



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:10 PM UTC

PDB ID : 3S8V / pdb_00003s8v
Title : Crystal structure of LRP6-Dkk1 complex
Authors : Cheng, Z.; Xu, W.
Deposited on : 2011-05-31
Resolution : 3.10 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

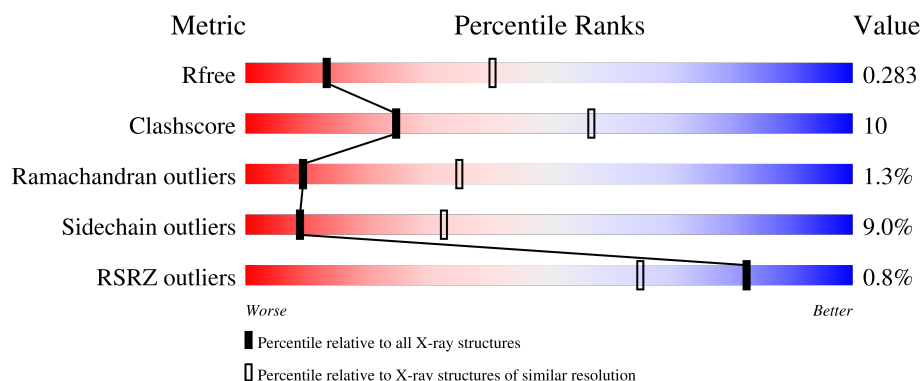
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	623	% 69% 24% . .
1	B	623	% 70% 25% . .
2	X	88	64% 16% . 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10177 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 Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	0	0
			4790	3011	846	908	25			
1	B	604	Total	C	N	O	S	0	0	0
			4818	3025	854	914	25			

There are 18 discrepancies between the modelled and reference sequences:

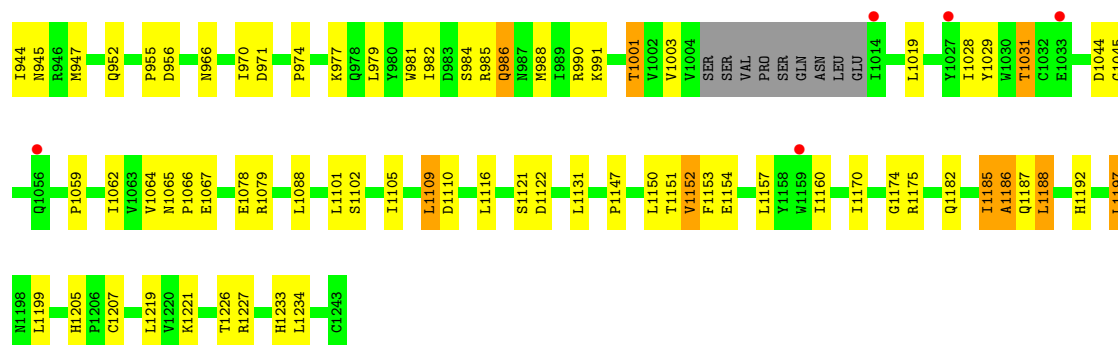
Chain	Residue	Modelled	Actual	Comment	Reference
A	621	HIS	-	expression tag	UNP O75581
A	622	HIS	-	expression tag	UNP O75581
A	623	HIS	-	expression tag	UNP O75581
A	624	HIS	-	expression tag	UNP O75581
A	625	HIS	-	expression tag	UNP O75581
A	626	HIS	-	expression tag	UNP O75581
A	627	HIS	-	expression tag	UNP O75581
A	628	HIS	-	expression tag	UNP O75581
A	1062	ILE	VAL	conflict	UNP O75581
B	621	HIS	-	expression tag	UNP O75581
B	622	HIS	-	expression tag	UNP O75581
B	623	HIS	-	expression tag	UNP O75581
B	624	HIS	-	expression tag	UNP O75581
B	625	HIS	-	expression tag	UNP O75581
B	626	HIS	-	expression tag	UNP O75581
B	627	HIS	-	expression tag	UNP O75581
B	628	HIS	-	expression tag	UNP O75581
B	1062	ILE	VAL	conflict	UNP O75581

