



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:17 am BST

PDB ID : 6DSZ
Title : Crystal structure of DDB1 in complex with DET1- and DDB1-associated protein 1 (DDA1)
Authors : Shabek, N.; Zheng, N.
Deposited on : 2018-06-14
Resolution : 3.09 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

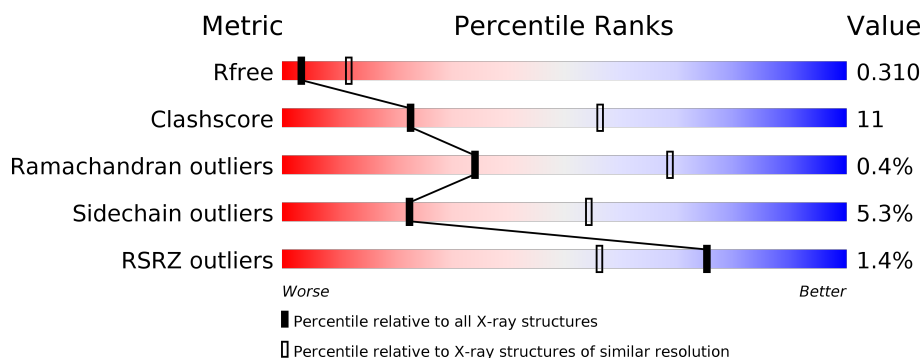
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 on 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	1140	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	1140	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>• 6%</div> </div> </div>
2	C	19	<div> <div></div> <div> <div>68%</div> <div>26%</div> <div>5%</div> </div> </div>
2	D	19	<div> <div></div> <div> <div>79%</div> <div>16%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34801 atoms, of which 17393 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1107	Total	C	H	N	O	S	0	0	0
			17329	5503	8655	1460	1664	47			
1	B	1072	Total	C	H	N	O	S	0	0	0
			16842	5356	8422	1418	1599	47			

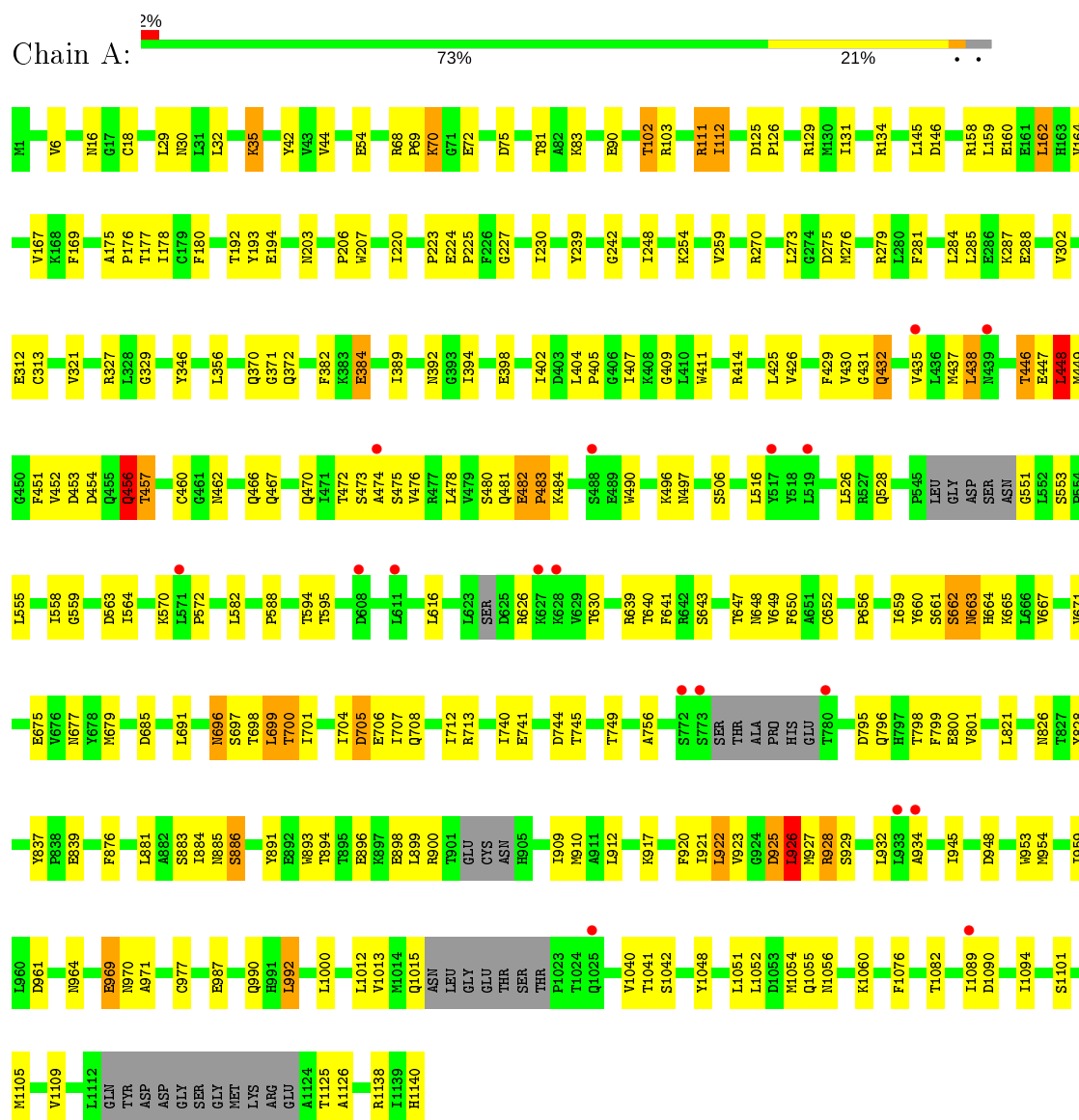
- Molecule 2 is a protein called DET1- and DDB1-associated protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	19	Total	C	H	N	O	S	0	0	0
			315	104	158	26	26	1			
2	D	19	Total	C	H	N	O	S	0	0	0
			315	104	158	26	26	1			

