



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:34 AM GMT

PDB ID : 2R7U
Title : Crystal Structure of Rotavirus SA11 VP1/RNA (AAAAGCC) Complex
Authors : Lu, X.; Harrison, S.C.; Tao, Y.J.; Patton, J.T.; Nibert, M.L.
Deposited on : 2007-09-10
Resolution : 3.10 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

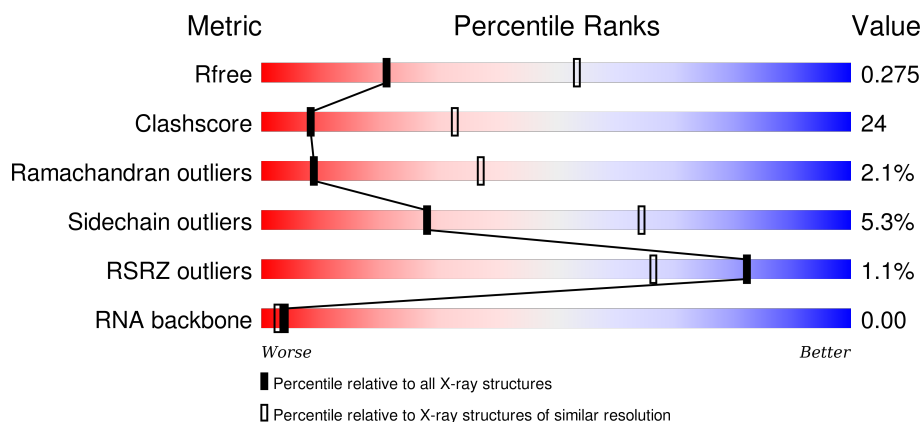
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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	X	7	 14% 57% 29%
2	A	1095	 52% 42% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8803 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(*AP*A*AP*AP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	5	Total	C	N	O	P	0	0	0
			104	48	21	31	4			


- 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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

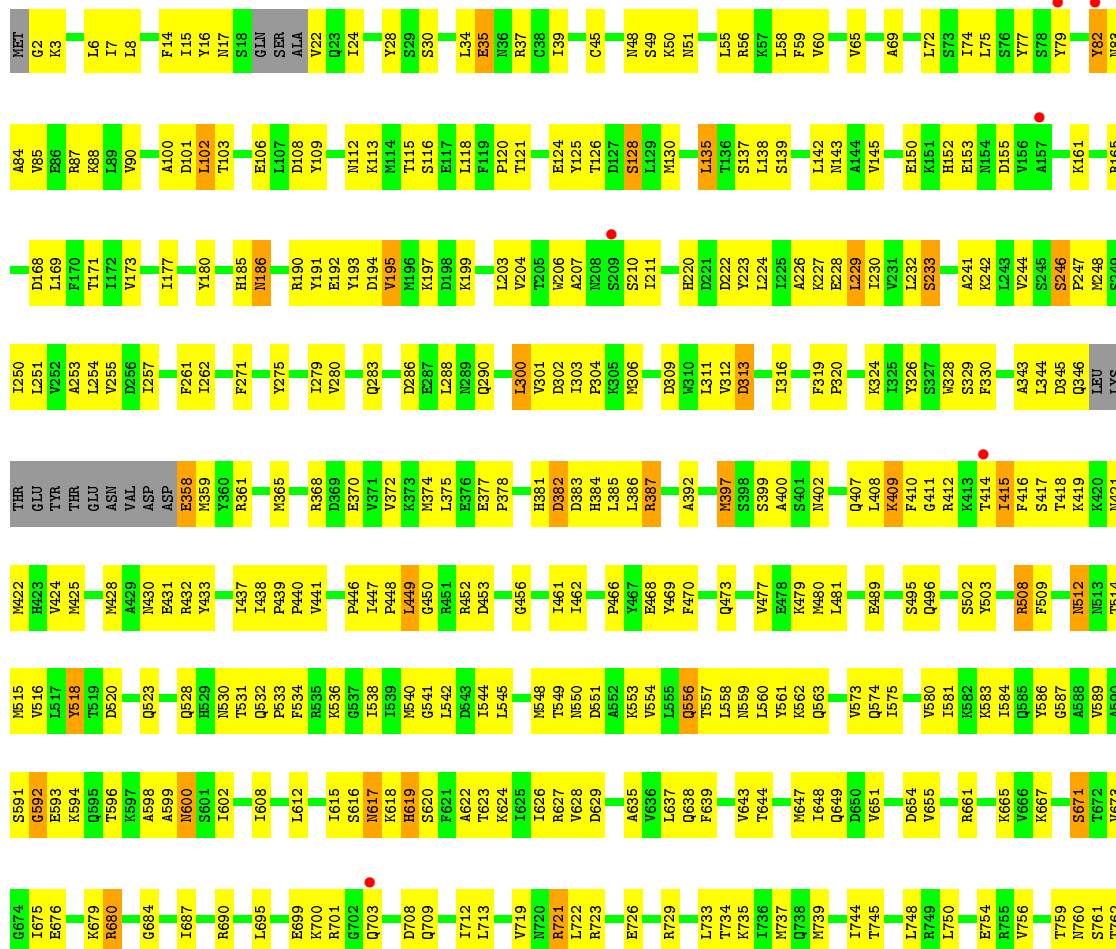
- Molecule 1: RNA (5'-R(*AP*A*AP*AP*GP*CP*C)-3')

Chain X: 



- Molecule 2: RNA-dependent RNA polymerase

Chain A: 



F763	K764	L847	R923	W1010
D770	F771	R851	D924	S1011
T777	T778	I854	S928	L1017
V779	D780	L857	A929	I1018
E781	V782	L858	I930	R1019
V783	I784	T859	S931	F1022
Q785	F788	L860	R932	K1023
M789	S790	L861	L933	G1024
L791	S796	Q862	S935	K1025
G797	I798	K863	Y939	I1026
A799	S869	P864	I944	P1027
T802	R870	V865	E945	A1028
A803	K871	T866	Y948	F1031
A804	T872	F867	I951	Y1036
T807	T873	K868	S952	A1037
F808	L878	S888	N956	K1047
K809	R879	L892	Q959	N1048
N810	D880	F893	I963	G1049
Y811	I881	I894	S964	S1053
V812	K882	Q895	G965	L1054
T813	P883	Y896	I966	F1055
E817	F884	Q897	I967	C1056
L820	F885	K898	P968	N1057
F821	T886	F899	K985	Y1058
S822	V887	P901	L989	P1059
K823	S888	Y902	E990	K1060
M824	L903	I908	S991	M1063
N825	Q909	Y909	Y992	I1064
S828	G912	G1002	Y993	K1065
