



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:27 AM UTC

PDB ID : 2R7T / pdb_00002r7t
Title : Crystal Structure of Rotavirus SA11 VP1/RNA (UGUGAACC) Complex
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Deposited on : 2007-09-10
Resolution : 3.00 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

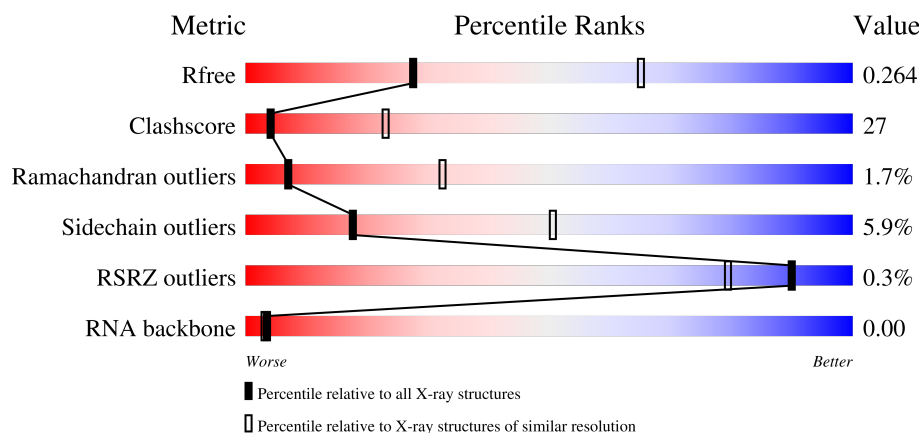
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	X	8	 88% 12%
2	A	1095	 47% 45% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8846 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 RNA chain called RNA (5'-R(*UP*GP*UP*GP*AP*AP*CP*C')-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	7	Total	C	N	O	P	0	0	0
			147	67	27	47	6			

- Molecule 2 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1073	Total	C	N	O	S	0	0	0
			8699	5579	1448	1634	38			

3 Residue-property plots

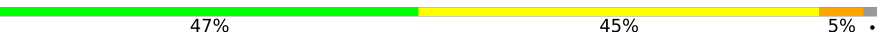
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

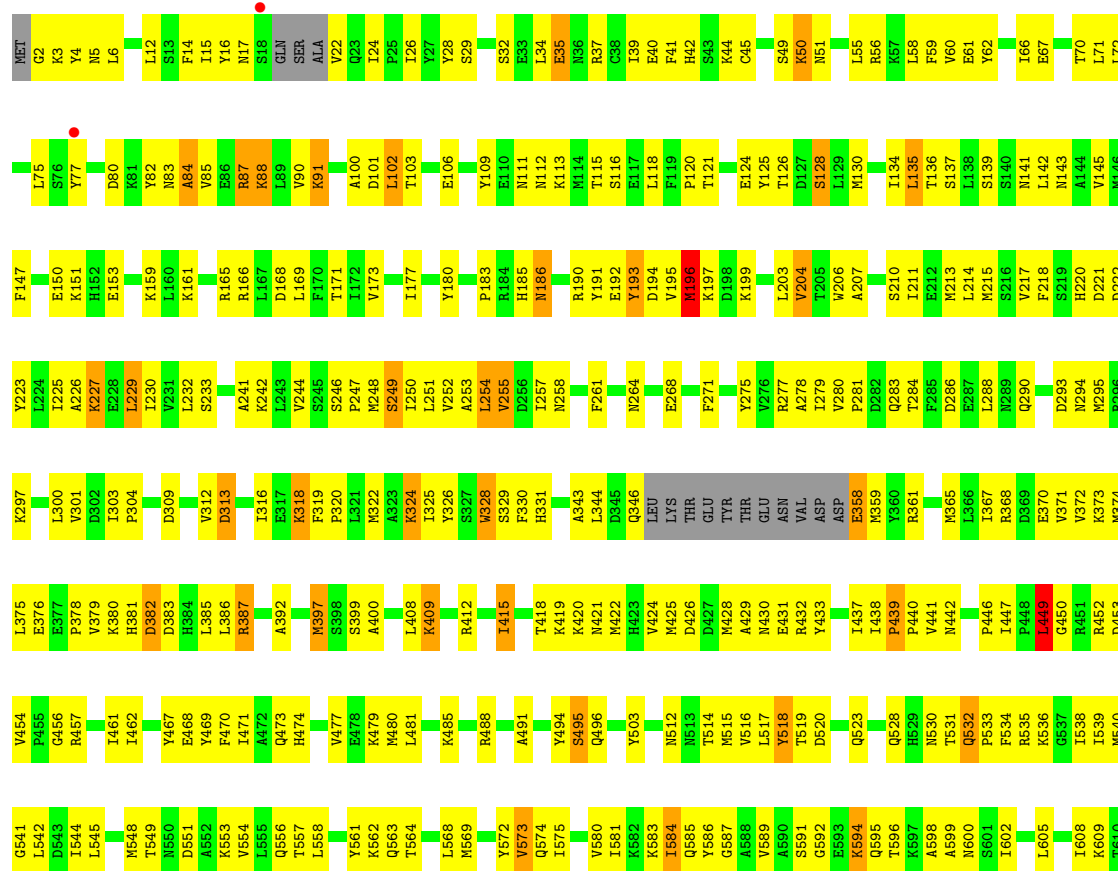
- Molecule 1: RNA (5'-R(*UP*GP*UP*GP*AP*AP*CP*C)-3')

Chain X: 



- Molecule 2: RNA-dependent RNA polymerase

Chain A: 



G1024	K1025	I1026	P1027	A1028	V1029	Y1036	A1037	K1047	N1048	G1049	S1053	L1054	F1055	C1056	N1057	Y1058	F1059	K1060	M1063	L1066	W1067	K1068	M1069	M1070	V1071	N1072	I1073	L1076	R1077	S1078	P1079	Y1080	F1086	Q1087	E1088	PRO	HIS	HIS	HIS	HIS	HIS									
V950	I951	S952	L953	H954	E957	I958	Q959	L962	I963	S964	I967	P968	K969	I970	D971	A972	D973	T974	Y975	G976	S977	S978	D984	K985	I988	L989	E990	S991	Y992	V993	S998	I999	N1000	C1003	Y1004	Q1005	L1006	F1007	D1008	F1009	P1012	K1016	L1017	I1018	R1019	I1020	P1021	K1023		
L858	T859	M860	L861	Q862	K863	P864	V865	T866	F867	K868	I872	T873	L878	R879	K882	P883	F884	F885	T886	V887	S888	L892	P893	I894	Q895	Y896	Q897	K898	F899	W900	T901	T902	L903	Y909	Y919	Q920	I921	E922	D923	D924	S928	A929	I930	S931	R932	L933	I934	V938	T944	E945
Y783	I784	Q785	R786	A787	F788	M789	S790	L791	Q794	I798	I802	A803	A804	T807	F808	K809	N810	Y811	V812	T813	E817	L820	F821	S822	K823	R824	N825	S828	R829	G830	I831	A832	K836	A837	K838	L839	N840	S841	Y842	A843	P844	I845	S846	L847	E848	K849	R850	R851	A852	Q853
S704	T705	Q706	W707	D708	Q709	I712	L713	Y714	Y717	I718	W719	W720	R721	L722	R723	E726	T727	D728	R729	E730	F731	I732	L733	T734	K735	I736	M737	Q738	M739	I744	T745	L748	R749	L750	E754	R755	V756	L757	T758	T762	F763	K764	F689	R690	A691	G692	L695	E699	K700	Q703
V611	L612	I615	S616	N617	K618	H619	S620	F621	A622	T623	I626	D629	A635	W636	L637	Q638	F639	I648	Q649	S652	N653	D654	Y659	K665	V666	K667	S671	T672	V673	G674	I675	E676	Y681	G684	I687	F688	F689	R690	A691	G692	L695	E699	K700	Q703						

