



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:55 PM GMT

PDB ID : 3S8V  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

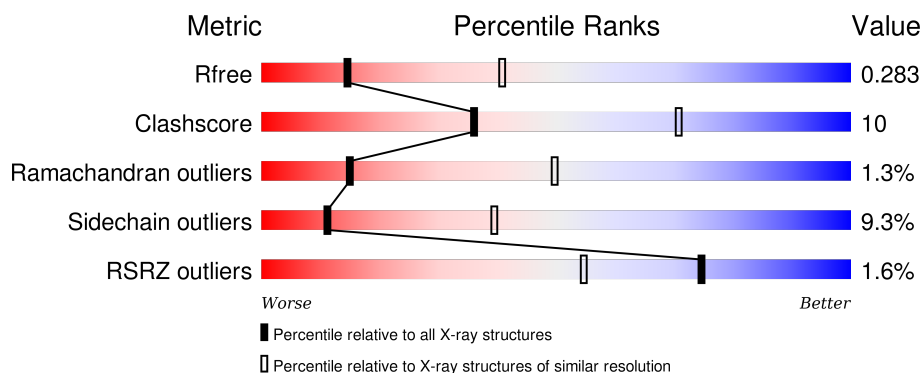
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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  $\geq 3$ , 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	623	<div> <div>2%</div> <div>70%</div> <div>22%</div> <div>• •</div> </div>
1	B	623	<div> <div>2%</div> <div>70%</div> <div>25%</div> <div>• •</div> </div>
2	X	88	<div> <div>2%</div> <div>63%</div> <div>18%</div> <div>• 17%</div> </div>

## 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			

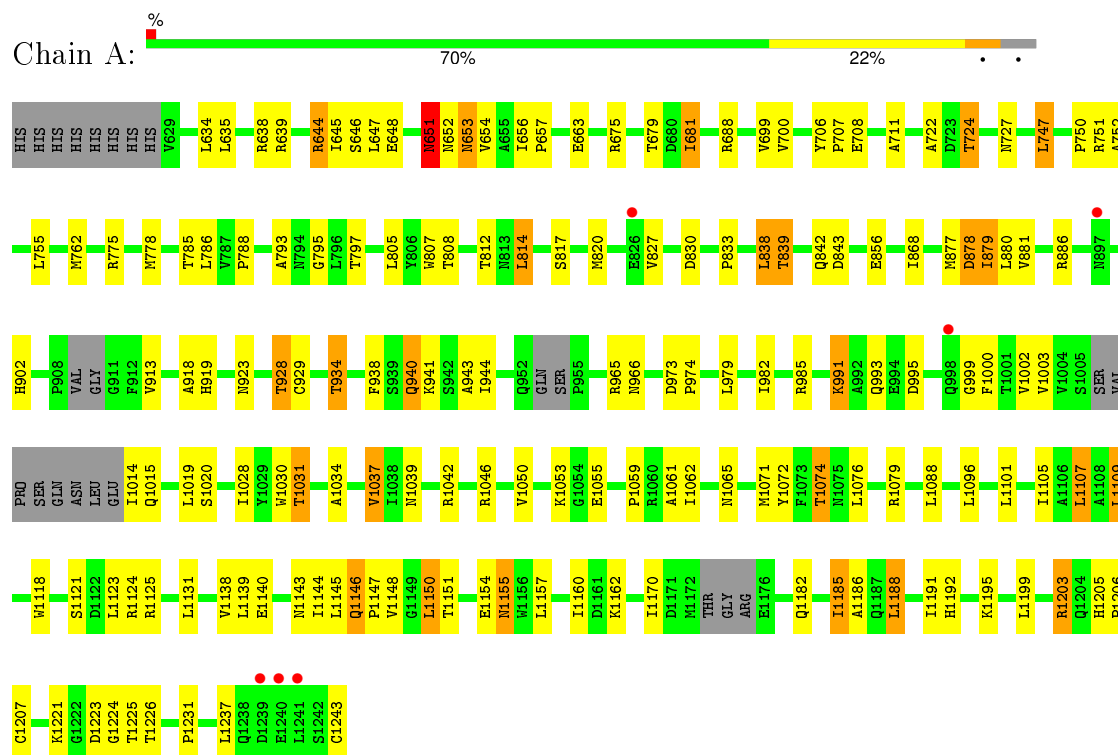
There are 4 discrepancies between the modelled and reference sequences:

