



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2018 – 10:58 AM EST

PDB ID : 5XBK
Title : Crystal structure of human Importin4
Authors : Song, J.J.; Yoon, J.
Deposited on : 2017-03-20
Resolution : 3.22 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
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)	:	rb-20030736

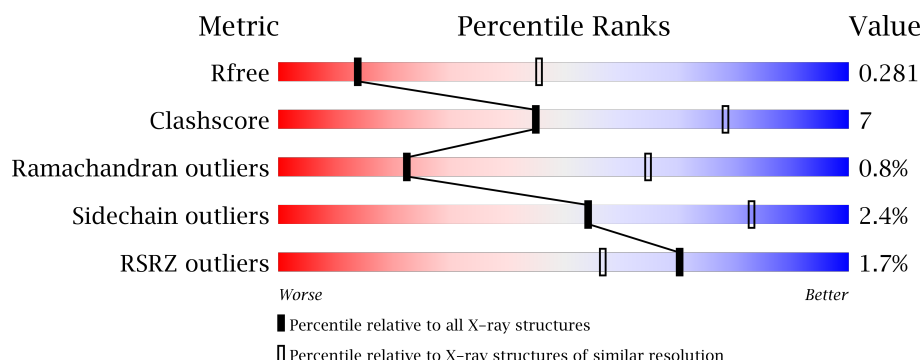
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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	1036 (3.24-3.20)
Clashscore	112137	1161 (3.24-3.20)
Ramachandran outliers	110173	1140 (3.24-3.20)
Sidechain outliers	110143	1139 (3.24-3.20)
RSRZ outliers	101464	1040 (3.24-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	416	
1	B	416	
1	C	416	
1	D	416	
2	E	18	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11162 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 Importin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	369	Total	C	N	O	S	0	0	0
			2785	1778	484	505	18			
1	A	366	Total	C	N	O	S	0	0	0
			2762	1769	477	499	17			
1	B	373	Total	C	N	O	S	0	0	0
			2817	1799	489	511	18			
1	C	368	Total	C	N	O	S	0	0	0
			2776	1770	483	505	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	666	GLY	-	expression tag	UNP Q8TEX9
D	667	SER	-	expression tag	UNP Q8TEX9
A	666	GLY	-	expression tag	UNP Q8TEX9
A	667	SER	-	expression tag	UNP Q8TEX9
B	666	GLY	-	expression tag	UNP Q8TEX9
B	667	SER	-	expression tag	UNP Q8TEX9
C	666	GLY	-	expression tag	UNP Q8TEX9
C	667	SER	-	expression tag	UNP Q8TEX9

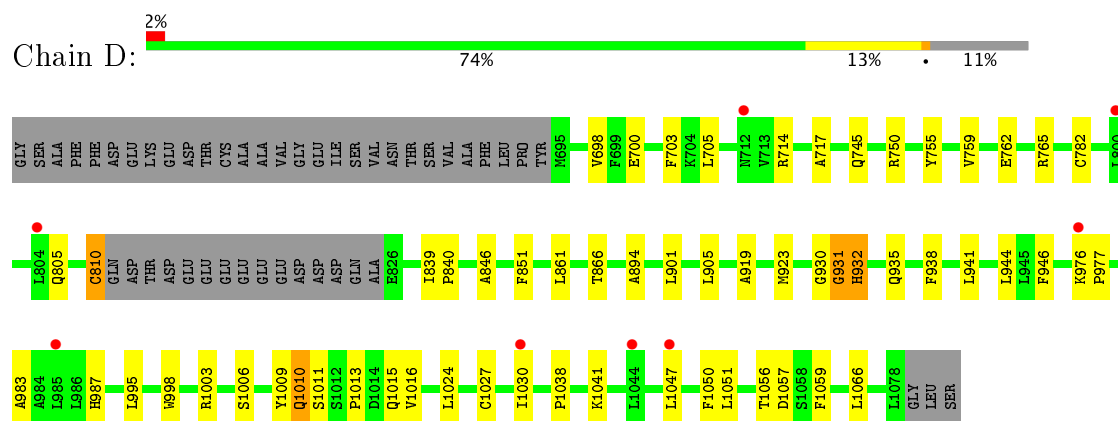
- Molecule 2 is a protein called histone H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			22	13	5	4			