R829	S916	C1003	I999	K1069
G830	Y919	Y1004	G1007	M1070
I831	E922	L1005	F1007	W1071
A832		L1006	F1009	N1072
K836				I1073
A837				B1077
K838				S1078
Y842				P1079
A843				Y1080
P844				E1088
				PRO
				HIS
				HIS
				HIS
				HIS
				HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.74Å 112.15Å 144.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-3.10) 92.5 (30.00-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.11Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.289 0.225 , 0.275	Depositor DCC
R_{free} test set	1688 reflections (7.86%)	DCC
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 23218 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8803	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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](#)

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	0.64	0/116	1.76	7/179 (3.9%)
2	A	0.45	1/8870 (0.0%)	0.66	2/11989 (0.0%)
All	All	0.45	1/8986 (0.0%)	0.69	9/12168 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	2	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	CYS	CB-SG	-6.35	1.71	1.82

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	824	ASN	N-CA-C	9.66	137.08	111.00
1	X	1106	C	C2'-C3'-O3'	8.14	127.41	109.50
1	X	1104	A	C2'-C3'-O3'	7.77	126.60	109.50
1	X	1105	G	C2'-C3'-O3'	7.58	126.17	109.50
1	X	1104	A	C4'-C3'-C2'	6.17	108.77	102.60
1	X	1106	C	C4'-C3'-C2'	6.07	108.67	102.60
2	A	825	ASN	N-CA-C	5.17	124.96	111.00
1	X	1103	A	C4'-C3'-C2'	5.11	107.70	102.60
1	X	1106	C	C4'-C3'-O3'	5.10	123.20	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	X	1105	G	C3'
1	X	1106	C	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	104	0	57	10	0
2	A	8699	0	8793	421	0
All	All	8803	0	8850	427	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 24.

