



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:39 pm GMT

PDB ID : 5F0O  
Title : Cohesin subunit Pds5 in complex with Scc1  
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Deposited on : 2015-11-27  
Resolution : 3.50 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

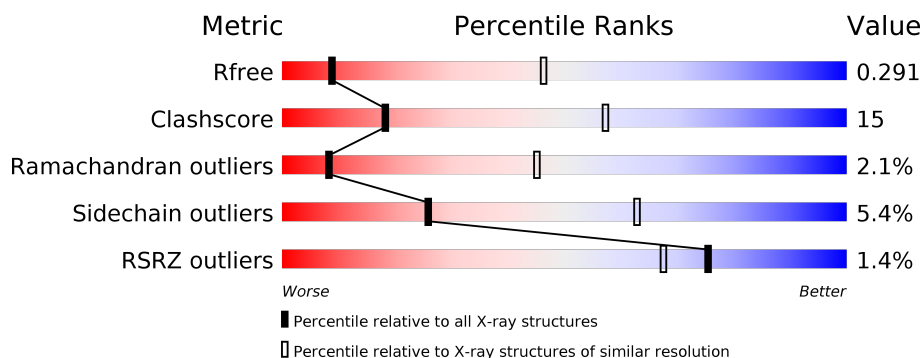
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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	1133	<div> <div></div> <div> <div></div> <div>57%</div> <div>31%</div> <div>•</div> <div>10%</div> </div> </div>
2	E	22	<div> <div>41%</div> <div>27%</div> <div>9%</div> <div>23%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8183 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.

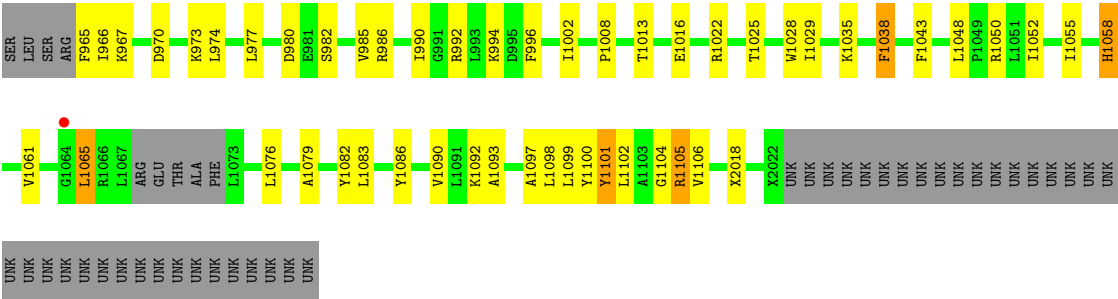
- Molecule 1 is a protein called cohesin subunit Pds5, KLTH0D07062p, KLTH0D07062p, KLTH0D07062p, cohesin subunit Pds5, KLTH0D07062p, KLTH0D07062p, KLTH0D07062p, cohesin subunit Pds5, KLTH0D07062p, KLTH0D07062p, KLTH0D07062p, cohesin subunit Pds5, KLTH0D07062p, KLTH0D07062p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1018	Total	C	N	O	S	0	0	0
			8045	5178	1343	1497	27			

- Molecule 2 is a protein called KLTH0G16610p.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	0	0	0
			138	88	22	28			





● Molecule 2: KLTH0G16610p



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.40Å 235.40Å 94.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.49 – 3.50 48.49 – 3.48	Depositor EDS
% Data completeness (in resolution range)	78.1 (44.49-3.50) 77.0 (48.49-3.48)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.232 , 0.291 0.232 , 0.291	Depositor DCC
$R_{free}$ test set	915 reflections (4.78%)	DCC
Wilson B-factor (Å <sup>2</sup> )	129.0	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 81.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.058 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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, 0.333 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	0.29	0/7994	0.50	2/10806 (0.0%)
2	E	0.29	0/138	0.51	0/187
All	All	0.29	0/8132	0.50	2/10993 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1065	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	329	LEU	CA-CB-CG	5.08	126.99	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	8045	0	8016	241	0
2	E	138	0	141	8	0
All	All	8183	0	8157	245	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 15.

