Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 11:47 AM EDT

PDB ID	:	2B5M
Title	:	Crystal Structure of DDB1
Authors	:	Li, T.; Chen, X.; Garbutt, K.C.; Zhou, P.; Zheng, N.
Deposited on	:	2005-09-28
Resolution	:	2.92 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

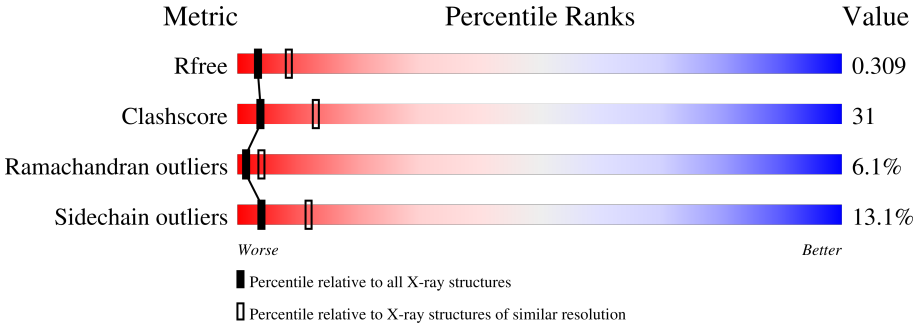
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1140	42% 40% 14% • •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8768 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 damage-specific DNA binding protein 1.

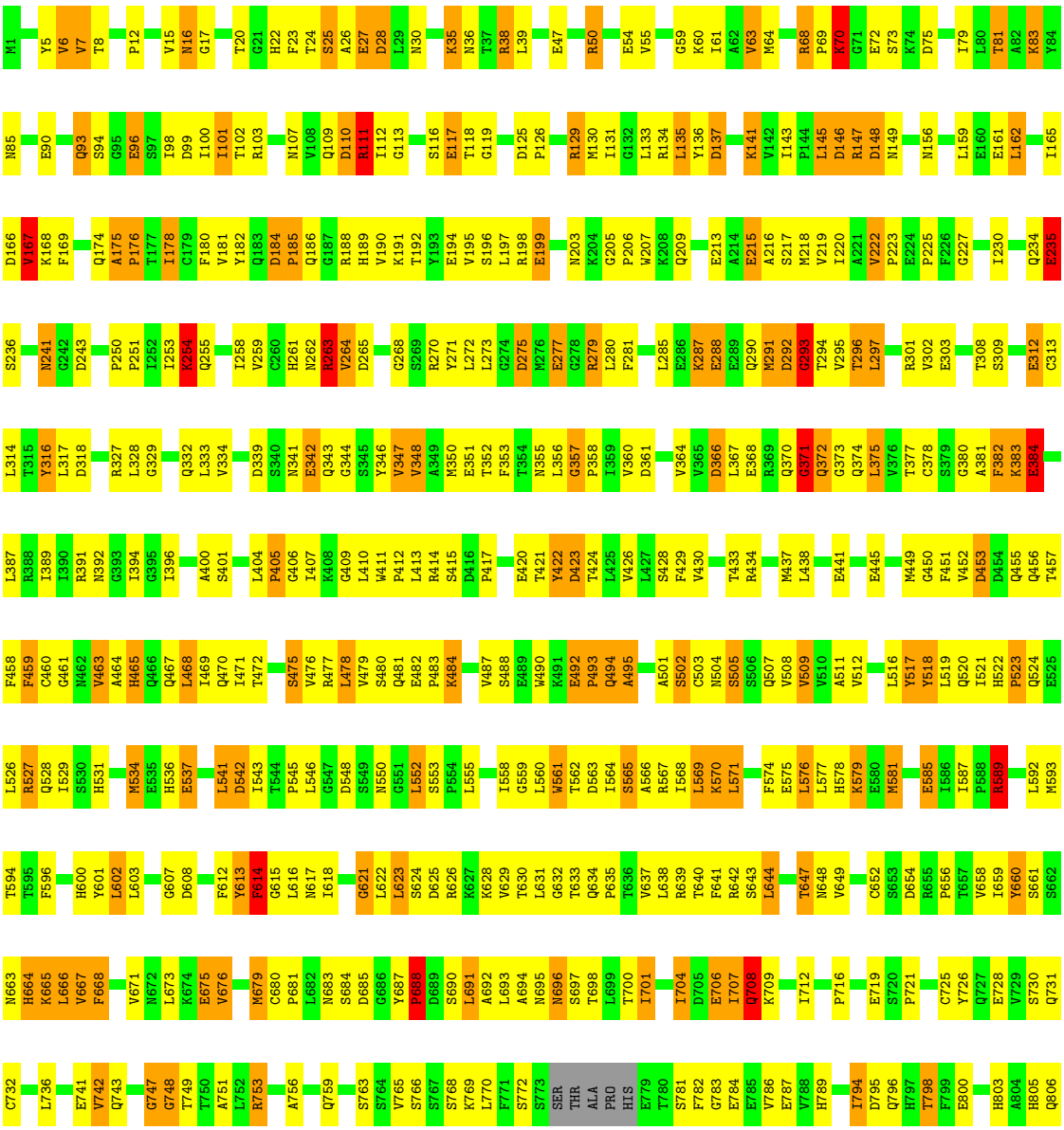
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1119	8768	5556	1477	1687	48	0	0	0

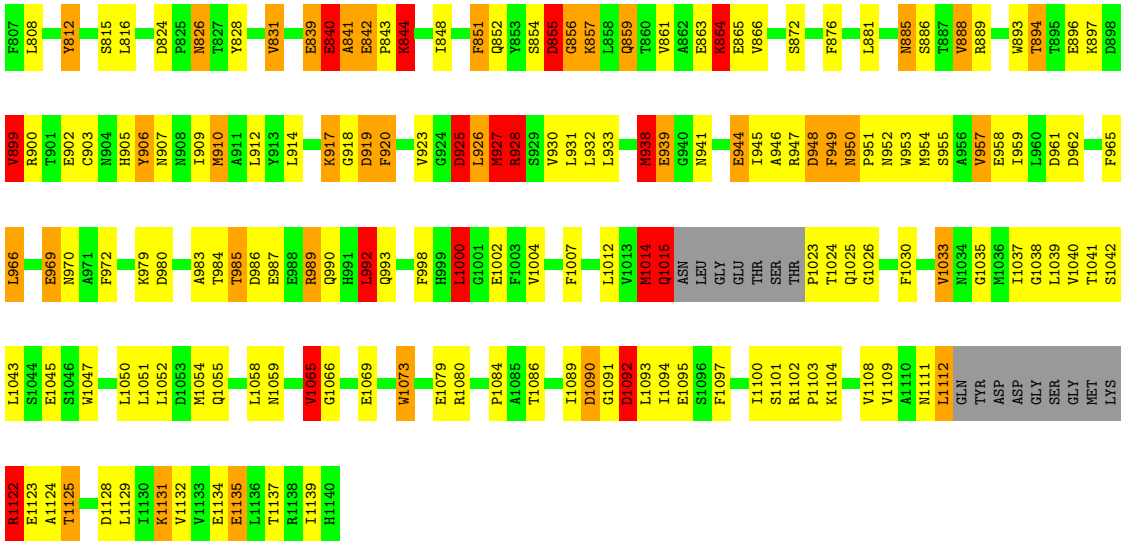
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: damage-specific DNA binding protein 1

Chain A: 42% 40% 14%




F807 L808 Y812 S815 L816 D824 P825 N826 T827 Y828 V831 E839 E840 A841 E842 P843 K844 I848 F851 Q852 Y853 S854 D855 G856 K857 L858 Q859 T860 V861 A862 E863 K864 E865 V866 S872 F876 L881 N885 S886 T887 V888 R889 W893 T894 T895 E896 K897 D898
V899 R900 T901 E902 C903 N904 H905 Y906 N907 N908 I909 M910 A911 L912 Y913 L914 K917 G918 D919 F920 V923 G924 D925 L926 M927 R928 S929 V930 L931 L932 L933 M938 E939 G940 N941 E944 I945 A946 R947 D948 F949 N950 P951 N952 W953 M954 S955 A956 V957 E958 I959 L960 D961 D962 F965
L966 E969 N970 A971 F972 K979 D980 A983 T984 T985 D986 E987 E988 R989 Q990 H991 L992 Q993 F998 H999 L1000 G1001 E1002 F1003 V1004 F1007 L1012 V1013 M1014 Q1015 ASN LEU GLY GLU THR SER THR P1023 T1024 Q1025 G1026 F1030 V1033 M1034 G1035 M1036 I1037 G1038 L1039 V1040 T1041 S1042
L1043 S1044 E1045 S1046 W1047 L1050 L1051 L1052 D1053 M1054 Q1055 L1058 N1059 V1065 G1066 E1069 W1073 E1079 R1080 P1084 A1085 T1086 I1089 D1090 G1091 D1092 L1093 I1094 E1095 S1096 F1097 I1100 S1101 R1102 P1103 K1104 V1108 V1109 A1110 N1111 L1112 GLN TYR ASP ASP GLY SER GLY MET LYS
R1122 E1123 A1124 T1125 D1128 L1129 I1130 K1131 V1132 V1133 E1134 E1135 L1136 T1137 R1138 I1139 H1140