All (427) 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:520:ASP:HB3	2:A:667:LYS:HG2	1.33	1.05
2:A:865:VAL:HG22	2:A:866:THR:H	1.20	1.05
2:A:101:ASP:OD1	2:A:103:THR:HG22	1.57	1.04
2:A:866:THR:HG22	2:A:867:PHE:H	1.29	0.96
2:A:385:LEU:HD23	2:A:479:LYS:HE2	1.49	0.95
2:A:556:GLN:HA	2:A:556:GLN:HE21	1.31	0.93
2:A:177:ILE:HD13	2:A:203:LEU:HD11	1.53	0.89
2:A:503:TYR:HB2	2:A:687:ILE:HD13	1.54	0.87
2:A:186:ASN:ND2	2:A:190:ARG:H	1.72	0.87
2:A:667:LYS:O	2:A:667:LYS:HG3	1.73	0.86
2:A:708:ASP:O	2:A:712:ILE:HG13	1.76	0.84
2:A:449:LEU:HD22	2:A:573:VAL:HG11	1.61	0.82
2:A:778:THR:O	2:A:782:VAL:HG23	1.80	0.82
1:X:1105:G:H5'	2:A:400:ALA:HB1	1.61	0.81
2:A:283:GLN:OE1	2:A:649:GLN:HG3	1.78	0.81
2:A:232:LEU:CD2	2:A:300:LEU:HG	2.13	0.79
2:A:473:GLN:HG2	2:A:561:TYR:CE1	2.18	0.79
2:A:24:ILE:HB	2:A:75:LEU:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:381:HIS:O	2:A:382:ASP:HB2	1.82	0.79
2:A:248:MET:O	2:A:248:MET:HE3	1.82	0.78
2:A:820:LEU:HB2	2:A:964:SER:O	1.83	0.77
2:A:135:LEU:HD22	2:A:709:GLN:NE2	1.98	0.77
2:A:449:LEU:HD22	2:A:573:VAL:CG1	2.15	0.77
2:A:6:LEU:H	2:A:6:LEU:HD22	1.51	0.75
2:A:385:LEU:HD23	2:A:479:LYS:CE	2.17	0.75
2:A:85:VAL:HG21	2:A:139:SER:OG	1.87	0.74
2:A:186:ASN:HD21	2:A:190:ARG:H	1.34	0.73
2:A:229:LEU:O	2:A:233:SER:HB3	1.87	0.73
2:A:866:THR:HG22	2:A:867:PHE:N	2.04	0.73
2:A:180:TYR:HB3	2:A:199:LYS:HG3	1.71	0.73
2:A:618:LYS:HD2	2:A:654:ASP:OD2	1.88	0.72
2:A:824:ASN:CG	2:A:828:SER:HB2	2.10	0.72
2:A:777:THR:HG21	2:A:882:LYS:HE3	1.70	0.71
2:A:2:GLY:HA2	2:A:754:GLU:OE2	1.90	0.71
2:A:886:THR:OG1	2:A:1055:PHE:HB3	1.89	0.71
2:A:226:ALA:O	2:A:230:ILE:HG13	1.91	0.71
2:A:473:GLN:HE22	2:A:593:GLU:HB3	1.55	0.70
2:A:972:ALA:O	2:A:976:VAL:HG23	1.91	0.70
2:A:279:ILE:HG22	2:A:648:ILE:HD12	1.73	0.70
2:A:865:VAL:HG22	2:A:866:THR:N	2.02	0.69
2:A:553:LYS:O	2:A:557:THR:HG22	1.91	0.69
2:A:622:ALA:HB3	2:A:638:GLN:HB3	1.73	0.69
2:A:762:THR:HA	2:A:1077:ARG:O	1.92	0.68
2:A:687:ILE:HG23	2:A:900:MET:HG3	1.75	0.68
2:A:397:MET:HA	2:A:470:PHE:HE2	1.58	0.68
2:A:247:PRO:O	2:A:251:LEU:HG	1.94	0.68
2:A:161:LYS:O	2:A:165:ARG:HG3	1.93	0.67
2:A:608:ILE:HD13	2:A:626:ILE:HG23	1.77	0.67
2:A:309:ASP:O	2:A:312:VAL:HG22	1.94	0.66
2:A:446:PRO:HG2	2:A:583:LYS:HD3	1.75	0.66
2:A:930:ILE:O	2:A:934:ILE:HG13	1.94	0.66
2:A:556:GLN:HE21	2:A:556:GLN:CA	2.04	0.66
2:A:438:ILE:HD12	2:A:563:GLN:HB3	1.77	0.66
1:X:1103:A:H2'	1:X:1103:A:N3	2.09	0.66
2:A:612:LEU:HD23	2:A:615:ILE:HD11	1.78	0.66
2:A:1023:LYS:O	2:A:1060:LYS:HG2	1.95	0.66
