



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:52 PM UTC

PDB ID : 3AGP / pdb_00003agp
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

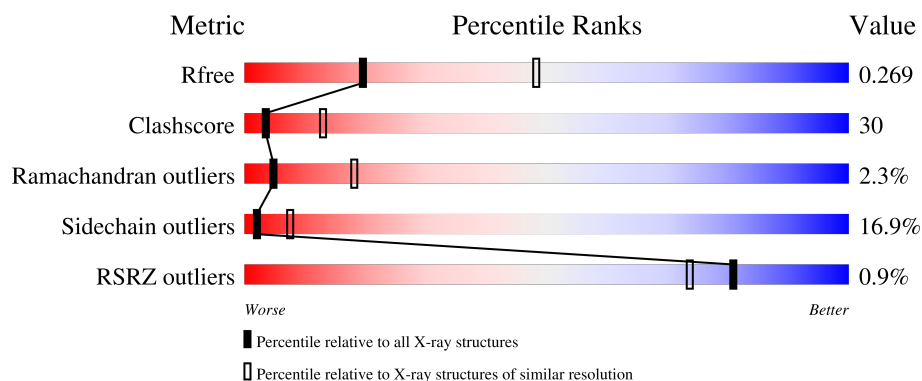
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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 $\leq 5\%$. 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	46% 37% 10% 7%

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 (CCD ID: CA) (formula: Ca).

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

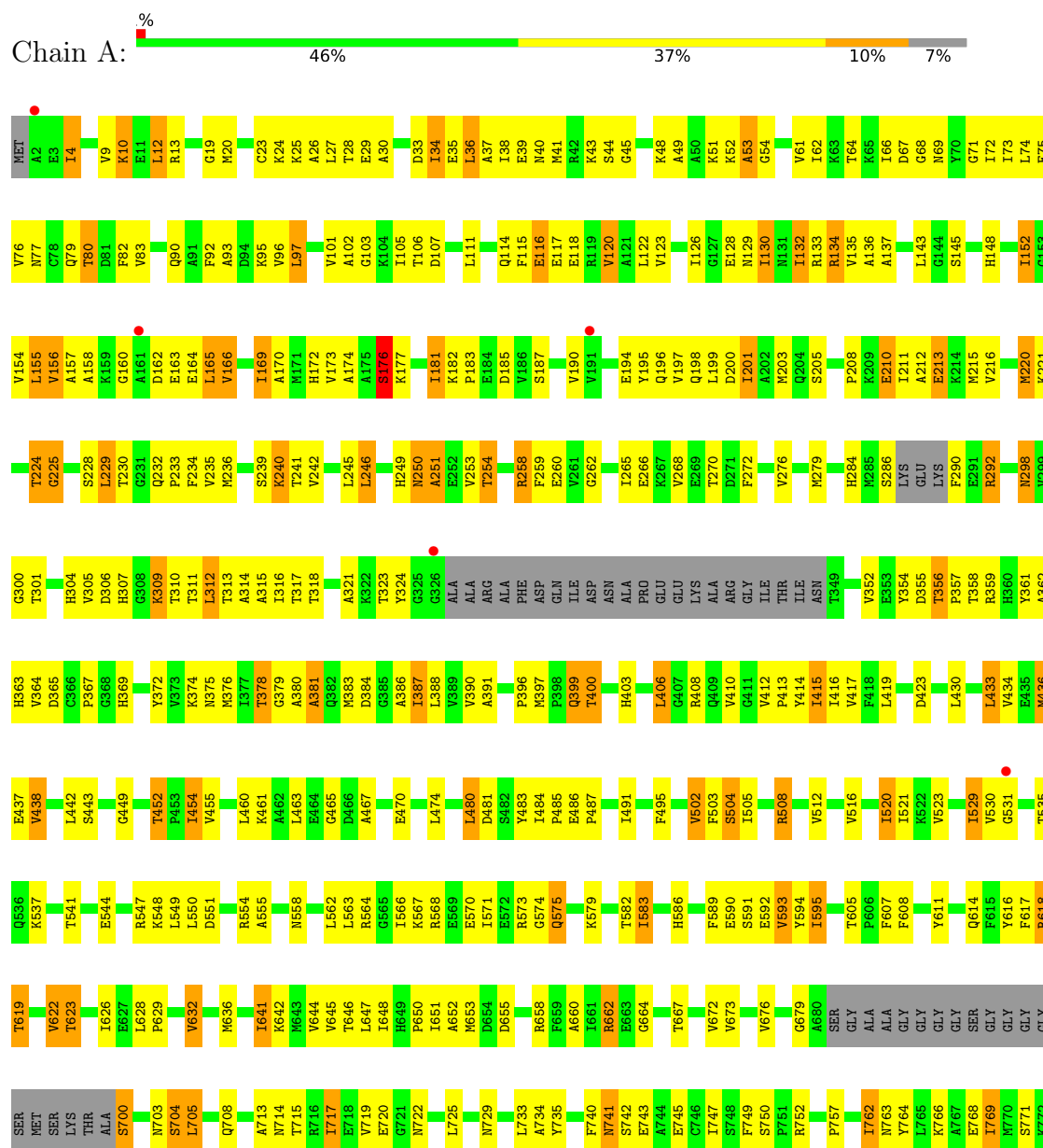
- Molecule 3 is water.