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.38Å 133.83Å 184.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.92 48.68 – 2.92	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.70-2.92) 92.0 (48.68-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.277 0.293 , 0.309	Depositor DCC
R_{free} test set	1591 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	57.4	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 21.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	8768	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.62	110/8928 (1.2%)	1.41	85/12091 (0.7%)

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	1	2

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1033	VAL	CB-CG1	-10.01	1.31	1.52
1	A	277	GLU	CD-OE1	9.55	1.36	1.25
1	A	1135	GLU	CD-OE2	8.49	1.34	1.25
1	A	841	ALA	CA-CB	8.46	1.70	1.52
1	A	857	LYS	CD-CE	8.37	1.72	1.51
1	A	660	TYR	CD2-CE2	8.22	1.51	1.39
1	A	1079	GLU	CD-OE2	7.93	1.34	1.25
1	A	334	VAL	CB-CG1	-7.78	1.36	1.52
1	A	613	TYR	CE1-CZ	7.68	1.48	1.38
1	A	808	LEU	C-O	-7.65	1.08	1.23
1	A	759	GLN	CG-CD	7.57	1.68	1.51
1	A	47	GLU	CD-OE2	7.43	1.33	1.25
1	A	844	LYS	CB-CG	7.42	1.72	1.52
1	A	1004	VAL	CB-CG1	-7.16	1.37	1.52
1	A	1079	GLU	CD-OE1	7.15	1.33	1.25
1	A	840	GLU	CG-CD	7.13	1.62	1.51
1	A	958	GLU	CD-OE2	7.08	1.33	1.25
1	A	667	VAL	CA-CB	7.01	1.69	1.54
1	A	939	GLU	CD-OE1	6.97	1.33	1.25
1	A	111	ARG	CG-CD	6.96	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	VAL	CB-CG1	-6.91	1.38	1.52
1	A	614	PHE	CE1-CZ	6.90	1.50	1.37
1	A	370	GLN	C-O	6.85	1.36	1.23
1	A	561	TRP	CB-CG	-6.81	1.38	1.50
1	A	938	MET	CG-SD	6.80	1.98	1.81
1	A	920	PHE	CE1-CZ	6.79	1.50	1.37
1	A	357	GLY	CA-C	-6.72	1.41	1.51
1	A	719	GLU	CG-CD	6.69	1.61	1.51
1	A	675	GLU	CD-OE1	6.66	1.32	1.25
1	A	364	VAL	CB-CG2	-6.62	1.39	1.52
1	A	1035	GLY	C-O	-6.55	1.13	1.23
1	A	920	PHE	CG-CD1	6.51	1.48	1.38
1	A	910	MET	CG-SD	-6.42	1.64	1.81
1	A	857	LYS	CG-CD	6.42	1.74	1.52
1	A	348	VAL	CB-CG2	-6.37	1.39	1.52
1	A	38	ARG	NE-CZ	-6.36	1.24	1.33
1	A	50	ARG	CG-CD	6.36	1.67	1.51
1	A	927	MET	SD-CE	6.29	2.13	1.77
1	A	1015	GLN	CG-CD	6.23	1.65	1.51
1	A	944	GLU	CD-OE2	6.22	1.32	1.25
1	A	12	PRO	C-O	6.22	1.35	1.23
1	A	346	TYR	CE1-CZ	-6.20	1.30	1.38
1	A	660	TYR	CD1-CE1	6.07	1.48	1.39
1	A	63	VAL	CB-CG1	-6.06	1.40	1.52
1	A	859	GLN	CG-CD	6.00	1.64	1.51
1	A	747	GLY	C-O	5.95	1.33	1.23
1	A	281	PHE	CE2-CZ	5.92	1.48	1.37
1	A	147	ARG	CG-CD	5.90	1.66	1.51
1	A	16	ASN	CB-CG	5.88	1.64	1.51
1	A	920	PHE	CG-CD2	5.84	1.47	1.38
1	A	382	PHE	CE1-CZ	-5.80	1.26	1.37
1	A	70	LYS	CB-CG	5.80	1.68	1.52
1	A	812	TYR	CD1-CE1	5.79	1.48	1.39
1	A	1073	TRP	CZ3-CH2	-5.76	1.30	1.40
1	A	287	LYS	CD-CE	5.76	1.65	1.51
1	A	888	VAL	CB-CG1	-5.76	1.40	1.52
1	A	676	VAL	CB-CG2	-5.69	1.40	1.52
1	A	741	GLU	CD-OE1	5.65	1.31	1.25
1	A	842	GLU	CD-OE2	5.64	1.31	1.25
1	A	1135	GLU	CD-OE1	5.63	1.31	1.25
1	A	728	GLU	CD-OE2	5.63	1.31	1.25
1	A	756	ALA	CA-CB	-5.61	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	GLY	C-O	-5.58	1.14	1.23
1	A	885	ASN	C-O	5.58	1.33	1.23
1	A	162	LEU	CB-CG	5.57	1.68	1.52
1	A	47	GLU	CD-OE1	5.56	1.31	1.25
1	A	1122	ARG	CB-CG	5.50	1.67	1.52
1	A	235	GLU	CD-OE2	5.49	1.31	1.25
1	A	660	TYR	CG-CD2	5.49	1.46	1.39
1	A	360	VAL	C-O	-5.46	1.12	1.23
1	A	68	ARG	NE-CZ	5.46	1.40	1.33
1	A	371	GLY	C-O	-5.45	1.15	1.23
1	A	928	ARG	CG-CD	5.44	1.65	1.51
1	A	736	LEU	C-O	-5.43	1.13	1.23
1	A	1065	VAL	CA-CB	-5.42	1.43	1.54
1	A	1095	GLU	CD-OE1	-5.41	1.19	1.25
1	A	347	VAL	CB-CG1	-5.38	1.41	1.52
1	A	222	VAL	CA-CB	-5.38	1.43	1.54
1	A	1122	ARG	CG-CD	5.37	1.65	1.51
1	A	368	GLU	CD-OE2	5.37	1.31	1.25
1	A	955	SER	CB-OG	-5.36	1.35	1.42
1	A	459	PHE	CE1-CZ	5.35	1.47	1.37
1	A	1090	ASP	C-O	-5.34	1.13	1.23
1	A	316	TYR	CD1-CE1	-5.33	1.31	1.39
1	A	742	VAL	CB-CG1	-5.30	1.41	1.52
1	A	920	PHE	CE2-CZ	5.28	1.47	1.37
1	A	920	PHE	CD2-CE2	5.27	1.49	1.39
1	A	581	MET	SD-CE	5.24	2.07	1.77
1	A	831	VAL	CA-CB	-5.22	1.43	1.54
1	A	111	ARG	CZ-NH1	5.22	1.39	1.33
1	A	989	ARG	NE-CZ	5.21	1.39	1.33
1	A	96	GLU	CD-OE1	5.20	1.31	1.25
1	A	716	PRO	CB-CG	-5.19	1.24	1.50
1	A	117	GLU	CD-OE2	5.17	1.31	1.25
1	A	328	LEU	C-O	-5.17	1.13	1.23
1	A	215	GLU	CD-OE1	-5.16	1.20	1.25
1	A	1090	ASP	CB-CG	-5.15	1.41	1.51
1	A	93	GLN	CD-NE2	5.15	1.45	1.32
1	A	350	MET	CG-SD	5.14	1.94	1.81
1	A	111	ARG	NE-CZ	5.14	1.39	1.33
1	A	851	PHE	CG-CD1	-5.12	1.31	1.38
1	A	1080	ARG	NE-CZ	5.12	1.39	1.33
1	A	1090	ASP	CA-C	-5.12	1.39	1.52
1	A	798	THR	C-O	-5.11	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	920	PHE	CB-CG	5.09	1.59	1.51
1	A	35	LYS	C-O	5.08	1.33	1.23
1	A	235	GLU	CD-OE1	5.08	1.31	1.25
1	A	1014	MET	CG-SD	5.08	1.94	1.81
1	A	613	TYR	CG-CD1	5.05	1.45	1.39
1	A	39	LEU	C-O	-5.03	1.13	1.23