All (245) 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:443:ARG:HG2	1:A:494:ILE:HD11	1.59	0.84
1:A:966:ILE:HG22	1:A:967:LYS:HG2	1.64	0.79
1:A:143:PRO:HB3	1:A:148:LEU:HD22	1.62	0.79
1:A:546:ARG:HE	2:E:139:LEU:HD22	1.49	0.77
1:A:417:PHE:O	1:A:459:ARG:NH2	2.17	0.77
1:A:214:LEU:H	1:A:263:HIS:HE1	1.31	0.76
1:A:410:ARG:NH1	1:A:444:GLU:OE1	2.19	0.76
1:A:432:ALA:HB1	1:A:480:VAL:HG21	1.66	0.75
1:A:512:LEU:HD21	1:A:528:LEU:HD22	1.69	0.74
1:A:1035:LYS:HG3	1:A:1038:PHE:HB2	1.70	0.72
1:A:986:ARG:NH1	1:A:1016:GLU:OE2	2.23	0.71
1:A:170:LEU:HD12	1:A:172:SER:H	1.55	0.71
1:A:471:THR:HG22	1:A:473:GLU:H	1.56	0.70
1:A:965:PHE:HB2	1:A:966:ILE:HA	1.74	0.70
1:A:112:LEU:HD11	1:A:129:ILE:HD12	1.74	0.68
1:A:1048:LEU:HD22	1:A:1099:LEU:HD12	1.75	0.68
1:A:158:LEU:HD13	1:A:164:ILE:HD13	1.76	0.68
1:A:211:CYS:O	1:A:263:HIS:NE2	2.28	0.66
1:A:214:LEU:H	1:A:263:HIS:CE1	2.11	0.66
1:A:143:PRO:HG3	1:A:148:LEU:HD13	1.76	0.66
1:A:158:LEU:HA	1:A:163:SER:HB2	1.75	0.66
1:A:920:VAL:HG11	1:A:974:LEU:HD23	1.77	0.65
1:A:219:LEU:HD23	1:A:267:PHE:HB2	1.79	0.64
1:A:141:GLN:NE2	1:A:183:ILE:O	2.30	0.64
1:A:208:ILE:HD13	1:A:260:LEU:HD12	1.78	0.64
1:A:1061:VAL:HG12	1:A:1065:LEU:HD22	1.81	0.63
1:A:982:SER:HB3	1:A:985:VAL:HG22	1.81	0.62
1:A:87:LEU:HA	1:A:92:ILE:HD13	1.81	0.62
1:A:946:ARG:NH1	1:A:980:ASP:OD1	2.33	0.61
1:A:622:SER:HB2	1:A:627:VAL:HG23	1.83	0.61
1:A:170:LEU:HB2	1:A:171:PRO:HD2	1.84	0.60
1:A:1008:PRO:HG2	1:A:1050:ARG:HB3	1.82	0.60
1:A:130:PHE:HA	1:A:133:PHE:HB2	1.84	0.60
1:A:175:GLN:HA	1:A:178:GLU:HB3	1.84	0.60
1:A:258:ASN:OD1	1:A:259:ARG:NH1	2.32	0.60
1:A:1055:ILE:HD11	1:A:1079:ALA:HA	1.83	0.59
1:A:208:ILE:HA	1:A:214:LEU:HD11	1.82	0.59
1:A:1058:HIS:HD2	1:A:1082:TYR:HE2	1.51	0.59
1:A:586:SER:HB2	1:A:595:VAL:HB	1.85	0.58
1:A:220:LYS:O	1:A:224:ASN:HB2	2.01	0.58
1:A:501:MET:HA	1:A:504:ASP:HB2	1.86	0.58
1:A:994:LYS:HD3	1:A:1025:THR:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:THR:HG21	1:A:696:LYS:HG3	1.86	0.57
1:A:464:SER:HA	1:A:468:ILE:HD12	1.86	0.57
1:A:486:SER:OG	1:A:533:ASN:OD1	2.23	0.57
1:A:448:ASP:N	1:A:448:ASP:OD1	2.38	0.57
1:A:417:PHE:CD2	1:A:438:LEU:HD13	2.40	0.56
1:A:445:THR:HG23	1:A:446:ARG:HD2	1.87	0.56
1:A:450:ARG:CZ	1:A:499:ILE:HD11	2.35	0.56
1:A:540:PHE:HE1	1:A:675:ILE:HD13	1.70	0.56
1:A:942:GLN:O	1:A:946:ARG:HG3	2.05	0.55
1:A:159:LEU:HD13	1:A:203:ILE:HD13	1.88	0.55
1:A:512:LEU:HD22	1:A:524:ARG:HB3	1.89	0.55
1:A:359:LYS:HD2	1:A:362:LEU:HD12	1.89	0.55
1:A:676:PHE:O	1:A:710:LYS:NZ	2.39	0.55
1:A:550:MET:HB3	1:A:671:ALA:HB2	1.89	0.54
1:A:886:LYS:O	1:A:890:ASN:ND2	2.27	0.54
1:A:917:PHE:CG	1:A:970:ASP:HB3	2.41	0.54
2:E:127:TYR:CD1	2:E:128:LEU:HG	2.41	0.54
1:A:725:ILE:HG21	1:A:765:PHE:HE1	1.72	0.54
1:A:965:PHE:HB2	1:A:966:ILE:HD13	1.90	0.54