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

3 Residue-property plots

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 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: Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase



PHE	I1188	R1088	D995	P920	E840	Y773
GLN	T1189	E1089	L996	G921	G841	D774
THR	T1192	S1090	R997	N922	M842	D775
LYS	R1193	K1093	P999	N923	L843	F776
VAL	D1194	H1094	L1003	F926	C846	S777
ALA	R1195	H1095	P1004	Q927	R847	L778
SER	E1196	Y1096	V1008	T930	F848	G779
LEU	R1197	V1099	E1012	G931	S849	I780
HIS	L1200	D1100	K1013	G932	T853	D781
GLU	R1210	Y1101	E1014	I933	T854	T782
ALA	G1211	T1102	T1015	I934	T855	E783
HIS	L1212	Y1105	S1016	R935	M856	A784
HIS	S1215	T1106	M1017	L938	M857	V785
HIS	N1216	R1109	Y1021	I943	S859	A786
ASP	GLY	I1110	T1022	D947	H862	W787
LEU	PRO	L1116	F1023	Q948	S863	E788
PRO	LEU	L1121	E1024	T949	S864	K789
ARG	GLY	Y1124	L1028	N951	F865	F790
PRO	SER	W1125	T1029	Q952	K866	L791
GLY	GLY	A1127	F1030	R953	F867	E794
ASP	SER	T1128	L1033	R954	A868	A795
SER	ALA	I1129	T1040	A955	L869	E796
ALA	ASP	D1130	L1041	Q871	P870	C797
ASP	LEU	R1136	D1042	G958	T874	A798
PHE	PHE	K1143	L1043	S959	V881	L799
A1234	I1235	Y1144	D1044	T961	S887	T800
R1241	R1242	K1150	S1046	N962	T892	N801
HIS	N1243	Q1151	E1047	L964	R893	A802
HIS	P1244	L1152	Y1048	A965	T894	L804
HIS	T1245	L1157	T1049	T966	S896	Y805
HIS	K1246	A1165	V1055	D967	D896	A806
HIS	I1247	L1166	I1056	L969	T897	P807
HIS	S1248	V1167	L1057	S970	F900	D808
HIS	R1249	I1172	P1068	A971	N901	Y809
HIS	S1250	R1173	V1067	L978	T905	S810
HIS	F1254	P1174	V1068	A979	V906	E811
HIS	S1263	F1175	V1072	L980	T906	D812
HIS	R1264	R1179	G1073	A999	T906	F813
HIS	VAL	L1182	F1074	G988	N909	N814
HIS	LEU	ALA	T1075	W989	S910	F815
HIS	ALA	PRO	T1076	F990	K911	S816
HIS	PRO	TYR	N1077	E991	T912	L817
HIS	TYR	VAL	T1078	V992	T913	T822
HIS	VAL	VAL	T1081	M994	T914	H823
					T915	M824
					T916	K828
					T917	K831
					T918	L832
					T919	T833
					T920	G834
					T921	D835
					T922	V836
					T923	P837
					T924	S838
					T925	V839

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 19.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.90-2.80) 97.9 (19.90-2.80)	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 0.210 , 0.269	Depositor DCC
R_{free} test set	2230 reflections (4.96%)	wwPDB-VP
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 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
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
F_o, F_c correlation	0.95	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.49	0/9443	0.90	16/12771 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	910	SER	N-CA-C	-7.27	104.54	113.41
1	A	1243	ASN	N-CA-C	7.01	119.76	110.36
1	A	1243	ASN	CA-C-N	6.93	128.50	119.84
1	A	1243	ASN	C-N-CA	6.93	128.50	119.84
1	A	251	ALA	N-CA-C	6.91	120.43	109.65
1	A	309	LYS	N-CA-C	-6.80	104.85	113.01
1	A	783	GLU	N-CA-C	-5.76	106.11	114.12
1	A	998	SER	CA-C-N	5.61	125.14	119.19
1	A	998	SER	C-N-CA	5.61	125.14	119.19
1	A	784	ALA	N-CA-C	-5.57	105.30	111.71
1	A	1050	VAL	N-CA-C	5.54	116.65	108.45
1	A	1173	ASN	CA-C-N	5.27	124.89	119.56
1	A	1173	ASN	C-N-CA	5.27	124.89	119.56
1	A	814	ASN	N-CA-C	5.26	118.19	110.30
1	A	971	ALA	N-CA-C	-5.22	102.33	110.10
1	A	769	ILE	N-CA-C	5.02	116.34	110.62

There are no chirality outliers.

There are no planarity outliers.

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	9274	0	9256	550	0
2	A	1	0	0	0	0
3	A	36	0	0	3	0
All	All	9311	0	9256	550	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 30.