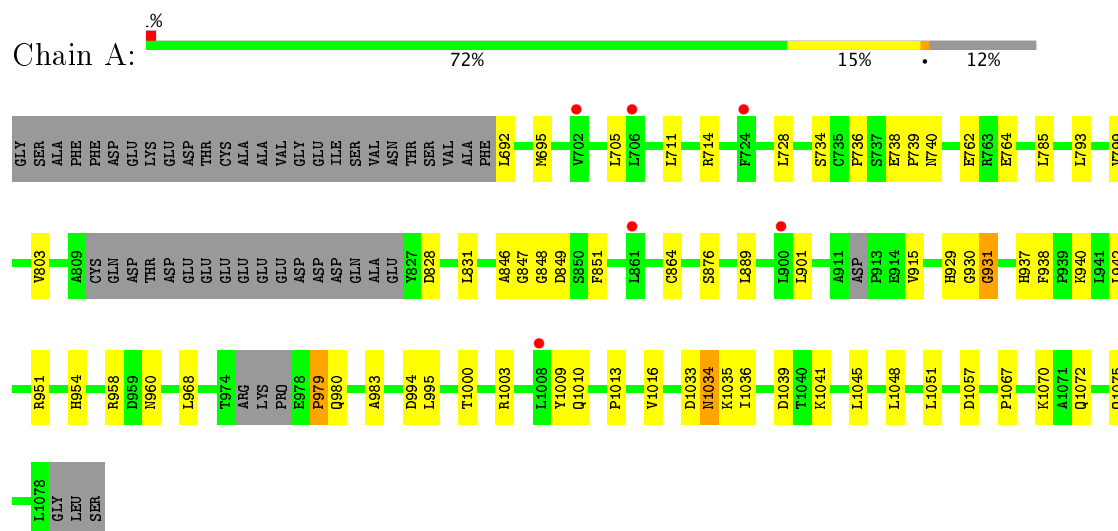
3 Residue-property plots [i](#)