1:A:428:CYS:O	1:A:430:PRO:HD3	2.07	0.54
1:A:928:SER:O	1:A:930:SER:N	2.39	0.54
1:A:692:ASN:O	1:A:696:LYS:HD2	2.06	0.53
1:A:808:LEU:HD23	1:A:815:PHE:HE1	1.73	0.53
1:A:416:THR:O	1:A:420:VAL:HG12	2.08	0.53
1:A:850:LEU:HD23	1:A:926:LEU:HB3	1.89	0.53
1:A:786:LYS:O	1:A:790:LEU:HD23	2.08	0.53
1:A:951:LEU:HB3	1:A:992:ARG:HH11	1.73	0.53
1:A:143:PRO:HG2	1:A:193:GLN:HG3	1.90	0.53
1:A:990:ILE:HG22	1:A:994:LYS:HE2	1.90	0.53
1:A:349:ASN:HD21	1:A:352:VAL:HB	1.74	0.53
1:A:407:HIS:HB3	1:A:446:ARG:NH1	2.24	0.53
1:A:205:GLY:HA3	1:A:256:TYR:CE1	2.44	0.53
1:A:779:LEU:HB2	1:A:871:TYR:HB3	1.90	0.52
1:A:913:LEU:HB3	1:A:966:ILE:HD11	1.89	0.52
1:A:406:ASP:OD2	1:A:408:THR:OG1	2.23	0.52
1:A:970:ASP:HA	1:A:973:LYS:HD2	1.92	0.52
1:A:1083:LEU:HD13	1:A:2018:UNK:HA	1.92	0.52
1:A:560:PHE:HD2	1:A:581:THR:HG21	1.75	0.52
1:A:457:VAL:HG22	1:A:484:ILE:HG23	1.91	0.52
1:A:595:VAL:HG13	1:A:663:VAL:HG11	1.92	0.51
1:A:956:ILE:HA	1:A:959:ILE:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:THR:HB	1:A:696:LYS:HE2	1.93	0.51
1:A:692:ASN:N	1:A:696:LYS:HZ2	2.08	0.51
1:A:546:ARG:NH2	1:A:670:ARG:HG2	2.27	0.50
1:A:889:ALA:O	1:A:893:LYS:HE2	2.11	0.50
1:A:885:LEU:HD22	1:A:916:PHE:HE1	1.77	0.50
1:A:435:PHE:O	1:A:439:VAL:HG23	2.12	0.50
1:A:554:LEU:HD21	1:A:667:LEU:HD22	1.94	0.50
1:A:1086:TYR:CZ	1:A:1090:VAL:HG21	2.47	0.50
1:A:797:TYR:O	1:A:801:VAL:HG23	2.12	0.50
1:A:516:LEU:HD22	1:A:520:GLU:HB3	1.94	0.49
1:A:1052:ILE:HD13	1:A:1106:VAL:HG21	1.93	0.49
1:A:514:LEU:O	1:A:628:ARG:NE	2.33	0.49
1:A:1025:THR:O	1:A:1029:ILE:HD12	2.13	0.49
1:A:815:PHE:O	1:A:819:VAL:HG23	2.12	0.49
1:A:927:VAL:HG11	1:A:934:ASN:HB3	1.95	0.49
1:A:142:GLU:N	1:A:143:PRO:HD2	2.27	0.49
1:A:845:ILE:HG21	1:A:911:ARG:HH21	1.77	0.49
1:A:812:SER:OG	1:A:813:LYS:N	2.46	0.48
1:A:914:LYS:HD3	1:A:966:ILE:HG21	1.95	0.48
1:A:547:GLN:HA	1:A:670:ARG:O	2.13	0.48
1:A:919:LEU:HG	1:A:926:LEU:HD21	1.95	0.48
1:A:1013:THR:HG22	1:A:1016:GLU:HB2	1.95	0.48
1:A:802:ALA:O	1:A:804:ALA:N	2.45	0.48
1:A:822:LEU:HD13	1:A:840:ILE:HD13	1.95	0.48
1:A:377:VAL:HG23	1:A:380:ILE:HD11	1.96	0.48
1:A:802:ALA:C	1:A:804:ALA:H	2.17	0.48
1:A:235:LEU:O	1:A:236:ASP:HB3	2.13	0.48
1:A:411:LEU:HD13	1:A:449:LEU:HG	1.96	0.48
1:A:417:PHE:HD2	1:A:438:LEU:HD13	1.79	0.48
1:A:906:HIS:O	1:A:906:HIS:ND1	2.46	0.48
1:A:88:ILE:HD11	1:A:121:TYR:CE1	2.49	0.48
1:A:710:LYS:O	1:A:713:ILE:HG22	2.14	0.47
1:A:504:ASP:OD1	1:A:546:ARG:NH1	2.46	0.47
1:A:604:GLU:O	1:A:606:ASN:N	2.47	0.47
1:A:702:LEU:O	1:A:706:ILE:HG13	2.13	0.47
1:A:137:LEU:HD22	1:A:155:ILE:HG13	1.95	0.47
1:A:496:ASP:HB3	1:A:499:ILE:HB	1.95	0.47
1:A:644:PHE:CD1	1:A:651:ILE:HD11	2.49	0.47
1:A:501:MET:HB2	1:A:666:VAL:HG11	1.97	0.47
1:A:123:ASP:HB3	1:A:171:PRO:HD3	1.96	0.47