- Molecule 2 is a protein called Dickkopf-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	73	Total	C	N	O	S	0	0	0
			569	345	116	98	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	179	GLY	-	expression tag	UNP O94907
X	180	PRO	-	expression tag	UNP O94907
X	181	GLY	-	expression tag	UNP O94907
X	182	SER	-	expression tag	UNP O94907



- Molecule 2: Dickkopf-related protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.38Å 105.05Å 161.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-3.10) 98.1 (30.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.240 , 0.292 0.236 , 0.283	Depositor DCC
R_{free} test set	1539 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10177	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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

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	0.46	0/4889	0.76	0/6630
1	B	0.46	0/4919	0.73	1/6674 (0.0%)
2	X	0.48	0/577	0.88	0/766
All	All	0.46	0/10385	0.76	1/14070 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	650	ASN	CB-CA-C	-5.10	110.68	116.54

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	4790	0	4676	96	0
1	B	4818	0	4705	90	0
2	X	569	0	558	14	0
All	All	10177	0	9939	198	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 10.

All (198) 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:A:1031:THR:HG23	1:A:1062:ILE:HD11	1.19	1.12
1:B:1031:THR:HG23	1:B:1062:ILE:HD11	1.36	1.03
1:A:679:THR:HG21	1:A:707:PRO:O	1.63	0.99
1:A:1019:LEU:HD12	1:A:1028:ILE:HD11	1.44	0.97
1:B:1031:THR:HG23	1:B:1062:ILE:CD1	1.94	0.97
1:B:1019:LEU:HD12	1:B:1028:ILE:HD11	1.44	0.95
1:A:795:GLY:O	1:A:807:TRP:HA	1.77	0.83
1:B:940:GLN:HA	1:B:1188:LEU:HA	1.63	0.81
2:X:215:LYS:H	2:X:218:GLN:HE21	1.29	0.79
1:B:985:ARG:O	1:B:986:GLN:HB2	1.85	0.77
1:B:1110:ASP:HB2	1:B:1152:VAL:HG21	1.65	0.77
1:B:793:ALA:HA	1:B:808:THR:O	1.86	0.75
1:A:934:THR:HG23	1:A:1195:LYS:HA	1.69	0.73
1:A:634:LEU:HD23	1:A:879:ILE:HD11	1.71	0.72
1:A:812:THR:HB	1:A:814:LEU:HD22	1.71	0.72
2:X:215:LYS:H	2:X:218:GLN:NE2	1.88	0.72
