE2	1:D:407:ILE:HD11	2.54	0.43
2:B:208:ILE:HD13	2:B:360:LEU:HD22	2.01	0.43
1:D:548:GLN:HA	1:D:551:ILE:HD12	2.00	0.43
1:A:184:VAL:HG12	1:A:218:LEU:HD11	2.01	0.43
2:E:120:ASP:HB2	3:F:72:ARG:CG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:C	1:A:104:ALA:HB3	2.39	0.42
2:B:73:LYS:HA	2:B:73:LYS:HD2	1.62	0.42
1:A:221:ASP:HB2	1:A:223:THR:HG23	2.01	0.42
2:E:33:HIS:HB3	2:E:35:PHE:HE2	1.84	0.42
1:A:169:ASP:HB3	1:A:188:THR:OG1	2.19	0.42
2:E:203:GLU:OE2	2:E:210:HIS:NE2	2.52	0.42
1:A:46:PHE:CE1	1:A:56:ILE:HG12	2.55	0.42
2:B:325:LEU:HD12	2:B:327:PHE:CE1	2.54	0.42
1:D:502:LYS:NZ	1:D:502:LYS:HB3	2.35	0.42
2:E:350:ILE:HG13	2:E:350:ILE:H	1.65	0.42
2:B:294:ARG:HD2	2:B:296:TYR:OH	2.20	0.42
2:B:85:HIS:CE1	2:B:89:THR:HG21	2.54	0.42
2:B:350:ILE:H	2:B:350:ILE:HG13	1.61	0.42
1:D:634:UNK:O	1:D:636:UNK:N	2.53	0.42
2:E:176:LEU:HD23	2:E:244:VAL:HA	2.01	0.42
1:D:375:ILE:HD11	1:D:422:VAL:HG21	2.02	0.42
1:D:88:LYS:C	1:D:104:ALA:HB3	2.40	0.42
2:E:295:MET:HG2	2:E:365:ARG:HE	1.85	0.42
1:A:63:LYS:NZ	1:A:65:ASP:O	2.53	0.41
1:A:248:TYR:CE2	1:A:284:PRO:HG3	2.49	0.41
1:D:193:ARG:HB2	1:D:195:TRP:CH2	2.54	0.41
1:D:372:LYS:HD2	1:D:416:VAL:O	2.19	0.41
3:F:36:ILE:O	3:F:41:GLN:NE2	2.46	0.41
2:B:162:LYS:HB3	2:B:163:PRO:HD3	2.02	0.41
1:A:312:ILE:HB	1:A:326:LEU:HD11	2.02	0.41
2:E:349:ASP:O	2:E:351:SER:N	2.47	0.41
2:B:284:ASN:OD1	2:B:286:SER:HB3	2.20	0.41
2:E:247:LEU:HD13	2:E:294:ARG:HG2	2.01	0.41
2:B:75:ASN:HA	2:B:105:ARG:HD2	2.03	0.41
3:C:48:LYS:HB2	3:C:48:LYS:HE2	1.75	0.41
1:A:137:LEU:HD22	2:B:237:GLU:OE2	2.20	0.41
1:D:398:LEU:HD13	1:D:406:GLU:HG2	2.02	0.41
1:A:90:LEU:H	1:A:104:ALA:HB2	1.85	0.41
2:E:258:PHE:HB2	3:F:71:LEU:HD22	2.02	0.41
1:A:37:GLN:HE21	1:A:82:VAL:HA	1.86	0.41
1:A:37:GLN:HG2	1:A:83:LEU:HB2	2.02	0.41
1:D:33:VAL:HB	1:D:315:ALA:HB1	2.02	0.41
1:A:253:GLU:OE2	1:A:272:ARG:HD2	2.21	0.41
1:A:88:LYS:HE2	1:A:104:ALA:O	2.21	0.41
1:A:19:TYR:HE1	1:A:466:LEU:HD21	1.84	0.41
2:E:45:TYR:CE2	2:E:119:GLN:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:GLY:HA2	2:E:39:ASN:O	2.21	0.41
2:E:37:LEU:HA	2:E:97:ILE:O	2.21	0.41
2:B:280:LEU:HD13	2:B:362:TYR:CZ	2.56	0.41
1:D:135:ALA:HB1	1:D:171:ILE:HD13	2.03	0.41
1:D:37:GLN:HG2	1:D:83:LEU:HB2	2.02	0.41
2:B:44:CYS:SG	3:C:76:GLY:CA	3.07	0.41
1:A:458:PRO:HG2	1:A:460:LEU:HD11	2.03	0.41
1:D:135:ALA:HB2	1:D:141:ILE:HG23	2.03	0.41
1:A:73:HIS:CE1	1:A:109:CYS:HB3	2.56	0.41
2:B:303:VAL:HG11	2:B:344:TYR:HE1	1.86	0.40
2:E:113:PHE:CE1	2:E:119:GLN:HG2	2.56	0.40
1:A:398:LEU:HD13	1:A:406:GLU:HG2	2.03	0.40
2:B:57:ARG:HB3	2:B:57:ARG:CZ	2.50	0.40
1:A:256:TRP:CZ2	1:A:272:ARG:NH1	2.74	0.40
2:B:33:HIS:HB3	2:B:35:PHE:HE2	1.86	0.40
2:E:355:GLU:H	2:E:355:GLU:HG2	1.78	0.40
1:A:526:PHE:CZ	1:A:528:LEU:HB3	2.57	0.40
1:D:19:TYR:HE1	1:D:466:LEU:HD21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	513/677 (76%)	474 (92%)	35 (7%)	4 (1%)	24	68
1	D	513/677 (76%)	474 (92%)	35 (7%)	4 (1%)	24	68
2	B	317/358 (88%)	298 (94%)	17 (5%)	2 (1%)	30	73
2	E	317/358 (88%)	298 (94%)	16 (5%)	3 (1%)	21	66
3	C	74/96 (77%)	73 (99%)	1 (1%)	0	100	100
3	F	74/96 (77%)	73 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1808/2262 (80%)	1690 (94%)	105 (6%)	13 (1%)	26 70

