



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:42 AM GMT

PDB ID : 2Y35
Title : CRYSTAL STRUCTURE OF XRN1-SUBSTRATE COMPLEX
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Deposited on : 2010-12-18
Resolution : 3.20 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
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

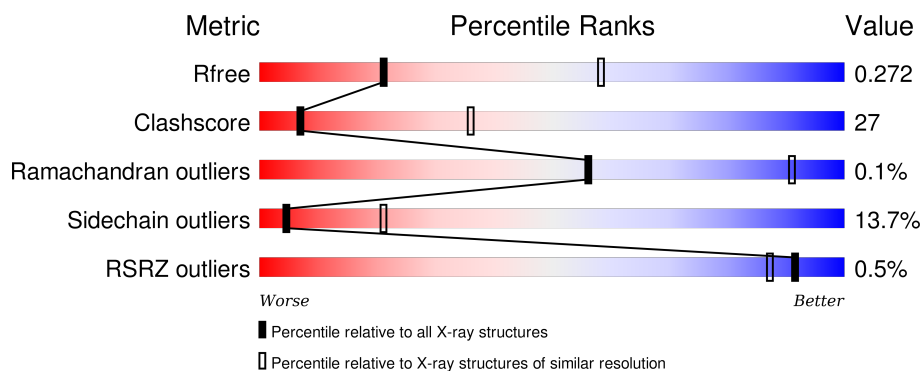
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	1140	
2	B	11	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8187 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 LD22664P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1026	Total	C	N	O	S	0	0	0
			8104	5231	1392	1443	38			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	ALA	ASP	ENGINEERED MUTATION	UNP Q9VWI1

- Molecule 2 is a DNA chain called DT11 (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	P	0	0	0
			65	30	6	25	4			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

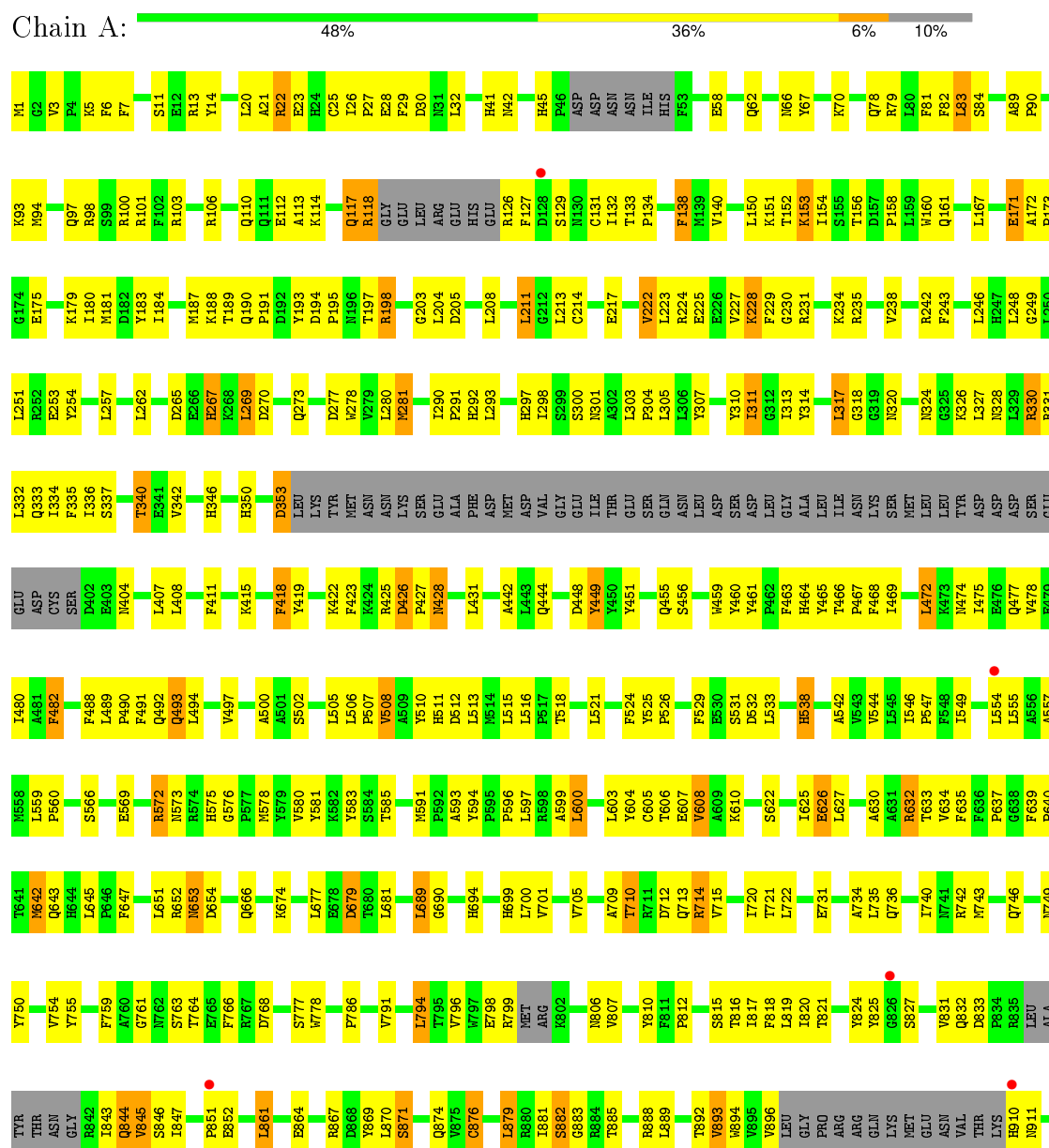
- Molecule 4 is water.