All (550) 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
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:H	1:A:399:GLN:HE21	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:914:ARG:HH22	1:A:1017:MET:HE2	1.40	0.86
1:A:558:ASN:HB3	1:A:1210:ARG:HG3	1.57	0.86
1:A:930:ILE:HD11	1:A:1021:TYR:HD2	1.40	0.86
1:A:700:SER:N	1:A:1179:ARG:HG2	1.91	0.86
1:A:947:ASP:OD1	1:A:949:THR:HB	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:824:MET:HE1	1:A:1040:ILE:CG1	2.11	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:210:GLU:CD	1:A:210:GLU:H	1.88	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:717:ILE:HD13	1:A:717:ILE:C	2.10	0.77
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:901:ASN:C	1:A:901:ASN:HD22	1.94	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: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
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: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:779:GLY:C	1:A:781:ASP:H	1.98	0.71
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: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:20:MET:HE3	1:A:20:MET:HA	1.74	0.69
1:A:93:ALA:HA	1:A:96:VAL:HG12	1.73	0.69
1:A:780:ILE:HD13	1:A:780:ILE:H	1.57	0.69
1:A:836:VAL:HG22	1:A:837:PRO:HD2	1.75	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:169:ILE:HD11	1:A:229:LEU:HD11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LYS:HE3	1:A:594:TYR:CZ	2.28	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:586:HIS:HB2	1:A:653:MET:HE2	1.74	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:148:HIS:HB3	1:A:152:ILE:HG22	1.75	0.67
1:A:930:ILE:HD11	1:A:1021:TYR:CB	2.24	0.67
1:A:949:THR:HG23	1:A:953:ARG:NH1	2.10	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:1173:ASN:C	1:A:1173:ASN:HD22	2.03	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:HD13	1:A:4:ILE:H	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:92:PHE:HE1	1:A:132:ILE:HD11	1.61	0.64
1:A:968:ASP:H	1:A:1081:THR:HG22	1.62	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:HE21	1:A:1151:GLN:H	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:611:TYR:HB3	1:A:626:ILE:HD11	1.79	0.63
1:A:1049:THR:HG22	1:A:1056:ILE:HB	1.78	0.63
1:A:130:ILE:O	1:A:130:ILE:HG12	1.96	0.63
1:A:775:ASP:OD2	1:A:1109:ARG:HD3	1.98	0.63
1:A:442:LEU:HD12	1:A:452:THR:HG21	1.81	0.63
1:A:824:MET:HE1	1:A:1040:ILE:HG12	1.80	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:784:ALA:O	1:A:788:GLU:HG3	1.99	0.63
1:A:853:THR:HG23	1:A:866:LYS:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:HG11	1:A:352:VAL:HG11	1.80	0.63
1:A:529:ILE:HG12	1:A:529:ILE:O	1.93	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:HG23	1:A:521:ILE:O	1.99	0.62
1:A:930:ILE:CD1	1:A:1021:TYR:HB3	2.27	0.62
1:A:148:HIS:HB3	1:A:152:ILE:CG2	2.29	0.61
1:A:1110:ILE:HD12	1:A:1116:LEU:HA	1.82	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:529:ILE:HD12	1:A:571:ILE:HG12	1.84	0.60
1:A:717:ILE:HD13	1:A:717:ILE:O	2.01	0.60
1:A:12:LEU:HD22	1:A:27:LEU:HD13	1.83	0.60
1:A:163:GLU:CD	1:A:163:GLU:H	2.09	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
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:41:MET:HA	1:A:44:SER:OG	2.02	0.59
1:A:399:GLN:HE21	1:A:399:GLN:N	1.92	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:25:LYS:O	1:A:28:THR:HG22	2.03	0.58
1:A:356:THR:HG23	1:A:357:PRO:HD2	1.86	0.58
1:A:967:VAL:HA	1:A:1081:THR:HG22	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:111:LEU:HD23	1:A:111:LEU:H	1.68	0.58
1:A:224:THR:HG23	1:A:225:GLY:N	2.17	0.58
1:A:806:ARG:N	1:A:807:PRO:HD2	2.13	0.58