2:A:50:LYS:O	2:A:50:LYS:HG2	1.95	0.66
2:A:145:VAL:HG21	2:A:211:ILE:HG23	1.77	0.65
2:A:120:PRO:HD2	2:A:124:GLU:OE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1106:C:H5'	1:X:1107:C:OP2	1.96	0.65
2:A:3:LYS:HA	2:A:6:LEU:HD23	1.77	0.64
2:A:863:LYS:O	2:A:863:LYS:HG3	1.97	0.64
2:A:324:LYS:O	2:A:328:TRP:HD1	1.80	0.64
2:A:385:LEU:CD2	2:A:479:LYS:HE2	2.27	0.64
2:A:439:PRO:HD3	2:A:468:GLU:HG2	1.79	0.64
2:A:254:LEU:HD23	2:A:280:VAL:HG21	1.78	0.64
2:A:989:LEU:O	2:A:993:VAL:HG23	1.97	0.64
2:A:250:ILE:HG21	2:A:288:LEU:HB2	1.79	0.64
2:A:409:LYS:HB2	2:A:409:LYS:HZ2	1.63	0.64
2:A:762:THR:HA	2:A:1078:SER:HB3	1.80	0.64
2:A:820:LEU:HD23	2:A:820:LEU:H	1.61	0.63
2:A:858:LEU:O	2:A:862:GLN:HG2	1.98	0.63
1:X:1105:G:H5'	2:A:400:ALA:CB	2.27	0.63
2:A:516:VAL:HG12	2:A:671:SER:O	1.97	0.63
2:A:784:ILE:HD12	2:A:788:PHE:CE2	2.33	0.63
2:A:222:ASP:OD1	2:A:324:LYS:NZ	2.28	0.62
2:A:804:ALA:HA	2:A:809:LYS:HE3	1.80	0.62
2:A:428:MET:HG2	2:A:433:TYR:CG	2.33	0.62
1:X:1103:A:H5''	1:X:1103:A:N3	2.13	0.62
2:A:437:ILE:O	2:A:439:PRO:HD3	1.99	0.62
2:A:887:VAL:HG22	2:A:1054:LEU:HD11	1.80	0.62
2:A:6:LEU:HD22	2:A:6:LEU:N	2.13	0.62
2:A:1019:ARG:HD2	2:A:1053:SER:OG	2.00	0.62
2:A:241:ALA:HB3	2:A:456:GLY:HA2	1.82	0.62
2:A:261:PHE:CE1	2:A:271:PHE:HB2	2.34	0.62
2:A:1018:ILE:HD12	2:A:1037:ALA:HB1	1.82	0.61
2:A:851:ARG:HH11	2:A:851:ARG:HG2	1.64	0.61
2:A:899:PHE:O	2:A:901:PRO:HD3	2.00	0.61
2:A:644:THR:OG1	2:A:647:MET:HG3	2.00	0.61
2:A:375:LEU:C	2:A:378:PRO:HD2	2.21	0.60
2:A:449:LEU:CD2	2:A:573:VAL:HG11	2.28	0.60
2:A:544:ILE:O	2:A:548:MET:HG3	2.01	0.60
2:A:892:LEU:HD22	2:A:1017:LEU:HD11	1.82	0.60
2:A:169:LEU:HD21	2:A:227:LYS:HB2	1.84	0.60
2:A:882:LYS:HB3	2:A:883:PRO:HD3	1.82	0.60
2:A:428:MET:HE1	2:A:811:TYR:HD1	1.65	0.60
2:A:1028:ALA:HB1	2:A:1070:MET:CE	2.31	0.60
2:A:721:ARG:HD2	2:A:726:GLU:HG3	1.84	0.60
2:A:116:SER:HB3	2:A:197:LYS:HG3	1.83	0.59
2:A:880:ASP:OD2	2:A:1069:LYS:HE2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1070:MET:O	2:A:1073:ILE:HG13	2.02	0.59
2:A:302:ASP:O	2:A:306:MET:HG3	2.02	0.59
2:A:242:LYS:O	2:A:246:SER:HB2	2.02	0.59
2:A:865:VAL:CG2	2:A:866:THR:H	2.03	0.58
2:A:190:ARG:HG2	2:A:701:ARG:NH2	2.18	0.58
2:A:402:ASN:OD1	2:A:466:PRO:HA	2.04	0.58
2:A:538:ILE:O	2:A:542:LEU:HG	2.04	0.58
2:A:1003:CYS:SG	2:A:1007:PHE:CZ	2.97	0.58
2:A:102:LEU:H	2:A:102:LEU:HD22	1.67	0.58
2:A:1024:GLY:O	2:A:1025:LYS:CB	2.51	0.58
2:A:461:ILE:HD11	2:A:586:TYR:CZ	2.39	0.58
2:A:368:ARG:O	2:A:372:VAL:HG23	2.03	0.58
