



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:21 AM GMT

PDB ID : 3AGP
Title : Structure of viral polymerase form I
Authors : Takeshita, D.; Tomita, K.
Deposited on : 2010-04-06
Resolution : 2.80 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

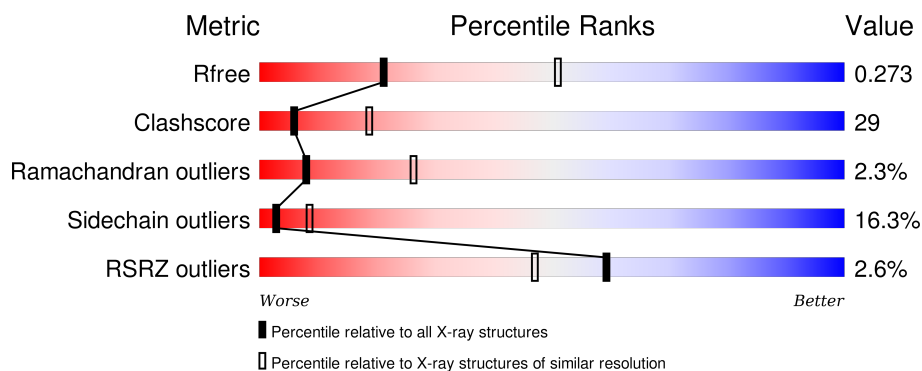
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	1289	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9311 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 Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1202	Total	C	N	O	S	0	0	0
			9274	5857	1603	1769	45			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	HIS	-	LINKER	UNP P0A6P3
A	1284	HIS	-	EXPRESSION TAG	UNP Q8LTE0
A	1285	HIS	-	EXPRESSION TAG	UNP Q8LTE0
A	1286	HIS	-	EXPRESSION TAG	UNP Q8LTE0
A	1287	HIS	-	EXPRESSION TAG	UNP Q8LTE0
A	1288	HIS	-	EXPRESSION TAG	UNP Q8LTE0
A	1289	HIS	-	EXPRESSION TAG	UNP Q8LTE0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		

ALA	I1182	T1076	F990	T912	K831
PRO	R1183	M1077	E991	D913	L832
TYR	Y1184	T1078	V992	R914	R833
GLY	V1185		I993	C915	G834
VAL		T1081	M994	I916	D835
PHE	I1188		D995	A917	V836
GLN		R1088	I996	I918	P837
GLY	T1192	E1089	R997	E919	S838
THR	R1193	S1090	S998	P920	V839
LYS	D1194		P999	G921	E840
VAL	R1195	K1093		W922	
ALA	E1196	H1094	L1003	N923	L843
SER	R1197	Y1095	P1004		
LEU		Y1096		F926	C846
HIS	L1200		V1008	Q927	R847
GLU		V1099			F848
ALA	R1210	D1100	E1012	I930	S849
HIS		V1101	K1013	G931	
HIS	S1215	T1102	I1014	G932	T853
HIS	M1216		S1015	I933	T854
ASP		Y1105	S1016	L934	T855
GLY		I1106	M1017	R935	R856
LEU					N857
PRO		R1109	Y1021	L938	R858
LEU		I1110	T1022		S859
ARG			F1023	D947	
GLY		L1116	E1024	Q948	H862
PRO				T949	P863
SER		N1121	L1028	I950	S864
GLY			I1029	N951	F865
CYS		Y1124	F1030	Q952	K866
ASP		R1125		R953	F867
SER		W1126	L1033	R954	A868
ALA		A1127		A955	L869
ASP		T1128	I1040		P870
LEU		I1129	L1041	G958	
LEU		D1130	D1042	S959	A871
PHE			L1043	V960	A872
	A1234		D1044	T961	C873
ALA	I1235	R1136	S1045	N962	T874
D1236			E1046	N963	
Q1237		K1143	S1046	L964	V881
L1238		Y1144	E1047	A965	
			V1048	T966	S887
R1241		K1150	T1049	V967	T892
S1242		Q1151	V1050	D968	R893
N1243		L1152		I969	I894
P1244			I1055	S895	S895
T1245			I1056	S970	D896
K1246		I1157	L1057		I897
I1247			P1058	L978	
S1248		A1165		A979	F900
R1249		L1166	L1065	L980	N901
S1250		V1167	R1066	C981	
		I1172	E1067	E982	
		N1173	V1068	L983	T905
F1254		P1174		L984	V906
			V1072		
S1263		F1175	G1073	P987	N909
R1264			F1074	G988	S910
VAL			T1075	W989	K911
LEU		R1179			

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	139.50Å 256.43Å 100.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.80 29.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.90-2.80) 98.2 (29.55-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.80Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.283 0.208 , 0.273	Depositor DCC
R_{free} test set	2231 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.0	EDS
Estimated twinning fraction	0.022 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 44108 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9311	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: CA

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	0.39	0/9443	0.56	0/12771

There are no bond length outliers.

There are no bond angle outliers.

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	9274	0	9256	530	0
2	A	1	0	0	0	0
3	A	36	0	0	3	0
All	All	9311	0	9256	530	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 29.