1:A:833:ILE:HG23	1:A:989:TRP:CE2	2.39	0.58
1:A:309:LYS:HE3	1:A:365:ASP:OD2	2.04	0.58
1:A:589:PHE:CD1	1:A:673:VAL:HG12	2.39	0.58
1:A:629:PRO:HG2	1:A:632:VAL:CG1	2.34	0.58
1:A:52:LYS:O	1:A:54:GLY:N	2.37	0.57
1:A:842:MET:HE1	1:A:930:ILE:HG22	1.85	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: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:162:ASP:O	1:A:166:VAL:HG22	2.04	0.57
1:A:798:ALA:HA	1:A:1012:GLU:HG2	1.86	0.57
1:A:132:ILE:HD12	1:A:132:ILE:N	2.19	0.56
1:A:1100:ASP:OD1	1:A:1102:THR:CG2	2.45	0.56
1:A:700:SER:O	1:A:1179:ARG:HD2	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
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:24:LYS:HG3	1:A:430:LEU:HD11	1.86	0.56
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: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:134:ARG:NH2	1:A:259:PHE:CD2	2.75	0.55
1:A:262:GLY:HA2	1:A:265:ILE:HD12	1.89	0.55
1:A:809:TYR:C	1:A:811:GLU:H	2.13	0.55
1:A:1243:ASN:CB	1:A:1244:PRO:HD2	2.36	0.55
1:A:384:ASP:O	1:A:413:PRO:HG2	2.06	0.55
1:A:857:ASN:H	1:A:857:ASN:ND2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:33:ASP:OD1	1:A:36:LEU:HB2	2.06	0.54
1:A:229:LEU:CD2	1:A:242:VAL:HG11	2.37	0.54
1:A:423:ASP:OD2	1:A:461:LYS:HE2	2.07	0.54
1:A:961:THR:CG2	1:A:963:ASN:H	2.13	0.54
1:A:961:THR:HG23	1:A:963:ASN:N	2.15	0.54
1:A:195:TYR:CD1	1:A:195:TYR:C	2.84	0.54
1:A:798:ALA:CA	1:A:1012:GLU:HG2	2.37	0.54
1:A:930:ILE:CD1	1:A:1021:TYR:CD2	2.88	0.54
1:A:508:ARG:HD3	1:A:562:LEU:HD21	1.89	0.54
1:A:413:PRO:HB2	1:A:414:TYR:CD1	2.42	0.54
1:A:558:ASN:HB3	1:A:1210:ARG:CG	2.33	0.54
1:A:4:ILE:HD13	1:A:4:ILE:N	2.22	0.54
1:A:617:PHE:O	1:A:618:ARG:HG2	2.06	0.54
1:A:1110:ILE:CD1	1:A:1116:LEU:HA	2.37	0.54
1:A:221:LYS:O	1:A:224:THR:HG23	2.08	0.53
1:A:734:ALA:HB1	1:A:1136:ARG:O	2.07	0.53
1:A:794:GLU:HA	1:A:794:GLU:OE1	2.07	0.53
1:A:1245:THR:O	1:A:1246:LYS:HD3	2.08	0.53
1:A:66:ILE:O	1:A:66:ILE:HD12	2.09	0.53
1:A:1017:MET:HA	1:A:1022:THR:HG21	1.89	0.53
1:A:417:VAL:HG12	1:A:454:ILE:HG23	1.91	0.53
1:A:574:GLY:HA2	1:A:619:THR:HG22	1.90	0.53
1:A:747:ILE:HG22	1:A:771:SER:HA	1.91	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:1055:ILE:C	1:A:1056:ILE:HD12	2.34	0.53
1:A:951:ASN:OD1	1:A:1049:THR:HG23	2.09	0.52
1:A:954:ARG:HH11	1:A:1049:THR:CG2	2.22	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: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:930:ILE:HA	1:A:933:ILE:HG23	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:LEU:HD23	1:A:1057:LEU:H	1.74	0.52
1:A:365:ASP:C	1:A:367:PRO:HD3	2.34	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:436:MET:HA	1:A:436:MET:HE2	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:12:LEU:HG	1:A:13:ARG:N	2.25	0.51
1:A:593:VAL:HG22	1:A:641:ILE:HG22	1.92	0.51
1:A:1173:ASN:ND2	1:A:1175:PHE:N	2.53	0.51
1:A:369:HIS:NE2	1:A:406:LEU:HD23	2.25	0.51
1:A:901:ASN:C	1:A:901:ASN:ND2	2.67	0.51
1:A:1021:TYR:CD1	1:A:1021:TYR:C	2.88	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:676:VAL:HG23	1:A:676:VAL:O	2.10	0.51
1:A:1024:GLU:OE1	1:A:1024:GLU:N	2.40	0.51
1:A:593:VAL:HG22	1:A:641:ILE:CG2	2.40	0.51
1:A:806:ARG:N	1:A:807:PRO:CD	2.68	0.51
1:A:853:THR:CG2	1:A:866:LYS:HE2	2.40	0.51
1:A:200:ASP:O	1:A:201:ILE:C	2.53	0.51
1:A:412:VAL:HG13	1:A:412:VAL:O	2.11	0.51
1:A:541:THR:CG2	1:A:564:ARG:HB3	2.36	0.51
1:A:987:PRO:HD2	3:A:2007:HOH:O	2.09	0.51
1:A:1182:ILE:HG13	1:A:1184:TYR:CE2	2.45	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:930:ILE:HD11	1:A:1021:TYR:CG	2.44	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
1:A:152:ILE:HB	1:A:260:GLU:HG3	1.93	0.51