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

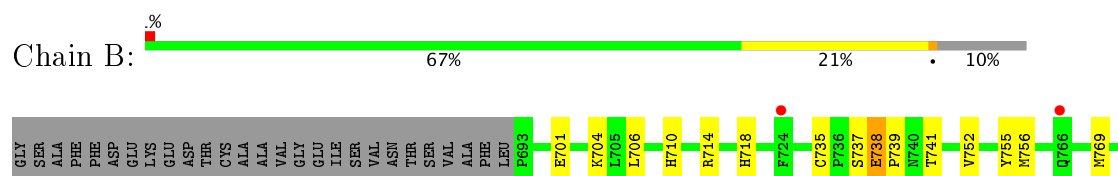
• Molecule 1: Importin-4

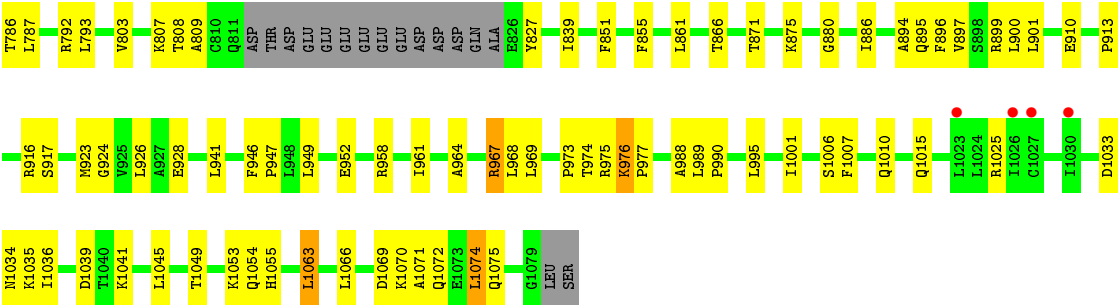


• Molecule 1: Importin-4

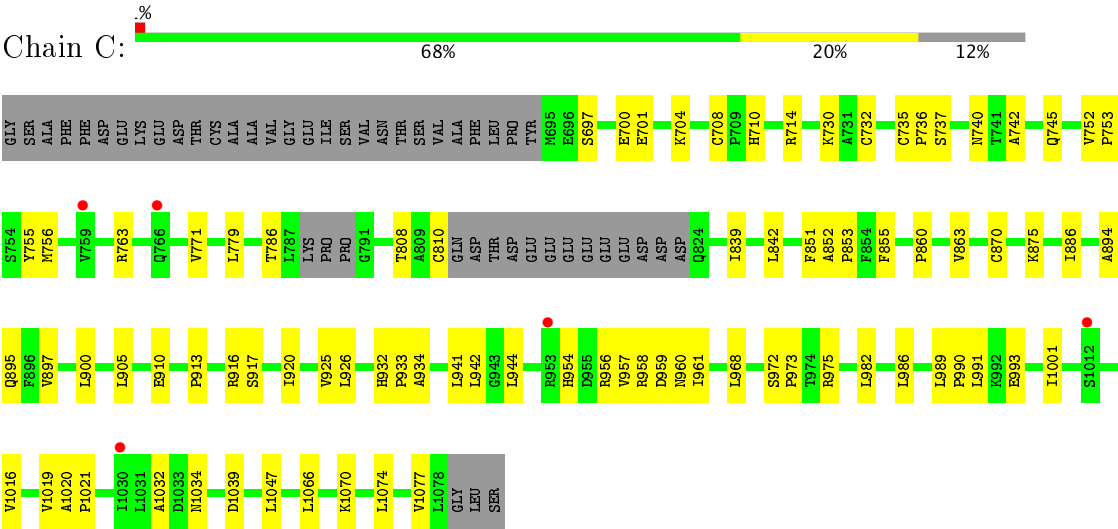


• Molecule 1: Importin-4





● Molecule 1: Importin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.02Å 108.54Å 124.86Å 90.00° 103.41° 90.00°	Depositor
Resolution (Å)	49.98 – 3.22 49.98 – 3.22	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.98-3.22) 98.1 (49.98-3.22)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.218 , 0.281 0.218 , 0.281	Depositor DCC
R_{free} test set	2671 reflections (9.94%)	DCC
Wilson B-factor (Å ²)	90.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11162	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.27	0/2813	0.43	0/3818
1	B	0.28	0/2871	0.43	0/3898
1	C	0.29	0/2825	0.45	0/3833
1	D	0.28	0/2837	0.44	0/3852
2	E	0.25	0/21	0.33	0/25
All	All	0.28	0/11367	0.44	0/15426

There are no bond length outliers.

There are no bond angle outliers.