1:A:486:SER:HB2	1:A:532:PHE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:PHE:O	1:A:920:VAL:HG23	2.15	0.47
1:A:980:ASP:HB3	1:A:985:VAL:HG23	1.96	0.47
1:A:113:ARG:HG3	1:A:161:TYR:CD2	2.50	0.46
1:A:90:ARG:HD3	1:A:91:LYS:HD2	1.97	0.46
1:A:445:THR:HG22	2:E:127:TYR:O	2.14	0.46
1:A:513:PRO:HG2	1:A:516:LEU:HG	1.97	0.46
1:A:841:VAL:HG11	1:A:908:PHE:HE1	1.80	0.46
1:A:380:ILE:N	1:A:381:PRO:HD2	2.31	0.46
1:A:365:MET:C	1:A:367:ASP:H	2.19	0.46
1:A:826:THR:O	1:A:894:VAL:HG21	2.16	0.46
2:E:127:TYR:HD1	2:E:128:LEU:HG	1.80	0.46
1:A:775:GLU:HA	1:A:814:HIS:CD2	2.51	0.46
1:A:220:LYS:HD3	1:A:271:ILE:HD11	1.98	0.46
1:A:659:ASN:O	1:A:663:VAL:HG23	2.16	0.46
1:A:822:LEU:HD22	1:A:833:LEU:HD21	1.98	0.46
1:A:561:CYS:HB3	1:A:611:TYR:CZ	2.51	0.46
1:A:810:LEU:HD13	1:A:843:LEU:HD21	1.97	0.46
1:A:261:GLY:O	1:A:265:ILE:HG13	2.16	0.46
1:A:504:ASP:CG	1:A:546:ARG:HH12	2.19	0.46
1:A:947:CYS:HB2	1:A:985:VAL:HG12	1.97	0.46
1:A:380:ILE:HD11	1:A:398:LEU:HD13	1.98	0.45
1:A:313:GLY:HA2	1:A:354:HIS:HE1	1.80	0.45
1:A:717:GLN:O	1:A:721:LEU:HB2	2.16	0.45
1:A:785:ILE:HG12	1:A:821:VAL:HG13	1.98	0.45
1:A:95:ASN:CG	1:A:96:LYS:H	2.19	0.45
1:A:108:LEU:O	1:A:112:LEU:HD12	2.16	0.45
1:A:597:GLN:HB2	1:A:655:PHE:HD2	1.80	0.45
1:A:908:PHE:O	1:A:912:THR:HG23	2.17	0.45
1:A:578:LEU:HA	1:A:581:THR:HG22	1.98	0.45
1:A:624:HIS:CE1	1:A:628:ARG:HD2	2.52	0.45
1:A:678:ILE:HA	1:A:713:ILE:HG13	1.98	0.45
1:A:980:ASP:OD1	1:A:985:VAL:HG21	2.17	0.45
1:A:108:LEU:O	1:A:111:ILE:HG22	2.16	0.45
1:A:625:LEU:HA	1:A:625:LEU:HD12	1.71	0.45
1:A:933:ASP:O	1:A:934:ASN:ND2	2.45	0.44
1:A:429:LEU:HD13	1:A:434:VAL:HG11	1.98	0.44
1:A:497:LEU:H	1:A:497:LEU:HD22	1.83	0.44
1:A:422:VAL:HG21	1:A:463:GLU:HG3	2.00	0.44
1:A:454:ILE:HA	1:A:457:VAL:HG12	1.99	0.44
1:A:773:ALA:HB1	1:A:801:VAL:HG11	1.99	0.44
1:A:951:LEU:HB3	1:A:992:ARG:NH1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:SER:HB2	1:A:428:CYS:O	2.17	0.44
1:A:809:ASP:CG	1:A:812:SER:HB2	2.38	0.44
1:A:866:SER:O	1:A:868:GLU:N	2.50	0.44
1:A:917:PHE:CD1	1:A:970:ASP:HB3	2.52	0.44
1:A:260:LEU:O	1:A:263:HIS:N	2.50	0.43
1:A:598:ILE:HG23	1:A:660:PHE:CD1	2.53	0.43
1:A:866:SER:O	1:A:869:ASP:N	2.42	0.43
1:A:935:TYR:CE1	1:A:936:PRO:HB3	2.53	0.43
1:A:305:TRP:O	1:A:309:PRO:HB3	2.18	0.43
1:A:492:TYR:CD1	2:E:139:LEU:HD21	2.53	0.43
1:A:1097:ALA:O	1:A:1101:TYR:HB2	2.18	0.43
1:A:798:LEU:HD12	1:A:829:GLN:OE1	2.18	0.43
1:A:885:LEU:HD22	1:A:916:PHE:CE1	2.54	0.43
1:A:977:LEU:HA	1:A:980:ASP:HB2	2.01	0.43
1:A:805:ILE:HG13	1:A:806:LEU:N	2.34	0.43
1:A:179:GLU:HA	1:A:182:ASN:HB2	2.01	0.43
1:A:358:TYR:O	1:A:361:TRP:HB3	2.19	0.43
1:A:250:LEU:HD21	1:A:307:TYR:HB3	2.00	0.43
1:A:522:VAL:HG11	1:A:683:SER:CB	2.49	0.43
1:A:854:VAL:HG11	1:A:941:TYR:CZ	2.54	0.43
1:A:996:PHE:HB3	1:A:1002:ILE:HG12	1.99	0.43