1:A:703:ASN:C	1:A:705:LEU:H	2.18	0.51
1:A:1045:SER:O	1:A:1048:VAL:HG13	2.10	0.51
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:416:ILE:HD12	1:A:480:LEU:HD12	1.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ILE:HG12	1:A:897:ILE:O	2.10	0.50
1:A:1030:PHE:HE2	1:A:1074:PHE:CE1	2.30	0.50
1:A:148:HIS:NE2	1:A:636:MET:HG3	2.26	0.50
1:A:158:ALA:HA	1:A:253:VAL:HA	1.94	0.50
1:A:279:MET:SD	1:A:311:THR:HG22	2.52	0.50
1:A:558:ASN:HD22	1:A:1210:ARG:HH21	1.60	0.50
1:A:862:HIS:CD2	1:A:864:SER:H	2.29	0.50
1:A:246:LEU:O	1:A:249:HIS:O	2.29	0.50
1:A:824:MET:HE1	1:A:1040:ILE:HG13	1.92	0.50
1:A:949:THR:CG2	1:A:953:ARG:NH1	2.75	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:359:ARG:HD2	1:A:361:TYR:OH	2.12	0.49
1:A:516:VAL:HG13	1:A:555:ALA:HA	1.94	0.49
1:A:579:LYS:O	1:A:582:THR:HB	2.12	0.49
1:A:714:ASN:ND2	1:A:1254:PHE:H	2.06	0.49
1:A:194:GLU:HA	1:A:197:VAL:HG12	1.94	0.49
1:A:399:GLN:H	1:A:399:GLN:NE2	1.96	0.49
1:A:232:GLN:O	1:A:242:VAL:HG23	2.11	0.49
1:A:1110:ILE:HD11	1:A:1116:LEU:CG	2.41	0.49
1:A:165:LEU:O	1:A:169:ILE:HG22	2.12	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:900:PHE:HE2	1:A:1008:VAL:HG12	1.77	0.49
1:A:930:ILE:HD13	1:A:931:GLY:N	2.28	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:H	1:A:132:ILE:CD1	2.26	0.49
1:A:1182:ILE:HD12	1:A:1183:ARG:N	2.28	0.49
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:12:LEU:HD11	1:A:23:CYS:SG	2.53	0.49
1:A:276:VAL:HG21	1:A:313:THR:HG23	1.95	0.49
1:A:967:VAL:CG2	1:A:1055:ILE:HB	2.36	0.49
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:914:ARG:HH12	1:A:1017:MET:HG3	1.78	0.48
1:A:220:MET:HA	1:A:220:MET:HE2	1.95	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:52:LYS:C	1:A:54:GLY:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1234:ALA:C	1:A:1235:ILE:HG12	2.39	0.48
1:A:181:ILE:HD13	1:A:181:ILE:C	2.39	0.48
1:A:356:THR:CG2	1:A:358:THR:HG22	2.43	0.48
1:A:954:ARG:HD3	1:A:1049:THR:HG21	1.95	0.48
1:A:80:THR:HB	1:A:128:GLU:OE1	2.14	0.48
1:A:199:LEU:HD23	1:A:199:LEU:O	2.13	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:43:LYS:C	1:A:45:GLY:H	2.20	0.48
1:A:66:ILE:HG22	1:A:71:GLY:HA3	1.95	0.48
1:A:990:PHE:O	1:A:994:MET:HG2	2.14	0.48
1:A:177:LYS:HG2	1:A:258:ARG:NH2	2.29	0.48
1:A:313:THR:O	1:A:317:THR:HG23	2.13	0.48
1:A:317:THR:HG22	1:A:354:TYR:HD1	1.79	0.48
1:A:617:PHE:C	1:A:618:ARG:HG2	2.38	0.48
1:A:1173:ASN:ND2	1:A:1173:ASN:C	2.70	0.48
1:A:10:LYS:HB3	1:A:433:LEU:HD11	1.96	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:64:THR:HG21	1:A:145:SER:HB2	1.96	0.47
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: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:783:GLU:OE1	1:A:905:THR:HG21	2.15	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:966:THR:HG22	1:A:1056:ILE:HG13	1.95	0.47
1:A:160:GLY:O	1:A:251:ALA:HB2	2.15	0.47
1:A:568:ARG:HD2	1:A:568:ARG:O	2.15	0.47
1:A:805:TYR:O	1:A:806:ARG:CB	2.63	0.47
1:A:284:HIS:CE1	1:A:318:THR:HG22	2.49	0.47
1:A:356:THR:HG21	1:A:481:ASP:CG	2.39	0.47
1:A:233:PRO:HA	1:A:241:THR:HA	1.97	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
1:A:1057:LEU:CD1	1:A:1065:LEU:HD22	2.45	0.46
1:A:101:VAL:O	1:A:102:ALA:C	2.57	0.46
1:A:795:ALA:O	1:A:799:LEU:HD22	2.14	0.46
1:A:968:ASP:N	1:A:1081:THR:HG22	2.29	0.46
1:A:134:ARG:CG	1:A:134:ARG:NH2	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ILE:CD1	1:A:554:ARG:HG3	2.42	0.46
1:A:779:GLY:C	1:A:781:ASP:N	2.65	0.46
1:A:41:MET:HA	1:A:44:SER:HG	1.80	0.46
1:A:210:GLU:CD	1:A:210:GLU:N	2.66	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:HG22	1:A:1235:ILE:O	2.15	0.46