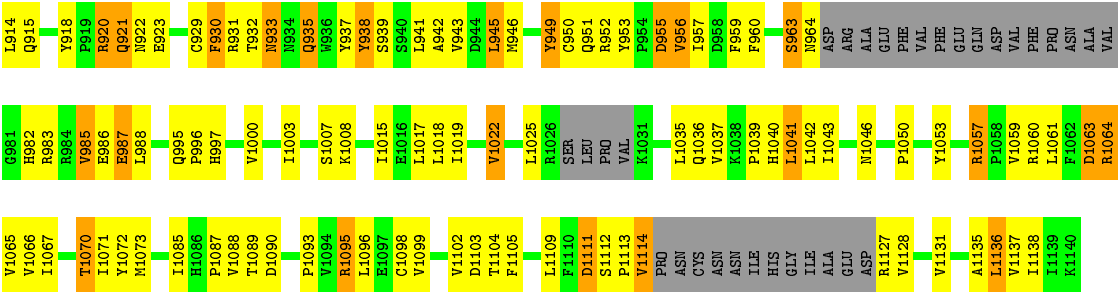
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		

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: LD22664P





● Molecule 2: DT11 (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.99Å 149.99Å 154.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.00 – 3.20 75.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (75.00-3.20) 99.1 (75.00-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.225 , 0.271 0.221 , 0.272	Depositor DCC
R_{free} test set	1179 reflections (4.00%)	DCC
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.4	EDS
Estimated twinning fraction	0.014 for -h,l,k 0.005 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 29504 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8187	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/8312	0.52	1/11327 (0.0%)
2	B	0.53	0/70	1.52	0/105
All	All	0.33	0/8382	0.54	1/11432 (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	A	228	LYS	N-CA-C	-5.48	96.21	111.00

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	8104	0	7817	422	0
2	B	65	0	36	7	0
3	A	1	0	0	0	0
4	A	17	0	0	1	0
All	All	8187	0	7853	425	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 27.