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	986	ASP	CB-CA-C	21.05	152.49	110.40
1	A	987	GLU	N-CA-CB	-18.34	77.60	110.60
1	A	842	GLU	N-CA-CB	-15.89	82.00	110.60
1	A	841	ALA	CB-CA-C	15.19	132.88	110.10
1	A	309	SER	N-CA-CB	-12.03	92.46	110.50
1	A	1015	GLN	N-CA-C	-11.06	81.14	111.00
1	A	542	ASP	CB-CG-OD2	10.47	127.72	118.30
1	A	147	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	986	ASP	N-CA-C	-9.62	85.03	111.00
1	A	137	ASP	CB-CG-OD2	9.51	126.86	118.30
1	A	961	ASP	CB-CG-OD2	9.04	126.44	118.30
1	A	38	ARG	NE-CZ-NH1	-8.66	115.97	120.30
1	A	925	ASP	CB-CG-OD2	8.57	126.02	118.30
1	A	948	ASP	CB-CG-OD2	8.51	125.95	118.30
1	A	1090	ASP	CB-CG-OD2	-8.38	110.76	118.30
1	A	688	PRO	N-CA-C	8.33	133.76	112.10
1	A	167	VAL	CB-CA-C	-7.84	96.51	111.40
1	A	309	SER	N-CA-C	-7.81	89.91	111.00
1	A	147	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	A	1014	MET	CA-C-N	-7.74	100.18	117.20
1	A	855	ASP	CB-CG-OD2	7.41	124.97	118.30
1	A	111	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	339	ASP	CB-CG-OD2	7.22	124.80	118.30
1	A	987	GLU	N-CA-C	7.20	130.44	111.00
1	A	162	LEU	CB-CG-CD2	7.14	123.14	111.00
1	A	243	ASP	CB-CG-OD2	6.98	124.58	118.30
1	A	542	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	A	184	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	308	THR	N-CA-C	-6.57	93.27	111.00
1	A	1015	GLN	N-CA-CB	6.53	122.35	110.60
1	A	275	ASP	CB-CA-C	-6.42	97.56	110.40
1	A	926	LEU	CA-CB-CG	6.39	130.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	962	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	68	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	64	MET	CG-SD-CE	6.30	110.28	100.20
1	A	453	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	28	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	1014	MET	C-N-CA	6.22	137.25	121.70
1	A	279	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	148	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	357	GLY	CA-C-O	-6.10	109.62	120.60
1	A	7	VAL	CB-CA-C	-6.09	99.83	111.40
1	A	666	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	563	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	899	VAL	CG1-CB-CG2	-5.93	101.41	110.90
1	A	146	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	548	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	691	LEU	CA-CB-CG	5.81	128.66	115.30
1	A	1014	MET	N-CA-C	5.80	126.67	111.00
1	A	391	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	925	ASP	OD1-CG-OD2	-5.78	112.33	123.30
1	A	552	LEU	CA-CB-CG	5.73	128.49	115.30
1	A	166	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	99	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	101	ILE	CG1-CB-CG2	-5.67	98.92	111.40
1	A	917	LYS	CD-CE-NZ	-5.67	98.66	111.70
1	A	927	MET	CG-SD-CE	-5.67	91.13	100.20
1	A	129	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	1080	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	361	ASP	CB-CG-OD1	5.62	123.35	118.30
1	A	992	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	293	GLY	N-CA-C	-5.55	99.22	113.10
1	A	534	MET	CG-SD-CE	5.51	109.02	100.20
1	A	925	ASP	CB-CA-C	-5.50	99.40	110.40
1	A	1084	PRO	N-CD-CG	-5.45	95.03	103.20
1	A	270	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	1000	LEU	CB-CG-CD1	-5.41	101.80	111.00
1	A	145	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	A	824	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	914	LEU	CA-CB-CG	5.32	127.55	115.30
1	A	375	LEU	CB-CG-CD1	-5.29	102.01	111.00
1	A	119	GLY	N-CA-C	5.26	126.26	113.10
1	A	111	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	384	GLU	N-CA-CB	-5.18	101.28	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118	THR	N-CA-CB	5.14	120.07	110.30
1	A	1090	ASP	N-CA-CB	5.12	119.83	110.60
1	A	213	GLU	OE1-CD-OE2	5.12	129.44	123.30
1	A	263	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	1092	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	541	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	A	589	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	251	PRO	N-CD-CG	-5.05	95.63	103.20
1	A	6	VAL	CB-CA-C	-5.03	101.84	111.40
1	A	313	CYS	CA-CB-SG	-5.01	104.98	114.00
1	A	795	ASP	CB-CG-OD2	5.00	122.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	841	ALA	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1023	PRO	Peptide
1	A	292	ASP	Peptide

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	8768	0	8744	542	0
All	All	8768	0	8744	542	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 31.