1:A:45:GLY:HA2	1:A:48:LYS:HD3	1.96	0.46
1:A:523:VAL:HG13	1:A:551:ASP:O	2.16	0.46
1:A:909:ASN:HB2	1:A:912:THR:HG22	1.98	0.46
1:A:1150:LYS:HD2	1:A:1150:LYS:H	1.81	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: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:111:LEU:HA	1:A:114:GLN:HB3	1.98	0.45
1:A:361:TYR:CZ	1:A:480:LEU:HB3	2.51	0.45
1:A:641:ILE:HD13	1:A:642:LYS:C	2.42	0.45
1:A:66:ILE:HD12	1:A:66:ILE:C	2.41	0.45
1:A:73:ILE:HG23	1:A:73:ILE:O	2.17	0.45
1:A:224:THR:O	1:A:225:GLY:C	2.60	0.45
1:A:786:ALA:O	1:A:789:LYS:HB2	2.15	0.45
1:A:745:GLU:O	1:A:745:GLU:HG2	2.17	0.45
1:A:36:LEU:HD23	1:A:40:ASN:HD21	1.82	0.45
1:A:417:VAL:HB	1:A:454:ILE:HD13	1.97	0.45
1:A:838:SER:HB2	1:A:840:GLU:CG	2.45	0.45
1:A:839:VAL:O	1:A:843:LEU:HD23	2.17	0.45
1:A:1003:LEU:HB3	1:A:1004:PRO:HD2	1.99	0.45
1:A:1183:ARG:NH2	1:A:1183:ARG:HB2	2.31	0.45
1:A:53:ALA:HA	1:A:129:ASN:ND2	2.32	0.45
1:A:157:ALA:C	1:A:254:THR:HG23	2.42	0.45
1:A:304:HIS:CD2	1:A:305:VAL:HG12	2.52	0.45
1:A:650:PRO:O	1:A:651:ILE:HG12	2.16	0.45
1:A:920:PRO:O	1:A:923:ASN:HB2	2.17	0.45
1:A:133:ARG:CG	1:A:134:ARG:H	2.12	0.45
1:A:324:TYR:CE2	1:A:357:PRO:HG3	2.52	0.45
1:A:833:ILE:HG21	1:A:833:ILE:HD13	1.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:486:GLU:HA	1:A:487:PRO:HD2	1.83	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:705:LEU:HD22	1:A:705:LEU:HA	1.75	0.44
1:A:749:PHE:CE1	1:A:766:LYS:HG2	2.52	0.44
1:A:773:TYR:HB3	1:A:776:PHE:CE1	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:67:ASP:O	1:A:69:ASN:N	2.50	0.44
1:A:794:GLU:OE1	1:A:1013:LYS:HD3	2.18	0.44
1:A:1151:GLN:H	1:A:1151:GLN:NE2	2.12	0.44
1:A:386:ALA:HB3	1:A:415:ILE:HG12	1.99	0.44
1:A:622:VAL:HG11	1:A:651:ILE:HG13	1.98	0.44
1:A:848:PHE:HD2	1:A:867:PHE:CZ	2.36	0.44
1:A:4:ILE:H	1:A:4:ILE:CD1	2.29	0.44
1:A:549:LEU:C	1:A:550:LEU:HD23	2.43	0.44
1:A:998:SER:HA	1:A:999:PRO:HD2	1.83	0.44
1:A:61:VAL:HG11	1:A:90:GLN:NE2	2.33	0.44
1:A:154:VAL:HG21	1:A:170:ALA:O	2.18	0.44
1:A:616:TYR:HB3	1:A:660:ALA:HB3	1.99	0.44
1:A:768:GLU:HB3	1:A:1105:TYR:CE1	2.52	0.44
1:A:833:ILE:HG23	1:A:989:TRP:NE1	2.33	0.44
1:A:1172:ILE:HD13	1:A:1172:ILE:HA	1.64	0.44
1:A:1234:ALA:O	1:A:1235:ILE:HG12	2.17	0.44
1:A:37:ALA:O	1:A:41:MET:HG3	2.18	0.44
1:A:495:PHE:CE2	1:A:521:ILE:HB	2.53	0.44
1:A:508:ARG:HE	1:A:562:LEU:HD11	1.81	0.44
1:A:833:ILE:CG2	1:A:989:TRP:NE1	2.81	0.44
1:A:901:ASN:HB2	1:A:918:ILE:O	2.18	0.44
1:A:301:THR:HA	1:A:387:ILE:HG23	1.99	0.43
1:A:836:VAL:HG22	1:A:837:PRO:CD	2.46	0.43
1:A:958:GLY:HA2	1:A:961:THR:HG22	2.00	0.43
1:A:460:LEU:O	1:A:463:LEU:HB2	2.18	0.43
1:A:484:ILE:HA	1:A:485:PRO:HD3	1.86	0.43
1:A:573:ARG:NH1	1:A:1241:ARG:HB2	2.33	0.43
1:A:713:ALA:HB2	1:A:1188:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:THR:HG23	1:A:855:THR:N	2.34	0.43
1:A:36:LEU:CD2	1:A:40:ASN:HD21	2.32	0.43
1:A:134:ARG:CZ	1:A:259:PHE:CD2	3.02	0.43
1:A:154:VAL:HG12	1:A:258:ARG:HB2	2.00	0.43
1:A:948:GLN:O	1:A:952:GLN:HG3	2.17	0.43
1:A:1021:TYR:C	1:A:1021:TYR:HD1	2.26	0.43
1:A:1247:ILE:N	1:A:1247:ILE:CD1	2.81	0.43
1:A:49:ALA:CB	1:A:123:VAL:HG11	2.44	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:1183:ARG:HB2	1:A:1183:ARG:HH21	1.84	0.43
1:A:35:GLU:HA	1:A:38:ILE:HG12	2.01	0.43
1:A:83:VAL:HG21	1:A:128:GLU:CD	2.44	0.43
1:A:115:PHE:O	1:A:118:GLU:N	2.52	0.43
1:A:846:CYS:SG	1:A:926:PHE:HA	2.59	0.43
1:A:782:THR:HG21	1:A:784:ALA:HB3	2.01	0.43
1:A:790:PHE:HB2	1:A:915:CYS:SG	2.59	0.43
1:A:848:PHE:O	1:A:849:SER:HB2	2.17	0.43
1:A:967:VAL:CA	1:A:1081:THR:HG22	2.46	0.43
1:A:1126:TRP:CD2	1:A:1126:TRP:O	2.72	0.43
1:A:465:GLY:HA2	1:A:470:GLU:OE1	2.19	0.43
1:A:449:GLY:O	1:A:452:THR:HG22	2.18	0.43