3 Residue-property plots

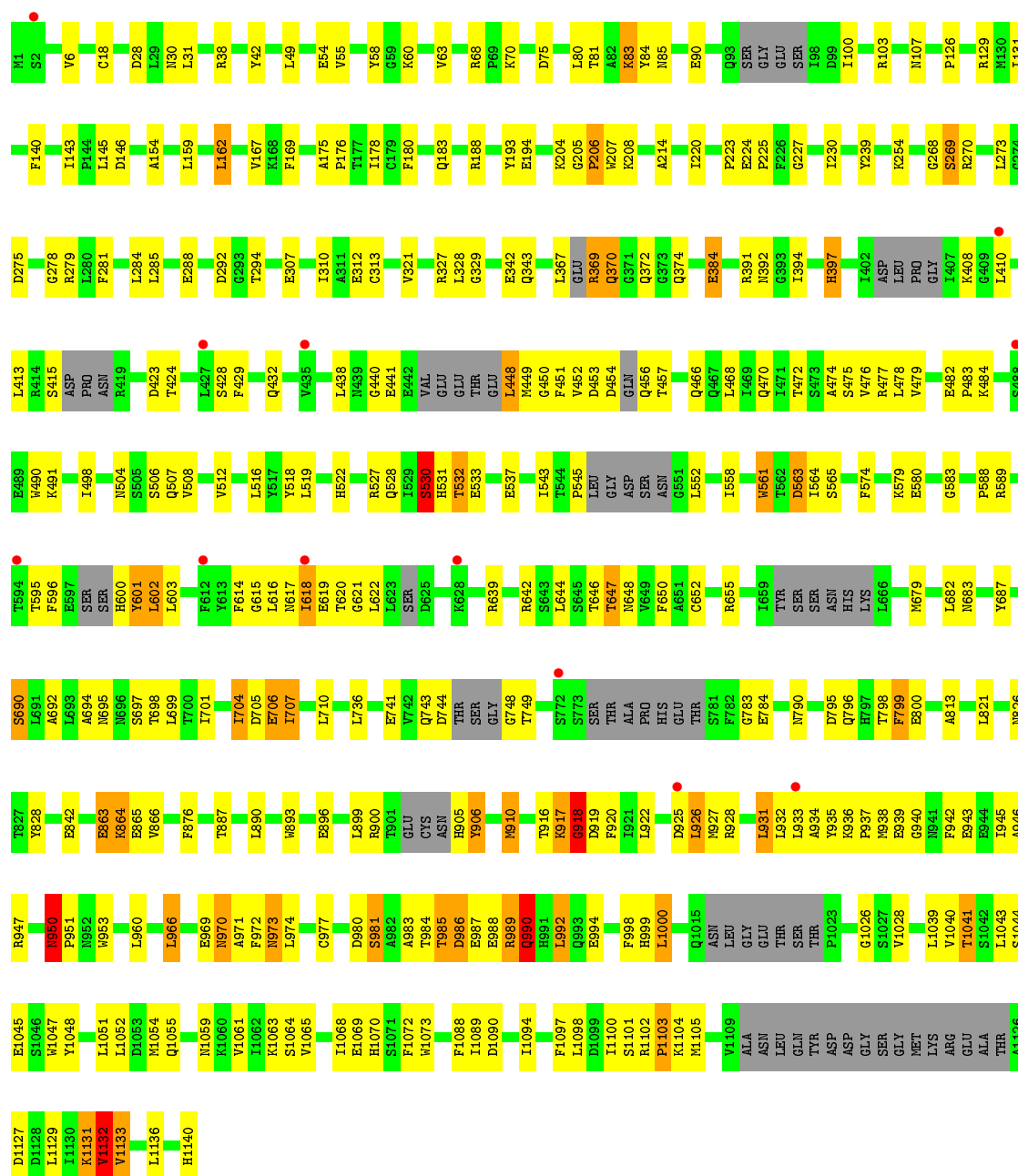
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA damage-binding protein 1



• Molecule 1: DNA damage-binding protein 1





- Molecule 2: DET1- and DDB1-associated protein 1

Chain C: 68% 26% 5%



- Molecule 2: DET1- and DDB1-associated protein 1

Chain D: 79% 16% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.20Å 219.18Å 89.32Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	47.80 – 3.09 47.80 – 3.09	Depositor EDS
% Data completeness (in resolution range)	88.7 (47.80-3.09) 88.7 (47.80-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.247 , 0.307 0.250 , 0.310	Depositor DCC
R_{free} test set	1997 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.587	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , -1.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	34801	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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	0.28	1/8830 (0.0%)	0.58	8/11954 (0.1%)
1	B	0.31	0/8563	0.73	24/11575 (0.2%)
2	C	0.35	0/161	0.66	0/214
2	D	0.31	0/161	0.45	0/214
All	All	0.30	1/17715 (0.0%)	0.66	32/23957 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	1	6
All	All	1	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	456	GLN	C-N	-5.98	1.20	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	983	ALA	N-CA-C	20.05	165.15	111.00
1	B	983	ALA	CB-CA-C	-18.70	82.05	110.10
1	B	983	ALA	C-N-CA	17.19	164.67	121.70
1	B	863	GLU	C-N-CA	14.91	158.97	121.70
1	B	864	LYS	N-CA-CB	13.06	134.11	110.60
1	B	985	THR	N-CA-C	12.93	145.92	111.00
1	A	456	GLN	C-N-CA	12.08	151.90	121.70
1	B	530	SER	CB-CA-C	-11.98	87.34	110.10
1	B	620	THR	N-CA-C	-10.69	82.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	GLN	O-C-N	-9.58	107.37	122.70
1	A	456	GLN	N-CA-C	9.11	135.59	111.00
1	B	986	ASP	N-CA-C	-8.96	86.82	111.00
1	B	985	THR	CB-CA-C	-8.86	87.67	111.60
1	A	457	THR	N-CA-C	-8.35	88.46	111.00
1	B	981	SER	N-CA-C	7.97	132.51	111.00
1	B	863	GLU	N-CA-C	-7.19	91.59	111.00
1	B	799	PHE	CB-CA-C	7.08	124.55	110.40
1	A	456	GLN	CB-CA-C	-6.85	96.70	110.40
1	A	287	LYS	CB-CA-C	-6.10	98.20	110.40
1	B	647	THR	N-CA-C	-6.01	94.78	111.00
1	B	1132	VAL	N-CA-C	-5.94	94.96	111.00
1	B	918	GLY	C-N-CA	5.93	136.52	121.70
1	B	440	GLY	N-CA-C	-5.65	98.97	113.10
1	B	990	GLN	CB-CA-C	5.54	121.49	110.40
1	A	457	THR	N-CA-CB	5.48	120.72	110.30
1	B	799	PHE	N-CA-C	-5.48	96.21	111.00
1	A	927	MET	N-CA-C	-5.38	96.47	111.00
1	B	918	GLY	N-CA-C	-5.37	99.68	113.10
1	B	1132	VAL	CB-CA-C	5.28	121.44	111.40
1	B	950	ASN	N-CA-C	-5.12	97.18	111.00
1	B	950	ASN	C-N-CD	5.09	139.10	128.40
1	B	926	LEU	CA-CB-CG	5.02	126.84	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	983	ALA	CA

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	448	LEU	Peptide
1	A	456	GLN	Mainchain,Peptide
1	A	705	ASP	Peptide
1	A	925	ASP	Peptide
1	A	926	LEU	Peptide
1	B	530	SER	Peptide
1	B	618	ILE	Peptide
1	B	863	GLU	Peptide
1	B	906	TYR	Peptide
1	B	918	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	970	ASN	Peptide

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	8674	8655	8663	186	0
1	B	8420	8422	8433	215	0
2	C	157	158	158	5	0
2	D	157	158	158	2	0
All	All	17408	17393	17412	399	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 11.