All (542) 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:1054:MET:SD	1:A:1054:MET:CE	2.05	1.45
1:A:581:MET:SD	1:A:581:MET:CE	2.07	1.43
1:A:927:MET:SD	1:A:927:MET:CE	2.13	1.37
1:A:781:SER:HB3	1:A:784:GLU:OE1	1.31	1.27
1:A:81:THR:HG21	1:A:85:ASN:HD22	1.07	1.09
1:A:781:SER:HB3	1:A:784:GLU:CD	1.75	1.04
1:A:910:MET:H	1:A:926:LEU:HD13	1.17	1.03
1:A:691:LEU:O	1:A:701:ILE:HA	1.61	1.00
1:A:707:ILE:O	1:A:708:GLN:O	1.81	0.97
1:A:24:THR:HG22	1:A:25:SER:OG	1.64	0.96
1:A:542:ASP:OD1	1:A:593:MET:HG2	1.66	0.95
1:A:413:LEU:HB3	1:A:424:THR:O	1.69	0.93
1:A:910:MET:N	1:A:926:LEU:HD13	1.82	0.92
1:A:389:ILE:HD12	1:A:389:ILE:N	1.88	0.89
1:A:81:THR:HG21	1:A:85:ASN:ND2	1.87	0.89
1:A:1051:LEU:HD22	1:A:1094:ILE:HD13	1.54	0.88
1:A:275:ASP:OD2	1:A:279:ARG:HD2	1.74	0.87
1:A:840:GLU:HB2	1:A:844:LYS:NZ	1.89	0.87
1:A:111:ARG:HA	1:A:111:ARG:HH11	1.38	0.87
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.09	0.87
1:A:664:HIS:ND1	1:A:664:HIS:O	2.09	0.86
1:A:781:SER:CB	1:A:784:GLU:OE1	2.23	0.85
1:A:1112:LEU:HB2	1:A:1122:ARG:HE	1.41	0.85
1:A:848:ILE:O	1:A:863:GLU:O	1.95	0.85
1:A:1101:SER:OG	1:A:1103:PRO:HD2	1.77	0.83
1:A:925:ASP:C	1:A:925:ASP:OD1	2.15	0.83
1:A:839:GLU:HG3	1:A:840:GLU:H	1.42	0.82
1:A:61:ILE:HD13	1:A:79:ILE:HD13	1.62	0.81
1:A:478:LEU:HD11	1:A:521:ILE:HG23	1.63	0.80
1:A:568:ILE:HD11	1:A:602:LEU:HD21	1.63	0.80
1:A:413:LEU:HD23	1:A:424:THR:CG2	2.12	0.79
1:A:1109:VAL:O	1:A:1109:VAL:HG12	1.83	0.79
1:A:919:ASP:CG	1:A:920:PHE:H	1.86	0.79
1:A:1112:LEU:HB2	1:A:1122:ARG:HB2	1.66	0.78
1:A:297:LEU:HD12	1:A:297:LEU:O	1.84	0.77
1:A:629:VAL:HG11	1:A:668:PHE:HE2	1.47	0.77
1:A:939:GLU:HB3	1:A:941:ASN:HD22	1.51	0.76
1:A:840:GLU:HB2	1:A:844:LYS:HZ1	1.51	0.76
1:A:568:ILE:O	1:A:577:LEU:HB2	1.87	0.74
1:A:1014:MET:SD	1:A:1015:GLN:N	2.60	0.74
1:A:372:GLN:OE1	1:A:372:GLN:C	2.25	0.74
1:A:110:ASP:OD2	1:A:141:LYS:NZ	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:HG22	1:A:477:ARG:NH2	2.03	0.74
1:A:928:ARG:HD2	1:A:953:TRP:CE3	2.23	0.74
1:A:131:ILE:HG13	1:A:145:LEU:HD11	1.68	0.74
1:A:629:VAL:HG11	1:A:668:PHE:CE2	2.23	0.73
1:A:602:LEU:HD23	1:A:616:LEU:HD22	1.69	0.73
1:A:396:ILE:HD11	1:A:673:LEU:HD11	1.71	0.72
1:A:23:PHE:H	1:A:30:ASN:HD22	1.36	0.72
1:A:24:THR:H	1:A:30:ASN:HD21	1.38	0.71
1:A:69:PRO:O	1:A:72:GLU:HB2	1.90	0.71
1:A:1131:LYS:O	1:A:1135:GLU:HG3	1.90	0.71
1:A:275:ASP:HB3	1:A:277:GLU:H	1.56	0.71
1:A:1039:LEU:HD21	1:A:1139:ILE:HG22	1.73	0.70
1:A:616:LEU:HD12	1:A:621:GLY:HA2	1.74	0.70
1:A:411:TRP:HB2	1:A:460:CYS:HB3	1.72	0.70
1:A:511:ALA:HB2	1:A:516:LEU:HD23	1.72	0.70
1:A:742:VAL:O	1:A:749:THR:HA	1.92	0.69
1:A:909:ILE:HG23	1:A:926:LEU:HB2	1.75	0.69
1:A:917:LYS:O	1:A:919:ASP:N	2.26	0.69
1:A:467:GLN:NE2	1:A:524:GLN:HA	2.09	0.68
1:A:503:CYS:HA	1:A:543:ILE:HD11	1.75	0.68
1:A:593:MET:HB3	1:A:602:LEU:HD22	1.74	0.68
1:A:725:CYS:SG	1:A:816:LEU:HD23	2.34	0.68
1:A:81:THR:HB	1:A:85:ASN:HB2	1.76	0.68
1:A:925:ASP:OD1	1:A:925:ASP:O	2.12	0.67
1:A:433:THR:OG1	1:A:455:GLN:O	2.12	0.67
1:A:639:ARG:HG2	1:A:679:MET:O	1.94	0.67
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.29	0.66
1:A:542:ASP:OD1	1:A:593:MET:CG	2.42	0.66
1:A:794:ILE:CD1	1:A:794:ILE:N	2.59	0.66
1:A:568:ILE:CD1	1:A:602:LEU:HD21	2.25	0.66
1:A:969:GLU:HG2	1:A:970:ASN:N	2.10	0.66
1:A:90:GLU:HB3	1:A:101:ILE:CG2	2.25	0.66
1:A:950:ASN:OD1	1:A:950:ASN:O	2.13	0.66
1:A:894:THR:HG22	1:A:896:GLU:H	1.61	0.65
1:A:234:GLN:O	1:A:236:SER:N	2.30	0.65
1:A:490:TRP:CD2	1:A:519:LEU:HD11	2.32	0.65
1:A:571:LEU:HD23	1:A:574:PHE:HE2	1.61	0.65
1:A:1014:MET:SD	1:A:1015:GLN:CA	2.85	0.65
1:A:979:LYS:NZ	1:A:989:ARG:NH2	2.46	0.64
1:A:504:ASN:HD21	1:A:507:GLN:HG2	1.63	0.64
1:A:569:LEU:HA	1:A:577:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLY:HA3	1:A:384:GLU:HG2	1.79	0.64
1:A:644:LEU:H	1:A:644:LEU:HD23	1.62	0.64
1:A:781:SER:CB	1:A:784:GLU:CD	2.61	0.64
1:A:854:SER:O	1:A:855:ASP:C	2.35	0.64
1:A:6:VAL:HG12	1:A:1040:VAL:HG22	1.79	0.63
1:A:23:PHE:H	1:A:30:ASN:ND2	1.96	0.63
1:A:642:ARG:HA	1:A:647:THR:HG22	1.80	0.63
1:A:654:ASP:HA	1:A:675:GLU:HG3	1.80	0.63
1:A:707:ILE:O	1:A:708:GLN:C	2.36	0.63
1:A:946:ALA:HA	1:A:990:GLN:OE1	1.98	0.63
1:A:25:SER:HB2	1:A:28:ASP:HB2	1.79	0.63
1:A:1097:PHE:CZ	1:A:1129:LEU:HD12	2.34	0.63
1:A:5:TYR:OH	1:A:1091:GLY:HA3	1.97	0.63
1:A:546:LEU:HD11	1:A:593:MET:HB2	1.81	0.63
1:A:396:ILE:CD1	1:A:673:LEU:HD11	2.29	0.63
1:A:332:GLN:HE21	1:A:352:THR:HG22	1.63	0.63
1:A:511:ALA:HB2	1:A:516:LEU:CD2	2.28	0.63
1:A:215:GLU:HG3	1:A:234:GLN:HE21	1.64	0.63
1:A:218:MET:HE3	1:A:261:HIS:HD2	1.64	0.63
1:A:292:ASP:C	1:A:293:GLY:O	2.35	0.62
1:A:482:GLU:HB3	1:A:483:PRO:HD3	1.79	0.62
1:A:679:MET:O	1:A:679:MET:SD	2.56	0.62
1:A:38:ARG:NH1	1:A:54:GLU:OE2	2.32	0.62
1:A:81:THR:CG2	1:A:85:ASN:HD22	1.99	0.62
1:A:494:GLN:O	1:A:495:ALA:HB3	1.99	0.62
1:A:519:LEU:HD23	1:A:528:GLN:N	2.14	0.62
1:A:558:ILE:CG2	1:A:567:ARG:HB2	2.29	0.62
1:A:660:TYR:CD1	1:A:707:ILE:HG23	2.33	0.62
1:A:938:MET:CE	1:A:939:GLU:OE2	2.47	0.62
1:A:601:TYR:CZ	1:A:666:LEU:HD21	2.33	0.62
1:A:191:LYS:HG2	1:A:192:THR:H	1.63	0.62
1:A:192:THR:HG21	1:A:206:PRO:HD2	1.81	0.62
1:A:1041:THR:HG22	1:A:1042:SER:N	2.14	0.62
1:A:569:LEU:HD22	1:A:576:LEU:HA	1.80	0.62
1:A:893:TRP:CE3	1:A:899:VAL:HG23	2.35	0.62
1:A:743:GLN:HG3	1:A:781:SER:O	2.00	0.62
1:A:131:ILE:HG22	1:A:133:LEU:HD13	1.82	0.61
1:A:568:ILE:HD11	1:A:602:LEU:CD2	2.29	0.61
1:A:130:MET:HA	1:A:145:LEU:HD13	1.83	0.61
1:A:577:LEU:O	1:A:578:HIS:HB2	2.01	0.60
1:A:660:TYR:CD2	1:A:707:ILE:HG12	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HD12	1:A:297:LEU:C	2.21	0.60
1:A:894:THR:HG22	1:A:896:GLU:N	2.15	0.60
1:A:341:ASN:OD1	1:A:342:GLU:O	2.20	0.60
1:A:407:ILE:HD12	1:A:694:ALA:HB1	1.83	0.60
1:A:692:ALA:HA	1:A:700:THR:O	2.01	0.60
1:A:747:GLY:O	1:A:748:GLY:O	2.20	0.60
1:A:16:ASN:HD22	1:A:35:LYS:C	2.05	0.60
1:A:464:ALA:O	1:A:467:GLN:OE1	2.20	0.60
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.84	0.60
1:A:478:LEU:HB3	1:A:487:VAL:CG2	2.31	0.59
1:A:478:LEU:HB3	1:A:487:VAL:HG22	1.83	0.59
1:A:501:ALA:O	1:A:502:SER:HB2	2.01	0.59
1:A:648:ASN:ND2	1:A:660:TYR:HA	2.17	0.59
1:A:839:GLU:HG3	1:A:840:GLU:N	2.16	0.59
1:A:366:ASP:N	1:A:366:ASP:OD1	2.34	0.59
1:A:394:ILE:HD11	1:A:707:ILE:O	2.03	0.59
1:A:585:GLU:CD	1:A:585:GLU:N	2.55	0.59
1:A:643:SER:HB2	1:A:644:LEU:HD23	1.85	0.59
1:A:783:GLY:O	1:A:784:GLU:HG3	2.02	0.59
1:A:928:ARG:HD2	1:A:953:TRP:CD2	2.38	0.59
1:A:939:GLU:O	1:A:941:ASN:ND2	2.36	0.59
1:A:660:TYR:CZ	1:A:707:ILE:HG13	2.38	0.59
1:A:692:ALA:C	1:A:693:LEU:HD12	2.23	0.59
1:A:1047:TRP:CZ3	1:A:1132:VAL:HG13	2.38	0.59
1:A:1123:GLU:OE2	1:A:1128:ASP:OD1	2.20	0.58
1:A:130:MET:SD	1:A:195:VAL:HG11	2.44	0.58
1:A:1051:LEU:HD22	1:A:1094:ILE:CD1	2.31	0.58
1:A:492:GLU:HG3	1:A:512:VAL:HG11	1.84	0.58
1:A:570:LYS:HG3	1:A:577:LEU:HD11	1.84	0.58
1:A:747:GLY:O	1:A:748:GLY:C	2.42	0.58
1:A:794:ILE:N	1:A:794:ILE:HD12	2.17	0.58
1:A:392:ASN:HD22	1:A:1012:LEU:HB3	1.68	0.58
1:A:852:GLN:NE2	1:A:859:GLN:OE1	2.37	0.58
1:A:342:GLU:N	1:A:342:GLU:OE1	2.37	0.58
1:A:131:ILE:HB	1:A:143:ILE:HB	1.84	0.58
1:A:329:GLY:HA3	1:A:384:GLU:CG	2.34	0.57
1:A:457:THR:HG1	1:A:470:GLN:HE21	1.51	0.57
1:A:516:LEU:O	1:A:531:HIS:HA	2.05	0.57
1:A:612:PHE:HE2	1:A:628:LYS:HG3	1.69	0.57
1:A:1015:GLN:CA	1:A:1015:GLN:OE1	2.52	0.57
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:HG2	1:A:192:THR:N	2.19	0.57
1:A:839:GLU:HG3	1:A:840:GLU:HG3	1.87	0.57
1:A:1014:MET:SD	1:A:1015:GLN:HA	2.45	0.57
1:A:250:PRO:HG2	1:A:253:ILE:HD12	1.85	0.57
1:A:188:ARG:NH1	1:A:216:ALA:O	2.38	0.56
1:A:753:ARG:HG2	1:A:753:ARG:HH11	1.69	0.56
1:A:5:TYR:CZ	1:A:1091:GLY:HA3	2.40	0.56
1:A:218:MET:CE	1:A:261:HIS:HD2	2.19	0.56
1:A:502:SER:OG	1:A:543:ILE:HG12	2.04	0.56
1:A:296:THR:OG1	1:A:297:LEU:N	2.39	0.56
1:A:840:GLU:HB2	1:A:844:LYS:HZ3	1.69	0.56
1:A:493:PRO:O	1:A:494:GLN:HG2	2.04	0.56
1:A:494:GLN:O	1:A:495:ALA:CB	2.53	0.56
1:A:1125:THR:HB	1:A:1128:ASP:CB	2.36	0.56
1:A:111:ARG:HA	1:A:111:ARG:NH1	2.14	0.56
1:A:509:VAL:HG12	1:A:541:LEU:HD13	1.87	0.56