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	2762	0	2844	33	1
1	B	2817	0	2894	56	0
1	C	2776	0	2851	52	1
1	D	2785	0	2866	34	0
2	E	22	0	23	1	0
All	All	11162	0	11478	168	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 7.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1025:ARG:HA	1:B:1066:LEU:HD21	1.71	0.71
1:C:917:SER:OG	1:C:960:ASN:ND2	2.22	0.71
1:A:714:ARG:HH22	1:A:764:GLU:HG3	1.57	0.70
1:B:894:ALA:HB3	1:C:895:GLN:HG3	1.75	0.67
1:C:958:ARG:HA	1:C:961:ILE:HD12	1.75	0.67
1:B:701:GLU:OE1	1:B:704:LYS:NZ	2.27	0.66
1:A:1033:ASP:O	1:A:1041:LYS:NZ	2.29	0.66
1:D:1027:CYS:HA	1:D:1030:ILE:HG12	1.79	0.64
1:C:886:ILE:HD11	1:C:900:LEU:HD13	1.80	0.64
1:B:928:GLU:HB2	1:B:967:ARG:HG2	1.79	0.63
1:D:700:GLU:OE1	1:D:750:ARG:NH2	2.32	0.63
1:B:995:LEU:HD11	1:B:1035:LYS:HD3	1.82	0.61
1:C:905:LEU:HD22	1:C:944:LEU:HD13	1.83	0.60
1:B:895:GLN:HG3	1:C:894:ALA:HB3	1.84	0.58
1:D:1009:TYR:HB2	1:D:1047:LEU:HD23	1.86	0.58
1:A:1036:ILE:HB	1:A:1041:LYS:HE3	1.86	0.58
1:B:1039:ASP:OD1	1:B:1039:ASP:N	2.33	0.57
1:B:923:MET:HE3	1:B:941:LEU:HD22	1.87	0.57
1:B:901:LEU:HD11	1:B:941:LEU:HD21	1.85	0.57
1:C:941:LEU:HD23	1:C:968:LEU:HD11	1.86	0.57
1:A:929:HIS:O	1:A:931:GLY:N	2.38	0.57
1:C:763:ARG:HD2	1:C:810:CYS:HA	1.86	0.57
1:C:957:VAL:HG12	1:C:961:ILE:HD11	1.86	0.56
1:C:941:LEU:HB3	1:C:968:LEU:HD21	1.87	0.56
1:B:1063:LEU:HD21	1:B:1074:LEU:HD23	1.88	0.55
1:D:894:ALA:HB2	1:D:931:GLY:HA3	1.89	0.55
1:B:735:CYS:O	1:B:737:SER:N	2.35	0.55
1:A:980:GLN:HB2	1:A:983:ALA:HB3	1.87	0.54
1:A:876:SER:HB3	1:A:915:VAL:HG22	1.89	0.54
1:A:1039:ASP:N	1:A:1039:ASP:OD1	2.41	0.54
1:D:1051:LEU:HB3	1:D:1059:PHE:HB2	1.88	0.54
1:B:976:LYS:NZ	1:B:1015:GLN:HB3	2.23	0.54
1:D:1016:VAL:HG23	1:D:1051:LEU:HD21	1.89	0.54
1:B:973:PRO:O	1:B:975:ARG:HG2	2.08	0.54
1:A:1072:GLN:HA	1:A:1075:GLN:HG2	1.90	0.54
1:B:706:LEU:HA	1:B:714:ARG:HG2	1.89	0.53
1:D:1010:GLN:HG3	1:B:1007:PHE:HB2	1.89	0.53
1:A:1045:LEU:HA	1:A:1048:LEU:HB2	1.91	0.53
1:B:897:VAL:HG22	1:B:926:LEU:HD11	1.90	0.53
1:A:1033:ASP:OD1	1:A:1034:ASN:N	2.42	0.52
1:B:1036:ILE:HB	1:B:1041:LYS:HZ2	1.73	0.52
1:D:1030:ILE:HD12	1:D:1041:LYS:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:969:LEU:HD22	1:B:977:PRO:HB3	1.91	0.52
1:A:1067:PRO:HG2	1:A:1070:LYS:HB2	1.92	0.52
1:D:977:PRO:O	1:D:1015:GLN:NE2	2.42	0.51
1:B:941:LEU:HD12	1:B:968:LEU:HD21	1.93	0.51
1:D:930:GLY:O	1:D:932:HIS:N	2.43	0.51
1:A:692:LEU:HD22	1:A:740:ASN:HB3	1.92	0.51
1:C:842:LEU:HD23	1:C:851:PHE:CE1	2.46	0.51
1:A:714:ARG:NH2	1:A:762:GLU:OE2	2.21	0.50
1:B:769:MET:SD	1:B:827:TYR:HB3	2.51	0.50
1:C:894:ALA:HB1	1:C:933:PRO:HG3	1.91	0.50