All (425) 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:591:MET:HB2	1:A:603:LEU:HD11	1.27	1.13
1:A:269:LEU:H	1:A:269:LEU:HD12	1.17	1.10
1:A:950:CYS:HA	1:A:957:ILE:HD11	1.35	1.08
1:A:227:VAL:HG12	1:A:228:LYS:O	1.53	1.08
1:A:313:ILE:HD11	1:A:334:ILE:HG22	1.36	1.07
1:A:101:ARG:HH12	1:A:133:THR:HB	1.19	1.03
1:A:546:ILE:HG22	1:A:547:PRO:HD2	1.47	0.95
1:A:101:ARG:NH1	1:A:133:THR:HB	1.85	0.89
2:B:2:DT:H2"	2:B:3:DT:H5"	1.52	0.89
1:A:1113:PRO:O	1:A:1114:VAL:HB	1.71	0.87
1:A:889:LEU:HD22	1:A:946:MET:HE3	1.57	0.86
1:A:710:THR:HG22	1:A:712:ASP:H	1.40	0.84
1:A:546:ILE:HG22	1:A:547:PRO:CD	2.09	0.83
1:A:1093:PRO:HG2	1:A:1099:VAL:HA	1.59	0.82
1:A:101:ARG:HG3	1:A:497:VAL:HG13	1.59	0.81
1:A:920:ARG:HG2	1:A:920:ARG:HH11	1.46	0.80
1:A:79:ARG:HH12	1:A:197:THR:HG22	1.46	0.79
1:A:181:MET:SD	1:A:211:LEU:HD13	2.22	0.79
1:A:150:LEU:O	1:A:154:ILE:HG22	1.82	0.79
1:A:1064:ARG:CG	1:A:1064:ARG:HH11	1.96	0.77
1:A:817:ILE:HD11	1:A:831:VAL:HB	1.67	0.77
1:A:227:VAL:CG1	1:A:228:LYS:O	2.30	0.77
1:A:581:TYR:HA	1:A:606:THR:O	1.85	0.77
1:A:815:SER:O	1:A:831:VAL:HG12	1.85	0.76
1:A:269:LEU:H	1:A:269:LEU:CD1	1.96	0.76
2:B:2:DT:C2'	2:B:3:DT:H5"	2.15	0.75
1:A:652:ARG:HG2	1:A:653:ASN:H	1.51	0.75
1:A:58:GLU:HG3	1:A:596:PRO:HB3	1.67	0.75
1:A:98:ARG:HH12	1:A:549:ILE:HG13	1.51	0.75
1:A:652:ARG:HH22	1:A:746:GLN:NE2	1.84	0.74
1:A:761:GLY:O	1:A:777:SER:HB3	1.87	0.73
1:A:1064:ARG:HG2	1:A:1064:ARG:HH11	1.53	0.73
1:A:456:SER:HB2	1:A:482:PHE:HB2	1.71	0.72
1:A:735:LEU:HD22	1:A:1096:LEU:HD21	1.70	0.72
1:A:953:TYR:HB3	1:A:956:VAL:HG21	1.70	0.72
1:A:694:HIS:CD2	1:A:794:LEU:HD11	2.25	0.72
1:A:889:LEU:HD22	1:A:946:MET:CE	2.20	0.71
1:A:97:GLN:O	1:A:101:ARG:HG2	1.91	0.71
1:A:494:LEU:HB3	1:A:506:LEU:HD21	1.70	0.71
1:A:500:ALA:HB1	1:A:515:LEU:HD21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLN:HG2	1:A:480:ILE:HD13	1.72	0.71
1:A:112:GLU:HG2	1:A:126:ARG:HH12	1.55	0.71
1:A:127:PHE:CE1	1:A:138:PHE:HE2	2.09	0.70
1:A:203:GLY:O	1:A:222:VAL:HG13	1.92	0.70
1:A:26:ILE:HD11	1:A:243:PHE:CD1	2.27	0.69
1:A:1072:TYR:CD2	1:A:1073:MET:HG3	2.28	0.69
1:A:642:MET:HE3	1:A:647:PHE:CZ	2.27	0.68
1:A:204:LEU:HD12	1:A:224:ARG:HE	1.58	0.68
1:A:1071:ILE:HD11	1:A:1135:ALA:CB	2.22	0.68
1:A:32:LEU:HD23	1:A:81:PHE:CE1	2.28	0.68
1:A:920:ARG:HG2	1:A:920:ARG:NH1	2.06	0.68
1:A:715:VAL:HG22	1:A:720:ILE:HG12	1.75	0.67
1:A:152:THR:O	1:A:156:THR:HG23	1.93	0.67
1:A:1019:ILE:O	1:A:1022:VAL:HG23	1.95	0.67
1:A:952:ARG:C	1:A:953:TYR:HD1	1.97	0.67
1:A:1019:ILE:HG23	1:A:1127:ARG:NH2	2.09	0.67
1:A:1066:VAL:HG12	1:A:1137:VAL:HG22	1.76	0.67
1:A:171:GLU:HG2	1:A:576:GLY:HA3	1.78	0.66
1:A:1050:PRO:HA	1:A:1053:TYR:CE1	2.29	0.66
1:A:467:PRO:HB2	1:A:472:LEU:HD21	1.75	0.66
1:A:591:MET:HB2	1:A:603:LEU:CD1	2.17	0.66
1:A:512:ASP:HA	1:A:516:LEU:HD13	1.76	0.66
1:A:180:ILE:O	1:A:184:ILE:HG13	1.95	0.66
1:A:593:ALA:HB2	1:A:599:ALA:HB2	1.76	0.66
1:A:831:VAL:HA	1:A:845:VAL:HG13	1.78	0.65
1:A:997:HIS:O	1:A:1000:VAL:HG22	1.95	0.65
1:A:21:ALA:HB1	1:A:25:CYS:HB2	1.78	0.65
1:A:538:HIS:N	1:A:538:HIS:CD2	2.64	0.65
1:A:852:GLU:OE1	1:A:1064:ARG:HG2	1.96	0.65
1:A:489:LEU:H	1:A:492:GLN:NE2	1.93	0.65
1:A:942:ALA:O	1:A:946:MET:HG3	1.97	0.65
1:A:933:ASN:CG	1:A:933:ASN:O	2.36	0.64
1:A:508:VAL:HA	1:A:511:HIS:CE1	2.33	0.64
1:A:154:ILE:HG13	1:A:160:TRP:O	1.97	0.64
1:A:819:LEU:HD23	1:A:824:TYR:HB2	1.79	0.64
1:A:114:LYS:HA	1:A:117:GLN:HE21	1.63	0.63
1:A:894:TRP:CZ3	1:A:911:ASN:HB2	2.33	0.63
1:A:70:LYS:HD3	1:A:229:PHE:CE2	2.33	0.63
1:A:317:LEU:H	1:A:317:LEU:HD12	1.62	0.63
1:A:513:LEU:HD22	1:A:521:LEU:HD12	1.78	0.63
1:A:303:LEU:O	1:A:307:TYR:CD1	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:TYR:HA	1:A:317:LEU:HD13	1.80	0.62
1:A:1067:ILE:HD12	1:A:1071:ILE:HD12	1.82	0.62