1:A:609:ARG:HB3	1:A:637:ARG:NH1	2.33	0.43
1:A:888:PHE:CD1	1:A:888:PHE:N	2.86	0.42
1:A:1102:LEU:O	1:A:1105:ARG:N	2.52	0.42
1:A:225:LYS:HA	1:A:225:LYS:HD3	1.86	0.42
1:A:785:ILE:HD12	1:A:785:ILE:HA	1.91	0.42
1:A:950:GLY:O	1:A:954:LEU:HD13	2.19	0.42
1:A:99:GLY:O	1:A:103:PHE:HB2	2.19	0.42
1:A:869:ASP:OD1	1:A:869:ASP:N	2.52	0.42
1:A:942:GLN:HA	1:A:945:LEU:HD12	2.00	0.42
2:E:127:TYR:CE1	2:E:128:LEU:HG	2.54	0.42
1:A:478:TRP:HA	1:A:481:VAL:HG22	2.01	0.42
1:A:558:ILE:HG21	1:A:615:LYS:HB2	2.01	0.42
1:A:1076:LEU:HD12	1:A:1079:ALA:HB3	2.02	0.42
1:A:1102:LEU:O	1:A:1104:GLY:N	2.53	0.42
1:A:130:PHE:HE2	1:A:166:ILE:HG22	1.85	0.42
1:A:316:THR:HG22	1:A:319:LEU:HD13	2.02	0.42
1:A:548:ASP:O	1:A:551:SER:HB3	2.19	0.42
1:A:619:ALA:O	1:A:673:PRO:HG3	2.19	0.42
1:A:877:ALA:HB3	1:A:941:TYR:OH	2.20	0.42
1:A:954:LEU:HB3	1:A:996:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ALA:HA	1:A:700:ARG:HB2	2.02	0.42
1:A:864:TRP:CZ3	1:A:985:VAL:HG13	2.55	0.41
1:A:143:PRO:CG	1:A:193:GLN:HG3	2.50	0.41
1:A:841:VAL:HG11	1:A:908:PHE:CE1	2.55	0.41
1:A:194:GLY:C	1:A:196:MET:H	2.24	0.41
1:A:703:ILE:HA	1:A:706:ILE:HD12	2.02	0.41
1:A:947:CYS:O	1:A:951:LEU:HG	2.20	0.41
1:A:501:MET:O	1:A:505:LEU:HD12	2.21	0.41
1:A:522:VAL:HG11	1:A:683:SER:HB3	2.02	0.41
1:A:806:LEU:CD1	1:A:840:ILE:HD11	2.50	0.41
1:A:986:ARG:HD2	1:A:1016:GLU:OE2	2.21	0.41
1:A:121:TYR:N	1:A:121:TYR:CD1	2.88	0.41
1:A:607:ASP:HB3	1:A:610:LEU:HG	2.02	0.41
1:A:951:LEU:HD22	1:A:992:ARG:HD2	2.01	0.41
1:A:891:LYS:HB3	1:A:908:PHE:HE2	1.85	0.41
1:A:913:LEU:HA	1:A:913:LEU:HD12	1.85	0.41
1:A:1028:TRP:HE3	1:A:1029:ILE:HG13	1.86	0.41
1:A:108:LEU:HD21	1:A:129:ILE:HG22	2.03	0.41
1:A:613:LEU:O	1:A:617:ALA:N	2.39	0.41
1:A:91:LYS:HD2	1:A:91:LYS:N	2.35	0.41
1:A:348:ILE:O	1:A:349:ASN:ND2	2.54	0.41
1:A:658:ASP:O	1:A:662:THR:OG1	2.26	0.41
1:A:844:LEU:HA	1:A:848:VAL:HG23	2.03	0.41
2:E:133:VAL:CG2	2:E:137:GLU:HB3	2.51	0.41
1:A:1055:ILE:HD12	1:A:1082:TYR:HB2	2.03	0.40
1:A:278:GLU:OE1	1:A:290:ALA:HB2	2.21	0.40
1:A:582:VAL:HG13	1:A:599:LEU:HD12	2.03	0.40
1:A:1035:LYS:HE2	1:A:1035:LYS:HB3	1.90	0.40
1:A:835:LYS:HG2	1:A:835:LYS:H	1.54	0.40
1:A:946:ARG:HG3	1:A:946:ARG:H	1.61	0.40
1:A:226:PHE:HE1	1:A:307:TYR:HD2	1.69	0.40
1:A:493:TYR:HE1	2:E:138:VAL:HG22	1.85	0.40
1:A:288:SER:OG	1:A:289:SER:N	2.53	0.40
1:A:652:GLU:H	1:A:654:ARG:HD2	1.87	0.40
1:A:778:PRO:HB2	1:A:871:TYR:HA	2.03	0.40
1:A:817:SER:O	1:A:821:VAL:HG23	2.22	0.40
1:A:1048:LEU:HD13	1:A:1086:TYR:CE1	2.56	0.40
1:A:162:ARG:O	1:A:165:VAL:HG22	2.21	0.40
1:A:589:PHE:CZ	1:A:667:LEU:HG	2.57	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	960/1133 (85%)	835 (87%)	108 (11%)	17 (2%)	10	48
2	E	15/22 (68%)	11 (73%)	1 (7%)	3 (20%)	0	1
All	All	975/1155 (84%)	846 (87%)	109 (11%)	20 (2%)	8	45