All (530) 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:491:ILE:HG22	1:A:555:ALA:HB3	1.36	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:ASP:OD1	1:A:1102:THR:HG22	1.59	1.02
1:A:133:ARG:HG2	1:A:134:ARG:H	1.25	1.01
1:A:854:THR:HG21	1:A:872:ALA:HB3	1.42	1.01
1:A:806:ARG:H	1:A:807:PRO:HD2	1.31	0.96
1:A:399:GLN:HE21	1:A:399:GLN:H	1.13	0.94
1:A:183:PRO:HD3	1:A:230:THR:HB	1.51	0.93
1:A:467:ALA:HA	1:A:470:GLU:HB2	1.53	0.91
1:A:930:ILE:HD11	1:A:1021:TYR:HB3	1.54	0.89
1:A:961:THR:HG23	1:A:963:ASN:H	1.33	0.89
1:A:930:ILE:HD11	1:A:1021:TYR:CD2	2.07	0.89
1:A:220:MET:O	1:A:224:THR:HG22	1.73	0.88
1:A:930:ILE:HD11	1:A:1021:TYR:HD2	1.40	0.86
1:A:558:ASN:HB3	1:A:1210:ARG:HG3	1.57	0.86
1:A:947:ASP:OD1	1:A:949:THR:HB	1.75	0.86
1:A:700:SER:N	1:A:1179:ARG:HG2	1.91	0.86
1:A:307:HIS:CD2	1:A:391:ALA:H	1.92	0.85
1:A:134:ARG:HH21	1:A:134:ARG:HG3	1.39	0.85
1:A:967:VAL:HG22	1:A:1055:ILE:HB	1.60	0.84
1:A:541:THR:HG21	1:A:564:ARG:HB3	1.59	0.83
1:A:372:TYR:HE1	1:A:410:VAL:HG21	1.44	0.82
1:A:224:THR:HG23	1:A:225:GLY:H	1.44	0.82
1:A:800:THR:HG22	1:A:803:ARG:NH1	1.93	0.82
1:A:800:THR:HG22	1:A:803:ARG:HH11	1.44	0.81
1:A:1173:ASN:ND2	1:A:1175:PHE:H	1.79	0.80
1:A:290:PHE:N	1:A:292:ARG:CZ	2.45	0.80
1:A:714:ASN:HD21	1:A:1254:PHE:H	1.30	0.79
1:A:520:ILE:HD11	1:A:554:ARG:HG3	1.63	0.79
1:A:358:THR:HG23	1:A:359:ARG:HG2	1.62	0.78
1:A:806:ARG:H	1:A:807:PRO:CD	1.95	0.78
1:A:198:GLN:HA	1:A:201:ILE:HG12	1.66	0.78
1:A:729:ASN:HD21	1:A:740:PHE:H	1.32	0.78
1:A:752:ARG:H	1:A:763:ASN:HD21	1.32	0.77
1:A:849:SER:HA	1:A:863:PRO:HG3	1.65	0.76
1:A:592:GLU:HG2	1:A:642:LYS:HG2	1.68	0.75
1:A:752:ARG:H	1:A:763:ASN:ND2	1.84	0.75
1:A:210:GLU:CD	1:A:210:GLU:H	1.88	0.75
1:A:103:GLY:O	1:A:105:ILE:HG13	1.86	0.75
1:A:92:PHE:CE1	1:A:132:ILE:HD11	2.21	0.75
1:A:801:ASN:HD22	1:A:1012:GLU:HG3	1.52	0.74
1:A:246:LEU:HD21	1:A:253:VAL:HG13	1.68	0.74
1:A:1129:ILE:O	1:A:1129:ILE:HG22	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ASP:HA	1:A:673:VAL:HG23	1.69	0.73
1:A:790:PHE:HD1	1:A:791:LEU:HD13	1.52	0.73
1:A:356:THR:HG22	1:A:358:THR:H	1.53	0.72
1:A:717:ILE:C	1:A:717:ILE:HD13	2.10	0.72
1:A:854:THR:HG21	1:A:872:ALA:CB	2.20	0.72
1:A:120:VAL:HA	1:A:123:VAL:HG12	1.71	0.72
1:A:133:ARG:HG2	1:A:134:ARG:N	2.03	0.72
1:A:134:ARG:HH21	1:A:134:ARG:CG	2.02	0.71
1:A:923:ASN:O	1:A:927:GLN:HG3	1.90	0.71
1:A:901:ASN:HD22	1:A:901:ASN:C	1.94	0.71
1:A:1110:ILE:HD11	1:A:1116:LEU:HG	1.71	0.71
1:A:544:GLU:HB3	1:A:549:LEU:HG	1.73	0.71
1:A:49:ALA:HB2	1:A:123:VAL:HG11	1.72	0.71
1:A:836:VAL:HG22	1:A:837:PRO:HD2	1.75	0.69
1:A:780:ILE:HD13	1:A:780:ILE:H	1.57	0.69
1:A:93:ALA:HA	1:A:96:VAL:HG12	1.73	0.69
1:A:854:THR:HG23	1:A:855:THR:HG23	1.74	0.69
1:A:1143:LYS:HD3	1:A:1144:TYR:CE1	2.28	0.69
1:A:374:LYS:HE3	1:A:594:TYR:CZ	2.28	0.69
1:A:169:ILE:HD11	1:A:229:LEU:HD11	1.75	0.69
1:A:529:ILE:HG12	1:A:529:ILE:O	1.93	0.69
1:A:583:ILE:HG12	1:A:652:ALA:HB1	1.74	0.68
1:A:301:THR:OG1	1:A:309:LYS:HB2	1.92	0.68
1:A:704:SER:O	1:A:708:GLN:HB2	1.93	0.68
1:A:965:ALA:HA	1:A:1088:ARG:NH2	2.08	0.68
1:A:117:GLU:O	1:A:120:VAL:HG22	1.94	0.68
1:A:930:ILE:HD11	1:A:1021:TYR:CB	2.24	0.67
1:A:148:HIS:HB3	1:A:152:ILE:HG22	1.75	0.67
1:A:949:THR:HG23	1:A:953:ARG:NH1	2.10	0.67
1:A:779:GLY:C	1:A:781:ASP:H	1.98	0.67
1:A:618:ARG:NH1	1:A:652:ALA:O	2.28	0.66
1:A:307:HIS:HD2	1:A:391:ALA:H	1.40	0.66
1:A:838:SER:HB2	1:A:840:GLU:HG3	1.77	0.66
1:A:212:ALA:O	1:A:216:VAL:HG23	1.95	0.66
1:A:470:GLU:O	1:A:474:LEU:HD12	1.95	0.65
1:A:502:VAL:HG11	1:A:571:ILE:HB	1.77	0.65
1:A:388:LEU:HB3	1:A:417:VAL:HG22	1.79	0.65
1:A:4:ILE:H	1:A:4:ILE:HD13	1.60	0.65
1:A:72:ILE:HG13	1:A:137:ALA:HB2	1.78	0.65
1:A:298:ASN:HB3	1:A:362:ALA:HB3	1.78	0.65
1:A:968:ASP:H	1:A:1081:THR:HG22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PHE:HE1	1:A:132:ILE:HD11	1.61	0.64
1:A:1173:ASN:HD22	1:A:1175:PHE:H	1.46	0.64
1:A:930:ILE:HD13	1:A:931:GLY:H	1.62	0.64
1:A:1151:GLN:H	1:A:1151:GLN:HE21	1.46	0.64
1:A:930:ILE:CD1	1:A:1021:TYR:HD2	2.11	0.64
1:A:1121:ASN:HD21	1:A:1167:VAL:H	1.44	0.64
1:A:1049:THR:HG22	1:A:1056:ILE:HB	1.78	0.63
1:A:611:TYR:HB3	1:A:626:ILE:HD11	1.79	0.63
1:A:775:ASP:OD2	1:A:1109:ARG:HD3	1.98	0.63
1:A:130:ILE:HG12	1:A:130:ILE:O	1.96	0.63
1:A:442:LEU:HD12	1:A:452:THR:HG21	1.81	0.63
1:A:356:THR:HG21	1:A:481:ASP:OD1	1.97	0.63
1:A:965:ALA:HA	1:A:1088:ARG:HH21	1.61	0.63
1:A:1157:ILE:HG12	1:A:1165:ALA:HB3	1.79	0.63
1:A:1157:ILE:HG22	1:A:1185:VAL:HG11	1.81	0.63
1:A:764:TYR:OH	1:A:1094:HIS:HD2	1.81	0.63
1:A:853:THR:HG23	1:A:866:LYS:HE2	1.80	0.63
1:A:784:ALA:O	1:A:788:GLU:HG3	1.99	0.63
1:A:276:VAL:HG11	1:A:352:VAL:HG11	1.80	0.63
1:A:801:ASN:ND2	1:A:1012:GLU:HG3	2.13	0.62
1:A:906:VAL:HG13	1:A:914:ARG:HB3	1.80	0.62
1:A:662:ARG:HD2	1:A:667:THR:HG22	1.81	0.62
1:A:741:ASN:HD22	1:A:742:SER:H	1.47	0.62
1:A:132:ILE:HD12	1:A:132:ILE:H	1.64	0.62
1:A:626:ILE:HG22	1:A:645:VAL:HG22	1.82	0.62
1:A:502:VAL:HG13	1:A:512:VAL:HG12	1.82	0.62
1:A:521:ILE:O	1:A:521:ILE:HG23	1.99	0.62
1:A:930:ILE:CD1	1:A:1021:TYR:HB3	2.27	0.62
1:A:1110:ILE:HD12	1:A:1116:LEU:HA	1.82	0.61
1:A:148:HIS:HB3	1:A:152:ILE:CG2	2.29	0.61
1:A:442:LEU:CD1	1:A:452:THR:HG21	2.30	0.61
1:A:704:SER:HB3	3:A:2003:HOH:O	2.01	0.61
1:A:304:HIS:ND1	1:A:397:MET:HG3	2.15	0.61
1:A:848:PHE:HE1	1:A:921:GLY:O	1.84	0.61
1:A:272:PHE:CZ	1:A:313:THR:HG21	2.36	0.60
1:A:1173:ASN:HD22	1:A:1173:ASN:C	2.03	0.60
1:A:717:ILE:O	1:A:717:ILE:HD13	2.01	0.60
1:A:529:ILE:HD12	1:A:571:ILE:HG12	1.84	0.60
1:A:12:LEU:HD22	1:A:27:LEU:HD13	1.83	0.60
1:A:166:VAL:HA	1:A:169:ILE:HG23	1.84	0.60
1:A:62:ILE:HG12	1:A:75:GLU:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1243:ASN:HB2	1:A:1244:PRO:HD2	1.84	0.59
1:A:980:LEU:HD22	1:A:1072:VAL:HB	1.84	0.59
1:A:743:GLU:HB2	1:A:778:LEU:HD22	1.83	0.59
1:A:304:HIS:HD2	1:A:306:ASP:H	1.50	0.59
1:A:399:GLN:HE21	1:A:399:GLN:N	1.92	0.59
1:A:41:MET:HA	1:A:44:SER:OG	2.02	0.59