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

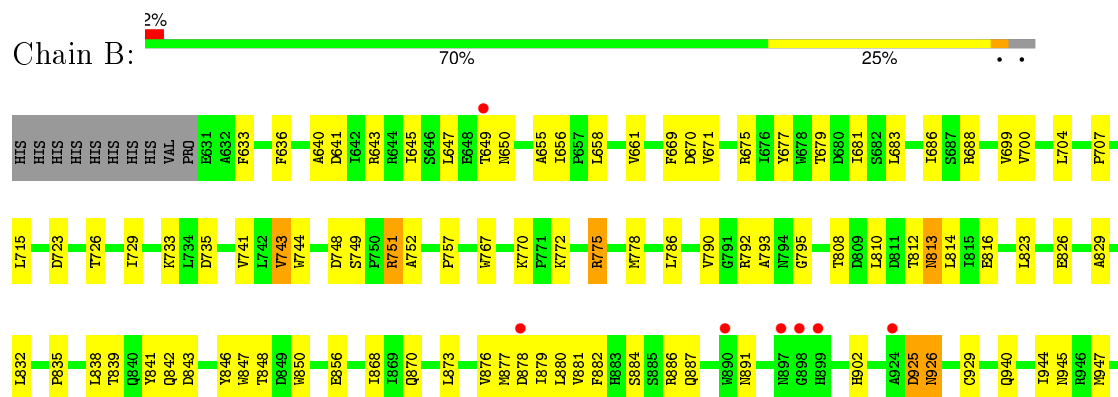
### 3 Residue-property plots

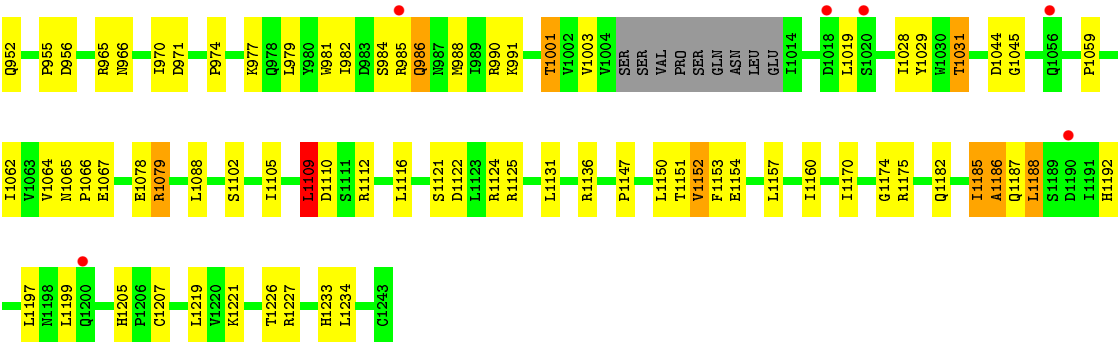
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Low-density lipoprotein receptor-related protein 6