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.65Å 112.53Å 143.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.4 (30.00-3.00) 87.4 (30.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.280 0.220 , 0.264	Depositor DCC
R_{free} test set	2025 reflections (7.93%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8846	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	X	0.45	0/164	2.28	17/254 (6.7%)
2	A	0.54	0/8870	1.04	40/11989 (0.3%)
All	All	0.54	0/9034	1.08	57/12243 (0.5%)

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	X	2	0

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	824	ASN	N-CA-C	25.26	138.82	111.28
1	X	1101	U	C2'-C3'-O3'	12.07	127.60	109.50
2	A	196	MET	N-CA-C	11.76	124.18	111.36
2	A	825	ASN	N-CA-C	11.22	123.51	111.28
1	X	1103	U	C2'-C3'-O3'	10.78	125.67	109.50
1	X	1102	G	C2'-C3'-O3'	10.61	125.42	109.50
2	A	823	LYS	CA-C-N	9.95	133.61	120.28
2	A	823	LYS	C-N-CA	9.95	133.61	120.28
2	A	254	LEU	N-CA-C	9.34	121.07	111.07
1	X	1107	C	C2'-C3'-O3'	9.03	123.05	109.50
2	A	757	LEU	N-CA-C	8.59	120.72	111.36
1	X	1105	A	C2'-C3'-O3'	8.54	126.51	113.70
2	A	67	GLU	N-CA-C	8.30	120.40	111.36
1	X	1102	G	C4'-C3'-O3'	8.14	121.61	109.40
1	X	1104	G	C2'-C3'-O3'	7.79	125.38	113.70
1	X	1106	A	C2'-C3'-O3'	7.60	125.10	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1026	ILE	CA-C-N	7.54	129.27	119.84
2	A	1026	ILE	C-N-CA	7.54	129.27	119.84
2	A	344	LEU	N-CA-C	7.45	119.40	111.28
1	X	1103	U	C4'-C3'-O3'	6.95	119.82	109.40
2	A	900	MET	CA-C-N	6.83	128.38	119.84
2	A	900	MET	C-N-CA	6.83	128.38	119.84
2	A	825	ASN	CA-C-N	-6.81	111.13	120.46
2	A	825	ASN	C-N-CA	-6.81	111.13	120.46
1	X	1101	U	C4'-C3'-O3'	6.68	119.43	109.40
2	A	1020	ILE	N-CA-C	6.66	114.75	108.15
2	A	823	LYS	N-CA-C	6.46	120.81	109.96
2	A	530	ASN	N-CA-C	6.37	118.22	111.28
2	A	328	TRP	N-CA-C	6.29	118.13	111.28
2	A	379	VAL	N-CA-C	6.22	117.00	110.72
1	X	1102	G	C4'-C3'-C2'	6.17	108.77	102.60
2	A	474	HIS	N-CA-C	6.16	118.00	111.28
1	X	1106	A	C4'-C3'-O3'	6.10	122.14	113.00
2	A	80	ASP	N-CA-C	-5.99	98.03	110.80
2	A	969	LYS	N-CA-C	5.93	117.75	111.28
2	A	32	SER	N-CA-C	5.83	118.11	111.11
2	A	88	LYS	CA-C-N	5.80	128.05	120.28
2	A	88	LYS	C-N-CA	5.80	128.05	120.28
1	X	1104	G	C4'-C3'-C2'	5.78	108.38	102.60
2	A	594	LYS	N-CA-C	-5.77	105.34	112.90
2	A	232	LEU	CA-C-N	5.55	127.72	120.28
2	A	232	LEU	C-N-CA	5.55	127.72	120.28
1	X	1105	A	C4'-C3'-O3'	5.54	121.31	113.00
2	A	88	LYS	N-CA-C	5.52	117.30	111.28
2	A	193	TYR	N-CA-C	5.50	117.28	111.28
2	A	15	ILE	N-CA-C	5.50	116.28	110.72
2	A	449	LEU	N-CA-C	5.50	118.37	109.40
2	A	975	TYR	N-CA-C	5.49	117.35	111.36
2	A	573	VAL	N-CA-C	5.49	117.31	108.85
2	A	204	VAL	N-CA-C	5.49	116.22	110.62
2	A	255	VAL	N-CA-C	5.30	117.27	109.63
1	X	1101	U	C4'-C3'-C2'	5.22	107.82	102.60
2	A	744	ILE	N-CA-C	-5.22	106.05	111.58
1	X	1104	G	C4'-C3'-O3'	5.15	120.73	113.00
1	X	1103	U	C4'-C3'-C2'	5.14	107.74	102.60
2	A	950	VAL	N-CA-C	5.10	115.87	110.72
2	A	137	SER	N-CA-C	5.07	118.02	110.52

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	X	1105	A	C3'
1	X	1106	A	C3'