All (399) 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:456:GLN:O	1:A:456:GLN:HG2	1.24	1.05
1:A:456:GLN:O	1:A:456:GLN:CG	2.05	1.02
1:B:799:PHE:O	1:B:800:GLU:HG3	1.63	0.99
1:A:407:ILE:CD1	1:A:699:LEU:CD1	2.44	0.95
1:A:398:GLU:CD	1:A:700:THR:HG21	1.87	0.94
1:B:984:THR:HG22	1:B:988:GLU:HG2	1.49	0.93
1:A:407:ILE:HD12	1:A:699:LEU:CD1	1.98	0.92
1:B:595:THR:OG1	1:B:600:HIS:ND1	2.13	0.82
1:B:1127:ASP:OD1	1:B:1131:LYS:NZ	2.14	0.81
1:B:188:ARG:NH1	1:B:214:ALA:O	2.16	0.79
1:B:391:ARG:NH2	1:B:705:ASP:OD2	2.16	0.78
1:A:407:ILE:CD1	1:A:699:LEU:HD11	2.14	0.78
1:B:985:THR:HG22	1:B:986:ASP:N	1.90	0.78
1:B:984:THR:HG22	1:B:988:GLU:CG	2.14	0.77
1:B:618:ILE:HB	1:B:619:GLU:HG2	1.67	0.76
1:B:980:ASP:OD1	1:B:981:SER:N	2.18	0.76
1:A:16:ASN:ND2	1:A:35:LYS:O	2.19	0.75
1:A:398:GLU:CD	1:A:700:THR:CG2	2.55	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLY:O	1:A:239:TYR:OH	2.04	0.75
1:B:946:ALA:HA	1:B:990:GLN:O	1.86	0.73
1:B:615:GLY:O	1:B:622:LEU:O	2.08	0.71
1:B:984:THR:CG2	1:B:988:GLU:HB2	2.22	0.70
1:A:407:ILE:HD11	1:A:699:LEU:HD13	1.73	0.70
1:B:1129:LEU:HA	1:B:1132:VAL:HG11	1.73	0.70
1:B:1129:LEU:HA	1:B:1132:VAL:CG1	2.22	0.69
1:B:798:THR:O	1:B:799:PHE:C	2.29	0.69
1:A:404:LEU:O	1:A:697:SER:O	2.09	0.69
1:A:158:ARG:NH1	1:A:160:GLU:OE1	2.25	0.69
1:B:227:GLY:O	1:B:239:TYR:OH	2.07	0.68
1:A:886:SER:O	1:A:909:ILE:N	2.21	0.68
1:A:954:MET:HA	1:A:969:GLU:HA	1.76	0.68
1:A:452:VAL:HG21	1:A:472:THR:HG21	1.76	0.68
1:A:697:SER:OG	1:A:698:THR:HG23	1.94	0.67
1:A:431:GLY:O	1:A:456:GLN:N	2.27	0.66
1:A:799:PHE:O	1:A:800:GLU:HG3	1.96	0.66
1:A:407:ILE:HD12	1:A:699:LEU:HD12	1.76	0.66
1:B:984:THR:HG22	1:B:988:GLU:CB	2.26	0.65
1:A:662:SER:OG	1:A:663:ASN:N	2.28	0.65
1:B:278:GLY:O	1:B:307:GLU:HB2	1.96	0.65
1:A:407:ILE:CD1	1:A:699:LEU:HD13	2.26	0.65
1:B:646:THR:O	1:B:647:THR:C	2.33	0.64
1:B:183:GLN:OE1	1:B:188:ARG:NH2	2.31	0.64
1:A:481:GLN:OE1	1:A:484:LYS:NZ	2.28	0.64
1:B:392:ASN:ND2	1:B:1140:HIS:OXT	2.31	0.64
1:A:432:GLN:HA	1:A:454:ASP:HA	1.80	0.64
1:A:398:GLU:CG	1:A:700:THR:HG21	2.28	0.63
1:A:912:LEU:HG	1:A:926:LEU:HD22	1.81	0.63
1:B:452:VAL:HG21	1:B:472:THR:HG21	1.79	0.63
1:B:415:SER:OG	1:B:484:LYS:NZ	2.32	0.63
1:A:677:ASN:ND2	1:A:696:ASN:OD1	2.31	0.62
1:A:675:GLU:OE1	1:B:900:ARG:NH1	2.32	0.62
1:A:923:VAL:CG2	1:A:959:ILE:HD11	2.29	0.62
1:A:446:THR:O	1:A:448:LEU:HD23	2.00	0.62
1:A:407:ILE:HD11	1:A:699:LEU:CD1	2.28	0.61
1:A:1125:THR:HG22	1:A:1126:ALA:H	1.65	0.61
1:A:392:ASN:ND2	1:A:1140:HIS:OXT	2.34	0.61
1:B:1044:SER:O	1:B:1047:TRP:N	2.27	0.61
1:A:961:ASP:OD2	1:A:964:ASN:ND2	2.33	0.61
1:B:936:LYS:O	1:B:938:MET:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:SER:OG	1:A:555:LEU:O	2.19	0.60
1:B:987:GLU:H	1:B:990:GLN:HB3	1.65	0.60
1:A:407:ILE:HG22	1:A:409:GLY:H	1.66	0.60
1:B:950:ASN:HD21	1:B:994:GLU:CD	2.05	0.60
1:A:506:SER:OG	1:A:551:GLY:O	2.20	0.59
1:A:18:CYS:N	1:A:313:CYS:SG	2.76	0.59
1:A:90:GLU:OE1	1:A:103:ARG:NE	2.35	0.59
1:B:518:TYR:HB3	1:B:530:SER:O	2.03	0.59
1:B:984:THR:HG22	1:B:988:GLU:HB2	1.83	0.59
1:A:696:ASN:OD1	1:A:696:ASN:N	2.35	0.58
1:B:448:LEU:N	1:B:448:LEU:HD13	2.18	0.58
1:B:821:LEU:HB3	1:B:893:TRP:HB2	1.87	0.57
1:B:456:GLN:HG2	1:B:457:THR:H	1.69	0.57
1:B:916:THR:HG22	1:B:918:GLY:H	1.70	0.56
1:B:707:ILE:O	1:B:707:ILE:HG13	2.06	0.56
1:B:706:GLU:HG2	1:B:707:ILE:N	2.21	0.56
1:B:532:THR:OG1	1:B:574:PHE:CD2	2.59	0.56
1:B:969:GLU:O	1:B:971:ALA:O	2.24	0.56
1:A:821:LEU:HB3	1:A:893:TRP:HB2	1.88	0.56
1:A:910:MET:O	1:A:926:LEU:O	2.23	0.55
1:A:516:LEU:HD11	1:A:558:ILE:HD12	1.88	0.55
1:B:1061:VAL:O	1:B:1061:VAL:HG12	2.06	0.55
1:A:691:LEU:HD12	1:A:704:ILE:HD11	1.88	0.55
1:B:31:LEU:HD23	1:B:49:LEU:HD21	1.88	0.55
1:B:83:LYS:HG2	1:B:1072:PHE:CE2	2.42	0.55
1:B:974:LEU:N	1:B:998:PHE:O	2.37	0.55
1:B:482:GLU:HB3	1:B:483:PRO:HD3	1.88	0.55
1:B:926:LEU:HG	1:B:928:ARG:H	1.72	0.54
1:A:472:THR:HG22	1:A:475:SER:O	2.06	0.54
1:A:457:THR:OG1	1:A:470:GLN:NE2	2.40	0.54
1:B:917:LYS:O	1:B:918:GLY:C	2.45	0.54
1:B:140:PHE:HB2	1:B:159:LEU:HD12	1.90	0.54
1:A:744:ASP:OD1	1:A:745:THR:N	2.40	0.54
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	1.88	0.54
1:B:81:THR:HB	1:B:83:LYS:O	2.08	0.54
1:A:456:GLN:O	1:A:457:THR:O	2.25	0.53
1:B:1098:LEU:HD11	1:B:1133:VAL:HG12	1.91	0.53
1:B:692:ALA:HA	1:B:701:ILE:HG22	1.91	0.53
1:A:275:ASP:OD2	1:A:279:ARG:NH1	2.41	0.53
1:B:743:GLN:HB2	1:B:783:GLY:H	1.73	0.53
1:A:284:LEU:HD11	2:C:4:PHE:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:THR:O	1:A:1138:ARG:NH2	2.38	0.53