2:A:744:ILE:HD13	2:A:748:LEU:HD22	1.85	0.58
2:A:286:ASP:O	2:A:290:GLN:HG3	2.04	0.58
2:A:428:MET:CE	2:A:811:TYR:HD1	2.17	0.57
2:A:651:VAL:O	2:A:655:VAL:HG23	2.04	0.57
2:A:514:THR:HG22	2:A:638:GLN:HG3	1.85	0.57
2:A:193:TYR:CZ	2:A:197:LYS:HD2	2.40	0.57
2:A:343:ALA:O	2:A:346:GLN:HG3	2.05	0.57
2:A:145:VAL:CG2	2:A:211:ILE:HG23	2.34	0.57
2:A:520:ASP:HB2	2:A:667:LYS:HE2	1.85	0.56
2:A:192:GLU:O	2:A:195:VAL:HG23	2.05	0.56
2:A:55:LEU:O	2:A:59:PHE:HD2	1.88	0.56
2:A:407:GLN:O	2:A:408:LEU:HD23	2.06	0.56
2:A:821:PHE:N	2:A:821:PHE:CD2	2.70	0.56
2:A:303:ILE:HB	2:A:304:PRO:HD3	1.88	0.56
2:A:414:THR:O	2:A:415:ILE:HD12	2.04	0.56
2:A:976:VAL:O	2:A:976:VAL:HG12	2.06	0.56
2:A:558:LEU:HD23	2:A:558:LEU:O	2.06	0.56
2:A:596:THR:O	2:A:600:ASN:HB2	2.06	0.55
2:A:319:PHE:N	2:A:320:PRO:CD	2.69	0.55
2:A:452:ARG:HD2	2:A:699:GLU:OE2	2.06	0.55
2:A:1059:PRO:O	2:A:1063:MET:HG3	2.05	0.55
2:A:177:ILE:CD1	2:A:203:LEU:HD11	2.32	0.55
2:A:326:TYR:OH	2:A:676:GLU:OE2	2.21	0.55
2:A:381:HIS:O	2:A:382:ASP:CB	2.53	0.55
2:A:928:SER:O	2:A:932:ARG:HG3	2.06	0.55
2:A:866:THR:CG2	2:A:867:PHE:H	2.11	0.55
1:X:1103:A:C2'	1:X:1103:A:N3	2.69	0.55
2:A:744:ILE:HG22	2:A:745:THR:HG23	1.89	0.55
2:A:667:LYS:O	2:A:667:LYS:CG	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:102:LEU:N	2:A:102:LEU:HD22	2.22	0.55
2:A:228:GLU:OE1	2:A:303:ILE:HG13	2.06	0.55
2:A:185:HIS:CD2	2:A:185:HIS:H	2.25	0.55
2:A:515:MET:HG2	2:A:639:PHE:HE2	1.71	0.55
2:A:721:ARG:HH11	2:A:721:ARG:CG	2.20	0.55
2:A:473:GLN:HG2	2:A:561:TYR:CD1	2.41	0.54
2:A:6:LEU:CD2	2:A:6:LEU:H	2.20	0.54
2:A:316:ILE:HD13	2:A:684:GLY:HA3	1.89	0.54
2:A:784:ILE:HG23	2:A:788:PHE:CE2	2.43	0.54
2:A:87:ARG:O	2:A:90:VAL:HG22	2.07	0.54
2:A:361:ARG:O	2:A:365:MET:HG2	2.07	0.54
2:A:8:LEU:HD23	2:A:74:ILE:HD12	1.89	0.54
2:A:22:VAL:HG22	2:A:77:TYR:HB2	1.90	0.54
2:A:591:SER:HB2	2:A:596:THR:HG21	1.89	0.54
2:A:959:GLN:HE21	2:A:973:ASP:HA	1.71	0.54
2:A:450:GLY:O	2:A:462:ILE:N	2.40	0.54
2:A:629:ASP:OD2	2:A:679:LYS:HD2	2.08	0.54
2:A:573:VAL:HG12	2:A:575:ILE:HG13	1.90	0.54
2:A:612:LEU:CD2	2:A:615:ILE:HD11	2.38	0.53
2:A:392:ALA:HB2	2:A:939:VAL:HG21	1.90	0.53
2:A:744:ILE:HD11	2:A:750:LEU:HB2	1.89	0.53
2:A:509:PHE:CD2	2:A:624:LYS:HB3	2.44	0.53
2:A:791:LEU:HD23	2:A:791:LEU:N	2.23	0.53
2:A:851:ARG:NH1	2:A:851:ARG:HG2	2.24	0.53
2:A:152:HIS:HA	2:A:155:ASP:OD1	2.08	0.53
2:A:591:SER:HB2	2:A:596:THR:CG2	2.39	0.53
2:A:878:LEU:HD22	2:A:1036:TYR:CD1	2.43	0.53
2:A:35:GLU:O	2:A:39:ILE:HG13	2.09	0.53