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	X	147	0	77	15	0
2	A	8699	0	8793	480	0
All	All	8846	0	8870	487	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (487) 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)
2:A:385:LEU:HD23	2:A:479:LYS:HE2	1.33	1.07
2:A:520:ASP:HB3	2:A:667:LYS:HG2	1.46	0.96
2:A:101:ASP:OD1	2:A:103:THR:HG22	1.67	0.94
2:A:734:THR:HA	2:A:737:MET:HE3	1.49	0.94
2:A:503:TYR:HB2	2:A:687:ILE:HD13	1.49	0.93
2:A:865:VAL:HG22	2:A:866:THR:H	1.31	0.93
2:A:186:ASN:ND2	2:A:190:ARG:H	1.70	0.89
2:A:735:LYS:O	2:A:739:MET:HG3	1.75	0.86
2:A:177:ILE:HD13	2:A:203:LEU:HD11	1.57	0.85
2:A:283:GLN:OE1	2:A:649:GLN:HG3	1.76	0.85
2:A:438:ILE:HD12	2:A:563:GLN:HB3	1.58	0.85
2:A:24:ILE:HB	2:A:75:LEU:HB2	1.61	0.82
2:A:135:LEU:HD22	2:A:709:GLN:HE21	1.43	0.82
2:A:721:ARG:HD2	2:A:726:GLU:HG3	1.61	0.82
2:A:254:LEU:HD23	2:A:280:VAL:HG21	1.63	0.81
2:A:248:MET:HE1	2:A:319:PHE:HZ	1.45	0.81
2:A:866:THR:HG22	2:A:867:PHE:H	1.45	0.81
2:A:999:ILE:HD11	2:A:1009:PHE:CZ	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3:LYS:HA	2:A:6:LEU:HD23	1.62	0.80
2:A:381:HIS:O	2:A:382:ASP:HB2	1.81	0.80
2:A:515:MET:HE3	2:A:639:PHE:CE2	2.18	0.79
2:A:186:ASN:HD21	2:A:190:ARG:H	1.29	0.78
2:A:778:THR:O	2:A:782:VAL:HG23	1.83	0.78
2:A:824:ASN:CG	2:A:828:SER:HB2	2.07	0.78
2:A:247:PRO:O	2:A:251:LEU:HG	1.83	0.78
2:A:744:ILE:HG22	2:A:745:THR:HG23	1.64	0.77
2:A:206:TRP:CD1	2:A:233:SER:HG	2.03	0.77
2:A:226:ALA:O	2:A:230:ILE:HG13	1.85	0.77
2:A:446:PRO:HG2	2:A:583:LYS:HD3	1.67	0.76
2:A:180:TYR:HB3	2:A:199:LYS:HG3	1.67	0.76
2:A:573:VAL:HG12	2:A:575:ILE:HG13	1.67	0.76
2:A:6:LEU:H	2:A:6:LEU:HD22	1.49	0.76
2:A:972:ALA:O	2:A:976:VAL:HG23	1.88	0.74
2:A:618:LYS:HD2	2:A:654:ASP:OD2	1.88	0.73
2:A:385:LEU:HD23	2:A:479:LYS:CE	2.17	0.72
2:A:608:ILE:HD13	2:A:626:ILE:HG23	1.72	0.72
2:A:886:THR:OG1	2:A:1055:PHE:HB3	1.89	0.72
2:A:248:MET:HE1	2:A:319:PHE:CZ	2.24	0.72
2:A:681:TYR:CZ	2:A:688:PHE:HB3	2.25	0.71
2:A:309:ASP:O	2:A:312:VAL:HG22	1.90	0.70
2:A:1059:PRO:O	2:A:1063:MET:HG3	1.91	0.70
2:A:928:SER:O	2:A:932:ARG:HG3	1.92	0.70
2:A:346:GLN:HG2	2:A:586:TYR:CE1	2.28	0.69
2:A:520:ASP:CB	2:A:667:LYS:HG2	2.21	0.69
2:A:420:LYS:O	2:A:424:VAL:HG23	1.92	0.69
2:A:882:LYS:HB3	2:A:883:PRO:HD3	1.73	0.69
2:A:777:THR:HG21	2:A:882:LYS:HE3	1.73	0.69
2:A:734:THR:CA	2:A:737:MET:HE3	2.23	0.69
2:A:286:ASP:O	2:A:290:GLN:HG3	1.91	0.69
2:A:865:VAL:HG22	2:A:866:THR:N	2.07	0.68
2:A:945:GLU:HG2	2:A:992:TYR:HE1	1.57	0.68
2:A:532:GLN:HG3	2:A:536:LYS:HE3	1.76	0.67
2:A:250:ILE:HG21	2:A:288:LEU:HB2	1.77	0.67
1:X:1105:A:H5'	2:A:400:ALA:HB1	1.77	0.67
2:A:295:MET:HE1	2:A:303:ILE:HG22	1.77	0.66
2:A:324:LYS:O	2:A:328:TRP:HD1	1.79	0.66
2:A:358:GLU:OE2	2:A:359:MET:HG2	1.96	0.66
2:A:820:LEU:H	2:A:820:LEU:HD23	1.59	0.66
2:A:575:ILE:HD12	2:A:584:ILE:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:VAL:HG21	2:A:139:SER:OG	1.97	0.65
2:A:556:GLN:HA	2:A:556:GLN:HE21	1.61	0.65
2:A:1023:LYS:O	2:A:1060:LYS:HG2	1.97	0.64
2:A:536:LYS:O	2:A:540:MET:HG3	1.96	0.64
2:A:885:PHE:CE1	2:A:1056:CYS:HB2	2.31	0.64
2:A:50:LYS:HG2	2:A:50:LYS:O	1.97	0.64
2:A:804:ALA:HA	2:A:809:LYS:HE3	1.79	0.64
1:X:1105:A:C4	2:A:462:ILE:HG21	2.32	0.64
2:A:843:ALA:HB3	2:A:844:PRO:HD3	1.81	0.63
2:A:206:TRP:HD1	2:A:233:SER:HG	1.46	0.63
2:A:387:ARG:HB3	2:A:387:ARG:HH11	1.63	0.63
2:A:622:ALA:HB3	2:A:638:GLN:HB3	1.80	0.62
1:X:1105:A:N3	2:A:592:GLY:HA2	2.14	0.62
2:A:820:LEU:HB2	2:A:964:SER:O	1.98	0.62
2:A:193:TYR:CE2	2:A:197:LYS:HD2	2.34	0.62
2:A:473:GLN:HG2	2:A:561:TYR:CE1	2.35	0.62
2:A:437:ILE:O	2:A:439:PRO:HD3	2.00	0.61
2:A:367:ILE:O	2:A:371:VAL:HG23	2.00	0.61
2:A:866:THR:HG22	2:A:867:PHE:N	2.16	0.61
2:A:1018:ILE:HD12	2:A:1037:ALA:HB1	1.83	0.60
2:A:591:SER:HB2	2:A:596:THR:CG2	2.32	0.60
2:A:485:LYS:NZ	2:A:495:SER:O	2.35	0.60
2:A:102:LEU:HD22	2:A:102:LEU:H	1.67	0.60
2:A:2:GLY:HA2	2:A:754:GLU:OE2	2.02	0.60
2:A:29:SER:OG	2:A:34:LEU:HD23	2.02	0.60
2:A:1024:GLY:O	2:A:1025:LYS:HB2	2.01	0.60
2:A:242:LYS:O	2:A:246:SER:HB2	2.02	0.60
2:A:516:VAL:HG21	2:A:675:ILE:CG2	2.32	0.59
2:A:544:ILE:O	2:A:548:MET:HG3	2.01	0.59
2:A:681:TYR:CZ	2:A:688:PHE:CB	2.85	0.59
2:A:744:ILE:HB	2:A:748:LEU:HD22	1.83	0.59
2:A:687:ILE:HG22	2:A:899:PHE:O	2.03	0.59
2:A:301:VAL:C	2:A:304:PRO:HD2	2.27	0.59
2:A:397:MET:HA	2:A:470:PHE:HE2	1.67	0.59
1:X:1106:A:H5"	1:X:1107:C:OP2	2.03	0.59
2:A:551:ASP:HB3	2:A:554:VAL:HB	1.84	0.59
2:A:608:ILE:HD11	2:A:635:ALA:HB2	1.85	0.59
2:A:598:ALA:O	2:A:602:ILE:HG13	2.03	0.59
2:A:764:LYS:HD3	2:A:1080:TYR:CG	2.38	0.59
2:A:246:SER:N	2:A:247:PRO:CD	2.67	0.58
2:A:134:ILE:HG23	2:A:136:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:135:LEU:HB3	2:A:706:GLN:HG2	1.86	0.58
2:A:591:SER:HB2	2:A:596:THR:HG21	1.85	0.58
2:A:316:ILE:HD13	2:A:684:GLY:HA3	1.84	0.58
2:A:762:THR:HA	2:A:1077:ARG:O	2.04	0.58
2:A:6:LEU:HD22	2:A:6:LEU:N	2.18	0.58
2:A:784:ILE:HD12	2:A:788:PHE:CE2	2.39	0.58
2:A:832:ALA:O	2:A:836:LYS:HG3	2.04	0.58
2:A:553:LYS:O	2:A:557:THR:HG22	2.02	0.58
2:A:312:VAL:HG23	2:A:313:ASP:N	2.19	0.57
2:A:581:ILE:O	2:A:581:ILE:HG22	2.04	0.57
2:A:518:TYR:H	2:A:518:TYR:HD2	1.49	0.57
2:A:343:ALA:O	2:A:346:GLN:HG3	2.04	0.57
2:A:477:VAL:HG21	2:A:594:LYS:HG3	1.85	0.57
2:A:241:ALA:HB3	2:A:456:GLY:HA2	1.86	0.57
2:A:865:VAL:CG2	2:A:866:THR:H	2.13	0.57
2:A:264:ASN:HD21	2:A:268:GLU:HG3	1.69	0.57
2:A:872:ILE:HG22	2:A:1073:ILE:HA	1.86	0.57
2:A:976:VAL:O	2:A:976:VAL:HG12	2.04	0.57