1:B:518:TYR:CB	1:B:530:SER:O	2.57	0.53
1:A:704:ILE:HG22	1:A:705:ASP:H	1.74	0.52
1:A:81:THR:HG22	1:A:83:LYS:H	1.74	0.52
1:A:929:SER:OG	1:A:948:ASP:O	2.23	0.52
1:B:920:PHE:O	1:B:934:ALA:HA	2.09	0.52
1:A:741:GLU:HB3	1:A:749:THR:HB	1.92	0.52
1:B:564:ILE:HB	1:B:583:GLY:HA3	1.90	0.52
1:A:466:GLN:HG3	1:A:466:GLN:O	2.10	0.52
1:A:1051:LEU:HA	1:A:1054:MET:HB2	1.91	0.52
1:A:398:GLU:CG	1:A:700:THR:CG2	2.87	0.52
1:B:38:ARG:NH1	1:B:54:GLU:OE2	2.31	0.51
1:A:476:VAL:HG22	1:A:490:TRP:HB3	1.93	0.51
1:A:648:ASN:HB3	1:A:659:ILE:O	2.10	0.51
1:B:194:GLU:HG3	1:B:205:GLY:HA2	1.91	0.51
1:B:68:ARG:HB3	1:B:75:ASP:HA	1.93	0.51
1:B:972:PHE:O	1:B:1000:LEU:N	2.43	0.51
1:B:408:LYS:N	1:B:428:SER:O	2.40	0.51
1:B:973:ASN:HA	1:B:999:HIS:HA	1.92	0.51
1:A:656:PRO:HB2	1:A:671:VAL:HB	1.92	0.51
1:B:275:ASP:OD2	1:B:279:ARG:NH1	2.44	0.51
1:A:426:VAL:HG22	1:A:435:VAL:HG13	1.93	0.51
1:A:923:VAL:HG23	1:A:959:ILE:HD11	1.93	0.51
1:B:865:GLU:CG	1:B:865:GLU:O	2.59	0.51
1:B:985:THR:HG22	1:B:986:ASP:CA	2.40	0.51
1:B:931:LEU:HA	1:B:947:ARG:HA	1.91	0.50
1:B:270:ARG:HG2	1:B:284:LEU:HD23	1.93	0.50
1:B:522:HIS:CG	1:B:527:ARG:HH12	2.30	0.50
1:B:927:MET:O	1:B:953:TRP:HA	2.11	0.50
1:B:984:THR:CG2	1:B:988:GLU:CB	2.86	0.50
1:B:985:THR:O	1:B:985:THR:CG2	2.42	0.50
1:A:925:ASP:OD2	1:A:954:MET:SD	2.70	0.50
1:B:167:VAL:HG13	1:B:180:PHE:HB3	1.93	0.50
1:B:601:TYR:N	1:B:601:TYR:CD1	2.80	0.50
1:A:389:ILE:HB	1:A:713:ARG:HB3	1.93	0.50
1:A:925:ASP:OD1	1:A:926:LEU:N	2.45	0.50
1:B:84:TYR:O	1:B:107:ASN:ND2	2.45	0.50
1:B:887:THR:HG23	1:B:906:TYR:HB3	1.94	0.50
1:A:987:GLU:O	1:A:990:GLN:N	2.45	0.49
1:B:1102:ARG:N	1:B:1103:PRO:HD2	2.27	0.49
1:B:987:GLU:H	1:B:990:GLN:CB	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:ASP:OD1	1:A:563:ASP:N	2.44	0.49
1:A:706:GLU:HG3	1:A:708:GLN:H	1.77	0.49
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.94	0.49
1:A:928:ARG:HH11	1:A:953:TRP:HA	1.77	0.49
1:B:744:ASP:N	1:B:748:GLY:O	2.32	0.49
1:A:1055:GLN:HG3	1:A:1094:ILE:HD11	1.94	0.49
1:B:639:ARG:O	1:B:650:PHE:N	2.34	0.49
1:A:473:SER:HB2	1:A:497:ASN:OD1	2.12	0.49
1:A:126:PRO:HD3	1:A:169:PHE:HB3	1.94	0.49
1:A:312:GLU:HG3	1:A:327:ARG:HE	1.78	0.49
1:A:398:GLU:HG2	1:A:700:THR:HG21	1.95	0.49
1:A:69:PRO:HD2	1:A:72:GLU:HG3	1.94	0.49
1:A:795:ASP:OD1	1:A:796:GLN:N	2.45	0.49
1:B:865:GLU:HG2	1:B:865:GLU:O	2.13	0.49
1:B:984:THR:OG1	1:B:985:THR:N	2.46	0.49
1:A:837:TYR:O	1:A:839:GLU:N	2.43	0.49
1:A:177:THR:HG21	1:A:206:PRO:HG2	1.94	0.48
1:B:1055:GLN:HG3	1:B:1094:ILE:HD11	1.94	0.48
1:B:423:ASP:O	1:B:438:LEU:HB2	2.13	0.48
1:B:988:GLU:HA	1:B:988:GLU:OE1	2.13	0.48
1:B:453:ASP:N	1:B:453:ASP:OD1	2.46	0.48
1:A:430:VAL:HG11	1:B:938:MET:HG2	1.95	0.48
1:A:697:SER:OG	1:A:698:THR:N	2.45	0.48
1:B:18:CYS:N	1:B:313:CYS:SG	2.86	0.48
1:B:476:VAL:HG22	1:B:490:TRP:HB3	1.94	0.48
1:B:707:ILE:CG1	1:B:707:ILE:O	2.61	0.48
1:B:565:SER:HA	1:B:580:GLU:O	2.14	0.48
1:A:430:VAL:HG21	1:B:939:GLU:HB2	1.94	0.48
1:A:482:GLU:CB	1:A:483:PRO:HD3	2.44	0.48
1:B:563:ASP:OD1	1:B:563:ASP:N	2.46	0.48
1:A:594:THR:HG22	1:A:595:THR:H	1.78	0.48
1:B:367:LEU:HD12	1:B:374:GLN:OE1	2.14	0.48
1:B:795:ASP:OD1	1:B:796:GLN:N	2.46	0.48
1:A:798:THR:O	1:A:799:PHE:C	2.52	0.48
1:A:68:ARG:HB3	1:A:75:ASP:HA	1.96	0.48
1:B:969:GLU:HG2	1:B:971:ALA:H	1.79	0.48
1:A:1109:VAL:O	1:A:1109:VAL:HG13	2.14	0.47
1:A:756:ALA:HB1	1:A:801:VAL:HG21	1.96	0.47
1:B:799:PHE:O	1:B:800:GLU:CG	2.49	0.47
1:A:480:SER:HB2	1:A:483:PRO:HD2	1.95	0.47
1:A:898:GLU:O	1:A:898:GLU:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:LEU:HD11	1:B:558:ILE:HD12	1.95	0.47
1:B:925:ASP:OD1	1:B:926:LEU:N	2.39	0.47
1:B:506:SER:HB2	1:B:552:LEU:HD21	1.97	0.47
1:B:950:ASN:ND2	1:B:994:GLU:OE2	2.47	0.47
1:A:70:LYS:HD3	1:A:70:LYS:H	1.80	0.47
1:A:917:LYS:HB2	1:A:959:ILE:HG21	1.96	0.47
1:B:876:PHE:HZ	1:B:920:PHE:HA	1.78	0.47
1:A:706:GLU:HG3	1:A:707:ILE:N	2.30	0.47
1:B:1051:LEU:HA	1:B:1054:MET:HB2	1.96	0.47
1:B:704:ILE:CG2	1:B:705:ASP:N	2.78	0.47
1:B:826:ASN:HB2	1:B:828:TYR:CZ	2.50	0.47
2:C:18:ARG:O	2:C:19:PHE:C	2.54	0.47
1:A:885:ASN:O	1:A:910:MET:HA	2.15	0.46
1:B:292:ASP:OD1	1:B:294:THR:OG1	2.28	0.46
1:A:102:THR:O	1:A:102:THR:OG1	2.33	0.46
1:B:126:PRO:HD3	1:B:169:PHE:HB3	1.97	0.46
1:B:1061:VAL:HG12	1:B:1104:LYS:HD3	1.96	0.46
1:B:269:SER:HA	1:B:285:LEU:HB2	1.97	0.46
1:B:1097:PHE:CZ	1:B:1105:MET:HG2	2.49	0.46
1:A:685:ASP:N	1:A:685:ASP:OD1	2.48	0.46
1:B:646:THR:OG1	1:B:648:ASN:OD1	2.27	0.46