1:A:960:VAL:HG22	1:A:961:THR:N	2.33	0.43
1:A:1057:LEU:HD23	1:A:1057:LEU:N	2.32	0.43
1:A:80:THR:CG2	1:A:82:PHE:HB2	2.49	0.43
1:A:95:LYS:C	1:A:97:LEU:H	2.27	0.43
1:A:181:ILE:HG13	1:A:253:VAL:HG23	2.01	0.43
1:A:795:ALA:O	1:A:798:ALA:HB3	2.19	0.43
1:A:79:GLN:HG2	1:A:128:GLU:HB3	2.01	0.42
1:A:240:LYS:HZ2	1:A:240:LYS:HB2	1.84	0.42
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:169:ILE:CD1	1:A:229:LEU:HD11	2.47	0.42
1:A:220:MET:HA	1:A:220:MET:CE	2.49	0.42
1:A:790:PHE:CD1	1:A:790:PHE:C	2.97	0.42
1:A:301:THR:HB	1:A:363:HIS:NE2	2.34	0.42
1:A:589:PHE:CZ	1:A:645:VAL:HB	2.54	0.42
1:A:996:LEU:HA	1:A:996:LEU:HD12	1.78	0.42
1:A:233:PRO:O	1:A:234:PHE:C	2.61	0.42
1:A:250:ASN:N	1:A:250:ASN:ND2	2.64	0.42
1:A:874:THR:HG22	1:A:923:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:ILE:HD12	1:A:38:ILE:C	2.43	0.42
1:A:172:HIS:CD2	1:A:172:HIS:C	2.97	0.42
1:A:35:GLU:HA	1:A:38:ILE:CG1	2.49	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:290:PHE:N	1:A:292:ARG:NE	2.68	0.42
1:A:307:HIS:CD2	1:A:391:ALA:N	2.75	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:135:VAL:HG22	1:A:136:ALA:N	2.35	0.42
1:A:156:VAL:CG1	1:A:166:VAL:HG12	2.48	0.42
1:A:658:ARG:HG3	1:A:658:ARG:NH1	2.34	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:502:VAL:O	1:A:1197:ARG:NH1	2.52	0.41
1:A:991:GLU:O	1:A:994:MET:N	2.52	0.41
1:A:1157:ILE:O	1:A:1167:VAL:HA	2.20	0.41
1:A:1200:LEU:HD23	1:A:1200:LEU:HA	1.83	0.41
1:A:122:LEU:O	1:A:123:VAL:C	2.62	0.41
1:A:172:HIS:O	1:A:176:SER:HB2	2.20	0.41
1:A:869:LEU:H	1:A:869:LEU:HD22	1.84	0.41
1:A:314:ALA:O	1:A:315:ALA:C	2.63	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:872:ALA:O	1:A:922:TRP:HB2	2.19	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:300:GLY:HA3	1:A:383:MET:SD	2.60	0.41
1:A:503:PHE:CD1	1:A:503:PHE:N	2.88	0.41
1:A:1121:ASN:O	1:A:1124:TYR:HB3	2.21	0.41
1:A:380:ALA:O	1:A:381:ALA:HB2	2.21	0.41
1:A:414:TYR:HB3	1:A:483:TYR:CE2	2.56	0.41
1:A:97:LEU:O	1:A:101:VAL:HG23	2.21	0.41
1:A:369:HIS:CE1	1:A:406:LEU:HD23	2.55	0.41
1:A:575:GLN:H	1:A:575:GLN:HG2	1.73	0.41
1:A:717:ILE:C	1:A:717:ILE:CD1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ILE:O	1:A:897:ILE:CG1	2.69	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:1173:ASN:HD21	1:A:1175:PHE:HB2	1.85	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:315:ALA:O	1:A:316:ILE:C	2.64	0.41
1:A:837:PRO:HD3	1:A:989:TRP:CE2	2.56	0.41
1:A:853:THR:O	1:A:854:THR:C	2.64	0.41
1:A:935:ARG:NH2	1:A:1024:GLU:OE2	2.45	0.41
1:A:949:THR:CG2	1:A:953:ARG:HH12	2.32	0.41
1:A:304:HIS:HB3	1:A:307:HIS:CG	2.55	0.41
1:A:30:ALA:HB1	1:A:36:LEU:HB3	2.03	0.40
1:A:195:TYR:OH	1:A:213:GLU:HG2	2.21	0.40
1:A:305:VAL:HG13	1:A:306:ASP:N	2.36	0.40
1:A:312:LEU:O	1:A:312:LEU:HD23	2.21	0.40
1:A:949:THR:HG23	1:A:953:ARG:HH12	1.86	0.40
1:A:1057:LEU:HD11	1:A:1065:LEU:HD22	2.03	0.40
1:A:236:MET:HG3	1:A:608:PHE:CZ	2.55	0.40
1:A:809:TYR:C	1:A:811:GLU:N	2.80	0.40
1:A:1066:ARG:HG2	1:A:1076:THR:HG21	2.03	0.40
1:A:120:VAL:HA	1:A:123:VAL:CG1	2.47	0.40
1:A:174:ALA:O	1:A:258:ARG:NH1	2.53	0.40
1:A:414:TYR:CE1	1:A:485:PRO:HG2	2.57	0.40
1:A:752:ARG:N	1:A:763:ASN:HD21	2.09	0.40
1:A:930:ILE:HD13	1:A:930:ILE:N	2.36	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:229:LEU:HD22	1:A:242:VAL:HG11	2.03	0.40
1:A:408:ARG:HD3	1:A:408:ARG:O	2.21	0.40
1:A:521:ILE:O	1:A:521:ILE:CG2	2.68	0.40
1:A:586:HIS:CB	1:A:653:MET:HE2	2.44	0.40
1:A:82:PHE:HE1	1:A:406:LEU:HB2	1.86	0.40
1:A:160:GLY:C	1:A:251:ALA:HB2	2.46	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	1192/1289 (92%)	1045 (88%)	120 (10%)	27 (2%)	5	18