2:A:28:TYR:HA	2:A:35:GLU:OE2	2.04	0.57
2:A:756:VAL:HG13	2:A:788:PHE:CZ	2.40	0.57
2:A:319:PHE:N	2:A:320:PRO:CD	2.68	0.57
2:A:922:GLU:OE2	2:A:991:SER:OG	2.18	0.57
2:A:621:PHE:CD1	2:A:637:LEU:HD22	2.39	0.56
2:A:318:LYS:HB2	2:A:318:LYS:NZ	2.20	0.56
2:A:331:HIS:NE2	2:A:692:GLY:HA2	2.20	0.56
2:A:821:PHE:N	2:A:821:PHE:CD2	2.73	0.56
2:A:370:GLU:O	2:A:374:MET:HG3	2.05	0.56
2:A:370:GLU:HA	2:A:373:LYS:HZ3	1.71	0.56
2:A:514:THR:HG22	2:A:638:GLN:HG3	1.88	0.56
2:A:477:VAL:HA	2:A:480:MET:CE	2.36	0.56
2:A:469:TYR:CD1	2:A:564:THR:HG22	2.40	0.56
2:A:375:LEU:C	2:A:378:PRO:HD2	2.31	0.56
2:A:449:LEU:HD22	2:A:573:VAL:CG1	2.35	0.56
2:A:549:THR:HG21	2:A:554:VAL:HG11	1.88	0.56
2:A:1024:GLY:O	2:A:1025:LYS:CB	2.53	0.56
2:A:860:MET:HE1	2:A:865:VAL:HG12	1.87	0.56
2:A:261:PHE:HD2	2:A:899:PHE:HB3	1.71	0.56
2:A:488:ARG:HG2	2:A:494:TYR:CE1	2.40	0.56
2:A:789:MET:HE2	2:A:1076:LEU:HD21	1.87	0.56
2:A:962:LEU:O	2:A:967:ILE:HB	2.06	0.55
2:A:419:LYS:HB2	2:A:422:MET:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:930:ILE:O	2:A:934:ILE:HG13	2.06	0.55
2:A:161:LYS:O	2:A:165:ARG:HG3	2.06	0.55
2:A:453:ASP:HB2	2:A:699:GLU:HG3	1.88	0.55
2:A:516:VAL:HG21	2:A:675:ILE:HG21	1.89	0.55
2:A:135:LEU:HD22	2:A:709:GLN:NE2	2.19	0.55
2:A:781:GLU:O	2:A:785:GLN:HG3	2.07	0.55
2:A:430:ASN:C	2:A:432:ARG:H	2.13	0.55
2:A:528:GLN:O	2:A:531:THR:HG22	2.07	0.55
2:A:984:ASP:O	2:A:988:ILE:HG12	2.07	0.55
2:A:1019:ARG:HD2	2:A:1053:SER:OG	2.07	0.55
1:X:1105:A:H5'	2:A:400:ALA:CB	2.36	0.54
2:A:409:LYS:HB2	2:A:409:LYS:NZ	2.23	0.54
2:A:900:MET:HE2	2:A:903:LEU:HG	1.89	0.54
2:A:933:LEU:HD23	2:A:962:LEU:HD22	1.89	0.54
2:A:365:MET:HE1	2:A:540:MET:HE1	1.89	0.54
2:A:558:LEU:O	2:A:558:LEU:HD23	2.08	0.54
2:A:177:ILE:CD1	2:A:203:LEU:HD11	2.34	0.54
2:A:312:VAL:HG23	2:A:313:ASP:H	1.72	0.54
2:A:72:LEU:CD2	2:A:864:PRO:HD3	2.38	0.54
2:A:324:LYS:O	2:A:328:TRP:CD1	2.60	0.54
2:A:803:ALA:HA	2:A:808:PHE:CD2	2.42	0.54
2:A:899:PHE:C	2:A:901:PRO:HD3	2.33	0.54
2:A:999:ILE:HD11	2:A:1009:PHE:CE2	2.43	0.54
2:A:539:ILE:HG23	2:A:562:LYS:HE3	1.90	0.53
2:A:884:PHE:CD1	2:A:1059:PRO:HD3	2.43	0.53
2:A:959:GLN:NE2	2:A:973:ASP:OD1	2.42	0.53
2:A:49:SER:C	2:A:51:ASN:H	2.16	0.53
2:A:945:GLU:HG2	2:A:992:TYR:CE1	2.41	0.53
2:A:951:ILE:HG12	2:A:985:LYS:HA	1.90	0.53
2:A:1003:CYS:SG	2:A:1007:PHE:CZ	3.02	0.53
2:A:878:LEU:HD22	2:A:1036:TYR:HD1	1.74	0.53
2:A:386:LEU:O	2:A:557:THR:HG21	2.08	0.53
2:A:454:VAL:CG1	2:A:457:ARG:HB3	2.38	0.53
2:A:136:THR:HB	2:A:739:MET:HE3	1.91	0.53
2:A:248:MET:HG2	2:A:326:TYR:CE1	2.43	0.53
2:A:708:ASP:O	2:A:712:ILE:HG13	2.08	0.53
2:A:244:VAL:CG1	2:A:329:SER:HB3	2.38	0.53
2:A:255:VAL:O	2:A:673:VAL:HG21	2.07	0.53
2:A:281:PRO:HG2	2:A:284:THR:OG1	2.08	0.53
2:A:116:SER:HB3	2:A:197:LYS:HG3	1.91	0.53
2:A:145:VAL:HG21	2:A:211:ILE:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:719:VAL:HG12	2:A:723:ARG:HD2	1.90	0.53
2:A:115:THR:HB	2:A:197:LYS:HA	1.91	0.53
2:A:399:SER:HB3	2:A:838:LYS:HB3	1.91	0.53
2:A:1012:PRO:O	2:A:1016:LYS:HG3	2.09	0.53
2:A:381:HIS:O	2:A:382:ASP:CB	2.56	0.53
2:A:503:TYR:CB	2:A:687:ILE:HD13	2.33	0.53
2:A:813:THR:O	2:A:817:GLU:HG3	2.09	0.53
2:A:368:ARG:HG3	2:A:541:GLY:N	2.24	0.52
1:X:1107:C:H5''	1:X:1107:C:C6	2.44	0.52
2:A:450:GLY:O	2:A:462:ILE:N	2.41	0.52
2:A:141:ASN:O	2:A:145:VAL:HG23	2.10	0.52
2:A:185:HIS:H	2:A:185:HIS:CD2	2.28	0.52
2:A:229:LEU:O	2:A:233:SER:HB3	2.10	0.52
2:A:313:ASP:N	2:A:313:ASP:OD2	2.42	0.52
2:A:951:ILE:HG13	2:A:985:LYS:HG2	1.92	0.52
2:A:217:VAL:HG13	2:A:222:ASP:HB2	1.90	0.52
2:A:824:ASN:OD1	2:A:828:SER:HB2	2.10	0.52
2:A:330:PHE:CE1	2:A:690:ARG:CZ	2.93	0.52
2:A:820:LEU:C	2:A:821:PHE:HD2	2.17	0.52
2:A:477:VAL:HA	2:A:480:MET:HE2	1.91	0.51
2:A:495:SER:OG	2:A:496:GLN:N	2.43	0.51
2:A:821:PHE:N	2:A:821:PHE:HD2	2.08	0.51
2:A:858:LEU:O	2:A:862:GLN:HG2	2.10	0.51
2:A:449:LEU:HD22	2:A:573:VAL:HG11	1.93	0.51
2:A:361:ARG:O	2:A:365:MET:HG2	2.09	0.51
2:A:22:VAL:HG22	2:A:77:TYR:HB2	1.91	0.51
2:A:83:ASN:O	2:A:85:VAL:N	2.36	0.51
2:A:397:MET:HA	2:A:470:PHE:CE2	2.45	0.51
2:A:428:MET:CE	2:A:811:TYR:HD1	2.24	0.51
2:A:439:PRO:HD3	2:A:468:GLU:HG2	1.93	0.51
2:A:705:THR:O	2:A:709:GLN:HG3	2.10	0.51
2:A:35:GLU:O	2:A:39:ILE:HG13	2.10	0.51
2:A:55:LEU:O	2:A:59:PHE:HD2	1.94	0.51
2:A:258:ASN:OD1	2:A:275:TYR:HD1	1.93	0.51
2:A:312:VAL:HG23	2:A:313:ASP:OD2	2.10	0.51
2:A:449:LEU:CD2	2:A:573:VAL:HG11	2.40	0.51
2:A:1070:MET:O	2:A:1073:ILE:HG13	2.10	0.51
2:A:87:ARG:O	2:A:90:VAL:HG22	2.11	0.51
2:A:246:SER:N	2:A:247:PRO:HD3	2.26	0.51
2:A:376:GLU:OE2	2:A:548:MET:HE1	2.11	0.51
2:A:532:GLN:HA	2:A:532:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:253:ALA:HB1	2:A:671:SER:HB2	1.93	0.51
2:A:4:TYR:HB3	2:A:754:GLU:OE1	2.11	0.51
2:A:430:ASN:O	2:A:432:ARG:N	2.44	0.51
2:A:518:TYR:CD2	2:A:518:TYR:N	2.78	0.51
2:A:909:TYR:CE2	2:A:1049:GLY:O	2.64	0.51
1:X:1102:G:N1	2:A:190:ARG:HD3	2.26	0.50
1:X:1105:A:C5'	2:A:400:ALA:HB1	2.40	0.50
2:A:894:ILE:O	2:A:894:ILE:HG13	2.10	0.50
2:A:887:VAL:HG22	2:A:1054:LEU:HD11	1.93	0.50
1:X:1102:G:H3'	1:X:1103:U:C6	2.47	0.50
2:A:14:PHE:CE2	2:A:147:PHE:HB2	2.46	0.50
2:A:383:ASP:O	2:A:387:ARG:HG3	2.12	0.50
2:A:892:LEU:HD22	2:A:1017:LEU:HD11	1.93	0.50
2:A:428:MET:HG2	2:A:433:TYR:CG	2.47	0.50
2:A:721:ARG:HH11	2:A:721:ARG:CG	2.24	0.50
2:A:370:GLU:HA	2:A:373:LYS:NZ	2.26	0.50
2:A:446:PRO:HB2	2:A:574:GLN:HG2	1.92	0.50
2:A:534:PHE:HZ	2:A:599:ALA:HB1	1.77	0.50