1:A:941:LEU:HD12	1:A:941:LEU:H	1.62	0.62
1:A:871:SER:HB3	1:A:874:GLN:HG3	1.80	0.61
1:A:995:GLN:HB3	1:A:996:PRO:HD2	1.83	0.61
1:A:327:LEU:H	1:A:444:GLN:HE22	1.48	0.61
1:A:303:LEU:HB2	1:A:304:PRO:HD3	1.82	0.61
1:A:442:ALA:HA	1:A:459:TRP:CH2	2.36	0.61
1:A:1007:SER:HB3	1:A:1087:PRO:HD2	1.82	0.61
1:A:953:TYR:HB3	1:A:956:VAL:CG2	2.30	0.61
1:A:817:ILE:HD13	1:A:1042:LEU:HD13	1.82	0.61
1:A:578:MET:HG2	1:A:610:LYS:O	2.01	0.61
1:A:213:LEU:HD22	1:A:251:LEU:CD2	2.31	0.61
1:A:253:GLU:OE1	1:A:642:MET:HG3	2.01	0.61
1:A:66:ASN:O	1:A:70:LYS:HG3	2.00	0.60
1:A:812:PRO:O	1:A:831:VAL:HG11	2.01	0.60
1:A:83:LEU:HD12	1:A:83:LEU:H	1.66	0.60
1:A:820:ILE:HG23	1:A:825:TYR:CE1	2.37	0.60
1:A:930:PHE:CD1	1:A:930:PHE:C	2.75	0.60
1:A:127:PHE:HE1	1:A:138:PHE:HE2	1.47	0.59
1:A:820:ILE:O	1:A:820:ILE:HG22	2.02	0.59
1:A:1:MET:HA	2:B:4:DT:OP1	2.02	0.59
2:B:2:DT:C3'	2:B:3:DT:H5''	2.31	0.59
1:A:594:TYR:O	1:A:597:LEU:N	2.35	0.59
1:A:228:LYS:C	1:A:230:GLY:H	2.05	0.59
1:A:310:TYR:O	1:A:313:ILE:HG22	2.03	0.59
1:A:110:GLN:O	1:A:113:ALA:HB3	2.02	0.59
1:A:101:ARG:HG3	1:A:497:VAL:CG1	2.32	0.59
1:A:851:PRO:HB2	1:A:1025:LEU:HD21	1.83	0.59
1:A:404:ASN:O	1:A:407:LEU:HB2	2.03	0.59
1:A:652:ARG:HH22	1:A:746:GLN:HE22	1.51	0.59
1:A:945:LEU:HD12	1:A:945:LEU:O	2.03	0.59
1:A:317:LEU:N	1:A:317:LEU:HD12	2.18	0.58
1:A:418:PHE:CE1	1:A:422:LYS:HB2	2.39	0.58
1:A:422:LYS:HB3	1:A:465:TYR:CE2	2.39	0.58
1:A:546:ILE:CG2	1:A:547:PRO:HD2	2.30	0.58
1:A:652:ARG:HG2	1:A:653:ASN:N	2.19	0.58
1:A:25:CYS:HB3	1:A:1095:ARG:HH22	1.69	0.58
1:A:1040:HIS:CE1	1:A:1041:LEU:HD12	2.38	0.58
1:A:269:LEU:N	1:A:269:LEU:HD12	2.02	0.57
1:A:493:GLN:HG3	1:A:494:LEU:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:TYR:O	1:A:423:PHE:HB2	2.03	0.57
1:A:952:ARG:HB3	1:A:953:TYR:CE1	2.39	0.57
1:A:262:LEU:HD21	1:A:311:ILE:HA	1.86	0.57
1:A:211:LEU:C	1:A:211:LEU:HD12	2.24	0.57
1:A:1071:ILE:HD11	1:A:1135:ALA:HB3	1.86	0.57
1:A:89:ALA:HB1	1:A:90:PRO:HD2	1.86	0.57
1:A:151:LYS:HE3	1:A:607:GLU:OE1	2.05	0.57
1:A:7:PHE:O	1:A:11:SER:HB2	2.05	0.56
1:A:952:ARG:C	1:A:953:TYR:CD1	2.78	0.56
1:A:42:ASN:ND2	1:A:228:LYS:HE2	2.20	0.56
1:A:939:SER:O	1:A:943:VAL:HG23	2.05	0.56
1:A:888:ARG:NH2	1:A:964:ASN:C	2.59	0.56
1:A:544:VAL:HG12	1:A:546:ILE:HG13	1.88	0.56
1:A:461:TYR:CE2	1:A:463:PHE:HB2	2.41	0.56
1:A:425:ARG:CZ	1:A:431:LEU:HD13	2.36	0.56
1:A:1018:LEU:O	1:A:1022:VAL:HG22	2.05	0.56
1:A:291:PRO:HB2	1:A:466:THR:HG23	1.88	0.55
1:A:709:ALA:HB3	1:A:755:TYR:HE1	1.70	0.55
1:A:546:ILE:CG2	1:A:547:PRO:CD	2.84	0.55
1:A:861:LEU:HD12	1:A:1017:LEU:CD1	2.36	0.55
1:A:1088:VAL:HG21	1:A:1105:PHE:HE1	1.71	0.55
1:A:938:TYR:CD1	1:A:938:TYR:N	2.73	0.55
1:A:297:HIS:O	1:A:300:SER:HB3	2.07	0.55
1:A:580:VAL:O	1:A:608:VAL:HG23	2.07	0.55
1:A:79:ARG:HH12	1:A:197:THR:CG2	2.18	0.55
1:A:62:GLN:HB2	1:A:596:PRO:HG3	1.89	0.55
1:A:959:PHE:O	1:A:963:SER:HB3	2.07	0.55
1:A:817:ILE:HD12	1:A:845:VAL:CG1	2.37	0.54
1:A:422:LYS:HB3	1:A:465:TYR:HE2	1.72	0.54
1:A:819:LEU:HD22	1:A:847:ILE:HG12	1.89	0.54
1:A:1088:VAL:HG21	1:A:1105:PHE:CE1	2.42	0.54
1:A:1060:ARG:O	1:A:1063:ASP:HB2	2.08	0.54
1:A:227:VAL:HG11	1:A:231:ARG:HB3	1.89	0.54
1:A:533:LEU:HG	1:A:542:ALA:HB2	1.90	0.54
1:A:1071:ILE:HD11	1:A:1135:ALA:HB1	1.88	0.54
1:A:451:TYR:HB3	1:A:622:SER:OG	2.07	0.54
1:A:843:ILE:HG22	1:A:845:VAL:HG22	1.90	0.54
1:A:833:ASP:O	1:A:844:GLN:HB2	2.07	0.54
1:A:622:SER:O	1:A:625:ILE:HG23	2.07	0.54
1:A:41:HIS:CE1	1:A:132:ILE:HD12	2.42	0.54
1:A:817:ILE:CD1	1:A:831:VAL:HB	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:LEU:HB3	1:A:506:LEU:CD2	2.39	0.53
1:A:626:GLU:HG3	1:A:632:ARG:HH22	1.73	0.53
1:A:953:TYR:N	1:A:953:TYR:CD1	2.76	0.53
1:A:500:ALA:HB1	1:A:515:LEU:CD2	2.38	0.53
1:A:572:ARG:HG3	1:A:572:ARG:O	2.08	0.53
1:A:818:PHE:HB2	1:A:1043:ILE:HB	1.91	0.53