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%)	825 (83%)	168 (17%)	2 7

All (168) 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	29	GLU
1	A	34	ILE
1	A	36	LEU
1	A	74	LEU
1	A	76	VAL
1	A	80	THR
1	A	97	LEU
1	A	120	VAL
1	A	130	ILE
1	A	132	ILE
1	A	134	ARG
1	A	143	LEU
1	A	152	ILE
1	A	155	LEU
1	A	156	VAL
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	203	MET
1	A	210	GLU
1	A	213	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	239	SER
1	A	240	LYS
1	A	245	LEU
1	A	246	LEU
1	A	250	ASN
1	A	254	THR
1	A	258	ARG
1	A	266	GLU
1	A	268	VAL
1	A	270	THR
1	A	286	SER
1	A	292	ARG
1	A	298	ASN
1	A	312	LEU
1	A	355	ASP
1	A	356	THR
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	406	LEU
1	A	415	ILE
1	A	419	LEU
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	480	LEU
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

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Mol	Chain	Res	Type
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
1	A	605	THR
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	700	SER
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	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

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Mol	Chain	Res	Type
1	A	869	LEU
1	A	873	CYS
1	A	881	VAL
1	A	887	SER
1	A	893	ARG
1	A	894	ILE
1	A	901	ASN
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	943	ILE
1	A	949	THR
1	A	950	ILE
1	A	960	VAL
1	A	961	THR
1	A	967	VAL
1	A	984	LEU
1	A	991	GLU
1	A	992	VAL
1	A	996	LEU
1	A	1008	VAL
1	A	1014	ILE
1	A	1016	SER
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	1050	VAL
1	A	1076	THR
1	A	1078	THR
1	A	1093	LYS
1	A	1102	THR
1	A	1106	ILE
1	A	1110	ILE
1	A	1116	LEU
1	A	1128	THR

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Mol	Chain	Res	Type
1	A	1151	GLN
1	A	1152	LEU
1	A	1172	ILE
1	A	1173	ASN
1	A	1182	ILE
1	A	1185	VAL
1	A	1189	THR
1	A	1200	LEU
1	A	1210	ARG
1	A	1212	LEU
1	A	1215	SER
1	A	1247	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	55	ASN
1	A	79	GLN
1	A	114	GLN
1	A	250	ASN
1	A	298	ASN
1	A	304	HIS
1	A	307	HIS
1	A	382	GLN
1	A	399	GLN
1	A	403	HIS
1	A	536	GLN
1	A	558	ASN
1	A	614	GLN
1	A	649	HIS
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

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Mol	Chain	Res	Type
1	A	963	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 oligosaccharides 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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1202/1289 (93%)	-0.31	11 (0%) 81 74	35, 75, 124, 148	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	326	GLY	4.3
1	A	1235	ILE	4.0
1	A	1216	ASN	3.9
1	A	807	PRO	2.9
1	A	2	ALA	2.5
1	A	191	VAL	2.4
1	A	778	LEU	2.4
1	A	531	GLY	2.1
1	A	780	ILE	2.1
1	A	161	ALA	2.0
1	A	1234	ALA	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	2001	1/1	0.95	0.10	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.