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	354	SER
2	E	354	SER
2	B	350	ILE
2	E	350	ILE
1	A	436	SER
2	E	353	ASN
1	D	436	SER
1	D	440	ALA
1	A	440	ALA
1	A	522	GLY
1	D	328	GLY
1	D	522	GLY
1	A	328	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	452/491 (92%)	417 (92%)	35 (8%)	16 55
1	D	452/491 (92%)	403 (89%)	49 (11%)	8 39
2	B	297/330 (90%)	266 (90%)	31 (10%)	9 40
2	E	297/330 (90%)	264 (89%)	33 (11%)	8 37
3	C	68/85 (80%)	61 (90%)	7 (10%)	9 40
3	F	68/85 (80%)	61 (90%)	7 (10%)	9 40
All	All	1634/1812 (90%)	1472 (90%)	162 (10%)	10 42

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	58	SER
1	A	63	LYS
1	A	84	CYS
1	A	88	LYS
1	A	106	LYS
1	A	111	SER
1	A	152	LEU
1	A	182	ILE
1	A	192	LEU
1	A	193	ARG
1	A	217	LEU
1	A	221	ASP
1	A	243	ARG
1	A	255	VAL
1	A	260	VAL
1	A	287	ARG
1	A	294	LYS
1	A	317	THR
1	A	325	THR
1	A	347	THR
1	A	366	CYS
1	A	373	ARG
1	A	423	ASP
1	A	442	TRP
1	A	457	ASP
1	A	459	LYS
1	A	476	ARG
1	A	502	LYS
1	A	528	LEU
1	A	531	ARG
1	A	536	GLU
1	A	538	GLU
1	A	548	GLN
1	A	555	VAL
2	B	32	GLU
2	B	60	ARG
2	B	67	LYS
2	B	69	GLN
2	B	72	LYS
2	B	100	LYS
2	B	101	LYS
2	B	105	ARG

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Mol	Chain	Res	Type
2	B	109	GLU
2	B	111	ASP
2	B	112	LEU
2	B	119	GLN
2	B	141	LYS
2	B	145	GLN
2	B	183	LEU
2	B	187	THR
2	B	213	ARG
2	B	214	ASP
2	B	258	PHE
2	B	264	LEU
2	B	278	LEU
2	B	280	LEU
2	B	298	LEU
2	B	325	LEU
2	B	334	LYS
2	B	336	ASP
2	B	340	ILE
2	B	341	GLU
2	B	346	LEU
2	B	350	ILE
2	B	360	LEU
3	C	1	MET
3	C	24	GLU
3	C	39	ASP
3	C	70	VAL
3	C	71	LEU
3	C	72	ARG
3	C	73	LEU
1	D	18	SER
1	D	25	VAL
1	D	29	ASN
1	D	34	ASN
1	D	58	SER
1	D	63	LYS
1	D	73	HIS
1	D	84	CYS
1	D	88	LYS
1	D	106	LYS
1	D	111	SER
1	D	138	ASP