1:A:828:ASP:HA	1:A:831:LEU:HB3	1.93	0.50
1:B:886:ILE:HD11	1:B:900:LEU:HD13	1.94	0.50
1:C:1066:LEU:HB3	1:C:1070:LYS:HB2	1.94	0.50
1:B:866:THR:HA	1:B:875:LYS:HG2	1.94	0.49
1:D:976:LYS:N	1:D:977:PRO:HD3	2.27	0.49
1:C:737:SER:HB2	1:C:740:ASN:HB2	1.94	0.49
1:C:870:CYS:O	1:C:875:LYS:NZ	2.45	0.49
1:A:1016:VAL:HG23	1:A:1051:LEU:HD21	1.95	0.49
1:A:1057:ASP:N	1:A:1057:ASP:OD1	2.46	0.49
1:B:718:HIS:O	1:B:755:TYR:OH	2.26	0.49
1:B:787:LEU:HD13	1:B:793:LEU:HD13	1.95	0.49
1:A:942:LEU:HD21	1:A:968:LEU:HD22	1.95	0.49
1:D:1057:ASP:OD1	1:D:1057:ASP:N	2.45	0.49
1:A:1033:ASP:OD1	1:A:1035:LYS:N	2.42	0.48
1:D:765:ARG:HG3	1:D:810:CYS:HB2	1.94	0.48
1:A:1000:THR:HA	1:A:1003:ARG:HH11	1.79	0.48
1:B:1054:GLN:O	1:B:1055:HIS:ND1	2.46	0.48
1:A:1013:PRO:O	1:A:1016:VAL:HG22	2.12	0.48
1:B:976:LYS:HE2	1:B:977:PRO:O	2.14	0.48
1:C:897:VAL:HG11	1:C:934:ALA:HA	1.95	0.48
1:A:846:ALA:HB3	1:A:851:PHE:HB2	1.96	0.48
1:C:860:PRO:HA	1:C:863:VAL:HG12	1.95	0.48
1:C:954:HIS:CD2	1:C:956:ARG:HB3	2.48	0.48
1:A:995:LEU:HD21	1:A:1035:LYS:HB3	1.96	0.47
1:B:910:GLU:O	1:B:916:ARG:NH1	2.48	0.47
1:D:1024:LEU:HB3	1:D:1066:LEU:HD11	1.95	0.47
1:D:1003:ARG:NH1	1:B:1010:GLN:O	2.45	0.47
1:D:1038:PRO:HB2	1:B:1053:LYS:HG3	1.97	0.47
1:D:846:ALA:HB3	1:D:851:PHE:HB2	1.97	0.47
1:B:738:GLU:HB3	1:B:739:PRO:HD3	1.97	0.47
1:C:735:CYS:O	1:C:737:SER:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:ASN:ND2	1:A:994:ASP:OD2	2.45	0.46
1:C:886:ILE:HG22	1:C:925:VAL:HG12	1.96	0.46
1:B:807:LYS:HA	1:B:807:LYS:HD3	1.72	0.46
1:C:1016:VAL:HG21	1:C:1047:LEU:HD22	1.97	0.46
1:C:842:LEU:HD23	1:C:851:PHE:HE1	1.80	0.46
1:B:989:LEU:HD21	1:B:1001:ILE:HG21	1.97	0.46
1:C:753:PRO:HA	1:C:756:MET:HG3	1.96	0.46
1:C:897:VAL:HG22	1:C:926:LEU:HD11	1.97	0.46
1:A:799:VAL:O	1:A:803:VAL:HG23	2.15	0.46
1:D:805:GLN:HE21	1:D:861:LEU:HD21	1.80	0.46
1:C:972:SER:OG	1:C:975:ARG:HB3	2.16	0.46
1:C:839:ILE:HG23	1:C:851:PHE:HZ	1.81	0.45
1:A:847:GLY:O	1:A:849:ASP:N	2.48	0.45
1:D:901:LEU:HD11	1:D:941:LEU:HD11	1.98	0.45
1:B:1074:LEU:HD12	1:B:1075:GLN:N	2.31	0.45
1:B:976:LYS:HE3	1:B:976:LYS:HB2	1.73	0.45
1:D:1013:PRO:HB2	1:D:1050:PHE:CE2	2.52	0.45
1:D:755:TYR:O	1:D:759:VAL:HG23	2.15	0.45
1:A:954:HIS:O	1:A:958:ARG:HG3	2.17	0.45
1:C:697:SER:O	1:C:701:GLU:HB2	2.17	0.45
1:A:695:MET:HG3	1:A:728:LEU:HD22	1.98	0.45
1:B:756:MET:HE1	1:B:792:ARG:HD3	1.99	0.45
1:B:1033:ASP:OD1	1:B:1034:ASN:N	2.50	0.45
1:D:919:ALA:O	1:D:923:MET:HG3	2.17	0.44
1:A:738:GLU:N	1:A:739:PRO:HD2	2.33	0.44
1:B:803:VAL:HG22	1:B:808:THR:HG21	1.99	0.44
1:B:946:PHE:HB3	1:B:947:PRO:HD3	2.00	0.44
1:C:942:LEU:HG	1:C:968:LEU:HD23	1.99	0.44