1:B:682:LEU:HB3	1:B:690:SER:O	2.16	0.46
1:A:926:LEU:O	1:A:926:LEU:HD23	2.16	0.46
1:B:977:CYS:HB3	1:B:992:LEU:HD13	1.98	0.46
1:A:570:LYS:HE2	1:A:572:PRO:HD2	1.98	0.46
1:A:1041:THR:HG22	1:A:1042:SER:H	1.81	0.46
1:A:111:ARG:HG2	1:A:112:ILE:HG23	1.97	0.46
1:A:398:GLU:OE2	1:A:700:THR:HG21	2.13	0.46
1:B:131:ILE:HG13	1:B:145:LEU:HD11	1.98	0.46
1:B:450:GLY:HA3	1:B:479:VAL:HG22	1.97	0.46
1:B:475:SER:HB3	1:B:491:LYS:HA	1.98	0.46
1:B:931:LEU:CD1	1:B:933:LEU:HD11	2.46	0.46
1:A:372:GLN:HG3	1:A:1012:LEU:O	2.15	0.45
1:B:1069:GLU:O	1:B:1072:PHE:N	2.47	0.45
1:A:923:VAL:HG21	1:A:959:ILE:CG1	2.46	0.45
1:B:989:ARG:O	1:B:989:ARG:HD3	2.16	0.45
1:A:466:GLN:O	1:A:481:GLN:HB2	2.16	0.45
1:A:659:ILE:HA	1:A:667:VAL:O	2.16	0.45
1:B:1064:SER:O	1:B:1064:SER:OG	2.33	0.45
1:A:134:ARG:HH11	1:A:164:VAL:HB	1.81	0.45
1:B:451:PHE:HA	1:B:470:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:PHE:HB2	1:B:601:TYR:OH	2.16	0.45
1:B:60:LYS:N	1:B:81:THR:HG23	2.32	0.45
1:B:927:MET:HB2	1:B:928:ARG:HE	1.81	0.45
1:A:663:ASN:O	1:A:664:HIS:HB2	2.16	0.45
1:B:83:LYS:O	1:B:85:ASN:N	2.48	0.45
1:B:985:THR:HG23	1:B:985:THR:O	2.17	0.45
1:A:704:ILE:HG22	1:A:705:ASP:N	2.32	0.45
1:B:953:TRP:HB2	1:B:970:ASN:OD1	2.17	0.45
1:A:125:ASP:HB3	1:A:129:ARG:H	1.82	0.45
1:A:178:ILE:HG22	1:A:193:TYR:HB2	1.99	0.45
1:B:432:GLN:HA	1:B:454:ASP:HA	1.98	0.45
1:B:601:TYR:HB3	1:B:614:PHE:O	2.17	0.45
1:A:407:ILE:HD12	1:A:699:LEU:HD11	1.81	0.45
1:B:220:ILE:HB	1:B:230:ILE:HB	1.97	0.45
1:A:1105:MET:O	1:A:1109:VAL:HG12	2.16	0.45
1:B:310:ILE:HG21	1:B:328:LEU:HD12	1.98	0.45
1:B:55:VAL:HG11	1:B:100:ILE:HG13	1.99	0.45
1:B:321:VAL:HG21	2:D:16:PHE:CD2	2.52	0.45
1:B:519:LEU:HA	1:B:527:ARG:O	2.17	0.45
1:B:646:THR:O	1:B:648:ASN:N	2.50	0.45
1:B:81:THR:HG22	1:B:83:LYS:N	2.31	0.45
1:B:926:LEU:HD12	1:B:927:MET:H	1.82	0.45
1:B:1026:GLY:H	1:B:1041:THR:HG22	1.81	0.44
1:B:1028:VAL:H	1:B:1039:LEU:HD12	1.82	0.44
1:A:1076:PHE:O	1:A:1082:THR:HA	2.17	0.44
1:B:799:PHE:C	1:B:800:GLU:HG3	2.36	0.44
1:A:917:LYS:HB2	1:A:959:ILE:HD13	1.99	0.44
1:B:543:ILE:O	1:B:545:PRO:HD3	2.18	0.44
1:B:984:THR:HG23	1:B:988:GLU:HB2	1.97	0.44
1:B:162:LEU:HD23	1:B:162:LEU:H	1.82	0.44
1:B:695:ASN:ND2	1:B:697:SER:OG	2.49	0.44
1:A:273:LEU:HB2	1:A:281:PHE:HB2	2.00	0.44
1:A:894:THR:HG22	1:A:896:GLU:H	1.81	0.44
1:B:273:LEU:HB2	1:B:281:PHE:HB2	2.00	0.44
1:B:369:ARG:C	1:B:370:GLN:HG3	2.38	0.44
1:B:448:LEU:CD1	1:B:448:LEU:N	2.81	0.44
1:B:595:THR:CB	1:B:600:HIS:ND1	2.81	0.44
1:B:441:GLU:HG3	1:B:687:TYR:CZ	2.53	0.44
1:A:220:ILE:HB	1:A:230:ILE:HB	1.99	0.44
1:A:798:THR:OG1	1:A:798:THR:O	2.35	0.44
1:B:698:THR:HG22	1:B:699:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:HG13	1:A:145:LEU:HD11	1.99	0.44
1:B:743:GLN:NE2	1:B:784:GLU:OE1	2.51	0.44
1:B:910:MET:O	1:B:926:LEU:HD13	2.16	0.44
1:A:1056:ASN:O	1:A:1060:LYS:HE2	2.17	0.44
1:A:472:THR:HG23	1:A:474:ALA:H	1.82	0.44
1:A:891:TYR:HB3	1:A:899:LEU:HD11	2.00	0.44
1:A:891:TYR:HB3	1:A:899:LEU:CD1	2.47	0.44
1:B:224:GLU:N	1:B:225:PRO:HD2	2.33	0.44
1:B:798:THR:OG1	1:B:798:THR:O	2.35	0.44
1:B:864:LYS:O	1:B:866:VAL:HG23	2.17	0.44
1:B:537:GLU:HB3	1:B:561:TRP:HB2	1.99	0.44
1:B:876:PHE:CZ	1:B:920:PHE:HA	2.53	0.44
1:A:453:ASP:OD1	1:A:453:ASP:N	2.50	0.43
1:A:664:HIS:O	1:A:665:LYS:HE3	2.18	0.43
1:A:926:LEU:HD21	1:A:928:ARG:HH22	1.83	0.43
1:B:600:HIS:HD2	1:B:617:ASN:O	2.00	0.43
1:A:640:THR:HA	1:A:649:VAL:HA	1.99	0.43
1:A:826:ASN:HB2	1:A:828:TYR:CZ	2.53	0.43
1:A:382:PHE:HE1	1:A:740:ILE:HD11	1.82	0.43
1:B:1104:LYS:O	1:B:1105:MET:HB3	2.19	0.43
1:B:466:GLN:HG3	1:B:466:GLN:O	2.18	0.43
1:B:472:THR:HG23	1:B:474:ALA:H	1.83	0.43
1:B:508:VAL:HB	1:B:519:LEU:HB2	2.00	0.43
1:B:490:TRP:NE1	1:B:528:GLN:OE1	2.50	0.43
1:A:194:GLU:HB2	1:A:203:ASN:HB2	1.99	0.43
1:A:248:ILE:HD11	1:A:302:VAL:HG23	1.99	0.43
1:A:356:LEU:HD21	1:A:712:ILE:HD13	2.01	0.43
1:A:876:PHE:CZ	1:A:920:PHE:HA	2.53	0.43
1:A:1048:TYR:O	1:A:1052:LEU:HB2	2.19	0.43
1:A:18:CYS:HA	1:A:32:LEU:O	2.18	0.43
1:A:429:PHE:O	1:A:456:GLN:HG3	2.19	0.43
1:A:934:ALA:HB2	1:A:945:ILE:HD11	1.99	0.43
1:A:917:LYS:N	1:A:959:ILE:HD12	2.33	0.43
1:B:6:VAL:O	1:B:1090:ASP:HA	2.18	0.43
1:B:394:ILE:HG21	1:B:704:ILE:HD13	2.00	0.43
1:A:660:TYR:CE2	1:A:707:ILE:HA	2.54	0.43
1:B:595:THR:OG1	1:B:600:HIS:CE1	2.71	0.43
1:B:429:PHE:O	1:B:456:GLN:HG3	2.18	0.43
1:B:890:LEU:HB2	1:B:942:PHE:HZ	1.83	0.43
1:A:1013:VAL:O	1:A:1015:GLN:N	2.52	0.43