1:A:491:PHE:CE2	1:A:507:PRO:HG2	2.43	0.53
1:A:1109:LEU:HD13	1:A:1128:VAL:HG23	1.90	0.53
1:A:489:LEU:HD12	1:A:492:GLN:NE2	2.24	0.53
1:A:98:ARG:HH22	1:A:524:PHE:HB3	1.74	0.53
1:A:921:GLN:O	1:A:922:ASN:HB3	2.09	0.53
1:A:798:GLU:O	1:A:799:ARG:CB	2.57	0.53
1:A:79:ARG:NH1	1:A:197:THR:HG22	2.19	0.52
1:A:914:LEU:HD21	1:A:949:TYR:HD2	1.74	0.52
1:A:735:LEU:HD13	1:A:786:PRO:HD3	1.90	0.52
1:A:265:ASP:HB2	1:A:267:HIS:NE2	2.24	0.52
1:A:931:ARG:HG3	1:A:935:GLN:O	2.08	0.52
1:A:138:PHE:C	1:A:138:PHE:CD1	2.82	0.52
1:A:213:LEU:HD22	1:A:251:LEU:HD23	1.90	0.52
1:A:41:HIS:CE1	2:B:1:DT:C5	2.98	0.52
1:A:694:HIS:HA	1:A:701:VAL:O	2.10	0.52
1:A:573:ASN:ND2	1:A:573:ASN:O	2.43	0.52
1:A:1064:ARG:NH1	1:A:1064:ARG:CG	2.63	0.52
1:A:278:TRP:HA	1:A:281:MET:HG3	1.92	0.52
1:A:869:TYR:C	1:A:870:LEU:HD23	2.30	0.52
1:A:277:ASP:O	1:A:281:MET:HG2	2.09	0.52
1:A:428:ASN:H	1:A:428:ASN:ND2	2.08	0.52
1:A:1066:VAL:HG12	1:A:1137:VAL:CG2	2.40	0.51
1:A:861:LEU:HD12	1:A:1017:LEU:HD11	1.92	0.51
1:A:134:PRO:HD2	1:A:493:GLN:HE22	1.74	0.51
1:A:864:GLU:O	1:A:867:ARG:HB2	2.10	0.51
1:A:404:ASN:O	1:A:408:LEU:HD13	2.09	0.51
1:A:681:LEU:HD21	1:A:715:VAL:HG23	1.93	0.51
1:A:759:PHE:HA	1:A:778:TRP:CE3	2.45	0.51
1:A:181:MET:SD	1:A:211:LEU:CD1	2.96	0.51
1:A:317:LEU:H	1:A:317:LEU:CD1	2.23	0.51
1:A:513:LEU:HD11	1:A:557:ALA:O	2.10	0.51
1:A:1111:ASP:HA	1:A:1127:ARG:NH1	2.26	0.51
1:A:820:ILE:HG23	1:A:825:TYR:HE1	1.74	0.51
1:A:418:PHE:C	1:A:418:PHE:HD1	2.14	0.51
1:A:194:ASP:HB3	1:A:197:THR:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:LEU:HD13	1:A:945:LEU:HG	1.92	0.50
1:A:205:ASP:OD1	1:A:208:LEU:HD13	2.10	0.50
1:A:353:ASP:OD1	1:A:353:ASP:N	2.43	0.50
1:A:161:GLN:HB3	1:A:583:TYR:CD2	2.45	0.50
1:A:138:PHE:HD1	1:A:138:PHE:C	2.13	0.50
1:A:941:LEU:H	1:A:941:LEU:CD1	2.25	0.50
1:A:930:PHE:CD1	1:A:937:TYR:HB2	2.46	0.50
1:A:806:ASN:ND2	1:A:807:VAL:H	2.10	0.50
1:A:42:ASN:OD1	1:A:228:LYS:NZ	2.39	0.50
1:A:456:SER:CB	1:A:482:PHE:HB2	2.39	0.50
1:A:418:PHE:CD1	1:A:422:LYS:HB2	2.47	0.50
1:A:882:SER:O	1:A:885:THR:HG22	2.12	0.50
1:A:941:LEU:HD12	1:A:941:LEU:N	2.27	0.50
1:A:812:PRO:HG2	1:A:815:SER:HB3	1.93	0.50
1:A:508:VAL:HA	1:A:511:HIS:ND1	2.26	0.49
1:A:418:PHE:C	1:A:418:PHE:CD1	2.85	0.49
1:A:524:PHE:C	1:A:526:PRO:HD3	2.33	0.49
1:A:533:LEU:HG	1:A:542:ALA:CB	2.42	0.49
1:A:228:LYS:C	1:A:230:GLY:N	2.65	0.49
1:A:953:TYR:O	1:A:956:VAL:HG23	2.13	0.49
1:A:132:ILE:O	1:A:132:ILE:HG22	2.11	0.49
1:A:82:PHE:HE1	1:A:84:SER:HB2	1.78	0.49
1:A:30:ASP:OD2	1:A:198:ARG:HG2	2.12	0.49
1:A:313:ILE:CD1	1:A:335:PHE:HA	2.42	0.49
1:A:234:LYS:O	1:A:234:LYS:HD3	2.11	0.49
1:A:1089:THR:HG22	1:A:1102:VAL:HG22	1.93	0.49
1:A:956:VAL:O	1:A:959:PHE:HB3	2.12	0.49
1:A:127:PHE:HE1	1:A:138:PHE:CE2	2.30	0.49
1:A:6:PHE:HD1	1:A:298:ILE:CD1	2.25	0.49
1:A:14:TYR:HB3	1:A:254:TYR:CD1	2.48	0.49
1:A:489:LEU:H	1:A:492:GLN:HE21	1.58	0.49
1:A:985:VAL:HG23	1:A:986:GLU:H	1.78	0.49
1:A:532:ASP:C	1:A:533:LEU:HD12	2.33	0.48
1:A:1109:LEU:HD11	1:A:1127:ARG:HD2	1.94	0.48
1:A:336:ILE:HG23	1:A:469:ILE:HG23	1.95	0.48
1:A:175:GLU:O	1:A:179:LYS:HG3	2.14	0.48
1:A:817:ILE:HD12	1:A:845:VAL:HG13	1.94	0.48
1:A:950:CYS:CA	1:A:957:ILE:HD11	2.26	0.48
1:A:1071:ILE:HD13	1:A:1131:VAL:HG13	1.96	0.48
1:A:652:ARG:NH2	1:A:746:GLN:HE22	2.10	0.48
1:A:310:TYR:HA	1:A:313:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:PRO:HA	1:A:1053:TYR:CZ	2.49	0.48
1:A:525:TYR:N	1:A:526:PRO:HD3	2.28	0.48
1:A:1046:ASN:HD21	1:A:1070:THR:H	1.61	0.48
1:A:42:ASN:CG	1:A:228:LYS:HZ1	2.16	0.48
1:A:945:LEU:C	1:A:945:LEU:HD12	2.34	0.48
1:A:766:PHE:CD2	1:A:1039:PRO:HB2	2.49	0.48
1:A:982:HIS:O	1:A:983:ARG:HD2	2.13	0.48
1:A:930:PHE:HD1	1:A:937:TYR:HB2	1.78	0.48
1:A:1035:LEU:HD12	1:A:1036:GLN:H	1.78	0.47