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Mol	Chain	Res	Type
1	D	152	LEU
1	D	169	ASP
1	D	181	THR
1	D	182	ILE
1	D	192	LEU
1	D	193	ARG
1	D	217	LEU
1	D	221	ASP
1	D	243	ARG
1	D	255	VAL
1	D	260	VAL
1	D	272	ARG
1	D	287	ARG
1	D	294	LYS
1	D	317	THR
1	D	325	THR
1	D	346	ILE
1	D	347	THR
1	D	358	LYS
1	D	373	ARG
1	D	375	ILE
1	D	412	LYS
1	D	423	ASP
1	D	429	LEU
1	D	442	TRP
1	D	457	ASP
1	D	459	LYS
1	D	476	ARG
1	D	502	LYS
1	D	528	LEU
1	D	531	ARG
1	D	536	GLU
1	D	538	GLU
1	D	548	GLN
1	D	555	VAL
1	D	559	MET
1	D	562	PHE
2	E	32	GLU
2	E	60	ARG
2	E	67	LYS
2	E	69	GLN
2	E	72	LYS

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Mol	Chain	Res	Type
2	E	100	LYS
2	E	101	LYS
2	E	105	ARG
2	E	109	GLU
2	E	111	ASP
2	E	112	LEU
2	E	119	GLN
2	E	141	LYS
2	E	145	GLN
2	E	183	LEU
2	E	186	GLU
2	E	187	THR
2	E	213	ARG
2	E	214	ASP
2	E	258	PHE
2	E	264	LEU
2	E	278	LEU
2	E	280	LEU
2	E	291	ASN
2	E	298	LEU
2	E	315	ILE
2	E	325	LEU
2	E	334	LYS
2	E	336	ASP
2	E	343	PHE
2	E	346	LEU
2	E	355	GLU
2	E	360	LEU
3	F	1	MET
3	F	24	GLU
3	F	39	ASP
3	F	70	VAL
3	F	71	LEU
3	F	72	ARG
3	F	73	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	105	HIS
2	B	173	GLN

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Mol	Chain	Res	Type
1	D	105	HIS
1	D	355	GLN
1	D	374	HIS
1	D	468	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	518/677 (76%)	0.01	10 (1%) 70 59	3, 43, 115, 232	0
1	D	518/677 (76%)	-0.07	8 (1%) 76 66	10, 58, 127, 231	0
2	B	321/358 (89%)	-0.02	5 (1%) 74 64	3, 22, 120, 195	0
2	E	321/358 (89%)	-0.09	3 (0%) 85 79	3, 27, 118, 195	0
3	C	76/96 (79%)	0.03	1 (1%) 79 70	3, 15, 48, 108	0
3	F	76/96 (79%)	-0.12	0 100 100	3, 23, 50, 56	0
All	All	1830/2262 (80%)	-0.04	27 (1%) 76 66	3, 39, 121, 232	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	333	ARG	7.4
1	A	454	ASP	4.7
1	A	331	ASN	3.3
1	D	429	LEU	3.2
2	B	348	SER	3.2
1	A	329	ILE	3.2
1	D	333	ARG	3.1
2	E	344	TYR	3.1
1	D	312	ILE	2.9
2	B	347	THR	2.8
1	D	268	TYR	2.8
2	B	366	GLU	2.7
1	A	429	LEU	2.7
1	D	270	GLY	2.6
1	D	61	GLN	2.5
2	E	31	ASN	2.5
1	A	287	ARG	2.5
3	C	61	ILE	2.4
1	A	334	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	312	ILE	2.3
1	D	460	LEU	2.2
1	A	332	PHE	2.1
2	B	357	GLY	2.1
2	E	67	LYS	2.0
1	D	234	ILE	2.0
1	A	156	ASN	2.0
2	B	344	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, 95^{th} 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
4	ZN	E	900	1/1	0.99	0.25	0.88	80,80,80,80	0
4	ZN	B	900	1/1	0.99	0.20	-0.66	82,82,82,82	0

6.5 Other polymers (i)

There are no such residues in this entry.