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	TYR
1	A	143	PRO
1	A	349	ASN
1	A	930	SER
1	A	90	ARG
1	A	605	LEU
1	A	802	ALA
1	A	867	ASP
1	A	929	GLU
2	E	134	THR
1	A	118	ASP
1	A	511	PHE
1	A	803	THR
1	A	174	SER
1	A	494	ILE
2	E	138	VAL
1	A	142	GLU
1	A	738	SER
1	A	1093	ALA
2	E	130	GLN

### 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	871/916 (95%)	824 (95%)	47 (5%)	26	63
2	E	16/21 (76%)	15 (94%)	1 (6%)	21	59
All	All	887/937 (95%)	839 (95%)	48 (5%)	26	63

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	84	ARG
1	A	90	ARG
1	A	94	ARG
1	A	97	ASP
1	A	101	ARG
1	A	103	PHE
1	A	113	ARG
1	A	144	GLU
1	A	157	ASN
1	A	169	ASP
1	A	193	GLN
1	A	226	PHE
1	A	260	LEU
1	A	262	ARG
1	A	267	PHE
1	A	319	LEU
1	A	356	ASP
1	A	374	GLN
1	A	392	ASP
1	A	412	SER
1	A	424	ARG
1	A	444	GLU
1	A	447	ARG
1	A	472	ASN
1	A	516	LEU
1	A	518	ASN
1	A	543	PHE
1	A	546	ARG
1	A	549	GLN
1	A	639	GLU