1:A:213:LEU:HD22	1:A:251:LEU:HD21	1.95	0.47
1:A:491:PHE:CD1	1:A:491:PHE:N	2.82	0.47
1:A:293:LEU:HD12	1:A:293:LEU:N	2.29	0.47
1:A:98:ARG:NH2	1:A:524:PHE:O	2.47	0.47
1:A:533:LEU:N	1:A:533:LEU:HD12	2.29	0.47
1:A:7:PHE:O	1:A:11:SER:CB	2.62	0.47
1:A:133:THR:OG1	1:A:134:PRO:HD2	2.15	0.47
1:A:94:MET:HE1	1:A:493:GLN:HA	1.97	0.47
1:A:464:HIS:HE1	1:A:546:ILE:O	1.97	0.47
1:A:960:PHE:HD1	1:A:960:PHE:H	1.63	0.47
1:A:327:LEU:HB2	1:A:444:GLN:NE2	2.29	0.47
1:A:1071:ILE:HG22	1:A:1071:ILE:O	2.13	0.47
1:A:538:HIS:H	1:A:538:HIS:CD2	2.31	0.47
1:A:529:PHE:CD1	1:A:529:PHE:O	2.68	0.47
1:A:448:ASP:O	1:A:449:TYR:C	2.52	0.47
1:A:27:PRO:HG2	1:A:29:PHE:CZ	2.50	0.47
1:A:591:MET:HE3	1:A:600:LEU:HB2	1.96	0.47
1:A:955:ASP:N	1:A:955:ASP:OD1	2.45	0.47
1:A:1037:VAL:HG11	1:A:1042:LEU:HD21	1.96	0.46
1:A:521:LEU:O	1:A:525:TYR:HD2	1.98	0.46
1:A:549:ILE:HD13	1:A:554:LEU:HD22	1.98	0.46
1:A:881:ILE:HB	1:A:885:THR:CG2	2.44	0.46
1:A:507:PRO:HB3	1:A:569:GLU:CD	2.36	0.46
1:A:346:HIS:CE1	1:A:350:HIS:CD2	3.04	0.46
1:A:1090:ASP:CB	1:A:1093:PRO:HG3	2.44	0.46
1:A:7:PHE:CE2	1:A:204:LEU:HD22	2.51	0.46
1:A:293:LEU:H	1:A:293:LEU:HD12	1.81	0.46
1:A:1057:ARG:HH21	1:A:1138:ILE:HD12	1.80	0.46
1:A:411:PHE:CE2	1:A:415:LYS:HE3	2.50	0.46
1:A:89:ALA:HB1	1:A:90:PRO:CD	2.45	0.46
1:A:524:PHE:CE1	1:A:549:ILE:HA	2.51	0.46
1:A:879:LEU:O	1:A:881:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:VAL:HG21	1:A:572:ARG:HD3	1.98	0.46
1:A:313:ILE:CD1	1:A:334:ILE:HG22	2.25	0.46
1:A:153:LYS:HD2	1:A:160:TRP:NE1	2.31	0.46
1:A:815:SER:OG	1:A:831:VAL:HG11	2.16	0.46
1:A:918:TYR:HB2	1:A:923:GLU:HB2	1.97	0.46
1:A:469:ILE:HA	1:A:472:LEU:HD23	1.96	0.45
1:A:14:TYR:HB3	1:A:254:TYR:CG	2.51	0.45
1:A:198:ARG:HB3	1:A:639:PHE:CZ	2.51	0.45
1:A:987:GLU:HG3	1:A:988:LEU:N	2.31	0.45
1:A:1088:VAL:HG22	1:A:1103:ASP:O	2.16	0.45
1:A:45:HIS:O	1:A:45:HIS:ND1	2.49	0.45
1:A:194:ASP:HB3	1:A:197:THR:CG2	2.47	0.45
1:A:491:PHE:HD1	1:A:491:PHE:N	2.14	0.45
1:A:158:PRO:HA	1:A:161:GLN:HG3	1.98	0.45
1:A:82:PHE:CE1	1:A:84:SER:HB2	2.52	0.45
1:A:603:LEU:O	1:A:604:TYR:HD1	2.00	0.45
1:A:93:LYS:HD2	1:A:175:GLU:OE2	2.16	0.45
1:A:103:ARG:HE	1:A:544:VAL:CG2	2.30	0.45
1:A:291:PRO:HB2	1:A:466:THR:CG2	2.46	0.45
1:A:6:PHE:HA	1:A:298:ILE:HD13	1.97	0.45
1:A:555:LEU:HD12	1:A:555:LEU:N	2.32	0.45
1:A:750:TYR:CD1	1:A:750:TYR:N	2.84	0.45
1:A:93:LYS:HZ2	1:A:97:GLN:HG2	1.82	0.45
1:A:194:ASP:O	1:A:197:THR:HG23	2.17	0.45
1:A:70:LYS:HE2	1:A:238:VAL:HG22	1.98	0.45
1:A:507:PRO:HB3	1:A:569:GLU:OE1	2.17	0.44
1:A:893:VAL:HG22	1:A:893:VAL:O	2.17	0.44
1:A:714:ARG:HD2	1:A:721:THR:OG1	2.18	0.44
1:A:820:ILE:HD11	1:A:1043:ILE:HG12	1.98	0.44
1:A:1061:LEU:C	1:A:1063:ASP:H	2.21	0.44
1:A:832:GLN:OE1	1:A:846:SER:HB2	2.17	0.44
1:A:876:CYS:SG	1:A:883:GLY:HA2	2.57	0.44
1:A:418:PHE:O	1:A:419:TYR:C	2.56	0.44
1:A:13:ARG:NH2	1:A:651:LEU:HD11	2.33	0.44
1:A:5:LYS:HG3	2:B:4:DT:OP2	2.18	0.44
1:A:198:ARG:H	1:A:198:ARG:HG2	1.52	0.44
1:A:731:GLU:O	1:A:734:ALA:HB3	2.17	0.44
1:A:489:LEU:O	1:A:490:PRO:C	2.56	0.44
1:A:911:ASN:OD1	1:A:915:GLN:OE1	2.36	0.44
1:A:1060:ARG:HB2	1:A:1063:ASP:OD2	2.17	0.44
1:A:632:ARG:N	1:A:632:ARG:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:SER:C	1:A:131:CYS:H	2.21	0.44
1:A:328:ASN:CG	1:A:331:ARG:HD2	2.38	0.44
1:A:889:LEU:HD23	1:A:889:LEU:O	2.18	0.44
1:A:652:ARG:NH1	1:A:654:ASP:OD2	2.49	0.44
1:A:127:PHE:CE1	1:A:138:PHE:CE2	2.97	0.44
1:A:488:PHE:O	1:A:575:HIS:HE1	2.01	0.44
1:A:722:LEU:H	1:A:722:LEU:HD12	1.83	0.44
1:A:290:ILE:HG22	1:A:291:PRO:HD2	1.99	0.44
1:A:475:ILE:O	1:A:478:VAL:HG23	2.17	0.44
1:A:930:PHE:O	1:A:930:PHE:CD1	2.71	0.43
1:A:938:TYR:HD1	1:A:938:TYR:N	2.15	0.43
1:A:918:TYR:HB3	1:A:921:GLN:HB2	2.00	0.43
1:A:153:LYS:HD2	1:A:160:TRP:CE2	2.53	0.43
1:A:100:ARG:HH21	2:B:1:DT:P	2.40	0.43