2:A:703:GLN:CD	2:A:703:GLN:N	2.69	0.50
2:A:372:VAL:HA	2:A:545:LEU:HD21	1.94	0.50
2:A:135:LEU:HB2	2:A:709:GLN:NE2	2.27	0.50
2:A:572:TYR:CE1	2:A:585:GLN:HB2	2.47	0.49
2:A:681:TYR:CE2	2:A:688:PHE:HB2	2.47	0.49
2:A:387:ARG:HB3	2:A:387:ARG:NH1	2.28	0.49
2:A:207:ALA:O	2:A:211:ILE:HG13	2.13	0.49
2:A:616:SER:O	2:A:617:ASN:C	2.54	0.49
2:A:784:ILE:HG23	2:A:788:PHE:CE2	2.48	0.49
2:A:920:GLN:OE1	2:A:920:GLN:HA	2.12	0.49
2:A:399:SER:O	2:A:419:LYS:HD2	2.12	0.49
2:A:798:ILE:O	2:A:802:ILE:HG22	2.12	0.49
2:A:897:GLN:OE1	2:A:897:GLN:N	2.37	0.49
2:A:989:LEU:O	2:A:993:VAL:HG23	2.12	0.49
2:A:473:GLN:HG2	2:A:561:TYR:CD1	2.48	0.49
2:A:424:VAL:O	2:A:428:MET:HG3	2.12	0.49
2:A:428:MET:HG2	2:A:433:TYR:CB	2.43	0.49
2:A:125:TYR:HB2	2:A:193:TYR:CD1	2.47	0.48
2:A:165:ARG:HE	2:A:220:HIS:HA	1.78	0.48
2:A:520:ASP:OD1	2:A:520:ASP:C	2.56	0.48
2:A:5:ASN:ND2	2:A:71:LEU:HD23	2.28	0.48
2:A:142:LEU:HD23	2:A:211:ILE:HD11	1.95	0.48
2:A:324:LYS:HG3	2:A:328:TRP:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:846:SER:OG	2:A:850:ARG:NH2	2.46	0.48
2:A:849:LYS:O	2:A:853:GLN:HG2	2.13	0.48
2:A:387:ARG:NH1	2:A:553:LYS:HG3	2.27	0.48
2:A:409:LYS:HB2	2:A:409:LYS:HZ3	1.77	0.48
2:A:919:TYR:CD1	2:A:919:TYR:C	2.92	0.48
2:A:4:TYR:C	2:A:4:TYR:CD2	2.92	0.48
2:A:681:TYR:CE2	2:A:688:PHE:CB	2.96	0.48
2:A:575:ILE:CD1	2:A:584:ILE:HG12	2.44	0.48
2:A:695:LEU:HG	2:A:713:LEU:CD1	2.44	0.48
1:X:1105:A:C5	2:A:462:ILE:HG21	2.48	0.48
1:X:1104:G:N3	1:X:1104:G:H2'	2.28	0.48
2:A:83:ASN:C	2:A:85:VAL:H	2.20	0.48
2:A:924:ASP:C	2:A:944:ILE:HD13	2.39	0.48
2:A:534:PHE:CZ	2:A:599:ALA:HB1	2.49	0.48
1:X:1107:C:H5''	1:X:1107:C:H6	1.78	0.47
2:A:532:GLN:CB	2:A:533:PRO:HD3	2.44	0.47
2:A:279:ILE:HG22	2:A:648:ILE:HD12	1.95	0.47
2:A:452:ARG:HD2	2:A:699:GLU:OE2	2.14	0.47
2:A:454:VAL:HG13	2:A:457:ARG:HB3	1.97	0.47
2:A:523:GLN:HB2	2:A:665:LYS:O	2.13	0.47
2:A:145:VAL:CG2	2:A:211:ILE:HG23	2.44	0.47
2:A:424:VAL:HG22	2:A:467:TYR:CD2	2.49	0.47
2:A:430:ASN:C	2:A:432:ARG:N	2.71	0.47
2:A:514:THR:HG22	2:A:638:GLN:HA	1.97	0.47
2:A:84:ALA:HB1	2:A:88:LYS:NZ	2.29	0.47
2:A:368:ARG:O	2:A:372:VAL:HG23	2.15	0.47
2:A:442:ASN:C	2:A:572:TYR:HB2	2.39	0.47
2:A:744:ILE:HD11	2:A:750:LEU:HB2	1.96	0.47
2:A:244:VAL:HG11	2:A:329:SER:HB3	1.97	0.47
2:A:409:LYS:H	2:A:409:LYS:HZ2	1.62	0.47
2:A:612:LEU:O	2:A:615:ILE:HG12	2.15	0.47
2:A:225:ILE:HD13	2:A:325:ILE:HG12	1.95	0.47
2:A:376:GLU:O	2:A:380:LYS:HG3	2.15	0.47
2:A:516:VAL:N	2:A:671:SER:O	2.47	0.47
2:A:605:LEU:O	2:A:609:LYS:HG3	2.15	0.47
2:A:699:GLU:OE1	2:A:700:LYS:HE2	2.14	0.47
1:X:1101:U:O4	2:A:415:ILE:HG13	2.14	0.47
2:A:102:LEU:HD22	2:A:102:LEU:N	2.30	0.47
2:A:210:SER:OG	2:A:230:ILE:HG23	2.15	0.47
2:A:420:LYS:CG	2:A:467:TYR:HB3	2.45	0.47
2:A:687:ILE:HG23	2:A:900:MET:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:794:GLN:HG2	2:A:853:GLN:OE1	2.15	0.47
2:A:4:TYR:HD1	2:A:733:LEU:HD22	1.79	0.47
2:A:169:LEU:HD21	2:A:227:LYS:HB2	1.96	0.47
2:A:295:MET:O	2:A:300:LEU:HB2	2.15	0.47
2:A:397:MET:O	2:A:838:LYS:NZ	2.41	0.47
2:A:470:PHE:HE1	2:A:594:LYS:HD3	1.80	0.47
2:A:887:VAL:HG12	2:A:888:SER:N	2.30	0.47
2:A:6:LEU:H	2:A:6:LEU:CD2	2.23	0.47
2:A:75:LEU:HD23	2:A:75:LEU:HA	1.79	0.47
2:A:215:MET:HE3	2:A:731:PHE:HB2	1.97	0.47
2:A:558:LEU:HD23	2:A:558:LEU:C	2.40	0.47
2:A:681:TYR:CD2	2:A:688:PHE:HB2	2.50	0.47
2:A:461:ILE:HD11	2:A:586:TYR:CZ	2.50	0.46
2:A:825:ASN:O	2:A:829:ARG:HG2	2.14	0.46
2:A:192:GLU:O	2:A:196:MET:HB2	2.16	0.46
2:A:789:MET:HE1	2:A:873:THR:HG21	1.97	0.46
2:A:75:LEU:HD22	2:A:748:LEU:HD21	1.98	0.46
2:A:428:MET:HE1	2:A:811:TYR:HD1	1.80	0.46
2:A:879:ARG:HG3	2:A:879:ARG:HH11	1.80	0.46
2:A:408:LEU:HD22	2:A:426:ASP:CG	2.41	0.46
2:A:865:VAL:HG13	2:A:866:THR:O	2.15	0.46
2:A:1000:ASN:O	2:A:1005:GLN:HB3	2.15	0.46
2:A:12:LEU:HD22	2:A:16:TYR:HE2	1.81	0.46
2:A:84:ALA:O	2:A:88:LYS:HG3	2.16	0.46
2:A:191:TYR:CE2	2:A:204:VAL:HG11	2.51	0.46
2:A:193:TYR:CZ	2:A:197:LYS:HD2	2.51	0.46
2:A:467:TYR:C	2:A:467:TYR:CD1	2.94	0.46
2:A:56:ARG:O	2:A:60:VAL:HG23	2.15	0.46
2:A:532:GLN:HB3	2:A:533:PRO:HD3	1.98	0.46
2:A:622:ALA:O	2:A:637:LEU:HA	2.16	0.46
2:A:952:SER:HB3	2:A:1071:TRP:CE3	2.52	0.45
2:A:168:ASP:O	2:A:171:THR:HB	2.16	0.45
2:A:519:THR:HG23	2:A:667:LYS:O	2.16	0.45
2:A:712:ILE:HD13	2:A:1086:PHE:CD2	2.50	0.45
2:A:62:TYR:O	2:A:66:ILE:HG12	2.16	0.45
2:A:261:PHE:CD2	2:A:899:PHE:HB3	2.49	0.45
2:A:556:GLN:HA	2:A:556:GLN:NE2	2.29	0.45
2:A:623:THR:CG2	2:A:626:ILE:HG13	2.46	0.45
2:A:1000:ASN:C	2:A:1005:GLN:HB3	2.41	0.45
2:A:126:THR:OG1	2:A:128:SER:HB3	2.17	0.45
2:A:252:VAL:HG23	2:A:253:ALA:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1106:A:O5'	1:X:1106:A:H8	2.00	0.45
2:A:213:MET:O	2:A:217:VAL:HG23	2.15	0.45
2:A:28:TYR:HD2	2:A:72:LEU:HB2	1.82	0.45
2:A:293:ASP:O	2:A:297:LYS:HG2	2.17	0.45
2:A:538:ILE:O	2:A:542:LEU:HG	2.17	0.45
2:A:659:TYR:CD1	2:A:666:VAL:HG21	2.52	0.45
2:A:515:MET:HG2	2:A:639:PHE:HE2	1.82	0.45
2:A:791:LEU:HD23	2:A:791:LEU:N	2.31	0.45
2:A:794:GLN:HG2	2:A:853:GLN:CD	2.42	0.45
2:A:803:ALA:HA	2:A:808:PHE:CE2	2.52	0.45
2:A:120:PRO:HD2	2:A:124:GLU:OE2	2.17	0.45
2:A:531:THR:HG21	2:A:587:GLY:O	2.17	0.45
2:A:667:LYS:O	2:A:667:LYS:HG3	2.16	0.45
2:A:899:PHE:O	2:A:901:PRO:HD3	2.17	0.45
2:A:824:ASN:CB	2:A:828:SER:HB2	2.47	0.44
2:A:253:ALA:CB	2:A:671:SER:HB2	2.48	0.44
2:A:667:LYS:NZ	2:A:676:GLU:OE1	2.51	0.44
2:A:837:ALA:O	2:A:840:ASN:ND2	2.49	0.44
2:A:161:LYS:HG2	2:A:165:ARG:CZ	2.47	0.44