2:A:470:PHE:HE1	2:A:594:LYS:HD3	1.74	0.52
2:A:370:GLU:O	2:A:374:MET:HG3	2.09	0.52
2:A:951:ILE:HG12	2:A:985:LYS:HA	1.91	0.52
2:A:449:LEU:HD13	2:A:573:VAL:HG13	1.90	0.52
2:A:191:TYR:CE2	2:A:204:VAL:HG11	2.44	0.52
2:A:733:LEU:O	2:A:737:MET:HE3	2.10	0.52
2:A:246:SER:N	2:A:247:PRO:CD	2.73	0.52
2:A:990:GLU:HG3	2:A:1031:PHE:CE1	2.45	0.52
2:A:528:GLN:O	2:A:531:THR:HG22	2.09	0.52
2:A:193:TYR:OH	2:A:197:LYS:HD2	2.10	0.52
2:A:549:THR:OG1	2:A:550:ASN:N	2.43	0.52
2:A:899:PHE:C	2:A:901:PRO:HD3	2.31	0.51
2:A:832:ALA:O	2:A:836:LYS:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:699:GLU:OE1	2:A:700:LYS:HE2	2.10	0.51
2:A:959:GLN:NE2	2:A:973:ASP:OD1	2.43	0.51
2:A:34:LEU:O	2:A:37:ARG:HB2	2.10	0.51
2:A:803:ALA:HA	2:A:808:PHE:CD2	2.45	0.51
2:A:358:GLU:OE2	2:A:359:MET:HG2	2.10	0.51
2:A:866:THR:O	2:A:867:PHE:HB2	2.10	0.51
2:A:612:LEU:HD23	2:A:615:ILE:CD1	2.41	0.51
1:X:1107:C:O5'	1:X:1107:C:H6	1.93	0.51
2:A:887:VAL:HG12	2:A:888:SER:N	2.26	0.51
2:A:999:ILE:HD11	2:A:1009:PHE:CZ	2.46	0.51
2:A:387:ARG:HH11	2:A:387:ARG:HB3	1.75	0.51
2:A:441:VAL:HB	2:A:447:ILE:CG1	2.40	0.51
2:A:824:ASN:OD1	2:A:828:SER:HB2	2.10	0.51
2:A:1024:GLY:O	2:A:1025:LYS:HB2	2.11	0.51
2:A:575:ILE:HD12	2:A:584:ILE:HG12	1.93	0.51
2:A:687:ILE:CG2	2:A:900:MET:HG3	2.40	0.51
2:A:884:PHE:CD1	2:A:1059:PRO:HD3	2.46	0.51
2:A:428:MET:HG2	2:A:433:TYR:CB	2.40	0.50
2:A:781:GLU:O	2:A:785:GLN:HG3	2.11	0.50
2:A:820:LEU:CB	2:A:964:SER:O	2.58	0.50
2:A:261:PHE:HD2	2:A:899:PHE:HB3	1.76	0.50
2:A:115:THR:HB	2:A:197:LYS:HA	1.93	0.50
2:A:879:ARG:HG3	2:A:879:ARG:HH11	1.77	0.50
2:A:735:LYS:O	2:A:739:MET:HG3	2.11	0.50
2:A:28:TYR:CD2	2:A:72:LEU:HB2	2.47	0.50
2:A:368:ARG:HG3	2:A:541:GLY:N	2.27	0.50
2:A:616:SER:O	2:A:617:ASN:C	2.50	0.49
2:A:516:VAL:HG21	2:A:675:ILE:CG2	2.42	0.49
2:A:72:LEU:HD12	2:A:756:VAL:CG2	2.42	0.49
2:A:842:TYR:CE2	2:A:844:PRO:HB2	2.47	0.49
2:A:100:ALA:CB	2:A:112:ASN:HB3	2.42	0.49
2:A:821:PHE:CE1	2:A:966:GLY:HA2	2.47	0.49
2:A:138:LEU:O	2:A:138:LEU:HD12	2.12	0.49
2:A:324:LYS:O	2:A:328:TRP:CD1	2.63	0.49
2:A:84:ALA:HB1	2:A:88:LYS:NZ	2.27	0.49
2:A:619:HIS:ND1	2:A:619:HIS:N	2.60	0.49
2:A:951:ILE:HG13	2:A:985:LYS:HG2	1.94	0.49
2:A:536:LYS:O	2:A:540:MET:HG3	2.11	0.49
2:A:556:GLN:NE2	2:A:556:GLN:CA	2.75	0.49
2:A:385:LEU:HD23	2:A:479:LYS:NZ	2.28	0.48
2:A:186:ASN:C	2:A:186:ASN:ND2	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:615:ILE:HG21	2:A:655:VAL:HG22	1.95	0.48
2:A:695:LEU:HG	2:A:713:LEU:CD1	2.43	0.48
2:A:616:SER:O	2:A:618:LYS:N	2.46	0.48