1:A:622:VAL:HG22	1:A:647:LEU:HD22	1.83	0.59
1:A:372:TYR:CE1	1:A:410:VAL:HG21	2.31	0.59
1:A:839:VAL:HG12	1:A:843:LEU:HD23	1.84	0.59
1:A:862:HIS:HD2	1:A:864:SER:H	1.51	0.58
1:A:790:PHE:CD1	1:A:791:LEU:HD13	2.35	0.58
1:A:549:LEU:HD23	1:A:550:LEU:N	2.18	0.58
1:A:967:VAL:HA	1:A:1081:THR:HG22	1.84	0.58
1:A:356:THR:HG23	1:A:357:PRO:HD2	1.86	0.58
1:A:25:LYS:O	1:A:28:THR:HG22	2.03	0.58
1:A:158:ALA:HB2	1:A:253:VAL:HG12	1.86	0.58
1:A:1047:GLU:HB3	1:A:1058:PRO:HD3	1.85	0.58
1:A:187:SER:HB3	1:A:190:VAL:CG1	2.34	0.58
1:A:817:LEU:HG	1:A:1068:VAL:HG23	1.86	0.58
1:A:806:ARG:N	1:A:807:PRO:HD2	2.13	0.58
1:A:224:THR:HG23	1:A:225:GLY:N	2.17	0.58
1:A:111:LEU:HD23	1:A:111:LEU:H	1.68	0.58
1:A:833:ILE:HG23	1:A:989:TRP:CE2	2.39	0.58
1:A:629:PRO:HG2	1:A:632:VAL:CG1	2.34	0.58
1:A:589:PHE:CD1	1:A:673:VAL:HG12	2.39	0.58
1:A:309:LYS:HE3	1:A:365:ASP:OD2	2.04	0.58
1:A:52:LYS:O	1:A:54:GLY:N	2.37	0.57
1:A:764:TYR:OH	1:A:1094:HIS:CD2	2.56	0.57
1:A:1093:LYS:HB3	1:A:1095:TYR:CE2	2.39	0.57
1:A:857:ASN:ND2	1:A:857:ASN:H	2.02	0.57
1:A:982:GLU:HB3	1:A:990:PHE:CE1	2.40	0.57
1:A:75:GLU:O	1:A:75:GLU:HG3	2.05	0.57
1:A:798:ALA:HA	1:A:1012:GLU:HG2	1.86	0.57
1:A:162:ASP:O	1:A:166:VAL:HG22	2.04	0.57
1:A:1100:ASP:OD1	1:A:1102:THR:CG2	2.45	0.56
1:A:132:ILE:N	1:A:132:ILE:HD12	2.19	0.56
1:A:700:SER:O	1:A:1179:ARG:HD2	2.05	0.56
1:A:836:VAL:CG2	1:A:837:PRO:HD2	2.34	0.56
1:A:988:GLY:O	1:A:992:VAL:HG12	2.05	0.56
1:A:38:ILE:HD12	1:A:39:GLU:N	2.20	0.56
1:A:73:ILE:HB	1:A:155:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LYS:HG2	1:A:185:ASP:OD2	2.05	0.56
1:A:614:GLN:HE22	1:A:664:GLY:H	1.54	0.56
1:A:24:LYS:HG3	1:A:430:LEU:HD11	1.86	0.56
1:A:80:THR:HG23	1:A:82:PHE:H	1.69	0.56
1:A:700:SER:N	1:A:1179:ARG:CG	2.67	0.56
1:A:722:ASN:HB3	1:A:725:LEU:HB3	1.87	0.55
1:A:729:ASN:ND2	1:A:740:PHE:H	2.03	0.55
1:A:156:VAL:HG12	1:A:166:VAL:HG12	1.87	0.55
1:A:187:SER:HB3	1:A:190:VAL:HG12	1.88	0.55
1:A:163:GLU:H	1:A:163:GLU:CD	2.09	0.55
1:A:134:ARG:NH2	1:A:259:PHE:CD2	2.75	0.55
1:A:1243:ASN:CB	1:A:1244:PRO:HD2	2.36	0.55
1:A:262:GLY:HA2	1:A:265:ILE:HD12	1.89	0.55
1:A:384:ASP:O	1:A:413:PRO:HG2	2.06	0.55
1:A:356:THR:HG22	1:A:358:THR:HG22	1.89	0.55
1:A:900:PHE:CE2	1:A:1008:VAL:HG12	2.42	0.55
1:A:79:GLN:NE2	1:A:129:ASN:H	2.04	0.55
1:A:504:SER:HB2	1:A:568:ARG:HG2	1.89	0.55
1:A:1121:ASN:ND2	1:A:1167:VAL:H	2.04	0.55
1:A:741:ASN:HD22	1:A:742:SER:N	2.05	0.55
1:A:961:THR:CG2	1:A:963:ASN:H	2.13	0.54
1:A:229:LEU:CD2	1:A:242:VAL:HG11	2.37	0.54
1:A:33:ASP:OD1	1:A:36:LEU:HB2	2.06	0.54
1:A:423:ASP:OD2	1:A:461:LYS:HE2	2.07	0.54
1:A:961:THR:HG23	1:A:963:ASN:N	2.15	0.54
1:A:930:ILE:CD1	1:A:1021:TYR:CD2	2.88	0.54
1:A:798:ALA:CA	1:A:1012:GLU:HG2	2.37	0.54
1:A:508:ARG:HD3	1:A:562:LEU:HD21	1.89	0.54
1:A:558:ASN:HB3	1:A:1210:ARG:CG	2.33	0.54
1:A:413:PRO:HB2	1:A:414:TYR:CD1	2.42	0.54
1:A:4:ILE:N	1:A:4:ILE:HD13	2.22	0.54
1:A:1110:ILE:CD1	1:A:1116:LEU:HA	2.37	0.54
1:A:617:PHE:O	1:A:618:ARG:HG2	2.06	0.54
1:A:221:LYS:O	1:A:224:THR:HG23	2.08	0.53
1:A:794:GLU:OE1	1:A:794:GLU:HA	2.07	0.53
1:A:734:ALA:HB1	1:A:1136:ARG:O	2.07	0.53
1:A:1245:THR:O	1:A:1246:LYS:HD3	2.08	0.53
1:A:1017:MET:HA	1:A:1022:THR:HG21	1.89	0.53
1:A:66:ILE:HD12	1:A:66:ILE:O	2.09	0.53
1:A:417:VAL:HG12	1:A:454:ILE:HG23	1.91	0.53
1:A:747:ILE:HG22	1:A:771:SER:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:GLY:HA2	1:A:619:THR:HG22	1.90	0.53
1:A:805:TYR:O	1:A:806:ARG:HB3	2.09	0.53
1:A:128:GLU:O	1:A:130:ILE:HG22	2.09	0.53
1:A:396:PRO:HG3	1:A:437:GLU:HB3	1.90	0.53
1:A:954:ARG:HH11	1:A:1049:THR:CG2	2.22	0.52
1:A:951:ASN:OD1	1:A:1049:THR:HG23	2.09	0.52
1:A:1096:TYR:O	1:A:1099:VAL:HG22	2.09	0.52
1:A:1247:ILE:HD13	1:A:1247:ILE:N	2.24	0.52
1:A:80:THR:HG22	1:A:83:VAL:H	1.74	0.52
1:A:930:ILE:HA	1:A:933:ILE:HG23	1.91	0.52
1:A:92:PHE:CZ	1:A:132:ILE:HD11	2.43	0.52
1:A:801:ASN:HA	1:A:979:ALA:HB2	1.90	0.52
1:A:187:SER:O	1:A:190:VAL:HG12	2.10	0.52
1:A:658:ARG:HG3	1:A:658:ARG:HH11	1.74	0.52
1:A:1057:LEU:HD23	1:A:1057:LEU:H	1.74	0.52
1:A:1173:ASN:HD22	1:A:1175:PHE:N	2.07	0.52
1:A:92:PHE:HB2	1:A:122:LEU:HD11	1.92	0.52
1:A:590:GLU:HB3	1:A:644:VAL:HG22	1.92	0.52
1:A:1193:ARG:HD2	1:A:1249:ARG:HH11	1.72	0.52
1:A:375:ASN:HA	1:A:378:THR:HG22	1.92	0.52
1:A:1173:ASN:ND2	1:A:1175:PHE:N	2.53	0.51
1:A:593:VAL:HG22	1:A:641:ILE:HG22	1.92	0.51
1:A:12:LEU:HG	1:A:13:ARG:N	2.25	0.51
1:A:369:HIS:NE2	1:A:406:LEU:HD23	2.25	0.51
1:A:48:LYS:O	1:A:51:LYS:HB3	2.11	0.51
1:A:566:ILE:HD11	1:A:570:GLU:HB2	1.92	0.51
1:A:1024:GLU:N	1:A:1024:GLU:OE1	2.40	0.51
1:A:676:VAL:HG23	1:A:676:VAL:O	2.10	0.51
1:A:806:ARG:N	1:A:807:PRO:CD	2.68	0.51
1:A:593:VAL:HG22	1:A:641:ILE:CG2	2.40	0.51
1:A:853:THR:CG2	1:A:866:LYS:HE2	2.40	0.51
1:A:20:MET:HE3	1:A:20:MET:HA	1.92	0.51
1:A:541:THR:CG2	1:A:564:ARG:HB3	2.36	0.51
1:A:1182:ILE:HG13	1:A:1184:TYR:CE2	2.45	0.51
1:A:412:VAL:O	1:A:412:VAL:HG13	2.11	0.51
1:A:987:PRO:HD2	3:A:2007:HOH:O	2.09	0.51
1:A:930:ILE:HD11	1:A:1021:TYR:CG	2.44	0.51
1:A:304:HIS:CD2	1:A:305:VAL:N	2.79	0.51
1:A:310:THR:O	1:A:313:THR:HG22	2.10	0.51
1:A:30:ALA:HB1	1:A:36:LEU:HD13	1.93	0.51
1:A:948:GLN:HG2	3:A:2017:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ILE:HB	1:A:260:GLU:HG3	1.93	0.51
1:A:1045:SER:O	1:A:1048:VAL:HG13	2.10	0.51
1:A:416:ILE:HD12	1:A:480:LEU:HD12	1.92	0.50
1:A:369:HIS:CD2	1:A:406:LEU:HD23	2.46	0.50
1:A:379:GLY:HA2	1:A:658:ARG:HH21	1.75	0.50
1:A:897:ILE:O	1:A:897:ILE:HG12	2.10	0.50
1:A:741:ASN:HD21	1:A:745:GLU:HB2	1.76	0.50
1:A:839:VAL:HG12	1:A:843:LEU:CD2	2.41	0.50
1:A:809:TYR:C	1:A:811:GLU:H	2.13	0.50
1:A:169:ILE:O	1:A:173:VAL:HG23	2.11	0.50
1:A:591:SER:HB2	1:A:672:VAL:O	2.11	0.50
1:A:1030:PHE:HE2	1:A:1074:PHE:CE1	2.30	0.50
1:A:558:ASN:HD22	1:A:1210:ARG:HH21	1.60	0.50
1:A:158:ALA:HA	1:A:253:VAL:HA	1.94	0.50
1:A:148:HIS:NE2	1:A:636:MET:HG3	2.26	0.50
1:A:862:HIS:CD2	1:A:864:SER:H	2.29	0.50
1:A:279:MET:SD	1:A:311:THR:HG22	2.52	0.50