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Mol	Chain	Res	Type
1	A	642	GLU
1	A	644	PHE
1	A	696	LYS
1	A	720	ASN
1	A	721	LEU
1	A	910	GLU
1	A	934	ASN
1	A	1022	ARG
1	A	1038	PHE
1	A	1043	PHE
1	A	1058	HIS
1	A	1092	LYS
1	A	1098	LEU
1	A	1100	TYR
1	A	1101	TYR
1	A	1105	ARG
2	E	127	TYR

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

Mol	Chain	Res	Type
1	A	354	HIS

### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2008:UNK	C	2009:UNK	N	32.25
1	A	1109:TYR	C	2000:UNK	N	24.42
1	A	17:UNK	C	80:LEU	N	12.97

## 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, 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	978/1133 (86%)	-0.02	14 (1%) 75 67	77, 121, 157, 178	0
2	E	17/22 (77%)	-0.06	0 100 100	98, 114, 127, 133	0
All	All	995/1155 (86%)	-0.02	14 (1%) 75 67	77, 121, 157, 178	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	ILE	3.5
1	A	93	LEU	2.9
1	A	203	ILE	2.7
1	A	183	ILE	2.6
1	A	141	GLN	2.5
1	A	92	ILE	2.5
1	A	1064	GLY	2.4
1	A	87	LEU	2.4
1	A	134	LEU	2.3
1	A	644	PHE	2.3
1	A	84	ARG	2.2
1	A	801	VAL	2.1
1	A	80	LEU	2.1
1	A	238	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.