2:A:734:THR:HA	2:A:737:MET:CE	2.43	0.48
2:A:722:LEU:HD21	2:A:771:PHE:CE1	2.48	0.48
2:A:419:LYS:HB2	2:A:422:MET:HG3	1.95	0.48
2:A:581:ILE:O	2:A:581:ILE:HG22	2.14	0.48
2:A:532:GLN:HG3	2:A:536:LYS:HE3	1.95	0.48
2:A:255:VAL:O	2:A:673:VAL:HG21	2.14	0.48
2:A:885:PHE:CE1	2:A:1056:CYS:HB2	2.48	0.48
2:A:385:LEU:HD13	2:A:939:VAL:HG23	1.96	0.48
2:A:186:ASN:C	2:A:186:ASN:HD22	2.16	0.48
2:A:3:LYS:O	2:A:7:ILE:HG12	2.13	0.48
2:A:967:ILE:N	2:A:967:ILE:HD12	2.29	0.48
2:A:409:LYS:H	2:A:409:LYS:HZ2	1.62	0.47
2:A:384:HIS:CE1	2:A:935:SER:O	2.67	0.47
2:A:512:ASN:N	2:A:512:ASN:HD22	2.12	0.47
2:A:109:TYR:HA	2:A:118:LEU:HD21	1.96	0.47
2:A:729:ARG:HE	2:A:770:ASP:CG	2.18	0.47
1:X:1105:G:O2'	2:A:592:GLY:O	2.31	0.47
2:A:206:TRP:CD1	2:A:233:SER:OG	2.68	0.47
2:A:1065:LYS:O	2:A:1069:LYS:HG3	2.14	0.47
2:A:580:VAL:HG12	2:A:581:ILE:N	2.30	0.47
2:A:49:SER:C	2:A:51:ASN:H	2.18	0.47
2:A:246:SER:N	2:A:247:PRO:HD3	2.30	0.47
2:A:165:ARG:NE	2:A:220:HIS:HA	2.29	0.47
2:A:554:VAL:O	2:A:558:LEU:HB2	2.14	0.47
2:A:15:ILE:HG22	2:A:16:TYR:CD1	2.49	0.47
2:A:261:PHE:CD2	2:A:899:PHE:HB3	2.50	0.47
2:A:244:VAL:CG1	2:A:329:SER:HB3	2.45	0.47
2:A:924:ASP:C	2:A:944:ILE:HD13	2.36	0.47
2:A:863:LYS:CG	2:A:863:LYS:O	2.61	0.47
2:A:518:TYR:N	2:A:518:TYR:CD2	2.83	0.46
2:A:897:GLN:N	2:A:897:GLN:OE1	2.42	0.46
2:A:514:THR:HG22	2:A:638:GLN:HA	1.97	0.46
2:A:598:ALA:O	2:A:602:ILE:HG13	2.15	0.46
2:A:1002:GLY:O	2:A:1005:GLN:HG2	2.15	0.46
2:A:968:PRO:HG2	2:A:971:ASP:HB2	1.98	0.46
2:A:523:GLN:HB2	2:A:665:LYS:O	2.15	0.46
2:A:446:PRO:HB2	2:A:574:GLN:HG2	1.97	0.46
2:A:882:LYS:HE2	2:A:1036:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:884:PHE:CG	2:A:1058:TYR:HD1	2.33	0.46
2:A:253:ALA:HB1	2:A:671:SER:HB2	1.97	0.46
2:A:477:VAL:O	2:A:481:LEU:HG	2.15	0.46
2:A:489:GLU:OE1	2:A:489:GLU:N	2.48	0.46
2:A:207:ALA:O	2:A:211:ILE:HG13	2.14	0.46
2:A:399:SER:HB3	2:A:838:LYS:HB3	1.97	0.46
2:A:58:LEU:N	2:A:58:LEU:HD22	2.31	0.46
2:A:14:PHE:CD1	2:A:150:GLU:OE1	2.69	0.46
2:A:312:VAL:HG23	2:A:313:ASP:N	2.31	0.46
2:A:948:TYR:OH	2:A:1070:MET:O	2.34	0.46
2:A:255:VAL:HG11	2:A:316:ILE:HB	1.97	0.46
2:A:24:ILE:HD12	2:A:45:CYS:HB3	1.97	0.45
2:A:165:ARG:HD3	2:A:223:TYR:CB	2.46	0.45
2:A:377:GLU:HB2	2:A:378:PRO:HD3	1.98	0.45
2:A:843:ALA:HB3	2:A:844:PRO:HD3	1.98	0.45
2:A:878:LEU:HD22	2:A:1036:TYR:HD1	1.81	0.45
2:A:84:ALA:O	2:A:88:LYS:HG3	2.16	0.45
2:A:430:ASN:O	2:A:432:ARG:N	2.49	0.45
2:A:798:ILE:O	2:A:802:ILE:HG22	2.16	0.45
2:A:790:SER:HB3	2:A:791:LEU:HD23	1.98	0.45