1:C:982:LEU:O	1:C:986:LEU:HB2	2.17	0.44
1:D:983:ALA:O	1:D:987:HIS:HB2	2.18	0.44
1:C:886:ILE:HD13	1:C:926:LEU:HD13	2.00	0.44
1:B:949:LEU:HD11	1:B:988:ALA:HB2	1.99	0.43
1:B:949:LEU:HB2	1:B:961:ILE:HG21	2.00	0.43
1:C:851:PHE:CE2	1:C:855:PHE:HB2	2.54	0.43
1:C:875:LYS:HE2	1:C:910:GLU:OE2	2.19	0.43
1:B:1072:GLN:C	1:B:1074:LEU:H	2.22	0.43
1:B:851:PHE:CE2	1:B:855:PHE:HB2	2.54	0.43
1:C:742:ALA:HA	1:C:745:GLN:HB2	2.01	0.43
1:C:745:GLN:OE1	1:C:745:GLN:N	2.51	0.43
1:C:700:GLU:O	1:C:704:LYS:HG2	2.18	0.43
1:D:995:LEU:HD22	1:D:998:TRP:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1066:LEU:HB2	1:B:1071:ALA:HB2	2.00	0.43
1:B:895:GLN:O	1:B:899:ARG:NH1	2.49	0.43
1:B:952:GLU:O	1:B:958:ARG:HD3	2.19	0.43
1:C:959:ASP:OD2	1:C:993:GLU:HB2	2.18	0.42
1:B:880:GLY:HA3	2:E:13:GLY:HA3	2.00	0.42
1:C:989:LEU:HD21	1:C:1001:ILE:HG21	2.00	0.42
1:C:779:LEU:HD21	1:C:842:LEU:HD12	2.01	0.42
1:C:913:PRO:O	1:C:917:SER:HB2	2.19	0.42
1:B:896:PHE:HA	1:B:899:ARG:HH11	1.84	0.42
1:C:920:ILE:HD13	1:C:961:ILE:HG12	2.00	0.42
1:A:734:SER:O	1:A:736:PRO:HD3	2.20	0.42
1:A:901:LEU:HD22	1:A:937:HIS:CD2	2.54	0.42
1:B:839:ILE:HG23	1:B:851:PHE:HZ	1.85	0.42
1:B:738:GLU:O	1:B:741:THR:OG1	2.26	0.42
1:B:990:PRO:HD3	1:B:1025:ARG:HH12	1.84	0.42
1:C:710:HIS:O	1:C:714:ARG:NH1	2.53	0.42
1:D:705:LEU:HD23	1:D:717:ALA:HB2	2.02	0.42
1:A:979:PRO:HB2	1:A:980:GLN:H	1.62	0.41
1:C:1020:ALA:N	1:C:1021:PRO:HD2	2.35	0.41
1:C:755:TYR:CD1	1:C:771:VAL:HG13	2.55	0.41
1:B:924:GLY:HA3	1:B:964:ALA:HA	2.02	0.41
1:C:730:LYS:HD2	1:C:730:LYS:HA	1.79	0.41
1:C:708:CYS:O	1:C:714:ARG:NH1	2.53	0.41
1:D:932:HIS:O	1:D:935:GLN:HG2	2.20	0.41
1:D:977:PRO:HB2	1:D:1015:GLN:OE1	2.20	0.41
1:B:1045:LEU:O	1:B:1049:THR:HG22	2.21	0.41
1:C:932:HIS:N	1:C:933:PRO:HD2	2.35	0.41
1:C:1032:ALA:O	1:C:1034:ASN:N	2.54	0.41
1:C:852:ALA:N	1:C:853:PRO:HD2	2.36	0.41
1:D:1013:PRO:O	1:D:1016:VAL:HG22	2.21	0.41
1:D:698:VAL:HG11	1:A:705:LEU:HD11	2.02	0.41
1:D:714:ARG:NH2	1:D:762:GLU:OE2	2.54	0.41
1:C:752:VAL:HG21	1:C:786:THR:HG23	2.03	0.41
1:A:848:GLY:HA2	1:A:889:LEU:HD23	2.02	0.41
1:D:839:ILE:HB	1:D:840:PRO:HD3	2.03	0.41
1:D:905:LEU:HD23	1:D:944:LEU:HD13	2.03	0.41
1:C:1074:LEU:HA	1:C:1077:VAL:HG22	2.03	0.40
1:C:959:ASP:OD1	1:C:991:LEU:HB3	2.21	0.40
1:B:1070:LYS:HA	1:B:1070:LYS:HD3	1.75	0.40
1:B:913:PRO:O	1:B:917:SER:HB2	2.21	0.40
1:D:1006:SER:O	1:B:1006:SER:OG	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:935:GLN:HA	1:D:938:PHE:CD1	2.55	0.40
1:C:910:GLU:O	1:C:916:ARG:NH1	2.53	0.40
1:B:752:VAL:HG21	1:B:786:THR:HG23	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:TYR:OH	1:C:1039:ASP:OD1[1_565]	2.19	0.01