1:A:522:HIS:HB2	1:A:527:ARG:NH1	2.20	0.56
1:A:1122:ARG:O	1:A:1122:ARG:HG3	2.05	0.56
1:A:1129:LEU:HD13	1:A:1129:LEU:O	2.06	0.56
1:A:16:ASN:ND2	1:A:35:LYS:O	2.33	0.55
1:A:116:SER:HB3	1:A:137:ASP:OD1	2.06	0.55
1:A:570:LYS:NZ	1:A:570:LYS:HB3	2.21	0.55
1:A:35:LYS:HB2	1:A:38:ARG:HB2	1.87	0.55
1:A:1026:GLY:O	1:A:1041:THR:HG23	2.06	0.55
1:A:125:ASP:OD1	1:A:126:PRO:HD2	2.06	0.55
1:A:567:ARG:HG2	1:A:579:LYS:HB2	1.88	0.55
1:A:458:PHE:HB3	1:A:501:ALA:CB	2.37	0.55
1:A:24:THR:H	1:A:30:ASN:ND2	2.05	0.55
1:A:615:GLY:HA3	1:A:624:SER:HB2	1.89	0.55
1:A:518:TYR:CD1	1:A:571:LEU:HD22	2.42	0.55
1:A:546:LEU:HD11	1:A:593:MET:SD	2.47	0.55
1:A:907:ASN:OD1	1:A:909:ILE:HD12	2.06	0.55
1:A:695:ASN:ND2	1:A:697:SER:H	2.04	0.55
1:A:649:VAL:HG23	1:A:659:ILE:HB	1.88	0.54
1:A:930:VAL:HG12	1:A:931:LEU:N	2.22	0.54
1:A:262:ASN:ND2	1:A:316:TYR:H	2.06	0.54
1:A:372:GLN:OE1	1:A:373:GLY:N	2.40	0.54
1:A:389:ILE:HD12	1:A:389:ILE:H	1.66	0.54
1:A:452:VAL:HG22	1:A:477:ARG:CZ	2.36	0.54
1:A:979:LYS:HZ2	1:A:989:ARG:NH2	2.05	0.54
1:A:509:VAL:CG2	1:A:571:LEU:HD11	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:O	1:A:405:PRO:O	2.26	0.54
1:A:455:GLN:HB3	1:A:472:THR:OG1	2.06	0.54
1:A:264:VAL:HG12	1:A:265:ASP:N	2.22	0.54
1:A:503:CYS:CA	1:A:543:ILE:HD11	2.37	0.54
1:A:467:GLN:HE22	1:A:524:GLN:HA	1.73	0.54
1:A:509:VAL:HG22	1:A:571:LEU:HD21	1.89	0.54
1:A:546:LEU:CD1	1:A:593:MET:HB2	2.38	0.54
1:A:907:ASN:OD1	1:A:909:ILE:CD1	2.56	0.54
1:A:659:ILE:HD13	1:A:668:PHE:HE1	1.73	0.54
1:A:223:PRO:C	1:A:225:PRO:HD2	2.29	0.53
1:A:429:PHE:O	1:A:456:GLN:HG3	2.08	0.53
1:A:687:TYR:CD1	1:A:701:ILE:HG13	2.43	0.53
1:A:984:THR:O	1:A:984:THR:OG1	2.18	0.53
1:A:667:VAL:HG21	1:A:707:ILE:CG2	2.39	0.53
1:A:1134:GLU:O	1:A:1137:THR:OG1	2.26	0.53
1:A:634:GLN:HB3	1:A:635:PRO:HD2	1.89	0.53
1:A:1102:ARG:N	1:A:1103:PRO:CD	2.71	0.53
1:A:268:GLY:O	1:A:285:LEU:HD22	2.08	0.53
1:A:912:LEU:HD12	1:A:928:ARG:HH22	1.72	0.53
1:A:919:ASP:CG	1:A:920:PHE:N	2.61	0.53
1:A:546:LEU:HD21	1:A:593:MET:HG3	1.90	0.53
1:A:770:LEU:HD13	1:A:865:GLU:HB2	1.91	0.53
1:A:596:PHE:CE2	1:A:648:ASN:HA	2.44	0.53
1:A:690:SER:O	1:A:691:LEU:HD23	2.09	0.53
1:A:507:GLN:CD	1:A:553:SER:H	2.12	0.53
1:A:585:GLU:N	1:A:585:GLU:OE2	2.41	0.53
1:A:614:PHE:CE1	1:A:626:ARG:HG3	2.44	0.53
1:A:413:LEU:HD23	1:A:424:THR:HG22	1.89	0.52
1:A:559:GLY:HA2	1:A:565:SER:O	2.10	0.52
1:A:615:GLY:CA	1:A:624:SER:HB2	2.38	0.52
1:A:643:SER:CB	1:A:644:LEU:HD23	2.39	0.52
1:A:1090:ASP:OD2	1:A:1090:ASP:N	2.41	0.52
1:A:24:THR:HG22	1:A:25:SER:HG	1.72	0.52
1:A:602:LEU:O	1:A:614:PHE:HB2	2.09	0.52
1:A:1094:ILE:CG2	1:A:1094:ILE:O	2.57	0.52
1:A:1014:MET:HA	1:A:1015:GLN:O	2.10	0.52
1:A:184:ASP:C	1:A:185:PRO:O	2.46	0.52
1:A:555:LEU:HD13	1:A:568:ILE:HG21	1.92	0.52
1:A:600:HIS:CD2	1:A:618:ILE:HG12	2.45	0.52
1:A:945:ILE:O	1:A:946:ALA:HB2	2.10	0.52
1:A:110:ASP:HB2	1:A:136:TYR:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:HG12	1:A:265:ASP:OD1	2.11	0.51
1:A:730:SER:HB2	1:A:732:CYS:SG	2.50	0.51
1:A:555:LEU:HD13	1:A:568:ILE:CG2	2.41	0.51
1:A:1055:GLN:HE22	1:A:1089:ILE:HA	1.75	0.51
1:A:206:PRO:O	1:A:207:TRP:HB3	2.10	0.51
1:A:463:VAL:HA	1:A:505:SER:O	2.10	0.51
1:A:564:ILE:N	1:A:564:ILE:HD12	2.25	0.51
1:A:1014:MET:SD	1:A:1014:MET:C	2.89	0.51
1:A:1108:VAL:O	1:A:1109:VAL:HB	2.09	0.51
1:A:1123:GLU:O	1:A:1124:ALA:HB3	2.09	0.51
1:A:413:LEU:HD23	1:A:424:THR:CB	2.40	0.51
1:A:1015:GLN:OE1	1:A:1015:GLN:C	2.49	0.51
1:A:5:TYR:HB2	1:A:1043:LEU:HD11	1.92	0.51
1:A:881:LEU:HD12	1:A:889:ARG:O	2.11	0.51
1:A:102:THR:O	1:A:102:THR:HG22	2.09	0.51
1:A:910:MET:O	1:A:910:MET:HG2	2.10	0.51
1:A:90:GLU:O	1:A:101:ILE:HG22	2.11	0.50
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.93	0.50
1:A:441:GLU:HA	1:A:687:TYR:CE2	2.47	0.50
1:A:1091:GLY:HA2	1:A:1094:ILE:HB	1.93	0.50
1:A:1125:THR:HB	1:A:1128:ASP:HB2	1.93	0.50
1:A:36:ASN:OD1	1:A:60:LYS:HG2	2.12	0.50
1:A:342:GLU:C	1:A:344:GLY:H	2.15	0.50
1:A:909:ILE:HA	1:A:926:LEU:HD22	1.94	0.50
1:A:1055:GLN:O	1:A:1059:ASN:ND2	2.44	0.50
1:A:576:LEU:HD13	1:A:577:LEU:N	2.26	0.50
1:A:275:ASP:HB2	1:A:279:ARG:H	1.76	0.50
1:A:317:LEU:O	1:A:318:ASP:HB2	2.10	0.50
1:A:358:PRO:HA	1:A:1033:VAL:O	2.12	0.50
1:A:558:ILE:HG22	1:A:567:ARG:HB2	1.92	0.50
1:A:347:VAL:HG12	1:A:348:VAL:N	2.27	0.50
1:A:351:GLU:OE2	1:A:353:PHE:HE2	1.95	0.50
1:A:480:SER:O	1:A:484:LYS:HA	2.12	0.49
1:A:589:ARG:HG3	1:A:635:PRO:HB2	1.93	0.49
1:A:928:ARG:HD3	1:A:953:TRP:HA	1.93	0.49
1:A:1041:THR:HG22	1:A:1042:SER:H	1.77	0.49
1:A:909:ILE:HA	1:A:926:LEU:CD2	2.42	0.49
1:A:81:THR:CG2	1:A:83:LYS:H	2.26	0.49
1:A:59:GLY:HA2	1:A:1073:TRP:CE3	2.46	0.49
1:A:110:ASP:HB2	1:A:136:TYR:CE1	2.48	0.49
1:A:261:HIS:HA	1:A:272:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:VAL:HG21	1:A:959:ILE:HG13	1.93	0.49
1:A:1125:THR:HB	1:A:1128:ASP:H	1.78	0.49
1:A:234:GLN:O	1:A:235:GLU:C	2.51	0.49
1:A:459:PHE:CD2	1:A:460:CYS:N	2.80	0.49
1:A:864:LYS:HD2	1:A:899:VAL:O	2.13	0.49
1:A:90:GLU:HB3	1:A:101:ILE:HG23	1.93	0.49
1:A:564:ILE:HD11	1:A:585:GLU:HA	1.95	0.49
1:A:660:TYR:CE1	1:A:707:ILE:HG13	2.47	0.49
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.95	0.49
1:A:614:PHE:HE1	1:A:626:ARG:HG3	1.77	0.49
1:A:641:PHE:HA	1:A:681:PRO:CG	2.43	0.49
1:A:1051:LEU:O	1:A:1054:MET:HB2	2.13	0.49
1:A:467:GLN:HE22	1:A:524:GLN:H	1.60	0.49
1:A:954:MET:HE3	1:A:957:VAL:HG23	1.94	0.49
1:A:927:MET:CE	1:A:927:MET:CG	2.90	0.49
1:A:1051:LEU:CD2	1:A:1094:ILE:HD13	2.35	0.49
1:A:182:TYR:HE2	1:A:191:LYS:HB2	1.78	0.48
1:A:617:ASN:ND2	1:A:622:LEU:HD13	2.28	0.48
1:A:667:VAL:HG21	1:A:707:ILE:HG21	1.96	0.48
1:A:392:ASN:HD22	1:A:1012:LEU:CB	2.26	0.48
1:A:185:PRO:O	1:A:186:GLN:HB2	2.12	0.48
1:A:656:PRO:HB2	1:A:671:VAL:HB	1.95	0.48
1:A:165:ILE:HG21	1:A:217:SER:HA	1.95	0.48
1:A:355:ASN:ND2	1:A:357:GLY:HA2	2.28	0.48
1:A:458:PHE:HB3	1:A:501:ALA:HB3	1.95	0.48
1:A:923:VAL:HG21	1:A:959:ILE:CG1	2.43	0.48
1:A:979:LYS:HZ3	1:A:989:ARG:NH2	2.10	0.48
1:A:637:VAL:HB	1:A:652:CYS:HB2	1.96	0.48
1:A:854:SER:O	1:A:856:GLY:N	2.47	0.48
1:A:864:LYS:HD2	1:A:899:VAL:HG12	1.94	0.48
1:A:933:LEU:HG	1:A:944:GLU:HA	1.96	0.48
1:A:576:LEU:HD13	1:A:577:LEU:C	2.35	0.48
1:A:507:GLN:NE2	1:A:553:SER:HB3	2.29	0.48
1:A:294:THR:CG2	1:A:295:VAL:H	2.27	0.48
1:A:743:GLN:HA	1:A:747:GLY:O	2.13	0.47
1:A:70:LYS:H	1:A:70:LYS:CD	2.27	0.47
1:A:38:ARG:HD2	1:A:54:GLU:OE1	2.14	0.47
1:A:413:LEU:HD23	1:A:424:THR:HB	1.95	0.47
1:A:659:ILE:HG22	1:A:666:LEU:HB3	1.96	0.47
1:A:789:HIS:ND1	1:A:812:TYR:HA	2.29	0.47
1:A:948:ASP:HB2	1:A:992:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:THR:C	1:A:422:TYR:CD1	2.88	0.47
1:A:826:ASN:ND2	1:A:852:GLN:OE1	2.48	0.47
1:A:222:VAL:HA	1:A:223:PRO:HD3	1.73	0.47
1:A:543:ILE:O	1:A:543:ILE:HG13	2.15	0.47
1:A:652:CYS:HB3	1:A:676:VAL:O	2.15	0.47
1:A:661:SER:HA	1:A:665:LYS:O	2.15	0.47
1:A:607:GLY:HA2	1:A:635:PRO:HB3	1.96	0.47
1:A:400:ALA:HB3	1:A:701:ILE:HD11	1.97	0.47
1:A:396:ILE:HD11	1:A:673:LEU:HD21	1.96	0.46
1:A:665:LYS:HB2	1:A:665:LYS:NZ	2.30	0.46
1:A:394:ILE:HD11	1:A:707:ILE:HA	1.97	0.46
1:A:765:VAL:HG12	1:A:806:GLN:HB3	1.98	0.46
1:A:174:GLN:O	1:A:175:ALA:HB2	2.15	0.46
1:A:290:GLN:O	1:A:291:MET:C	2.53	0.46
1:A:168:LYS:HE2	1:A:219:VAL:O	2.15	0.46
1:A:478:LEU:HD21	1:A:521:ILE:CG2	2.46	0.46
1:A:558:ILE:O	1:A:566:ALA:HA	2.15	0.46
1:A:184:ASP:O	1:A:185:PRO:O	2.33	0.46
1:A:459:PHE:HE2	1:A:461:GLY:HA3	1.80	0.46
1:A:509:VAL:HG21	1:A:571:LEU:HD11	1.98	0.46
1:A:107:ASN:OD1	1:A:109:GLN:HB2	2.16	0.46
1:A:367:LEU:HB2	1:A:374:GLN:OE1	2.15	0.46
1:A:377:THR:O	1:A:387:LEU:HA	2.16	0.46
1:A:1051:LEU:HA	1:A:1054:MET:HB2	1.98	0.46
1:A:182:TYR:OH	1:A:209:GLN:NE2	2.49	0.46
1:A:343:GLN:HE21	1:A:343:GLN:HA	1.81	0.46
1:A:706:GLU:HA	1:A:707:ILE:HD12	1.98	0.46
1:A:979:LYS:HZ3	1:A:989:ARG:HH21	1.62	0.46
1:A:1047:TRP:HZ3	1:A:1132:VAL:HG13	1.79	0.46
1:A:881:LEU:HD11	1:A:888:VAL:CG1	2.45	0.45
1:A:917:LYS:C	1:A:919:ASP:N	2.70	0.45
1:A:690:SER:HB3	1:A:701:ILE:HB	1.98	0.45
1:A:909:ILE:HG12	1:A:926:LEU:HD22	1.98	0.45
1:A:148:ASP:O	1:A:149:ASN:HB3	2.16	0.45