2:A:611:VAL:O	2:A:615:ILE:HG23	2.17	0.44
2:A:714:TYR:OH	2:A:770:ASP:OD1	2.22	0.44
2:A:847:LEU:HD23	2:A:850:ARG:NH1	2.32	0.44
2:A:165:ARG:HD3	2:A:223:TYR:CB	2.47	0.44
2:A:762:THR:HA	2:A:1078:SER:HB3	2.00	0.44
2:A:24:ILE:HD12	2:A:45:CYS:HB3	2.00	0.44
2:A:166:ARG:NH2	2:A:218:PHE:CE1	2.85	0.44
2:A:278:ALA:HB2	2:A:673:VAL:HG11	2.00	0.44
2:A:616:SER:C	2:A:618:LYS:N	2.75	0.44
2:A:134:ILE:CG2	2:A:136:THR:HG22	2.46	0.44
2:A:217:VAL:HG13	2:A:222:ASP:CB	2.48	0.44
2:A:1068:LYS:HA	2:A:1068:LYS:HD2	1.83	0.44
2:A:580:VAL:HG12	2:A:581:ILE:N	2.32	0.44
2:A:733:LEU:C	2:A:737:MET:HE3	2.42	0.44
2:A:824:ASN:ND2	2:A:824:ASN:O	2.51	0.44
2:A:186:ASN:ND2	2:A:186:ASN:C	2.76	0.43
2:A:261:PHE:CE1	2:A:271:PHE:HB2	2.52	0.43
2:A:823:LYS:HE3	2:A:825:ASN:ND2	2.33	0.43
2:A:944:ILE:HG23	2:A:945:GLU:N	2.33	0.43
2:A:50:LYS:O	2:A:50:LYS:CG	2.65	0.43
2:A:283:GLN:HG3	2:A:284:THR:N	2.32	0.43
2:A:412:ARG:O	2:A:412:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:439:PRO:HA	2:A:440:PRO:HD3	1.82	0.43
2:A:151:LYS:HA	2:A:151:LYS:HD3	1.83	0.43
2:A:421:ASN:O	2:A:425:MET:HG3	2.18	0.43
2:A:491:ALA:HB3	2:A:629:ASP:HB2	2.00	0.43
2:A:851:ARG:HH11	2:A:851:ARG:HG2	1.83	0.43
2:A:34:LEU:O	2:A:37:ARG:HB2	2.18	0.43
2:A:88:LYS:O	2:A:91:LYS:HG3	2.19	0.43
2:A:392:ALA:HB2	2:A:939:VAL:HG21	2.01	0.43
2:A:842:TYR:CE2	2:A:844:PRO:HB2	2.53	0.43
2:A:954:HIS:HB2	2:A:957:GLU:OE2	2.18	0.43
2:A:22:VAL:CG2	2:A:77:TYR:HB2	2.48	0.43
2:A:303:ILE:HB	2:A:304:PRO:HD3	2.01	0.43
2:A:847:LEU:O	2:A:851:ARG:HG3	2.18	0.43
2:A:72:LEU:HD23	2:A:861:LEU:O	2.19	0.43
2:A:727:THR:O	2:A:728:ASP:C	2.62	0.43
2:A:787:ALA:O	2:A:790:SER:HB3	2.19	0.43
2:A:829:ARG:HG3	2:A:830:GLY:N	2.33	0.43
2:A:397:MET:HE1	2:A:471:ILE:HG13	1.99	0.43
2:A:438:ILE:HD13	2:A:564:THR:HG23	2.01	0.43
2:A:446:PRO:HB2	2:A:574:GLN:CG	2.49	0.43
2:A:221:ASP:O	2:A:225:ILE:HG13	2.18	0.43
2:A:930:ILE:HG23	2:A:931:SER:N	2.34	0.42
2:A:1058:TYR:HA	2:A:1059:PRO:HD3	1.89	0.42
2:A:28:TYR:CZ	2:A:784:ILE:HG12	2.54	0.42
2:A:109:TYR:HA	2:A:118:LEU:HD21	2.01	0.42
2:A:258:ASN:OD1	2:A:275:TYR:CD1	2.70	0.42
2:A:376:GLU:CG	2:A:380:LYS:HE2	2.49	0.42
2:A:612:LEU:HD23	2:A:615:ILE:HD11	2.01	0.42
2:A:667:LYS:O	2:A:667:LYS:CG	2.67	0.42
2:A:744:ILE:CB	2:A:748:LEU:HD22	2.48	0.42
2:A:825:ASN:HA	2:A:828:SER:HB3	2.01	0.42
2:A:959:GLN:CD	2:A:973:ASP:OD1	2.63	0.42
2:A:130:MET:SD	2:A:130:MET:C	3.03	0.42
2:A:225:ILE:CD1	2:A:325:ILE:HG12	2.49	0.42
2:A:322:MET:HE2	2:A:322:MET:N	2.34	0.42
2:A:860:MET:HE1	2:A:865:VAL:CG1	2.49	0.42
2:A:1058:TYR:HD2	2:A:1063:MET:HG2	1.83	0.42
2:A:257:ILE:O	2:A:275:TYR:HA	2.20	0.42
2:A:387:ARG:HH11	2:A:387:ARG:CB	2.30	0.42
2:A:863:LYS:O	2:A:863:LYS:HG3	2.18	0.42
2:A:967:ILE:HD12	2:A:967:ILE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1023:LYS:HD2	2:A:1058:TYR:O	2.20	0.42
2:A:26:ILE:HD12	2:A:42:HIS:CE1	2.54	0.42
2:A:165:ARG:HD3	2:A:223:TYR:HB2	2.01	0.42
2:A:264:ASN:ND2	2:A:268:GLU:HG3	2.32	0.42
2:A:303:ILE:N	2:A:304:PRO:CD	2.83	0.42
2:A:477:VAL:O	2:A:481:LEU:HG	2.20	0.42
2:A:568:LEU:O	2:A:569:MET:C	2.63	0.42
2:A:173:VAL:O	2:A:177:ILE:HG12	2.20	0.42
2:A:758:THR:HG22	2:A:766:PHE:O	2.19	0.42
2:A:784:ILE:HD13	2:A:784:ILE:HA	1.84	0.42
2:A:791:LEU:HD21	2:A:860:MET:HE3	2.00	0.42
2:A:1029:VAL:HG13	2:A:1066:LEU:HD23	2.02	0.42
2:A:186:ASN:H	2:A:186:ASN:HD22	1.66	0.41
2:A:619:HIS:ND1	2:A:619:HIS:N	2.67	0.41
2:A:40:GLU:O	2:A:44:LYS:HG3	2.20	0.41
2:A:248:MET:HE2	2:A:252:VAL:HG13	2.01	0.41
2:A:520:ASP:HB2	2:A:667:LYS:HE2	2.01	0.41
2:A:531:THR:HB	2:A:589:VAL:HG23	2.02	0.41
2:A:83:ASN:HB3	2:A:84:ALA:H	1.56	0.41
2:A:319:PHE:N	2:A:320:PRO:HD2	2.36	0.41
2:A:429:ALA:C	2:A:430:ASN:OD1	2.63	0.41
2:A:277:ARG:HG2	2:A:277:ARG:HH11	1.85	0.41
2:A:376:GLU:HG3	2:A:380:LYS:HE2	2.02	0.41
2:A:536:LYS:HG2	2:A:569:MET:HE1	2.02	0.41
2:A:1018:ILE:HD12	2:A:1037:ALA:CB	2.49	0.41
2:A:28:TYR:CE2	2:A:70:THR:HB	2.56	0.41
2:A:535:ARG:HB2	2:A:569:MET:SD	2.60	0.41
2:A:842:TYR:HD2	2:A:845:ILE:HG13	1.84	0.41
2:A:962:LEU:O	2:A:967:ILE:HD13	2.21	0.41
2:A:100:ALA:O	2:A:102:LEU:HD22	2.20	0.41
2:A:392:ALA:HB2	2:A:939:VAL:CG2	2.51	0.41
2:A:735:LYS:HD2	2:A:735:LYS:HA	1.88	0.41
2:A:165:ARG:NE	2:A:220:HIS:HA	2.35	0.41
2:A:428:MET:HG2	2:A:433:TYR:HB2	2.03	0.41
2:A:985:LYS:HB3	2:A:985:LYS:HE2	1.89	0.41
1:X:1102:G:H3'	1:X:1103:U:C5	2.55	0.41
2:A:61:GLU:OE2	2:A:62:TYR:CE2	2.74	0.41
2:A:439:PRO:CD	2:A:468:GLU:HG2	2.51	0.41
2:A:549:THR:HG21	2:A:554:VAL:CG1	2.51	0.41
2:A:675:ILE:O	2:A:675:ILE:HG13	2.14	0.41
2:A:681:TYR:CE1	2:A:688:PHE:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:804:ALA:O	2:A:809:LYS:HE3	2.20	0.41
2:A:2:GLY:HA2	2:A:754:GLU:CD	2.46	0.41
2:A:14:PHE:CD1	2:A:150:GLU:OE1	2.74	0.41
2:A:183:PRO:HG2	2:A:204:VAL:HG22	2.02	0.41
2:A:968:PRO:HG2	2:A:971:ASP:HB2	2.03	0.41
2:A:150:GLU:O	2:A:153:GLU:HB2	2.21	0.40
2:A:214:LEU:HA	2:A:217:VAL:HG23	2.03	0.40
2:A:1054:LEU:HD12	2:A:1054:LEU:HA	1.92	0.40
2:A:249:SER:O	2:A:252:VAL:HG22	2.21	0.40
2:A:290:GLN:O	2:A:294:ASN:ND2	2.55	0.40
2:A:441:VAL:HB	2:A:447:ILE:HD11	2.02	0.40
2:A:717:TYR:OH	2:A:729:ARG:HG3	2.21	0.40
2:A:111:ASN:O	2:A:113:LYS:N	2.46	0.40
2:A:674:GLY:C	2:A:675:ILE:CG2	2.95	0.40
2:A:1020:ILE:O	2:A:1020:ILE:HG22	2.20	0.40
2:A:41:PHE:HE1	2:A:58:LEU:HB3	1.87	0.40
2:A:804:ALA:CA	2:A:809:LYS:HE3	2.49	0.40
2:A:837:ALA:C	2:A:839:LEU:N	2.79	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	
2	A	1067/1095 (97%)	966 (90%)	83 (8%)	18 (2%)	7	32