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	358/416 (86%)	325 (91%)	30 (8%)	3 (1%)	22	65
1	B	369/416 (89%)	347 (94%)	19 (5%)	3 (1%)	22	65
1	C	362/416 (87%)	335 (92%)	24 (7%)	3 (1%)	22	65
1	D	365/416 (88%)	341 (93%)	21 (6%)	3 (1%)	22	65
2	E	2/18 (11%)	1 (50%)	1 (50%)	0	100	100
All	All	1456/1682 (87%)	1349 (93%)	95 (6%)	12 (1%)	22	65

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	932	HIS
1	D	931	GLY
1	A	930	GLY
1	B	809	ALA
1	A	979	PRO
1	B	974	THR

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Mol	Chain	Res	Type
1	D	782	CYS
1	A	931	GLY
1	B	738	GLU
1	C	973	PRO
1	C	1019	VAL
1	C	736	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/334 (87%)	283 (97%)	9 (3%)	45	78
1	B	298/334 (89%)	290 (97%)	8 (3%)	50	81
1	C	293/334 (88%)	290 (99%)	3 (1%)	80	93
1	D	295/334 (88%)	287 (97%)	8 (3%)	50	81
2	E	1/13 (8%)	1 (100%)	0	100	100
All	All	1179/1349 (87%)	1151 (98%)	28 (2%)	54	83

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	703	PHE
1	D	745	GLN
1	D	810	CYS
1	D	866	THR
1	D	946	PHE
1	D	1010	GLN
1	D	1011	SER
1	D	1056	THR
1	A	711	LEU
1	A	785	LEU
1	A	793	LEU
1	A	864	CYS
1	A	938	PHE

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Mol	Chain	Res	Type
1	A	940	LYS
1	A	951	ARG
1	A	1010	GLN
1	A	1034	ASN
1	B	710	HIS
1	B	861	LEU
1	B	871	THR
1	B	967	ARG
1	B	976	LYS
1	B	1063	LEU
1	B	1069	ASP
1	B	1074	LEU
1	C	732	CYS
1	C	808	THR
1	C	990	PRO

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

Mol	Chain	Res	Type
1	C	960	ASN

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 ⓘ

There are no ligands in this entry.

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, 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	366/416 (87%)	-0.11	6 (1%) 72 60	63, 83, 123, 175	0
1	B	373/416 (89%)	-0.08	6 (1%) 72 60	60, 77, 126, 176	0
1	C	368/416 (88%)	-0.08	5 (1%) 75 63	61, 79, 125, 172	0
1	D	369/416 (88%)	-0.09	8 (2%) 62 48	60, 84, 124, 203	0
2	E	4/18 (22%)	-0.41	0 100 100	73, 89, 105, 111	0
All	All	1480/1682 (87%)	-0.09	25 (1%) 70 57	60, 81, 125, 203	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1030	ILE	5.7
1	D	985	LEU	5.0
1	B	1027	CYS	3.6
1	D	976	LYS	3.3
1	D	800	LEU	3.3
1	A	900	LEU	3.2
1	D	712	ASN	3.1
1	A	724	PHE	2.9
1	C	766	GLN	2.8
1	D	804	LEU	2.6
1	B	1023	LEU	2.5
1	C	953	ARG	2.3
1	D	1030	ILE	2.3
1	A	1008	LEU	2.3
1	B	724	PHE	2.2
1	D	1044	LEU	2.2
1	C	1012	SER	2.1
1	C	1030	ILE	2.1
1	D	1047	LEU	2.1
1	A	706	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	861	LEU	2.0
1	A	702	VAL	2.0
1	C	759	VAL	2.0
1	B	766	GLN	2.0
1	B	1026	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.