1:A:367:LEU:HA	1:A:367:LEU:HD23	1.76	0.45
1:A:706:GLU:O	1:A:707:ILE:HG13	2.16	0.45
1:A:63:VAL:O	1:A:79:ILE:HA	2.16	0.45
1:A:294:THR:HG22	1:A:295:VAL:N	2.32	0.45
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.73	0.45
1:A:534:MET:HE2	1:A:560:LEU:HD11	1.98	0.45
1:A:687:TYR:N	1:A:688:PRO:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:THR:CG2	1:A:295:VAL:N	2.80	0.45
1:A:695:ASN:OD1	1:A:698:THR:HB	2.16	0.45
1:A:184:ASP:O	1:A:185:PRO:C	2.55	0.45
1:A:536:HIS:ND1	1:A:562:THR:HB	2.33	0.45
1:A:926:LEU:HD12	1:A:927:MET:SD	2.57	0.45
1:A:1058:LEU:HD11	1:A:1097:PHE:HB2	1.99	0.45
1:A:254:LYS:O	1:A:254:LYS:HD3	2.18	0.44
1:A:378:CYS:HB3	1:A:721:PRO:HB2	1.98	0.44
1:A:828:TYR:CE2	1:A:861:VAL:HG21	2.52	0.44
1:A:966:LEU:HD13	1:A:1007:PHE:CE2	2.53	0.44
1:A:60:LYS:HE2	1:A:972:PHE:CE1	2.52	0.44
1:A:396:ILE:CG1	1:A:396:ILE:O	2.65	0.44
1:A:409:GLY:HA3	1:A:428:SER:OG	2.17	0.44
1:A:134:ARG:C	1:A:135:LEU:HD23	2.38	0.44
1:A:679:MET:SD	1:A:679:MET:C	2.95	0.44
1:A:175:ALA:O	1:A:176:PRO:C	2.56	0.44
1:A:468:LEU:HD11	1:A:481:GLN:OE1	2.17	0.44
1:A:518:TYR:CD1	1:A:571:LEU:CD2	3.00	0.44
1:A:1051:LEU:HB3	1:A:1094:ILE:CD1	2.48	0.44
1:A:133:LEU:HB3	1:A:135:LEU:HD21	2.00	0.44
1:A:452:VAL:HG11	1:A:455:GLN:HG3	2.00	0.44
1:A:504:ASN:ND2	1:A:507:GLN:HG2	2.31	0.44
1:A:529:ILE:HG22	1:A:529:ILE:O	2.17	0.44
1:A:433:THR:HB	1:A:452:VAL:O	2.18	0.44
1:A:511:ALA:CB	1:A:516:LEU:HD23	2.43	0.44
1:A:578:HIS:CD2	1:A:623:LEU:HG	2.52	0.44
1:A:612:PHE:HE2	1:A:628:LYS:CG	2.29	0.44
1:A:928:ARG:NE	1:A:928:ARG:H	2.16	0.44
1:A:263:ARG:HA	1:A:271:TYR:CD2	2.52	0.44
1:A:451:PHE:CE1	1:A:479:VAL:HG21	2.52	0.44
1:A:472:THR:HG22	1:A:475:SER:O	2.18	0.44
1:A:507:GLN:HE21	1:A:571:LEU:HD13	1.83	0.44
1:A:667:VAL:O	1:A:668:PHE:HD1	2.01	0.44
1:A:753:ARG:HG2	1:A:753:ARG:NH1	2.31	0.44
1:A:1065:VAL:HG12	1:A:1066:GLY:N	2.32	0.44
1:A:25:SER:O	1:A:26:ALA:C	2.56	0.43
1:A:665:LYS:HB2	1:A:665:LYS:HZ3	1.83	0.43
1:A:932:LEU:HD13	1:A:965:PHE:CZ	2.53	0.43
1:A:220:ILE:HB	1:A:230:ILE:HB	1.99	0.43
1:A:223:PRO:O	1:A:225:PRO:HD2	2.19	0.43
1:A:356:LEU:HD21	1:A:712:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:CYS:C	1:A:905:HIS:H	2.22	0.43
1:A:695:ASN:O	1:A:696:ASN:C	2.56	0.43
1:A:185:PRO:O	1:A:186:GLN:CB	2.64	0.43
1:A:414:ARG:HA	1:A:422:TYR:HA	1.99	0.43
1:A:433:THR:O	1:A:453:ASP:HA	2.19	0.43
1:A:458:PHE:CB	1:A:501:ALA:HB2	2.49	0.43
1:A:508:VAL:HG12	1:A:509:VAL:N	2.33	0.43
1:A:93:GLN:HB2	1:A:98:ILE:HG23	1.99	0.43
1:A:658:VAL:CG1	1:A:659:ILE:N	2.82	0.43
1:A:894:THR:CG2	1:A:896:GLU:HB2	2.48	0.43
1:A:542:ASP:O	1:A:593:MET:HE3	2.18	0.43
1:A:840:GLU:OE1	1:A:844:LYS:HE3	2.19	0.43
1:A:25:SER:O	1:A:27:GLU:N	2.52	0.43
1:A:255:GLN:OE1	1:A:279:ARG:NH2	2.52	0.43
1:A:297:LEU:C	1:A:297:LEU:CD1	2.88	0.43
1:A:639:ARG:HG3	1:A:640:THR:N	2.34	0.43
1:A:660:TYR:OH	1:A:704:ILE:CG2	2.67	0.43
1:A:905:HIS:O	1:A:906:TYR:HB3	2.19	0.43
1:A:253:ILE:O	1:A:255:GLN:N	2.51	0.43
1:A:600:HIS:NE2	1:A:618:ILE:HD13	2.33	0.43
1:A:196:SER:OG	1:A:199:GLU:HG2	2.19	0.42
1:A:839:GLU:CG	1:A:840:GLU:OE2	2.67	0.42
1:A:893:TRP:CZ3	1:A:899:VAL:HG23	2.54	0.42
1:A:949:PHE:HD1	1:A:949:PHE:H	1.65	0.42
1:A:520:GLN:HB2	1:A:527:ARG:HB3	2.01	0.42
1:A:534:MET:CE	1:A:560:LEU:HD11	2.49	0.42
1:A:592:LEU:O	1:A:603:LEU:N	2.38	0.42
1:A:706:GLU:CA	1:A:707:ILE:HD12	2.49	0.42
1:A:1041:THR:CG2	1:A:1042:SER:N	2.82	0.42
1:A:55:VAL:HG11	1:A:100:ILE:HG13	2.01	0.42
1:A:275:ASP:OD2	1:A:279:ARG:HB2	2.19	0.42
1:A:478:LEU:HD21	1:A:521:ILE:HG23	2.01	0.42
1:A:517:TYR:N	1:A:517:TYR:CD1	2.87	0.42
1:A:643:SER:OG	1:A:644:LEU:HD23	2.19	0.42
1:A:931:LEU:HB2	1:A:933:LEU:HD11	2.01	0.42
1:A:8:THR:HG1	1:A:1092:ASP:CG	2.23	0.42
1:A:507:GLN:NE2	1:A:553:SER:H	2.18	0.42
1:A:608:ASP:O	1:A:633:THR:O	2.37	0.42
1:A:886:SER:C	1:A:909:ILE:O	2.58	0.42
1:A:949:PHE:CD1	1:A:949:PHE:N	2.87	0.42
1:A:159:LEU:CD2	1:A:161:GLU:HB2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:PRO:HD2	1:A:380:GLY:HA2	2.02	0.42
1:A:371:GLY:HA3	1:A:1014:MET:HE1	2.00	0.42
1:A:492:GLU:O	1:A:494:GLN:N	2.51	0.42
1:A:816:LEU:HD12	1:A:831:VAL:HG22	2.01	0.42
1:A:909:ILE:HA	1:A:926:LEU:HD13	2.01	0.42
1:A:1097:PHE:HA	1:A:1100:ILE:HD12	2.02	0.42
1:A:1139:ILE:HD13	1:A:1139:ILE:HG21	1.60	0.42
1:A:312:GLU:HG3	1:A:327:ARG:HE	1.84	0.42
1:A:413:LEU:HD23	1:A:424:THR:HG21	1.98	0.42
1:A:938:MET:HE3	1:A:939:GLU:OE2	2.19	0.42
1:A:135:LEU:HD23	1:A:135:LEU:N	2.35	0.42
1:A:156:ASN:HD22	1:A:156:ASN:HA	1.51	0.42
1:A:381:ALA:O	1:A:382:PHE:C	2.57	0.42
1:A:537:GLU:HB3	1:A:561:TRP:CG	2.55	0.42
1:A:1102:ARG:HB2	1:A:1103:PRO:HD3	2.01	0.42
1:A:1108:VAL:H	1:A:1108:VAL:HG23	1.64	0.42
1:A:490:TRP:HB2	1:A:526:LEU:HD13	2.02	0.42
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.85	0.42
1:A:763:SER:O	1:A:803:HIS:HE1	2.03	0.42
1:A:23:PHE:N	1:A:30:ASN:ND2	2.66	0.42
1:A:301:ARG:NH1	1:A:303:GLU:OE2	2.53	0.42
1:A:642:ARG:HH22	1:A:683:ASN:CB	2.32	0.42
1:A:706:GLU:OE2	1:A:707:ILE:HD12	2.20	0.42
1:A:798:THR:HB	1:A:800:GLU:HG3	2.02	0.42
1:A:1125:THR:O	1:A:1129:LEU:HB2	2.20	0.42
1:A:275:ASP:HB3	1:A:277:GLU:N	2.31	0.41
1:A:522:HIS:CB	1:A:527:ARG:NH1	2.83	0.41
1:A:909:ILE:HA	1:A:926:LEU:CD1	2.49	0.41
1:A:194:GLU:HB2	1:A:203:ASN:HB2	2.01	0.41
1:A:815:SER:HB3	1:A:872:SER:HA	2.01	0.41
1:A:192:THR:HB	1:A:205:GLY:HA3	2.03	0.41
1:A:643:SER:H	1:A:647:THR:HG22	1.85	0.41
1:A:939:GLU:HB3	1:A:941:ASN:ND2	2.28	0.41
1:A:413:LEU:CB	1:A:424:THR:O	2.55	0.41
1:A:629:VAL:CG1	1:A:668:PHE:HE2	2.25	0.41
1:A:165:ILE:HB	1:A:181:VAL:O	2.20	0.41
1:A:410:LEU:HB3	1:A:680:CYS:SG	2.61	0.41
1:A:459:PHE:CZ	1:A:503:CYS:O	2.73	0.41
1:A:642:ARG:HH22	1:A:683:ASN:CG	2.24	0.41
1:A:932:LEU:C	1:A:933:LEU:HD12	2.40	0.41
1:A:347:VAL:CG1	1:A:348:VAL:N	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LEU:HD12	1:A:1037:ILE:HD13	2.03	0.41
1:A:415:SER:HB2	1:A:423:ASP:OD2	2.21	0.41
1:A:507:GLN:OE1	1:A:552:LEU:HA	2.20	0.41
1:A:920:PHE:N	1:A:920:PHE:CD2	2.85	0.41
1:A:1104:LYS:O	1:A:1108:VAL:HG23	2.19	0.41
1:A:110:ASP:O	1:A:111:ARG:C	2.59	0.41
1:A:222:VAL:O	1:A:227:GLY:HA2	2.21	0.41
1:A:938:MET:HE2	1:A:939:GLU:OE2	2.20	0.41
1:A:145:LEU:N	1:A:145:LEU:CD1	2.84	0.41
1:A:467:GLN:HE22	1:A:524:GLN:CA	2.34	0.41
1:A:706:GLU:OE2	1:A:707:ILE:CD1	2.69	0.41
1:A:169:PHE:CE2	1:A:178:ILE:HD12	2.55	0.41
1:A:190:VAL:HG13	1:A:190:VAL:O	2.21	0.41
1:A:215:GLU:CB	1:A:234:GLN:HG3	2.50	0.41
1:A:347:VAL:C	1:A:348:VAL:HG23	2.41	0.41
1:A:458:PHE:HB3	1:A:501:ALA:HB2	2.01	0.41
1:A:464:ALA:O	1:A:465:HIS:HB2	2.20	0.41
1:A:569:LEU:HA	1:A:577:LEU:HD22	2.02	0.41
1:A:768:SER:C	1:A:769:LYS:HD3	2.41	0.41
1:A:805:HIS:CD2	1:A:851:PHE:CZ	3.09	0.41
1:A:1030:PHE:CE1	1:A:1038:GLY:HA3	2.52	0.41
1:A:207:TRP:CZ3	1:A:241:ASN:ND2	2.88	0.41
1:A:375:LEU:O	1:A:389:ILE:HA	2.21	0.41
1:A:421:THR:C	1:A:422:TYR:CG	2.94	0.41
1:A:471:ILE:HD11	1:A:503:CYS:HB2	2.03	0.41
1:A:280:LEU:CD1	1:A:314:LEU:HD21	2.51	0.40
1:A:383:LYS:HE2	1:A:384:GLU:OE2	2.21	0.40
1:A:537:GLU:OE2	1:A:561:TRP:CE2	2.75	0.40
1:A:926:LEU:O	1:A:928:ARG:NH2	2.54	0.40
1:A:1030:PHE:CE2	1:A:1038:GLY:HA3	2.53	0.40
1:A:569:LEU:HB3	1:A:575:GLU:O	2.21	0.40
1:A:909:ILE:HG22	1:A:910:MET:N	2.37	0.40
1:A:107:ASN:OD1	1:A:109:GLN:CB	2.69	0.40
1:A:285:LEU:N	1:A:285:LEU:HD12	2.36	0.40
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.84	0.40
1:A:631:LEU:HD23	1:A:631:LEU:HA	1.86	0.40
1:A:839:GLU:HG3	1:A:840:GLU:CG	2.52	0.40
1:A:258:ILE:HD13	1:A:273:LEU:HD13	2.02	0.40
1:A:342:GLU:C	1:A:344:GLY:N	2.74	0.40
1:A:389:ILE:N	1:A:389:ILE:CD1	2.64	0.40
1:A:612:PHE:CE2	1:A:628:LYS:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:LEU:HD23	1:A:947:ARG:HB2	2.02	0.40
1:A:1112:LEU:HB3	1:A:1122:ARG:HH21	1.87	0.40
1:A:413:LEU:HD22	1:A:426:VAL:HG23	2.03	0.40
1:A:469:ILE:HG21	1:A:503:CYS:SG	2.62	0.40
1:A:478:LEU:HD12	1:A:526:LEU:CD2	2.52	0.40
1:A:504:ASN:HB3	1:A:543:ILE:O	2.21	0.40
1:A:786:VAL:HG12	1:A:787:GLU:N	2.36	0.40
1:A:902:GLU:O	1:A:905:HIS:HB2	2.21	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	1111/1140 (98%)	888 (80%)	155 (14%)	68 (6%)	1 4