1:A:246:LEU:O	1:A:249:HIS:O	2.29	0.50
1:A:949:THR:CG2	1:A:953:ARG:NH1	2.75	0.50
1:A:779:GLY:C	1:A:781:ASP:N	2.65	0.50
1:A:586:HIS:HB2	1:A:653:MET:CE	2.42	0.50
1:A:892:ILE:HG23	1:A:922:TRP:CZ2	2.47	0.50
1:A:516:VAL:HG13	1:A:555:ALA:HA	1.94	0.49
1:A:714:ASN:ND2	1:A:1254:PHE:H	2.06	0.49
1:A:359:ARG:HD2	1:A:361:TYR:OH	2.12	0.49
1:A:579:LYS:O	1:A:582:THR:HB	2.12	0.49
1:A:195:TYR:C	1:A:195:TYR:CD1	2.84	0.49
1:A:399:GLN:NE2	1:A:399:GLN:H	1.96	0.49
1:A:194:GLU:HA	1:A:197:VAL:HG12	1.94	0.49
1:A:1110:ILE:HD11	1:A:1116:LEU:CG	2.41	0.49
1:A:232:GLN:O	1:A:242:VAL:HG23	2.11	0.49
1:A:165:LEU:O	1:A:169:ILE:HG22	2.12	0.49
1:A:930:ILE:HD13	1:A:931:GLY:N	2.28	0.49
1:A:376:MET:HG3	1:A:410:VAL:CG2	2.43	0.49
1:A:796:GLU:O	1:A:800:THR:HG23	2.11	0.49
1:A:914:ARG:HH22	1:A:1017:MET:CE	2.26	0.49
1:A:900:PHE:HE2	1:A:1008:VAL:HG12	1.77	0.49
1:A:181:ILE:HG22	1:A:185:ASP:OD1	2.12	0.49
1:A:434:VAL:O	1:A:438:VAL:HG12	2.12	0.49
1:A:132:ILE:CD1	1:A:132:ILE:H	2.26	0.49
1:A:1182:ILE:HD12	1:A:1183:ARG:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:HG2	1:A:164:GLU:H	1.76	0.49
1:A:205:SER:O	1:A:757:PRO:HG2	2.13	0.49
1:A:967:VAL:CG2	1:A:1055:ILE:HB	2.36	0.49
1:A:276:VAL:HG21	1:A:313:THR:HG23	1.95	0.49
1:A:12:LEU:HD11	1:A:23:CYS:SG	2.53	0.49
1:A:914:ARG:HH12	1:A:1017:MET:HG3	1.78	0.48
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.60	0.48
1:A:208:PRO:HG2	1:A:211:ILE:HD13	1.94	0.48
1:A:400:THR:HA	1:A:403:HIS:CD2	2.48	0.48
1:A:25:LYS:HG3	1:A:26:ALA:N	2.28	0.48
1:A:954:ARG:HD3	1:A:1049:THR:HG21	1.95	0.48
1:A:356:THR:CG2	1:A:358:THR:HG22	2.43	0.48
1:A:199:LEU:HD23	1:A:199:LEU:O	2.13	0.48
1:A:80:THR:HB	1:A:128:GLU:OE1	2.14	0.48
1:A:126:ILE:O	1:A:304:HIS:HE1	1.96	0.48
1:A:978:LEU:HD23	1:A:1014:ILE:HG12	1.95	0.48
1:A:1055:ILE:C	1:A:1056:ILE:HD12	2.34	0.48
1:A:990:PHE:O	1:A:994:MET:HG2	2.14	0.48
1:A:66:ILE:HG22	1:A:71:GLY:HA3	1.95	0.48
1:A:317:THR:HG22	1:A:354:TYR:HD1	1.79	0.48
1:A:313:THR:O	1:A:317:THR:HG23	2.13	0.48
1:A:177:LYS:HG2	1:A:258:ARG:NH2	2.29	0.48
1:A:163:GLU:HG2	1:A:164:GLU:N	2.29	0.48
1:A:822:ILE:HB	1:A:984:LEU:CD1	2.44	0.48
1:A:10:LYS:HB3	1:A:433:LEU:HD11	1.96	0.48
1:A:323:THR:O	1:A:324:TYR:CD2	2.67	0.47
1:A:502:VAL:CG1	1:A:512:VAL:HG12	2.42	0.47
1:A:64:THR:HG21	1:A:145:SER:HB2	1.96	0.47
1:A:703:ASN:O	1:A:705:LEU:N	2.45	0.47
1:A:655:ASP:HA	1:A:673:VAL:CG2	2.41	0.47
1:A:365:ASP:C	1:A:367:PRO:HD3	2.34	0.47
1:A:783:GLU:OE1	1:A:905:THR:HG21	2.15	0.47
1:A:966:THR:HG22	1:A:1056:ILE:HG13	1.95	0.47
1:A:148:HIS:CE1	1:A:636:MET:HG3	2.50	0.47
1:A:894:ILE:HD11	1:A:897:ILE:HB	1.96	0.47
1:A:805:TYR:O	1:A:806:ARG:CB	2.63	0.47
1:A:568:ARG:HD2	1:A:568:ARG:O	2.15	0.47
1:A:160:GLY:O	1:A:251:ALA:HB2	2.15	0.47
1:A:284:HIS:CE1	1:A:318:THR:HG22	2.49	0.47
1:A:749:PHE:CE2	1:A:766:LYS:HE2	2.50	0.47
1:A:1150:LYS:HD2	1:A:1150:LYS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:PRO:HA	1:A:241:THR:HA	1.97	0.47
1:A:1057:LEU:CD1	1:A:1065:LEU:HD22	2.45	0.46
1:A:1021:TYR:C	1:A:1021:TYR:CD1	2.88	0.46
1:A:968:ASP:N	1:A:1081:THR:HG22	2.29	0.46
1:A:795:ALA:O	1:A:799:LEU:HD22	2.14	0.46
1:A:134:ARG:NH2	1:A:134:ARG:CG	2.67	0.46
1:A:520:ILE:CD1	1:A:554:ARG:HG3	2.42	0.46
1:A:200:ASP:O	1:A:201:ILE:C	2.53	0.46
1:A:833:ILE:HG22	1:A:834:GLY:N	2.29	0.46
1:A:1195:ARG:HB2	1:A:1247:ILE:HG22	1.97	0.46
1:A:1235:ILE:O	1:A:1235:ILE:HG22	2.15	0.46
1:A:45:GLY:HA2	1:A:48:LYS:HD3	1.96	0.46
1:A:703:ASN:C	1:A:705:LEU:H	2.18	0.46
1:A:523:VAL:HG13	1:A:551:ASP:O	2.16	0.46
1:A:1150:LYS:H	1:A:1150:LYS:HD2	1.81	0.46
1:A:909:ASN:HB2	1:A:912:THR:HG22	1.98	0.46
1:A:116:GLU:O	1:A:120:VAL:HG13	2.15	0.46
1:A:318:THR:O	1:A:321:ALA:HB3	2.15	0.46
1:A:909:ASN:HB3	1:A:911:LYS:H	1.81	0.46
1:A:629:PRO:HD3	1:A:642:LYS:O	2.15	0.46
1:A:1129:ILE:CG2	1:A:1129:ILE:O	2.58	0.45
1:A:115:PHE:O	1:A:117:GLU:N	2.48	0.45
1:A:1247:ILE:HG22	1:A:1248:SER:N	2.31	0.45
1:A:629:PRO:HG2	1:A:632:VAL:HG12	1.97	0.45
1:A:735:TYR:CG	1:A:762:ILE:HG13	2.52	0.45
1:A:361:TYR:CZ	1:A:480:LEU:HB3	2.51	0.45
1:A:914:ARG:HH22	1:A:1017:MET:HE3	1.82	0.45
1:A:111:LEU:HA	1:A:114:GLN:HB3	1.98	0.45
1:A:73:ILE:HG23	1:A:73:ILE:O	2.17	0.45
1:A:786:ALA:O	1:A:789:LYS:HB2	2.15	0.45
1:A:745:GLU:HG2	1:A:745:GLU:O	2.17	0.45
1:A:838:SER:HB2	1:A:840:GLU:CG	2.45	0.45
1:A:417:VAL:HB	1:A:454:ILE:HD13	1.97	0.45
1:A:36:LEU:HD23	1:A:40:ASN:HD21	1.82	0.45
1:A:43:LYS:C	1:A:45:GLY:H	2.20	0.45
1:A:1173:ASN:ND2	1:A:1173:ASN:C	2.70	0.45
1:A:839:VAL:O	1:A:843:LEU:HD23	2.17	0.45
1:A:1183:ARG:HB2	1:A:1183:ARG:NH2	2.31	0.45
1:A:1003:LEU:HB3	1:A:1004:PRO:HD2	1.99	0.45
1:A:304:HIS:CD2	1:A:305:VAL:HG12	2.52	0.45
1:A:920:PRO:O	1:A:923:ASN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ALA:HA	1:A:129:ASN:ND2	2.32	0.45
1:A:650:PRO:O	1:A:651:ILE:HG12	2.16	0.45
1:A:846:CYS:HG	1:A:926:PHE:HD1	1.62	0.45
1:A:133:ARG:CG	1:A:134:ARG:H	2.12	0.45
1:A:960:VAL:CG2	1:A:961:THR:N	2.78	0.45
1:A:1050:VAL:HG22	1:A:1055:ILE:HA	1.98	0.45
1:A:324:TYR:CE2	1:A:357:PRO:HG3	2.52	0.45
1:A:848:PHE:O	1:A:849:SER:HB2	2.17	0.45
1:A:833:ILE:HD13	1:A:833:ILE:HG21	1.66	0.45
1:A:800:THR:O	1:A:804:LEU:HB2	2.16	0.45
1:A:955:ALA:HB2	1:A:1090:SER:HB3	1.98	0.45
1:A:486:GLU:HA	1:A:487:PRO:HD2	1.83	0.45
1:A:773:TYR:HB3	1:A:776:PHE:CE1	2.52	0.44
1:A:705:LEU:HA	1:A:705:LEU:HD22	1.75	0.44
1:A:749:PHE:CE1	1:A:766:LYS:HG2	2.52	0.44
1:A:1041:LEU:HB2	1:A:1043:LEU:HD12	1.99	0.44
1:A:80:THR:CG2	1:A:82:PHE:H	2.29	0.44
1:A:62:ILE:HG12	1:A:75:GLU:CB	2.46	0.44
1:A:567:LYS:HB2	1:A:570:GLU:HG3	1.99	0.44
1:A:870:PRO:HB2	1:A:895:SER:HB3	1.99	0.44
1:A:794:GLU:OE1	1:A:1013:LYS:HD3	2.18	0.44
1:A:67:ASP:O	1:A:69:ASN:N	2.50	0.44
1:A:1151:GLN:H	1:A:1151:GLN:NE2	2.12	0.44
1:A:848:PHE:HD2	1:A:867:PHE:CZ	2.36	0.44
1:A:622:VAL:HG11	1:A:651:ILE:HG13	1.98	0.44
1:A:386:ALA:HB3	1:A:415:ILE:HG12	1.99	0.44
1:A:4:ILE:CD1	1:A:4:ILE:H	2.29	0.44
1:A:998:SER:HA	1:A:999:PRO:HD2	1.83	0.44