1:B:947:MET:HB3	1:B:956:ASP:HB3	1.72	0.71
1:B:1031:THR:CG2	1:B:1062:ILE:HD11	2.19	0.71
1:A:881:VAL:HG13	1:A:886:ARG:HD2	1.72	0.71
1:A:1031:THR:HG23	1:A:1062:ILE:CD1	2.12	0.70
1:A:1105:ILE:CD1	1:A:1121:SER:HB2	2.21	0.70
1:A:1160:ILE:HG23	1:A:1188:LEU:HG	1.73	0.70
1:A:1151:THR:HG21	1:A:1192:HIS:HA	1.77	0.67
1:B:656:ILE:HG22	1:B:658:LEU:HG	1.77	0.66
1:B:636:PHE:HB3	1:B:879:ILE:HG22	1.78	0.66
1:B:675:ARG:HD3	1:B:688:ARG:HD2	1.78	0.65
1:B:1182:GLN:HG2	1:B:1185:ILE:HD11	1.80	0.64
1:B:671:VAL:HG11	1:B:884:SER:HB3	1.78	0.64
1:A:1206:PRO:HB2	1:A:1226:THR:CG2	2.28	0.64
1:A:856:GLU:HG2	1:A:868:ILE:HG12	1.80	0.63
1:A:923:ASN:HD22	1:A:928:THR:HB	1.64	0.63
1:A:1061:ALA:HB3	1:A:1074:THR:HB	1.81	0.63
1:B:679:THR:HG22	1:B:686:ILE:HG12	1.81	0.62
1:A:1188:LEU:H	1:A:1188:LEU:HD23	1.64	0.62
1:B:795:GLY:HA3	1:B:838:LEU:HB3	1.82	0.62
1:B:810:LEU:HB3	2:X:229:HIS:CE1	2.34	0.62
1:B:640:ALA:HA	1:B:661:VAL:HG22	1.82	0.62
1:A:1188:LEU:H	1:A:1188:LEU:CD2	2.13	0.61
1:B:1019:LEU:HD12	1:B:1028:ILE:CD1	2.27	0.61
1:B:1065:ASN:HB2	1:B:1109:LEU:HD11	1.81	0.61
1:B:1185:ILE:HG22	1:B:1186:ALA:N	2.15	0.61
1:B:832:LEU:HB3	1:B:835:PRO:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:LEU:HD12	1:B:757:PRO:HB2	1.84	0.60
1:A:663:GLU:HB3	1:A:681:ILE:HD13	1.84	0.59
1:B:1151:THR:HG21	1:B:1192:HIS:HA	1.84	0.59
1:A:1105:ILE:HD13	1:A:1121:SER:HB2	1.85	0.59
1:A:805:LEU:O	1:A:817:SER:HA	2.01	0.59
1:A:1164:GLN:HG2	1:A:1166:MET:HE3	1.85	0.58
1:A:1155:ASN:HD22	1:A:1155:ASN:N	2.02	0.58
1:A:1031:THR:CG2	1:A:1062:ILE:HD11	2.13	0.58
1:A:1146:GLN:HG2	1:A:1162:LYS:HB3	1.86	0.58
1:A:663:GLU:HB3	1:A:681:ILE:CD1	2.34	0.57
1:A:965:ARG:HD3	1:A:985:ARG:NH2	2.21	0.56
2:X:215:LYS:N	2:X:218:GLN:HE21	2.02	0.56
1:A:1124:ARG:HD3	1:A:1145:LEU:HA	1.88	0.56
1:B:699:VAL:HG12	1:B:700:VAL:HG23	1.88	0.56
1:A:708:GLU:HB3	1:A:751:ARG:HD2	1.89	0.55
1:A:1042:ARG:HD2	1:A:1046:ARG:HB3	1.87	0.54
1:A:762:MET:HB3	1:A:778:MET:HG2	1.90	0.54
1:A:722:ALA:HB1	1:A:750:PRO:HB2	1.89	0.53
1:B:1153:PHE:HD2	1:B:1154:GLU:HG3	1.72	0.53
1:B:775:ARG:HD3	1:B:786:LEU:HD13	1.90	0.53
1:B:974:PRO:HB2	1:B:1197:LEU:HB2	1.90	0.53