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	GLU
1	A	291	MET
1	A	405	PRO
1	A	417	PRO
1	A	430	VAL
1	A	494	GLN
1	A	495	ALA
1	A	502	SER
1	A	505	SER
1	A	523	PRO
1	A	684	SER
1	A	696	ASN
1	A	706	GLU

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Mol	Chain	Res	Type
1	A	707	ILE
1	A	708	GLN
1	A	839	GLU
1	A	951	PRO
1	A	952	ASN
1	A	1024	THR
1	A	1065	VAL
1	A	287	LYS
1	A	371	GLY
1	A	406	GLY
1	A	463	VAL
1	A	623	LEU
1	A	632	GLY
1	A	748	GLY
1	A	751	ALA
1	A	772	SER
1	A	841	ALA
1	A	864	LYS
1	A	894	THR
1	A	906	TYR
1	A	918	GLY
1	A	938	MET
1	A	950	ASN
1	A	985	THR
1	A	146	ASP
1	A	254	LYS
1	A	450	GLY
1	A	475	SER
1	A	493	PRO
1	A	826	ASN
1	A	876	PHE
1	A	897	LYS
1	A	919	ASP
1	A	983	ALA
1	A	1025	GLN
1	A	175	ALA
1	A	199	GLU
1	A	288	GLU
1	A	412	PRO
1	A	664	HIS
1	A	856	GLY
1	A	885	ASN