1:A:833:ILE:HG23	1:A:989:TRP:NE1	2.33	0.44
1:A:154:VAL:HG21	1:A:170:ALA:O	2.18	0.44
1:A:1234:ALA:O	1:A:1235:ILE:HG12	2.17	0.44
1:A:768:GLU:HB3	1:A:1105:TYR:CE1	2.52	0.44
1:A:1172:ILE:HA	1:A:1172:ILE:HD13	1.64	0.44
1:A:61:VAL:HG11	1:A:90:GLN:NE2	2.33	0.44
1:A:616:TYR:HB3	1:A:660:ALA:HB3	1.99	0.44
1:A:901:ASN:HB2	1:A:918:ILE:O	2.18	0.44
1:A:833:ILE:CG2	1:A:989:TRP:NE1	2.81	0.44
1:A:495:PHE:CE2	1:A:521:ILE:HB	2.53	0.44
1:A:37:ALA:O	1:A:41:MET:HG3	2.18	0.44
1:A:52:LYS:C	1:A:54:GLY:H	2.21	0.44
1:A:508:ARG:HE	1:A:562:LEU:HD11	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:GLY:HA2	1:A:961:THR:HG22	2.00	0.43
1:A:836:VAL:HG22	1:A:837:PRO:CD	2.46	0.43
1:A:301:THR:HA	1:A:387:ILE:HG23	1.99	0.43
1:A:1234:ALA:C	1:A:1235:ILE:HG12	2.39	0.43
1:A:181:ILE:C	1:A:181:ILE:HD13	2.39	0.43
1:A:460:LEU:O	1:A:463:LEU:HB2	2.18	0.43
1:A:854:THR:HG23	1:A:855:THR:N	2.34	0.43
1:A:484:ILE:HA	1:A:485:PRO:HD3	1.86	0.43
1:A:713:ALA:HB2	1:A:1188:ILE:HD12	2.01	0.43
1:A:573:ARG:NH1	1:A:1241:ARG:HB2	2.33	0.43
1:A:134:ARG:CZ	1:A:259:PHE:CD2	3.02	0.43
1:A:36:LEU:CD2	1:A:40:ASN:HD21	2.32	0.43
1:A:1247:ILE:N	1:A:1247:ILE:CD1	2.81	0.43
1:A:948:GLN:O	1:A:952:GLN:HG3	2.17	0.43
1:A:154:VAL:HG12	1:A:258:ARG:HB2	2.00	0.43
1:A:49:ALA:CB	1:A:123:VAL:HG11	2.44	0.43
1:A:1183:ARG:HB2	1:A:1183:ARG:HH21	1.84	0.43
1:A:106:THR:HG23	1:A:107:ASP:N	2.33	0.43
1:A:1033:LEU:HD12	1:A:1033:LEU:HA	1.63	0.43
1:A:115:PHE:O	1:A:118:GLU:N	2.52	0.43
1:A:617:PHE:C	1:A:618:ARG:HG2	2.38	0.43
1:A:35:GLU:HA	1:A:38:ILE:HG12	2.01	0.43
1:A:846:CYS:SG	1:A:926:PHE:HA	2.59	0.43
1:A:967:VAL:CA	1:A:1081:THR:HG22	2.46	0.43
1:A:790:PHE:HB2	1:A:915:CYS:SG	2.59	0.43
1:A:782:THR:HG21	1:A:784:ALA:HB3	2.01	0.43
1:A:1126:TRP:O	1:A:1126:TRP:CD2	2.72	0.43
1:A:465:GLY:HA2	1:A:470:GLU:OE1	2.19	0.43
1:A:824:MET:HE1	1:A:1040:ILE:HD11	2.00	0.43
1:A:960:VAL:HG22	1:A:961:THR:N	2.33	0.43
1:A:449:GLY:O	1:A:452:THR:HG22	2.18	0.43
1:A:1057:LEU:N	1:A:1057:LEU:HD23	2.32	0.43
1:A:795:ALA:O	1:A:798:ALA:HB3	2.19	0.43
1:A:181:ILE:HG13	1:A:253:VAL:HG23	2.01	0.43
1:A:80:THR:CG2	1:A:82:PHE:HB2	2.49	0.43
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.71	0.42
1:A:964:LEU:O	1:A:1088:ARG:NH2	2.52	0.42
1:A:79:GLN:HG2	1:A:128:GLU:HB3	2.01	0.42
1:A:220:MET:CE	1:A:220:MET:HA	2.49	0.42
1:A:169:ILE:CD1	1:A:229:LEU:HD11	2.47	0.42
1:A:589:PHE:CZ	1:A:645:VAL:HB	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:HB	1:A:363:HIS:NE2	2.34	0.42
1:A:820:SER:O	1:A:824:MET:HE2	2.19	0.42
1:A:996:LEU:HD12	1:A:996:LEU:HA	1.78	0.42
1:A:874:THR:HG22	1:A:923:ASN:OD1	2.19	0.42
1:A:250:ASN:ND2	1:A:250:ASN:N	2.64	0.42
1:A:954:ARG:NH1	1:A:1049:THR:HB	2.34	0.42
1:A:1192:THR:HG22	1:A:1250:SER:HA	2.01	0.42
1:A:307:HIS:CD2	1:A:391:ALA:N	2.75	0.42
1:A:290:PHE:N	1:A:292:ARG:NE	2.68	0.42
1:A:356:THR:HG21	1:A:481:ASP:CG	2.39	0.42
1:A:199:LEU:HA	1:A:216:VAL:HG21	2.01	0.42
1:A:276:VAL:HG23	1:A:314:ALA:HB2	2.02	0.42
1:A:35:GLU:HA	1:A:38:ILE:CG1	2.49	0.42
1:A:505:ILE:HG21	1:A:508:ARG:HD2	2.00	0.42
1:A:824:MET:O	1:A:828:LYS:HG3	2.19	0.42
1:A:77:ASN:O	1:A:130:ILE:HA	2.20	0.42
1:A:595:ILE:HD13	1:A:607:PHE:HE2	1.85	0.42
1:A:623:THR:O	1:A:648:ILE:HG22	2.19	0.42
1:A:156:VAL:CG1	1:A:166:VAL:HG12	2.48	0.42
1:A:773:TYR:CE2	1:A:775:ASP:HB3	2.55	0.42
1:A:982:GLU:HB3	1:A:990:PHE:CZ	2.54	0.42
1:A:658:ARG:NH1	1:A:658:ARG:HG3	2.34	0.42
1:A:135:VAL:HG22	1:A:136:ALA:N	2.35	0.42
1:A:502:VAL:O	1:A:1197:ARG:NH1	2.52	0.41
1:A:1157:ILE:O	1:A:1167:VAL:HA	2.20	0.41
1:A:991:GLU:O	1:A:994:MET:N	2.52	0.41
1:A:1200:LEU:HD23	1:A:1200:LEU:HA	1.83	0.41
1:A:101:VAL:O	1:A:102:ALA:C	2.57	0.41
1:A:869:LEU:H	1:A:869:LEU:HD22	1.84	0.41
1:A:172:HIS:O	1:A:176:SER:HB2	2.20	0.41
1:A:872:ALA:O	1:A:922:TRP:HB2	2.19	0.41
1:A:777:SER:O	1:A:779:GLY:N	2.53	0.41
1:A:865:PHE:HA	1:A:868:ALA:HB3	2.01	0.41
1:A:641:ILE:HD13	1:A:642:LYS:N	2.35	0.41
1:A:93:ALA:HA	1:A:96:VAL:CG1	2.47	0.41
1:A:1121:ASN:O	1:A:1124:TYR:HB3	2.21	0.41
1:A:503:PHE:CD1	1:A:503:PHE:N	2.88	0.41
1:A:300:GLY:HA3	1:A:383:MET:SD	2.60	0.41
1:A:414:TYR:HB3	1:A:483:TYR:CE2	2.56	0.41
1:A:380:ALA:O	1:A:381:ALA:HB2	2.21	0.41
1:A:369:HIS:CE1	1:A:406:LEU:HD23	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ILE:CG1	1:A:897:ILE:O	2.69	0.41
1:A:97:LEU:O	1:A:101:VAL:HG23	2.21	0.41
1:A:575:GLN:H	1:A:575:GLN:HG2	1.73	0.41
1:A:1173:ASN:HD21	1:A:1175:PHE:HB2	1.85	0.41
1:A:323:THR:O	1:A:323:THR:HG22	2.21	0.41
1:A:741:ASN:ND2	1:A:742:SER:H	2.15	0.41
1:A:586:HIS:HB2	1:A:653:MET:HE3	2.03	0.41
1:A:949:THR:CG2	1:A:953:ARG:HH12	2.32	0.41
1:A:641:ILE:HD13	1:A:642:LYS:C	2.42	0.41
1:A:837:PRO:HD3	1:A:989:TRP:CE2	2.56	0.41
1:A:9:VAL:HA	1:A:12:LEU:HD23	2.02	0.41
1:A:35:GLU:O	1:A:38:ILE:HG13	2.21	0.41
1:A:935:ARG:NH2	1:A:1024:GLU:OE2	2.45	0.41
1:A:304:HIS:HB3	1:A:307:HIS:CG	2.55	0.41
1:A:224:THR:O	1:A:225:GLY:C	2.60	0.40
1:A:949:THR:HG23	1:A:953:ARG:HH12	1.86	0.40
1:A:305:VAL:HG13	1:A:306:ASP:N	2.36	0.40
1:A:30:ALA:HB1	1:A:36:LEU:HB3	2.03	0.40
1:A:66:ILE:HD12	1:A:66:ILE:C	2.41	0.40
1:A:1057:LEU:HD11	1:A:1065:LEU:HD22	2.03	0.40
1:A:195:TYR:OH	1:A:213:GLU:HG2	2.21	0.40
1:A:312:LEU:O	1:A:312:LEU:HD23	2.21	0.40
1:A:236:MET:HG3	1:A:608:PHE:CZ	2.55	0.40
1:A:1066:ARG:HG2	1:A:1076:THR:HG21	2.03	0.40
1:A:930:ILE:HD13	1:A:930:ILE:N	2.36	0.40
1:A:752:ARG:N	1:A:763:ASN:HD21	2.09	0.40
1:A:210:GLU:CD	1:A:210:GLU:N	2.66	0.40
1:A:120:VAL:HA	1:A:123:VAL:CG1	2.47	0.40
1:A:414:TYR:CE1	1:A:485:PRO:HG2	2.57	0.40
1:A:174:ALA:O	1:A:258:ARG:NH1	2.53	0.40
1:A:157:ALA:C	1:A:254:THR:HG23	2.42	0.40
1:A:229:LEU:HD22	1:A:242:VAL:HG11	2.03	0.40
1:A:521:ILE:O	1:A:521:ILE:CG2	2.68	0.40
1:A:37:ALA:HA	1:A:40:ASN:OD1	2.20	0.40
1:A:211:ILE:O	1:A:215:MET:HG3	2.22	0.40
1:A:408:ARG:O	1:A:408:ARG:HD3	2.21	0.40
1:A:82:PHE:HE1	1:A:406:LEU:HB2	1.86	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	1192/1289 (92%)	1045 (88%)	120 (10%)	27 (2%)	8	26