1:A:1155:ASN:HD22	1:A:1155:ASN:H	1.55	0.53
1:B:985:ARG:O	1:B:986:GLN:CB	2.55	0.53
1:B:715:LEU:HD13	1:B:891:ASN:HB2	1.91	0.53
1:A:986:GLN:HG2	1:A:988:MET:HE3	1.90	0.52
1:B:1205:HIS:HD2	1:B:1207:CYS:H	1.58	0.52
1:A:797:THR:HG21	1:A:839:THR:HA	1.91	0.52
1:B:1150:LEU:HD12	1:B:1157:LEU:HD11	1.91	0.52
2:X:223:HIS:HE1	2:X:232:GLU:HG3	1.75	0.52
1:A:944:ILE:HG21	1:A:979:LEU:HD21	1.92	0.52
1:B:633:PHE:HA	1:B:647:LEU:HG	1.92	0.52
1:A:651:ASN:ND2	1:A:652:ASN:H	2.07	0.52
1:A:653:ASN:HD22	1:A:653:ASN:C	2.18	0.52
1:A:1188:LEU:HD23	1:A:1188:LEU:N	2.25	0.52
1:A:795:GLY:HA3	1:A:838:LEU:HB3	1.91	0.51
1:A:918:ALA:O	1:A:919:HIS:HB2	2.09	0.51
1:A:1160:ILE:HG12	1:A:1188:LEU:HD12	1.93	0.51
1:B:636:PHE:HE2	1:B:645:ILE:CD1	2.22	0.51
1:B:755:LEU:HB3	1:B:778:MET:HE1	1.93	0.51
1:B:767:TRP:CE2	1:B:792:ARG:HB3	2.45	0.51
1:A:663:GLU:O	1:A:681:ILE:HD13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:ILE:HD11	1:A:1121:SER:HB2	1.92	0.51
1:B:850:TRP:HZ2	1:B:877:MET:HB3	1.77	0.50
1:B:1233:HIS:CD2	1:B:1234:LEU:HG	2.47	0.50
1:A:940:GLN:HG3	1:A:943:ALA:HB3	1.92	0.50
1:B:940:GLN:HE21	1:B:945:ASN:ND2	2.09	0.50
1:A:1065:ASN:HB2	1:A:1109:LEU:HD11	1.93	0.50
1:B:681:ILE:HG22	1:B:707:PRO:HD2	1.93	0.50
2:X:203:ARG:HB2	2:X:235:GLN:HE21	1.75	0.50
1:B:940:GLN:HE21	1:B:945:ASN:HD21	1.59	0.50
1:A:1015:GLN:HG2	1:A:1034:ALA:HB2	1.94	0.49
1:A:1150:LEU:HD12	1:A:1157:LEU:HD21	1.94	0.49
1:B:813:ASN:HD21	1:B:835:PRO:HD2	1.77	0.49
1:A:1051:VAL:HG21	1:A:1071:MET:HE1	1.93	0.49
1:A:644:ARG:HB2	1:A:656:ILE:HD11	1.94	0.48
1:A:706:TYR:HB2	1:A:724:THR:HG22	1.94	0.48
1:B:986:GLN:HB3	1:B:988:MET:HG2	1.96	0.48
1:B:1031:THR:HG22	1:B:1059:PRO:HB2	1.95	0.48
1:B:881:VAL:HG13	1:B:886:ARG:HD2	1.96	0.48
1:A:751:ARG:HG3	1:A:752:ALA:N	2.29	0.48
1:B:966:ASN:HB3	1:B:984:SER:HB2	1.94	0.47
1:B:814:LEU:CD1	1:B:816:GLU:HG3	2.44	0.47
1:A:747:LEU:HD22	1:A:750:PRO:HD3	1.96	0.47
1:A:775:ARG:HB3	1:A:786:LEU:HD13	1.96	0.47
1:B:1121:SER:HA	1:B:1147:PRO:HD2	1.97	0.47
1:A:675:ARG:HD3	1:A:688:ARG:HD2	1.97	0.47
1:A:708:GLU:HG2	1:A:751:ARG:NH1	2.29	0.46