1:A:502:SER:HB3	1:A:505:LEU:HD12	2.00	0.43
1:A:90:PRO:O	1:A:94:MET:HG3	2.19	0.43
1:A:93:LYS:HD3	1:A:97:GLN:NE2	2.33	0.43
1:A:705:VAL:HG13	1:A:754:VAL:HG13	2.00	0.43
1:A:1065:VAL:HB	1:A:1136:LEU:HG	1.99	0.43
1:A:1096:LEU:O	1:A:1099:VAL:HG12	2.19	0.43
1:A:1095:ARG:HB3	1:A:1098:CYS:SG	2.59	0.43
1:A:172:ALA:HA	1:A:173:PRO:HD3	1.79	0.43
1:A:634:VAL:CG1	1:A:635:PHE:N	2.82	0.43
1:A:559:LEU:N	1:A:560:PRO:HD2	2.34	0.43
1:A:640:PRO:HB3	1:A:699:HIS:HA	2.01	0.43
1:A:118:ARG:HB2	1:A:118:ARG:HE	1.48	0.43
1:A:573:ASN:CG	1:A:573:ASN:O	2.56	0.43
1:A:183:TYR:HE2	1:A:187:MET:HE3	1.83	0.43
1:A:490:PRO:O	1:A:493:GLN:HG3	2.19	0.42
1:A:1090:ASP:HB3	1:A:1093:PRO:HG3	2.01	0.42
1:A:418:PHE:CD2	1:A:468:PHE:HZ	2.37	0.42
1:A:249:GLY:O	1:A:253:GLU:HG3	2.18	0.42
1:A:114:LYS:NZ	1:A:118:ARG:HH11	2.16	0.42
1:A:459:TRP:CE3	1:A:460:TYR:HA	2.54	0.42
1:A:861:LEU:O	1:A:861:LEU:HD23	2.18	0.42
1:A:763:SER:HB2	1:A:777:SER:HB2	2.01	0.42
1:A:952:ARG:HB3	1:A:953:TYR:CD1	2.54	0.42
1:A:127:PHE:CZ	1:A:138:PHE:HE2	2.35	0.42
1:A:184:ILE:O	1:A:188:LYS:HG3	2.18	0.42
1:A:270:ASP:HB3	1:A:273:GLN:HB2	2.01	0.42
1:A:549:ILE:HG21	1:A:554:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:ILE:O	1:A:1019:ILE:HG13	2.18	0.42
1:A:190:GLN:HA	1:A:191:PRO:HD3	1.80	0.42
1:A:305:LEU:HD23	1:A:342:VAL:HG13	2.02	0.42
1:A:639:PHE:N	1:A:639:PHE:CD1	2.87	0.42
1:A:488:PHE:HD1	1:A:488:PHE:H	1.68	0.42
1:A:42:ASN:CG	1:A:228:LYS:NZ	2.72	0.42
1:A:277:ASP:O	1:A:280:LEU:HB3	2.20	0.42
1:A:820:ILE:CG2	1:A:820:ILE:O	2.67	0.42
1:A:474:ASN:ND2	1:A:477:GLN:HE21	2.17	0.42
1:A:679:ASP:OD2	1:A:749:ASN:ND2	2.44	0.42
1:A:223:LEU:C	1:A:223:LEU:HD12	2.40	0.42
1:A:546:ILE:HG22	1:A:547:PRO:N	2.35	0.42
1:A:327:LEU:N	1:A:444:GLN:HE22	2.15	0.42
1:A:824:TYR:HB3	1:A:827:SER:OG	2.20	0.41
1:A:722:LEU:HD12	1:A:722:LEU:N	2.35	0.41
1:A:21:ALA:O	1:A:242:ARG:HB2	2.20	0.41
1:A:651:LEU:HD21	1:A:666:GLN:CD	2.40	0.41
1:A:488:PHE:N	1:A:488:PHE:CD1	2.88	0.41
1:A:544:VAL:HG12	1:A:546:ILE:CG1	2.49	0.41
1:A:821:THR:HG22	1:A:1041:LEU:HD22	2.02	0.41
1:A:426:ASP:HA	1:A:427:PRO:HD3	1.77	0.41
1:A:193:TYR:OH	1:A:217:GLU:OE2	2.35	0.41
1:A:488:PHE:O	1:A:575:HIS:CE1	2.73	0.41
1:A:101:ARG:CG	1:A:497:VAL:HG13	2.42	0.41
1:A:28:GLU:OE2	1:A:78:GLN:HG3	2.20	0.41
1:A:167:LEU:O	1:A:578:MET:HB2	2.20	0.41
1:A:213:LEU:HD23	1:A:278:TRP:CZ3	2.55	0.41
1:A:950:CYS:SG	1:A:957:ILE:HD13	2.60	0.41
1:A:759:PHE:CE1	1:A:761:GLY:N	2.88	0.41
1:A:324:ASN:OD1	1:A:622:SER:HB2	2.20	0.41
1:A:330:ARG:O	1:A:333:GLN:HB3	2.20	0.41
1:A:852:GLU:OE1	1:A:1064:ARG:NH1	2.54	0.41
1:A:14:TYR:HB3	1:A:254:TYR:CE1	2.56	0.41
1:A:326:LYS:NZ	4:A:2009:HOH:O	2.53	0.41
1:A:812:PRO:O	1:A:831:VAL:CG1	2.69	0.41
1:A:817:ILE:HD12	1:A:845:VAL:HG11	2.03	0.41
1:A:188:LYS:HE2	1:A:627:LEU:HD11	2.02	0.41
1:A:198:ARG:HH11	1:A:198:ARG:CG	2.33	0.41
1:A:1057:ARG:NH2	1:A:1138:ILE:HD12	2.35	0.41
1:A:689:LEU:CD1	1:A:690:GLY:N	2.84	0.41
1:A:1008:LYS:HB2	1:A:1085:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:SER:O	1:A:340:THR:HB	2.20	0.41
1:A:889:LEU:HA	1:A:960:PHE:HE2	1.86	0.40
1:A:1090:ASP:HB2	1:A:1093:PRO:HG3	2.03	0.40
1:A:889:LEU:CD2	1:A:946:MET:HE3	2.40	0.40
1:A:914:LEU:HD22	1:A:945:LEU:HD11	2.04	0.40
1:A:132:ILE:CG2	1:A:132:ILE:O	2.68	0.40
1:A:448:ASP:HB3	1:A:455:GLN:CG	2.52	0.40
1:A:318:GLY:HA3	1:A:331:ARG:HH21	1.86	0.40
1:A:645:LEU:HA	1:A:645:LEU:HD23	1.74	0.40
1:A:45:HIS:CG	1:A:45:HIS:O	2.72	0.40
1:A:988:LEU:H	1:A:988:LEU:HD23	1.87	0.40
1:A:22:ARG:O	1:A:23:GLU:C	2.60	0.40
1:A:817:ILE:HG23	1:A:1042:LEU:HB3	2.03	0.40
1:A:794:LEU:HD12	1:A:794:LEU:H	1.86	0.40
1:A:689:LEU:CD1	1:A:689:LEU:C	2.90	0.40
1:A:195:PRO:HB2	1:A:630:ALA:HB2	2.02	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	1006/1140 (88%)	923 (92%)	82 (8%)	1 (0%)	56 91