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ALA
1	A	778	LEU
1	A	806	ARG
1	A	970	SER
1	A	19	GLY
1	A	34	ILE
1	A	68	GLY
1	A	618	ARG
1	A	780	ILE
1	A	809	TYR
1	A	854	THR
1	A	895	SER
1	A	1074	PHE
1	A	116	GLU
1	A	176	SER
1	A	1263	SER
1	A	381	ALA
1	A	547	ARG
1	A	704	SER
1	A	1130	ASP
1	A	813	PHE
1	A	868	ALA
1	A	679	GLY
1	A	201	ILE
1	A	225	GLY
1	A	1235	ILE
1	A	531	GLY

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	993/1060 (94%)	831 (84%)	162 (16%)	3 8

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	10	LYS
1	A	12	LEU
1	A	13	ARG
1	A	24	LYS
1	A	29	GLU
1	A	34	ILE
1	A	36	LEU
1	A	39	GLU
1	A	74	LEU
1	A	76	VAL
1	A	80	THR
1	A	130	ILE
1	A	134	ARG
1	A	141	ASP
1	A	143	LEU
1	A	151	ARG
1	A	152	ILE
1	A	155	LEU
1	A	165	LEU
1	A	166	VAL
1	A	169	ILE
1	A	176	SER
1	A	181	ILE
1	A	196	GLN
1	A	200	ASP
1	A	210	GLU
1	A	220	MET
1	A	224	THR
1	A	228	SER