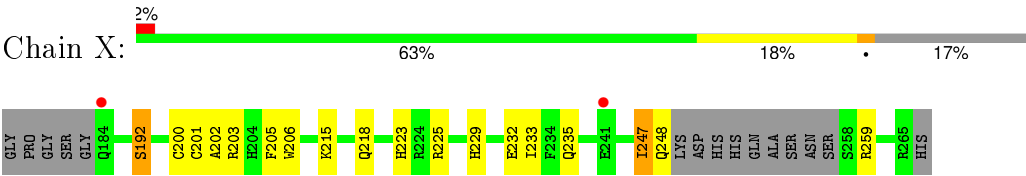


- Molecule 1: Low-density lipoprotein receptor-related protein 6





● 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, $\alpha$ , $\beta$ , $\gamma$	94.38Å 105.05Å 161.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 29.63 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-3.10) 97.4 (29.63-3.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	1490 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.7	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 30357 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10177	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.36	0/4889	0.57	0/6630
1	B	0.36	0/4919	0.55	1/6674 (0.0%)
2	X	0.37	0/577	0.55	0/766
All	All	0.36	0/10385	0.56	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	1109	LEU	CA-CB-CG	5.38	127.66	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	4790	0	4676	94	0
1	B	4818	0	4705	88	0
2	X	569	0	558	14	0
All	All	10177	0	9939	194	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 (194) 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:B:1031:THR:HG23	1:B:1062:ILE:CD1	1.94	0.97
1:A:1019:LEU:HD12	1:A:1028:ILE:HD11	1.44	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:1031:THR:CG2	1:B:1062:ILE:HD11	2.19	0.71
1:B:947:MET:HB3	1:B:956:ASP:HB3	1.72	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:1160:ILE:HG23	1:A:1188:LEU:HG	1.73	0.70
1:A:1105:ILE:CD1	1:A:1121:SER:HB2	2.21	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:HD23	1:A:1188:LEU:H	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:CD2	1:A:1188:LEU:H	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: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
2:X:215:LYS:N	2:X:218:GLN:HE21	2.02	0.56
1:A:965:ARG:HD3	1:A:985:ARG:NH2	2.21	0.56
1:B:699:VAL:HG12	1:B:700:VAL:HG23	1.88	0.56
1:A:1124:ARG:HD3	1:A:1145:LEU:HA	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:974:PRO:HB2	1:B:1197:LEU:HB2	1.90	0.53
1:B:775:ARG:HD3	1:B:786:LEU:HD13	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: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
2:X:223:HIS:HE1	2:X:232:GLU:HG3	1.75	0.52
1:B:1150:LEU:HD12	1:B:1157:LEU:HD11	1.91	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:1188:LEU:N	1:A:1188:LEU:HD23	2.25	0.52
1:A:651:ASN:ND2	1:A:652:ASN:H	2.07	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:767:TRP:CE2	1:B:792:ARG:HB3	2.45	0.51
1:A:1105:ILE:HD11	1:A:1121:SER:HB2	1.92	0.51
1:A:663:GLU:O	1:A:681:ILE:HD13	2.10	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:B:940:GLN:HE21	1:B:945:ASN:ND2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:GLN:HG3	1:A:943:ALA:HB3	1.92	0.50
1:B:681:ILE:HG22	1:B:707:PRO:HD2	1.93	0.50
1:A:1065:ASN:HB2	1:A:1109:LEU:HD11	1.93	0.50
1:A:805:LEU:HG	1:A:820:MET:HE1	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:B:813:ASN:HD21	1:B:835:PRO:HD2	1.77	0.49
1:A:1150:LEU:HD12	1:A:1157:LEU:HD21	1.94	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:1031:THR:HG22	1:B:1059:PRO:HB2	1.95	0.48
1:B:986:GLN:HB3	1:B:988:MET:HG2	1.96	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:A:653:ASN:C	1:A:653:ASN:HD22	2.18	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:B:636:PHE:HE2	1:B:645:ILE:HD11	1.81	0.46
1:A:793:ALA:HA	1:A:808:THR:O	2.15	0.46
1:A:940:GLN:HA	1:A:1188:LEU:HA	1.98	0.46
2:X:233:ILE:HA	2:X:233:ILE:HD13	1.81	0.46
1:B:1044:ASP:OD1	1:B:1045:GLY:N	2.49	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
1:B:744:TRP:CE2	1:B:955:PRO:HD3	2.52	0.45
1:B:835:PRO:HA	1:B:848:THR:O	2.15	0.45
1:A:1155:ASN:ND2	1:A:1155:ASN:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1029:TYR:CD2	1:B:1064:VAL:HG11	2.52	0.45
1:A:1199:LEU:O	1:A:1203:ARG:HG2	2.17	0.45
1:A:1185:ILE:HG22	1:A:1188:LEU:HD22	1.99	0.44
1:A:965:ARG:HE	1:A:965:ARG:HA	1.82	0.44
1:A:1205:HIS:CD2	1:A:1207:CYS:H	2.35	0.44
1:B:636:PHE:CB	1:B:879:ILE:HG22	2.45	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
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: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:A:639:ARG:HD2	2:X:206:TRP:CE2	2.53	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:729:ILE:HB	1:B:743:VAL:HG13	1.99	0.43
1:B:643:ARG:NH1	1:B:655:ALA:HB2	2.34	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:877:MET:O	1:A:878:ASP:O	2.36	0.43
1:A:711:ALA:HB3	1:A:755:LEU:HG	2.00	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:813:ASN:ND2	1:B:835:PRO:HD2	2.34	0.42
1:B:733:LYS:HB2	1:B:735:ASP:OD2	2.18	0.42
1:A:645:ILE:HG22	1:A:652:ASN:O	2.19	0.42
1:B:645:ILE:HD13	1:B:870:GLN:HG3	2.01	0.42
1:B:838:LEU:HA	1:B:846:TYR:O	2.19	0.42
1:A:656:ILE:HA	1:A:657:PRO:HD3	1.81	0.42
1:B:814:LEU:HD13	1:B:816:GLU:HG3	2.00	0.42
2:X:192:SER:HA	2:X:201:CYS:HB2	2.02	0.42
1:B:700:VAL:HG12	1:B:704:LEU:HD11	2.01	0.42
1:A:646:SER:OG	1:A:648:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:792:ARG:O	1:B:810:LEU:HB2	2.20	0.41
1:A:1002:VAL:HG12	1:A:1003:VAL:HG23	2.01	0.41
1:B:1205:HIS:CD2	1:B:1207:CYS:H	2.36	0.41
1:B:1116:LEU:HB2	1:B:1131:LEU:HD23	2.02	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:B:829:ALA:HB1	1:B:832:LEU:HD23	2.02	0.41
1:A:965:ARG:NE	1:A:965:ARG:HA	2.36	0.41
2:X:247:ILE:HD13	2:X:248:GLN:N	2.35	0.41
1:A:938:PHE:HB3	1:A:1191:ILE:HG13	2.02	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:B:633:PHE:CE1	1:B:882:PHE:HD1	2.38	0.41
1:A:979:LEU:O	1:A:991:LYS:HA	2.21	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
2:X:203:ARG:H	2:X:235:GLN:CG	2.33	0.40
1:B:1066:PRO:HD2	1:B:1067:GLU:OE1	2.20	0.40
1:B:723:ASP:HB3	1:B:726:THR:OG1	2.21	0.40
1:B:841:TYR:HB2	1:B:881:VAL:HG11	2.04	0.40
1:A:1071:MET:HB3	1:A:1088:LEU:HD23	2.03	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 ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	590/623 (95%)	529 (90%)	50 (8%)	11 (2%)	10	40
1	B	600/623 (96%)	540 (90%)	55 (9%)	5 (1%)	24	63
2	X	69/88 (78%)	65 (94%)	4 (6%)	0	100	100
All	All	1259/1334 (94%)	1134 (90%)	109 (9%)	16 (1%)	15	50