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	768	ASP

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	851/1025 (83%)	734 (86%)	117 (14%)	4 21

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	20	LEU
1	A	22	ARG
1	A	67	TYR
1	A	83	LEU
1	A	106	ARG
1	A	117	GLN
1	A	118	ARG
1	A	138	PHE
1	A	153	LYS
1	A	171	GLU
1	A	189	THR
1	A	198	ARG
1	A	211	LEU
1	A	214	CYS
1	A	222	VAL
1	A	225	GLU
1	A	235	ARG
1	A	246	LEU
1	A	248	LEU
1	A	257	LEU
1	A	267	HIS
1	A	269	LEU
1	A	281	MET
1	A	292	HIS
1	A	301	ASN
1	A	311	ILE
1	A	317	LEU
1	A	320	ASN
1	A	330	ARG

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Mol	Chain	Res	Type
1	A	332	LEU
1	A	340	THR
1	A	353	ASP
1	A	418	PHE
1	A	426	ASP
1	A	428	ASN
1	A	449	TYR
1	A	472	LEU
1	A	482	PHE
1	A	493	GLN
1	A	508	VAL
1	A	510	TYR
1	A	518	THR
1	A	531	SER
1	A	538	HIS
1	A	566	SER
1	A	572	ARG
1	A	585	THR
1	A	600	LEU
1	A	605	CYS
1	A	608	VAL
1	A	626	GLU
1	A	632	ARG
1	A	633	THR
1	A	637	PRO
1	A	642	MET
1	A	643	GLN
1	A	653	ASN
1	A	674	LYS
1	A	677	LEU
1	A	679	ASP
1	A	689	LEU
1	A	700	LEU
1	A	710	THR
1	A	713	GLN
1	A	714	ARG
1	A	736	GLN
1	A	740	ILE
1	A	742	ARG
1	A	743	MET
1	A	764	THR
1	A	791	VAL

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Mol	Chain	Res	Type
1	A	794	LEU
1	A	796	VAL
1	A	810	TYR
1	A	816	THR
1	A	844	GLN
1	A	845	VAL
1	A	861	LEU
1	A	871	SER
1	A	876	CYS
1	A	879	LEU
1	A	882	SER
1	A	892	THR
1	A	893	VAL
1	A	896	VAL
1	A	910	HIS
1	A	920	ARG
1	A	921	GLN
1	A	929	CYS
1	A	930	PHE
1	A	932	THR
1	A	933	ASN
1	A	935	GLN
1	A	938	TYR
1	A	945	LEU
1	A	949	TYR
1	A	951	GLN
1	A	955	ASP
1	A	956	VAL
1	A	963	SER
1	A	985	VAL
1	A	987	GLU
1	A	1003	ILE
1	A	1022	VAL
1	A	1041	LEU
1	A	1057	ARG
1	A	1059	VAL
1	A	1063	ASP
1	A	1064	ARG
1	A	1070	THR
1	A	1095	ARG
1	A	1104	THR
1	A	1111	ASP

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Mol	Chain	Res	Type
1	A	1112	SER
1	A	1114	VAL
1	A	1136	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	66	ASN
1	A	78	GLN
1	A	97	GLN
1	A	117	GLN
1	A	130	ASN
1	A	143	GLN
1	A	178	HIS
1	A	190	GLN
1	A	346	HIS
1	A	350	HIS
1	A	417	ASN
1	A	437	HIS
1	A	438	HIS
1	A	444	GLN
1	A	464	HIS
1	A	474	ASN
1	A	492	GLN
1	A	534	ASN
1	A	538	HIS
1	A	573	ASN
1	A	575	HIS
1	A	665	ASN
1	A	676	GLN
1	A	694	HIS
1	A	738	HIS
1	A	746	GLN
1	A	806	ASN
1	A	844	GLN
1	A	921	GLN
1	A	935	GLN
1	A	995	GLN
1	A	1046	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is 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 [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	1026/1140 (90%)	-0.11	5 (0%) 91 87	29, 75, 131, 178	0
2	B	4/11 (36%)	0.11	0 100 100	116, 122, 151, 164	0
All	All	1030/1151 (89%)	-0.11	5 (0%) 91 87	29, 75, 131, 178	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	826	GLY	3.6
1	A	554	LEU	2.5
1	A	128	ASP	2.3
1	A	910	HIS	2.2
1	A	851	PRO	2.1

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, 95th 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(\AA^2)	Q<0.9
3	MG	A	2141	1/1	0.95	0.04	-4.49	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.