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Mol	Chain	Res	Type
1	A	229	LEU
1	A	235	VAL
1	A	237	GLU
1	A	239	SER
1	A	240	LYS
1	A	250	ASN
1	A	254	THR
1	A	258	ARG
1	A	270	THR
1	A	286	SER
1	A	292	ARG
1	A	298	ASN
1	A	307	HIS
1	A	312	LEU
1	A	355	ASP
1	A	364	VAL
1	A	378	THR
1	A	387	ILE
1	A	390	VAL
1	A	399	GLN
1	A	400	THR
1	A	433	LEU
1	A	436	MET
1	A	438	VAL
1	A	443	SER
1	A	452	THR
1	A	454	ILE
1	A	455	VAL
1	A	502	VAL
1	A	504	SER
1	A	508	ARG
1	A	520	ILE
1	A	529	ILE
1	A	530	VAL
1	A	535	THR
1	A	537	LYS
1	A	548	LYS
1	A	563	LEU
1	A	575	GLN
1	A	583	ILE
1	A	593	VAL
1	A	595	ILE

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Mol	Chain	Res	Type
1	A	605	THR
1	A	614	GLN
1	A	619	THR
1	A	622	VAL
1	A	623	THR
1	A	628	LEU
1	A	632	VAL
1	A	641	ILE
1	A	646	THR
1	A	662	ARG
1	A	705	LEU
1	A	715	THR
1	A	717	ILE
1	A	719	VAL
1	A	720	GLU
1	A	733	LEU
1	A	741	ASN
1	A	750	SER
1	A	762	ILE
1	A	769	ILE
1	A	780	ILE
1	A	791	LEU
1	A	794	GLU
1	A	796	GLU
1	A	799	LEU
1	A	800	THR
1	A	806	ARG
1	A	809	TYR
1	A	816	SER
1	A	822	ILE
1	A	831	LYS
1	A	832	LEU
1	A	833	ILE
1	A	839	VAL
1	A	857	ASN
1	A	859	SER
1	A	869	LEU
1	A	873	CYS
1	A	881	VAL
1	A	887	SER
1	A	894	ILE
1	A	901	ASN