1:B:944:ILE:HG21	1:B:979:LEU:HD21	1.96	0.46
2:X:247:ILE:HD11	2:X:259:ARG:HB2	1.98	0.46
1:B:1221:LYS:HD2	1:B:1227:ARG:HH11	1.79	0.46
1:A:793:ALA:HA	1:A:808:THR:O	2.15	0.46
1:B:636:PHE:HE2	1:B:645:ILE:HD11	1.81	0.46
1:A:940:GLN:HA	1:A:1188:LEU:HA	1.98	0.46
1:B:1044:ASP:OD1	1:B:1045:GLY:N	2.49	0.46
2:X:233:ILE:HD13	2:X:233:ILE:HA	1.81	0.46
1:A:839:THR:HG21	1:A:881:VAL:H	1.81	0.46
1:A:923:ASN:ND2	1:A:928:THR:HB	2.31	0.46
1:A:991:LYS:HD2	1:A:1000:PHE:HB3	1.98	0.46
1:B:1102:SER:HB3	1:B:1122:ASP:HB2	1.98	0.46
1:A:699:VAL:HG12	1:A:700:VAL:HG23	1.98	0.45
1:B:847:TRP:CE2	1:B:856:GLU:HB2	2.51	0.45
1:A:1155:ASN:N	1:A:1155:ASN:ND2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:TRP:CE2	1:B:955:PRO:HD3	2.52	0.45
1:A:1155:ASN:H	1:A:1155:ASN:ND2	2.14	0.45
1:B:835:PRO:HA	1:B:848:THR:O	2.15	0.45
1:B:636:PHE:CE2	1:B:645:ILE:HD11	2.52	0.45
1:B:925:ASP:O	1:B:926:ASN:HB2	2.17	0.45
1:A:1031:THR:CG2	1:A:1059:PRO:HB2	2.47	0.45
1:A:1199:LEU:O	1:A:1203:ARG:HG2	2.17	0.45
1:B:1029:TYR:CD2	1:B:1064:VAL:HG11	2.52	0.45
1:A:965:ARG:HA	1:A:965:ARG:HE	1.82	0.44
1:A:1185:ILE:HG22	1:A:1188:LEU:HD22	1.99	0.44
1:A:1205:HIS:CD2	1:A:1207:CYS:H	2.35	0.44
1:A:1037:VAL:HG23	1:A:1053:LYS:HB3	1.99	0.44
1:A:1072:TYR:OH	1:A:1131:LEU:HB3	2.17	0.44
1:B:636:PHE:CB	1:B:879:ILE:HG22	2.45	0.44
2:X:205:PHE:HA	2:X:233:ILE:HG23	1.99	0.44
1:B:902:HIS:CE1	1:B:929:CYS:HB2	2.53	0.44
1:A:639:ARG:HD2	2:X:206:TRP:CE2	2.53	0.44
1:A:1140:GLU:HB3	1:A:1144:ILE:HD11	1.99	0.44
1:B:1066:PRO:HA	1:B:1088:LEU:HD11	1.98	0.44
1:B:1031:THR:HG23	1:B:1062:ILE:HD12	1.90	0.44
1:A:1237:LEU:HD23	1:A:1243:CYS:HA	2.00	0.44
1:A:679:THR:HG23	1:A:707:PRO:HG2	2.00	0.44
1:A:1030:TRP:CE2	1:A:1039:ASN:HB3	2.53	0.44
1:A:1144:ILE:HG21	1:A:1147:PRO:HG3	1.99	0.43
1:B:643:ARG:NH1	1:B:655:ALA:HB2	2.34	0.43
1:B:729:ILE:HB	1:B:743:VAL:HG13	1.99	0.43
1:A:1154:GLU:HB3	1:A:1155:ASN:HD22	1.82	0.43
1:B:990:ARG:HG3	1:B:1001:THR:HA	2.00	0.43
1:A:711:ALA:HB3	1:A:755:LEU:HG	2.00	0.43
1:A:877:MET:O	1:A:878:ASP:O	2.36	0.43
1:B:970:ILE:HG22	1:B:981:TRP:HB3	1.99	0.43
1:B:677:TYR:CE1	1:B:688:ARG:HD3	2.54	0.43