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	382	ASP
2	A	822	SER
2	A	978	SER

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Mol	Chain	Res	Type
2	A	1025	LYS
2	A	106	GLU
2	A	112	ASN
2	A	431	GLU
2	A	495	SER
2	A	82	TYR
2	A	102	LEU
2	A	1027	PRO
2	A	397	MET
2	A	84	ALA
2	A	128	SER
2	A	807	THR
2	A	865	VAL
2	A	864	PRO
2	A	439	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	975/996 (98%)	917 (94%)	58 (6%)	18	50

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	17	ASN
2	A	35	GLU
2	A	50	LYS
2	A	87	ARG
2	A	91	LYS
2	A	121	THR
2	A	135	LEU
2	A	143	ASN
2	A	159	LYS
2	A	186	ASN
2	A	194	ASP

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Mol	Chain	Res	Type
2	A	195	VAL
2	A	196	MET
2	A	227	LYS
2	A	229	LEU
2	A	249	SER
2	A	313	ASP
2	A	318	LYS
2	A	324	LYS
2	A	358	GLU
2	A	387	ARG
2	A	409	LYS
2	A	415	ILE
2	A	418	THR
2	A	449	LEU
2	A	512	ASN
2	A	517	LEU
2	A	518	TYR
2	A	532	GLN
2	A	584	ILE
2	A	595	GLN
2	A	600	ASN
2	A	619	HIS
2	A	620	SER
2	A	652	SER
2	A	671	SER
2	A	695	LEU
2	A	708	ASP
2	A	721	ARG
2	A	784	ILE
2	A	791	LEU
2	A	821	PHE
2	A	824	ASN
2	A	868	LYS
2	A	872	ILE
2	A	892	LEU
2	A	895	GLN
2	A	900	MET
2	A	922	GLU
2	A	939	VAL
2	A	970	ILE
2	A	998	SER
2	A	1019	ARG