1:A:652:CYS:SG	1:A:679:MET:HB3	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1102:ARG:H	1:B:1103:PRO:HD2	1.84	0.43
1:B:518:TYR:O	1:B:528:GLN:HA	2.19	0.43
1:B:564:ILE:HG23	1:B:588:PRO:HG3	2.01	0.43
1:A:162:LEU:H	1:A:162:LEU:HD23	1.83	0.43
1:A:922:LEU:O	1:A:932:LEU:HD12	2.19	0.43
1:B:1048:TYR:CE2	1:B:1052:LEU:HD12	2.54	0.43
1:A:270:ARG:NH2	2:C:7:GLY:O	2.39	0.43
1:B:270:ARG:NH2	2:D:7:GLY:O	2.49	0.43
1:B:413:LEU:HB3	1:B:424:THR:HB	2.01	0.42
1:B:504:ASN:OD1	1:B:507:GLN:HG2	2.19	0.42
1:B:652:CYS:SG	1:B:679:MET:HB3	2.59	0.42
1:A:224:GLU:N	1:A:225:PRO:HD2	2.34	0.42
1:A:321:VAL:HG11	2:C:16:PHE:CE2	2.54	0.42
1:A:482:GLU:HB2	1:A:483:PRO:HD3	2.00	0.42
1:A:881:LEU:HD21	1:A:922:LEU:HD21	2.01	0.42
1:B:342:GLU:C	1:B:343:GLN:HG2	2.40	0.42
1:A:230:ILE:HD11	1:A:285:LEU:HD21	2.01	0.42
1:A:451:PHE:CE2	1:A:470:GLN:HB2	2.55	0.42
1:A:582:LEU:HD21	1:A:626:ARG:HG3	2.00	0.42
1:B:602:LEU:HD22	1:B:603:LEU:N	2.34	0.42
1:A:447:GLU:OE2	1:A:453:ASP:HA	2.20	0.42
1:A:639:ARG:O	1:A:650:PHE:N	2.37	0.42
1:A:926:LEU:HG	1:A:928:ARG:NH1	2.34	0.42
1:B:413:LEU:HD11	1:B:468:LEU:HD23	2.00	0.42
1:B:936:LYS:HE2	1:B:943:GLU:HB2	2.02	0.42
1:A:6:VAL:HG12	1:A:1040:VAL:HG22	2.02	0.42
1:A:1101:SER:O	1:A:1105:MET:HB2	2.20	0.42
1:A:346:TYR:CE2	2:C:2:ALA:HB2	2.55	0.42
1:B:931:LEU:HD12	1:B:933:LEU:CD1	2.49	0.42
1:A:969:GLU:C	1:A:971:ALA:H	2.23	0.42
1:B:6:VAL:HG12	1:B:1040:VAL:HG22	2.02	0.42
1:B:312:GLU:HG3	1:B:327:ARG:HE	1.84	0.42
1:B:498:ILE:HA	1:B:512:VAL:HG22	2.01	0.42
1:A:30:ASN:HA	1:A:42:TYR:O	2.20	0.42
1:A:564:ILE:HG13	1:A:588:PRO:HD3	2.01	0.42
1:B:893:TRP:HE3	1:B:899:LEU:HB3	1.85	0.42
1:A:641:PHE:HZ	1:A:660:TYR:HE1	1.67	0.42
1:B:986:ASP:HA	1:B:990:GLN:HB2	2.01	0.42
1:A:876:PHE:HZ	1:A:920:PHE:HA	1.85	0.42
1:B:998:PHE:HB2	1:B:1088:PHE:CG	2.54	0.42
1:B:175:ALA:HB1	1:B:176:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:LEU:HD22	1:B:621:GLY:HA2	2.02	0.42
1:B:736:LEU:HD13	1:B:813:ALA:HB1	2.01	0.42
1:A:1048:TYR:CE2	1:A:1052:LEU:HD12	2.55	0.41
1:A:6:VAL:O	1:A:1090:ASP:HA	2.19	0.41
1:B:329:GLY:HA3	1:B:384:GLU:HG2	2.02	0.41
1:B:90:GLU:OE1	1:B:103:ARG:NE	2.52	0.41
1:B:934:ALA:HB2	1:B:945:ILE:HD11	2.02	0.41
1:A:920:PHE:O	1:A:934:ALA:HA	2.20	0.41
1:B:1132:VAL:O	1:B:1136:LEU:HG	2.20	0.41
1:B:922:LEU:O	1:B:932:LEU:HD12	2.20	0.41
1:A:29:LEU:HB3	1:A:44:VAL:HB	2.03	0.41
1:B:58:TYR:HB3	1:B:1073:TRP:HB2	2.03	0.41
1:A:207:TRP:CB	1:A:242:GLY:HA2	2.50	0.41
1:A:370:GLN:HG3	1:A:371:GLY:H	1.84	0.41
1:B:30:ASN:HA	1:B:42:TYR:O	2.20	0.41
1:B:1100:ILE:HG22	1:B:1101:SER:H	1.84	0.41
1:A:643:SER:N	1:A:647:THR:HG21	2.35	0.41
1:B:1051:LEU:HB2	1:B:1089:ILE:HD13	2.02	0.41
1:B:410:LEU:HD11	1:B:694:ALA:HB2	2.02	0.41
1:B:905:HIS:CE1	1:B:940:GLY:O	2.74	0.41
1:A:425:LEU:H	1:A:438:LEU:HD21	1.84	0.41
1:A:467:GLN:HB3	1:A:478:LEU:HD22	2.03	0.41
1:B:397:HIS:N	1:B:397:HIS:ND1	2.69	0.41
1:A:977:CYS:HB3	1:A:992:LEU:HD13	2.02	0.41
1:B:920:PHE:HB3	1:B:935:TYR:O	2.20	0.41
1:A:411:TRP:HB3	1:A:460:CYS:O	2.21	0.41
1:B:206:PRO:O	1:B:207:TRP:HB3	2.20	0.41
1:A:402:ILE:HG22	1:A:404:LEU:CD2	2.50	0.41
1:A:643:SER:H	1:A:647:THR:HG21	1.86	0.41
1:B:896:GLU:O	1:B:896:GLU:HG2	2.21	0.41
1:A:414:ARG:H	1:A:462:ASN:HD21	1.68	0.41
1:A:476:VAL:HG23	1:A:526:LEU:HD13	2.03	0.41
1:B:920:PHE:CD1	1:B:935:TYR:HD2	2.38	0.41
1:B:960:LEU:HD21	1:B:966:LEU:HD12	2.03	0.41
1:A:175:ALA:HB1	1:A:176:PRO:HD2	2.03	0.40
1:A:192:THR:HG22	1:A:206:PRO:HD2	2.03	0.40
1:A:394:ILE:O	1:A:671:VAL:HA	2.21	0.40
1:A:700:THR:C	1:A:701:ILE:CG1	2.89	0.40
1:B:1094:ILE:O	1:B:1097:PHE:HB3	2.20	0.40
1:B:143:ILE:HG12	1:B:154:ALA:HB2	2.03	0.40
1:B:81:THR:HG22	1:B:83:LYS:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ILE:HG12	1:A:559:GLY:N	2.36	0.40
1:B:63:VAL:HB	1:B:80:LEU:HB3	2.02	0.40
1:B:60:LYS:H	1:B:81:THR:HG23	1.86	0.40
1:A:329:GLY:HA3	1:A:384:GLU:HG2	2.04	0.40
1:A:665:LYS:HA	1:A:665:LYS:HE2	2.02	0.40
1:B:1059:ASN:OD1	1:B:1070:HIS:HB3	2.22	0.40
1:B:268:GLY:O	1:B:285:LEU:HD22	2.21	0.40
1:B:931:LEU:HD13	1:B:933:LEU:HD11	2.04	0.40
1:A:259:VAL:HG21	1:A:276:MET:HG3	2.04	0.40
1:B:178:ILE:HG22	1:B:193:TYR:HB2	2.02	0.40
1:B:230:ILE:HD11	1:B:285:LEU:HD21	2.03	0.40
1:B:741:GLU:HB3	1:B:749:THR:HB	2.04	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	1093/1140 (96%)	931 (85%)	157 (14%)	5 (0%)	29	64
1	B	1040/1140 (91%)	885 (85%)	151 (14%)	4 (0%)	34	69
2	C	17/19 (90%)	12 (71%)	5 (29%)	0	100	100
2	D	17/19 (90%)	13 (76%)	4 (24%)	0	100	100
All	All	2167/2318 (94%)	1841 (85%)	317 (15%)	9 (0%)	34	69