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 ⓘ

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%)	10	34
1	B	527/546 (96%)	479 (91%)	48 (9%)	12	40
2	X	64/75 (85%)	60 (94%)	4 (6%)	22	58
All	All	1116/1167 (96%)	1012 (91%)	104 (9%)	11	39

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	635	LEU
1	A	638	ARG
1	A	644	ARG
1	A	647	LEU
1	A	651	ASN
1	A	653	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	838	LEU
1	A	839	THR
1	A	842	GLN
1	A	843	ASP
1	A	913	VAL
1	A	928	THR
1	A	934	THR
1	A	940	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
1	A	1076	LEU
1	A	1096	LEU
1	A	1101	LEU
1	A	1107	LEU
1	A	1109	LEU
1	A	1123	LEU
1	A	1125	ARG
1	A	1138	VAL
1	A	1139	LEU
1	A	1143	ASN
1	A	1146	GLN

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Mol	Chain	Res	Type
1	A	1150	LEU
1	A	1155	ASN
1	A	1170	ILE
1	A	1185	ILE
1	A	1188	LEU
1	A	1203	ARG
1	A	1221	LYS
1	A	1223	ASP
1	A	1225	THR
1	B	641	ASP
1	B	649	THR
1	B	650	ASN
1	B	683	LEU
1	B	741	VAL
1	B	743	VAL
1	B	748	ASP
1	B	749	SER
1	B	751	ARG
1	B	770	LYS
1	B	772	LYS
1	B	775	ARG
1	B	778	MET
1	B	790	VAL
1	B	812	THR
1	B	813	ASN
1	B	823	LEU
1	B	826	GLU
1	B	839	THR
1	B	868	ILE
1	B	878	ASP
1	B	880	LEU
1	B	925	ASP
1	B	952	GLN
1	B	965	ARG
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	1079	ARG

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Mol	Chain	Res	Type
1	B	1105	ILE
1	B	1109	LEU
1	B	1112	ARG
1	B	1124	ARG
1	B	1125	ARG
1	B	1136	ARG
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	1199	LEU
1	B	1219	LEU
1	B	1226	THR
2	X	192	SER
2	X	200	CYS
2	X	225	ARG
2	X	247	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) 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	824	ASN
1	A	872	HIS
1	A	923	ASN
1	A	952	GLN
1	A	993	GLN
1	A	1015	GLN
1	A	1143	ASN
1	A	1155	ASN
1	A	1205	HIS
1	A	1211	ASN
1	A	1216	HIS
1	B	727	ASN
1	B	738	HIS
1	B	813	ASN
1	B	945	ASN

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Mol	Chain	Res	Type
1	B	1163	GLN
1	B	1205	HIS
2	X	184	GLN
2	X	218	GLN
2	X	223	HIS
2	X	235	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	600/623 (96%)	-0.21	6 (1%) 84 69	45, 80, 113, 143	0
1	B	604/623 (96%)	-0.06	13 (2%) 65 42	45, 90, 113, 141	0
2	X	73/88 (82%)	0.01	2 (2%) 58 34	65, 86, 107, 122	0
All	All	1277/1334 (95%)	-0.12	21 (1%) 74 55	45, 86, 113, 143	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	899	HIS	5.3
1	B	898	GLY	4.8
2	X	241	GLU	3.5
1	B	1056	GLN	2.9
1	A	1241	LEU	2.8
1	B	878	ASP	2.7
1	A	998	GLN	2.6
1	B	890	TRP	2.5
1	A	1239	ASP	2.5
1	B	897	ASN	2.4
1	B	1200	GLN	2.4
1	B	1018	ASP	2.2
1	B	1020	SER	2.2
1	B	1190	ASP	2.2
1	B	985	ARG	2.2
1	A	1240	GLU	2.1
1	A	826	GLU	2.1
2	X	184	GLN	2.1
1	B	649	THR	2.1
1	A	897	ASN	2.0
1	B	924	ALA	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.