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Mol	Chain	Res	Type
2	A	1022	PHE
2	A	1027	PRO
2	A	1047	LYS
2	A	1054	LEU
2	A	1088	GLU

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

Mol	Chain	Res	Type
2	A	36	ASN
2	A	48	ASN
2	A	51	ASN
2	A	63	ASN
2	A	68	ASN
2	A	185	HIS
2	A	186	ASN
2	A	289	ASN
2	A	308	GLN
2	A	381	HIS
2	A	473	GLN
2	A	496	GLN
2	A	512	ASN
2	A	528	GLN
2	A	529	HIS
2	A	556	GLN
2	A	563	GLN
2	A	574	GLN
2	A	579	ASN
2	A	604	ASN
2	A	617	ASN
2	A	646	GLN
2	A	653	ASN
2	A	706	GLN
2	A	709	GLN
2	A	760	ASN
2	A	824	ASN
2	A	825	ASN
2	A	853	GLN
2	A	895	GLN
2	A	908	GLN
2	A	959	GLN
2	A	1034	HIS

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Mol	Chain	Res	Type
2	A	1048	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	7/8 (87%)	6 (85%)	5 (71%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	1102	G
1	X	1103	U
1	X	1104	G
1	X	1105	A
1	X	1106	A
1	X	1107	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1101	U
1	X	1102	G
1	X	1103	U
1	X	1105	A
1	X	1106	A

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](#)

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](#)

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	X	7/8 (87%)	-0.09	0	100 100	45, 56, 71, 77	0
2	A	1073/1095 (97%)	-0.26	3 (0%)	90 79	13, 46, 75, 111	0
All	All	1080/1103 (97%)	-0.26	3 (0%)	90 79	13, 46, 75, 111	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	824	ASN	3.7
2	A	18	SER	2.1
2	A	77	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.