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	PRO
1	A	482	GLU
1	A	970	ASN

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Mol	Chain	Res	Type
1	B	1065	VAL
1	B	223	PRO
1	B	937	PRO
1	A	223	PRO
1	A	483	PRO
1	B	1103	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	971/999 (97%)	933 (96%)	38 (4%)	32	65
1	B	941/999 (94%)	880 (94%)	61 (6%)	17	47
2	C	17/17 (100%)	16 (94%)	1 (6%)	19	50
2	D	17/17 (100%)	14 (82%)	3 (18%)	2	8
All	All	1946/2032 (96%)	1843 (95%)	103 (5%)	22	54

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	54	GLU
1	A	70	LYS
1	A	102	THR
1	A	111	ARG
1	A	112	ILE
1	A	146	ASP
1	A	159	LEU
1	A	162	LEU
1	A	254	LYS
1	A	288	GLU
1	A	384	GLU
1	A	432	GLN
1	A	437	MET
1	A	438	LEU

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Mol	Chain	Res	Type
1	A	446	THR
1	A	448	LEU
1	A	449	MET
1	A	496	LYS
1	A	528	GLN
1	A	616	LEU
1	A	661	SER
1	A	662	SER
1	A	663	ASN
1	A	696	ASN
1	A	699	LEU
1	A	700	THR
1	A	883	SER
1	A	884	ILE
1	A	886	SER
1	A	900	ARG
1	A	921	ILE
1	A	922	LEU
1	A	926	LEU
1	A	928	ARG
1	A	969	GLU
1	A	992	LEU
1	A	1000	LEU
1	B	28	ASP
1	B	70	LYS
1	B	83	LYS
1	B	129	ARG
1	B	146	ASP
1	B	162	LEU
1	B	204	LYS
1	B	206	PRO
1	B	208	LYS
1	B	254	LYS
1	B	269	SER
1	B	288	GLU
1	B	369	ARG
1	B	370	GLN
1	B	372	GLN
1	B	384	GLU
1	B	397	HIS
1	B	448	LEU
1	B	449	MET