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Mol	Chain	Res	Type
1	A	465	HIS
1	A	621	GLY
1	A	840	GLU
1	A	855	ASP
1	A	998	PHE
1	A	113	GLY
1	A	484	LYS
1	A	509	VAL
1	A	264	VAL
1	A	185	PRO
1	A	545	PRO
1	A	112	ILE
1	A	293	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	982/999 (98%)	853 (87%)	129 (13%)	4 12

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	20	THR
1	A	22	HIS
1	A	25	SER
1	A	27	GLU
1	A	50	ARG
1	A	68	ARG
1	A	70	LYS
1	A	73	SER
1	A	75	ASP
1	A	81	THR
1	A	83	LYS
1	A	94	SER

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Mol	Chain	Res	Type
1	A	96	GLU
1	A	103	ARG
1	A	110	ASP
1	A	111	ARG
1	A	117	GLU
1	A	129	ARG
1	A	135	LEU
1	A	141	LYS
1	A	147	ARG
1	A	162	LEU
1	A	167	VAL
1	A	176	PRO
1	A	178	ILE
1	A	189	HIS
1	A	197	LEU
1	A	198	ARG
1	A	241	ASN
1	A	254	LYS
1	A	259	VAL
1	A	263	ARG
1	A	288	GLU
1	A	296	THR
1	A	297	LEU
1	A	302	VAL
1	A	312	GLU
1	A	342	GLU
1	A	366	ASP
1	A	372	GLN
1	A	383	LYS
1	A	384	GLU
1	A	401	SER
1	A	420	GLU
1	A	422	TYR
1	A	423	ASP
1	A	434	ARG
1	A	437	MET
1	A	438	LEU
1	A	445	GLU
1	A	449	MET
1	A	468	LEU
1	A	476	VAL
1	A	478	LEU

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Mol	Chain	Res	Type
1	A	488	SER
1	A	492	GLU
1	A	517	TYR
1	A	518	TYR
1	A	527	ARG
1	A	537	GLU
1	A	550	ASN
1	A	565	SER
1	A	569	LEU
1	A	570	LYS
1	A	571	LEU
1	A	576	LEU
1	A	579	LYS
1	A	585	GLU
1	A	587	ILE
1	A	589	ARG
1	A	594	THR
1	A	602	LEU
1	A	613	TYR
1	A	614	PHE
1	A	625	ASP
1	A	630	THR
1	A	638	LEU
1	A	644	LEU
1	A	647	THR
1	A	663	ASN
1	A	665	LYS
1	A	668	PHE
1	A	679	MET
1	A	685	ASP
1	A	688	PRO
1	A	701	ILE
1	A	704	ILE
1	A	708	GLN
1	A	709	LYS
1	A	753	ARG
1	A	766	SER
1	A	782	PHE
1	A	794	ILE
1	A	840	GLU
1	A	842	GLU
1	A	843	PRO

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Mol	Chain	Res	Type
1	A	844	LYS
1	A	857	LYS
1	A	864	LYS
1	A	866	VAL
1	A	899	VAL
1	A	900	ARG
1	A	925	ASP
1	A	927	MET
1	A	928	ARG
1	A	949	PHE
1	A	957	VAL
1	A	966	LEU
1	A	969	GLU
1	A	980	ASP
1	A	985	THR
1	A	992	LEU
1	A	993	GLN
1	A	1000	LEU
1	A	1014	MET
1	A	1015	GLN
1	A	1045	GLU
1	A	1050	LEU
1	A	1052	LEU
1	A	1069	GLU
1	A	1086	THR
1	A	1092	ASP
1	A	1093	LEU
1	A	1111	ASN
1	A	1112	LEU
1	A	1122	ARG
1	A	1125	THR
1	A	1131	LYS

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

Mol	Chain	Res	Type
1	A	16	ASN
1	A	30	ASN
1	A	85	ASN
1	A	156	ASN
1	A	186	GLN
1	A	189	HIS

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Mol	Chain	Res	Type
1	A	209	GLN
1	A	234	GLN
1	A	241	ASN
1	A	261	HIS
1	A	262	ASN
1	A	332	GLN
1	A	343	GLN
1	A	392	ASN
1	A	399	HIS
1	A	455	GLN
1	A	456	GLN
1	A	467	GLN
1	A	617	ASN
1	A	648	ASN
1	A	663	ASN
1	A	670	ASN
1	A	677	ASN
1	A	683	ASN
1	A	695	ASN
1	A	708	GLN
1	A	727	GLN
1	A	796	GLN
1	A	797	HIS
1	A	941	ASN
1	A	1055	GLN
1	A	1059	ASN
1	A	1070	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.