1:A:1182:GLN:HG3	1:A:1185:ILE:HD11	2.01	0.43
1:B:671:VAL:HG22	1:B:882:PHE:HE2	1.83	0.42
1:B:733:LYS:HB2	1:B:735:ASP:OD2	2.18	0.42
1:B:813:ASN:ND2	1:B:835:PRO:HD2	2.34	0.42
1:B:908:PRO:C	1:B:910:GLY:H	2.27	0.42
1:A:645:ILE:HG22	1:A:652:ASN:O	2.19	0.42
1:A:656:ILE:HA	1:A:657:PRO:HD3	1.81	0.42
1:B:645:ILE:HD13	1:B:870:GLN:HG3	2.01	0.42
1:B:814:LEU:HD13	1:B:816:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:838:LEU:HA	1:B:846:TYR:O	2.19	0.42
2:X:192:SER:HA	2:X:201:CYS:HB2	2.02	0.42
1:A:646:SER:OG	1:A:648:GLU:HB2	2.20	0.42
1:B:700:VAL:HG12	1:B:704:LEU:HD11	2.01	0.42
1:A:1107:LEU:HD12	1:A:1118:TRP:HB3	2.02	0.42
1:B:842:GLN:HB3	1:B:843:ASP:H	1.62	0.42
2:X:202:ALA:HB1	2:X:235:GLN:HG3	2.02	0.42
1:A:1002:VAL:HG12	1:A:1003:VAL:HG23	2.01	0.41
1:B:792:ARG:O	1:B:810:LEU:HB2	2.20	0.41
1:B:1116:LEU:HB2	1:B:1131:LEU:HD23	2.02	0.41
1:B:1205:HIS:CD2	1:B:1207:CYS:H	2.36	0.41
1:A:902:HIS:CE1	1:A:929:CYS:HB2	2.56	0.41
1:A:724:THR:O	1:A:727:ASN:ND2	2.53	0.41
1:A:973:ASP:HA	1:A:974:PRO:HD3	1.89	0.41
1:B:1078:GLU:HG3	1:B:1079:ARG:CZ	2.50	0.41
1:A:814:LEU:HB2	1:A:830:ASP:HA	2.01	0.41
1:A:938:PHE:HB3	1:A:1191:ILE:HG13	2.02	0.41
1:A:965:ARG:HA	1:A:965:ARG:NE	2.36	0.41
1:B:829:ALA:HB1	1:B:832:LEU:HD23	2.02	0.41
2:X:247:ILE:HD13	2:X:248:GLN:N	2.35	0.41
1:A:839:THR:OG1	1:A:880:LEU:HA	2.21	0.41
1:A:941:LYS:HG2	1:A:966:ASN:HA	2.03	0.41
1:B:873:LEU:HB3	1:B:876:VAL:HG21	2.01	0.41
1:A:979:LEU:O	1:A:991:LYS:HA	2.21	0.41
1:B:633:PHE:CE1	1:B:882:PHE:HD1	2.38	0.41
1:B:751:ARG:HB3	1:B:752:ALA:H	1.44	0.41
1:B:670:ASP:HB2	1:B:677:TYR:HE2	1.86	0.40
1:B:723:ASP:HB3	1:B:726:THR:OG1	2.21	0.40
1:B:1066:PRO:HD2	1:B:1067:GLU:OE1	2.20	0.40
2:X:203:ARG:H	2:X:235:GLN:CG	2.33	0.40
1:A:1071:MET:HB3	1:A:1088:LEU:HD23	2.03	0.40
1:B:841:TYR:HB2	1:B:881:VAL:HG11	2.04	0.40
1:B:669:PHE:O	1:B:887:GLN:NE2	2.47	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	590/623 (95%)	529 (90%)	50 (8%)	11 (2%)	6	27
1	B	600/623 (96%)	540 (90%)	55 (9%)	5 (1%)	16	47
2	X	69/88 (78%)	65 (94%)	4 (6%)	0	100	100
All	All	1259/1334 (94%)	1134 (90%)	109 (9%)	16 (1%)	9	35