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Mol	Chain	Res	Type
1	B	477	ARG
1	B	478	LEU
1	B	531	HIS
1	B	532	THR
1	B	533	GLU
1	B	561	TRP
1	B	563	ASP
1	B	579	LYS
1	B	589	ARG
1	B	601	TYR
1	B	602	LEU
1	B	642	ARG
1	B	644	LEU
1	B	655	ARG
1	B	683	ASN
1	B	690	SER
1	B	704	ILE
1	B	706	GLU
1	B	707	ILE
1	B	710	LEU
1	B	790	ASN
1	B	842	GLU
1	B	910	MET
1	B	917	LYS
1	B	919	ASP
1	B	931	LEU
1	B	950	ASN
1	B	951	PRO
1	B	966	LEU
1	B	973	ASN
1	B	989	ARG
1	B	990	GLN
1	B	992	LEU
1	B	1000	LEU
1	B	1041	THR
1	B	1043	LEU
1	B	1045	GLU
1	B	1063	LYS
1	B	1068	ILE
1	B	1131	LYS
1	B	1132	VAL
1	B	1133	VAL

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Mol	Chain	Res	Type
2	C	16	PHE
2	D	1	MET
2	D	16	PHE
2	D	19	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	877	ASN
1	A	950	ASN
1	B	107	ASN
1	B	950	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](#)

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	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	456:GLN	C	457:THR	N	1.20

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1107/1140 (97%)	0.08	18 (1%) 72 51	13, 48, 87, 129	0
1	B	1072/1140 (94%)	0.09	12 (1%) 80 64	13, 49, 87, 106	0
2	C	19/19 (100%)	0.04	0 100 100	32, 44, 72, 75	0
2	D	19/19 (100%)	-0.07	0 100 100	32, 46, 63, 76	0
All	All	2217/2318 (95%)	0.09	30 (1%) 75 56	13, 48, 87, 129	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	SER	3.5
1	B	435	VAL	3.5
1	B	427	LEU	3.2
1	A	435	VAL	3.1
1	B	925	ASP	3.1
1	A	933	LEU	2.8
1	A	628	LYS	2.8
1	A	474	ALA	2.7
1	B	410	LEU	2.6
1	A	1025	GLN	2.6
1	A	934	ALA	2.6
1	B	933	LEU	2.5
1	B	2	SER	2.5
1	B	772	SER	2.5
1	B	488	SER	2.4
1	B	628	LYS	2.4
1	A	772	SER	2.3
1	A	627	LYS	2.3
1	B	618	ILE	2.3
1	A	517	TYR	2.3
1	A	608	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	773	SER	2.2
1	A	519	LEU	2.2
1	A	780	THR	2.2
1	A	571	LEU	2.1
1	A	439	ASN	2.1
1	B	612	PHE	2.1
1	A	611	LEU	2.1
1	B	594	THR	2.1
1	A	1089	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.