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Mol	Chain	Res	Type
1	A	905	THR
1	A	906	VAL
1	A	910	SER
1	A	916	ILE
1	A	930	ILE
1	A	933	ILE
1	A	938	LEU
1	A	949	THR
1	A	950	ILE
1	A	961	THR
1	A	962	ASN
1	A	967	VAL
1	A	991	GLU
1	A	992	VAL
1	A	996	LEU
1	A	997	ARG
1	A	1008	VAL
1	A	1012	GLU
1	A	1014	ILE
1	A	1016	SER
1	A	1021	TYR
1	A	1028	LEU
1	A	1033	LEU
1	A	1040	ILE
1	A	1044	ASP
1	A	1048	VAL
1	A	1049	THR
1	A	1076	THR
1	A	1077	ASN
1	A	1078	THR
1	A	1089	GLU
1	A	1093	LYS
1	A	1102	THR
1	A	1106	ILE
1	A	1110	ILE
1	A	1116	LEU
1	A	1128	THR
1	A	1151	GLN
1	A	1152	LEU
1	A	1172	ILE
1	A	1173	ASN
1	A	1182	ILE

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Mol	Chain	Res	Type
1	A	1185	VAL
1	A	1200	LEU
1	A	1210	ARG
1	A	1215	SER
1	A	1247	ILE
1	A	1249	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	77	ASN
1	A	79	GLN
1	A	114	GLN
1	A	250	ASN
1	A	304	HIS
1	A	307	HIS
1	A	399	GLN
1	A	403	HIS
1	A	536	GLN
1	A	558	ASN
1	A	614	GLN
1	A	714	ASN
1	A	729	ASN
1	A	741	ASN
1	A	763	ASN
1	A	857	ASN
1	A	862	HIS
1	A	871	GLN
1	A	901	ASN
1	A	946	ASN
1	A	948	GLN
1	A	952	GLN
1	A	963	ASN
1	A	1077	ASN
1	A	1094	HIS
1	A	1121	ASN
1	A	1122	ASN
1	A	1151	GLN
1	A	1155	ASN
1	A	1173	ASN
1	A	1178	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 ⓘ

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	1202/1289 (93%)	-0.15	31 (2%) 59 47	35, 75, 124, 148	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	807	PRO	4.6
1	A	1234	ALA	4.3
1	A	701	SER	4.0
1	A	161	ALA	3.8
1	A	810	SER	3.7
1	A	700	SER	3.5
1	A	4	ILE	3.2
1	A	285	MET	3.1
1	A	268	VAL	3.0
1	A	1216	ASN	3.0
1	A	6	ALA	2.8
1	A	780	ILE	2.8
1	A	255	GLY	2.7
1	A	24	LYS	2.7
1	A	266	GLU	2.7
1	A	326	GLY	2.6
1	A	808	ASP	2.6
1	A	702	ARG	2.6
1	A	191	VAL	2.5
1	A	192	GLU	2.5
1	A	489	ARG	2.5
1	A	296	HIS	2.4
1	A	1236	ASP	2.4
1	A	1237	GLN	2.4
1	A	252	GLU	2.3
1	A	778	LEU	2.2
1	A	186	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	56	VAL	2.1
1	A	181	ILE	2.1
1	A	1238	LEU	2.1
1	A	269	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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
2	CA	A	2001	1/1	0.97	0.22	-	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.