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1174	GLY
1	A	878	ASP
1	A	879	ILE
1	B	926	ASN
1	B	986	GLN
1	A	999	GLY
1	A	1186	ALA
1	A	1224	GLY
1	B	1186	ALA
1	A	651	ASN
1	B	1185	ILE
1	A	833	PRO
1	A	1079	ARG
1	A	788	PRO
1	A	1231	PRO
1	A	1148	VAL

5.3.2 Protein sidechains [i](#)

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	525/546 (96%)	473 (90%)	52 (10%)	7	29
1	B	527/546 (96%)	483 (92%)	44 (8%)	10	35
2	X	64/75 (85%)	60 (94%)	4 (6%)	16	45
All	All	1116/1167 (96%)	1016 (91%)	100 (9%)	9	33

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	635	LEU
1	A	647	LEU
1	A	651	ASN
1	A	654	VAL
1	A	681	ILE
1	A	724	THR
1	A	747	LEU
1	A	785	THR
1	A	814	LEU
1	A	827	VAL
1	A	832	LEU
1	A	838	LEU
1	A	839	THR
1	A	842	GLN
1	A	843	ASP
1	A	880	LEU
1	A	913	VAL
1	A	928	THR
1	A	934	THR
1	A	940	GLN
1	A	952	GLN
1	A	982	ILE
1	A	991	LYS
1	A	993	GLN
1	A	995	ASP
1	A	1014	ILE
1	A	1020	SER
1	A	1031	THR
1	A	1037	VAL
1	A	1050	VAL
1	A	1055	GLU
1	A	1074	THR

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Mol	Chain	Res	Type
1	A	1076	LEU
1	A	1079	ARG
1	A	1096	LEU
1	A	1101	LEU
1	A	1107	LEU
1	A	1123	LEU
1	A	1125	ARG
1	A	1136	ARG
1	A	1138	VAL
1	A	1139	LEU
1	A	1143	ASN
1	A	1146	GLN
1	A	1148	VAL
1	A	1155	ASN
1	A	1170	ILE
1	A	1185	ILE
1	A	1188	LEU
1	A	1220	VAL
1	A	1221	LYS
1	A	1225	THR
1	B	641	ASP
1	B	649	THR
1	B	650	ASN
1	B	667	LEU
1	B	683	LEU
1	B	741	VAL
1	B	743	VAL
1	B	748	ASP
1	B	749	SER
1	B	770	LYS
1	B	772	LYS
1	B	778	MET
1	B	790	VAL
1	B	812	THR
1	B	823	LEU
1	B	826	GLU
1	B	832	LEU
1	B	834	HIS
1	B	839	THR
1	B	868	ILE
1	B	878	ASP
1	B	913	VAL

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Mol	Chain	Res	Type
1	B	925	ASP
1	B	952	GLN
1	B	971	ASP
1	B	977	LYS
1	B	982	ILE
1	B	991	LYS
1	B	1001	THR
1	B	1003	VAL
1	B	1031	THR
1	B	1101	LEU
1	B	1105	ILE
1	B	1109	LEU
1	B	1152	VAL
1	B	1160	ILE
1	B	1170	ILE
1	B	1175	ARG
1	B	1187	GLN
1	B	1188	LEU
1	B	1197	LEU
1	B	1199	LEU
1	B	1219	LEU
1	B	1226	THR
2	X	192	SER
2	X	200	CYS
2	X	233	ILE
2	X	247	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	651	ASN
1	A	653	ASN
1	A	727	ASN
1	A	738	HIS
1	A	789	ASN
1	A	824	ASN
1	A	872	HIS
1	A	899	HIS
1	A	923	ASN
1	A	952	GLN
1	A	986	GLN
1	A	987	ASN

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Mol	Chain	Res	Type
1	A	1143	ASN
1	A	1155	ASN
1	A	1216	HIS
1	B	652	ASN
1	B	727	ASN
1	B	738	HIS
1	B	813	ASN
1	B	834	HIS
1	B	872	HIS
1	B	897	ASN
1	B	945	ASN
1	B	966	ASN
1	B	993	GLN
1	B	1163	GLN
1	B	1205	HIS
1	B	1211	ASN
2	X	184	GLN
2	X	218	GLN
2	X	223	HIS
2	X	235	GLN
2	X	248	GLN
2	X	261	HIS
2	X	264	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	600/623 (96%)	0.03	4 (0%) 84 68	45, 80, 113, 143	0
1	B	604/623 (96%)	0.10	6 (0%) 79 61	45, 90, 113, 141	0
2	X	73/88 (82%)	0.11	0 100 100	65, 86, 107, 122	0
All	All	1277/1334 (95%)	0.07	10 (0%) 82 65	45, 86, 113, 143	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1062	ILE	3.4
1	A	795	GLY	3.2
1	B	1027	TYR	2.9
1	A	1160	ILE	2.8
1	B	1056	GLN	2.8
1	A	911	GLY	2.3
1	B	1159	TRP	2.3
1	B	909	VAL	2.3
1	B	1033	GLU	2.1
1	B	1014	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 oligosaccharides 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.