2:A:909:TYR:CE2	2:A:1049:GLY:O	2.70	0.45
2:A:759:THR:O	2:A:761:SER:N	2.50	0.45
2:A:409:LYS:HZ2	2:A:409:LYS:CB	2.28	0.45
2:A:959:GLN:NE2	2:A:973:ASP:HA	2.31	0.45
2:A:608:ILE:HD11	2:A:635:ALA:HB2	1.99	0.45
2:A:612:LEU:O	2:A:615:ILE:HG12	2.17	0.45
2:A:922:GLU:OE2	2:A:991:SER:OG	2.24	0.45
2:A:168:ASP:O	2:A:171:THR:HB	2.16	0.45
2:A:28:TYR:HD2	2:A:72:LEU:HB2	1.82	0.45
2:A:375:LEU:O	2:A:378:PRO:HD2	2.16	0.45
2:A:324:LYS:HG3	2:A:328:TRP:CD1	2.52	0.45
2:A:415:ILE:HG23	2:A:416:PHE:N	2.32	0.45
2:A:784:ILE:HD12	2:A:788:PHE:CZ	2.52	0.45
2:A:383:ASP:O	2:A:387:ARG:HG3	2.18	0.44
2:A:30:SER:N	2:A:780:ASP:OD1	2.43	0.44
2:A:417:SER:OG	2:A:419:LYS:HG2	2.18	0.44
2:A:430:ASN:C	2:A:432:ARG:H	2.21	0.44
2:A:573:VAL:CG1	2:A:574:GLN:N	2.81	0.44
2:A:313:ASP:N	2:A:313:ASP:OD2	2.49	0.44
2:A:559:ASN:O	2:A:562:LYS:HB3	2.18	0.44
2:A:622:ALA:O	2:A:637:LEU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:161:LYS:HG2	2:A:165:ARG:CZ	2.47	0.44
2:A:854:ILE:O	2:A:858:LEU:HG	2.18	0.44
2:A:1018:ILE:HD12	2:A:1037:ALA:CB	2.45	0.44
2:A:919:TYR:C	2:A:919:TYR:CD1	2.91	0.44
2:A:126:THR:OG1	2:A:128:SER:HB3	2.18	0.44
2:A:989:LEU:HD23	2:A:989:LEU:C	2.37	0.44
2:A:439:PRO:CD	2:A:468:GLU:HG2	2.46	0.44
2:A:28:TYR:CZ	2:A:784:ILE:HG12	2.52	0.44
2:A:643:VAL:HA	2:A:647:MET:SD	2.58	0.44
2:A:477:VAL:HA	2:A:480:MET:CE	2.48	0.44
2:A:421:ASN:O	2:A:425:MET:HG3	2.17	0.44
2:A:470:PHE:CE1	2:A:594:LYS:HD3	2.52	0.44
2:A:28:TYR:HA	2:A:35:GLU:OE2	2.18	0.44
2:A:8:LEU:HA	2:A:737:MET:SD	2.58	0.44
2:A:829:ARG:HG3	2:A:830:GLY:N	2.33	0.44
2:A:248:MET:CE	2:A:251:LEU:HB2	2.48	0.44
2:A:789:MET:HE1	2:A:873:THR:HG21	2.00	0.44
2:A:135:LEU:HA	2:A:135:LEU:HD12	1.78	0.44
2:A:161:LYS:HE3	2:A:161:LYS:HB2	1.88	0.44
2:A:253:ALA:CB	2:A:671:SER:HB2	2.48	0.44
2:A:56:ARG:O	2:A:60:VAL:HG23	2.17	0.44
2:A:530:ASN:O	2:A:533:PRO:HD2	2.18	0.44
2:A:622:ALA:N	2:A:638:GLN:O	2.50	0.43
2:A:397:MET:HA	2:A:470:PHE:CE2	2.44	0.43
2:A:516:VAL:N	2:A:671:SER:O	2.47	0.43
2:A:142:LEU:HD23	2:A:211:ILE:HD11	2.00	0.43
2:A:616:SER:C	2:A:618:LYS:N	2.71	0.43
2:A:439:PRO:HA	2:A:440:PRO:HD3	1.78	0.43
2:A:137:SER:HB2	2:A:185:HIS:CD2	2.53	0.43
2:A:358:GLU:HG3	2:A:359:MET:N	2.33	0.43
2:A:898:LYS:HE2	2:A:912:GLN:NE2	2.34	0.43
2:A:822:SER:OG	2:A:823:LYS:N	2.50	0.43
2:A:150:GLU:O	2:A:153:GLU:HB2	2.19	0.43
2:A:125:TYR:CG	2:A:126:THR:N	2.86	0.43
2:A:763:PHE:CE1	2:A:857:LEU:HD13	2.54	0.43
2:A:514:THR:CG2	2:A:638:GLN:HG3	2.49	0.43
2:A:1028:ALA:HB1	2:A:1070:MET:HE3	1.99	0.43
2:A:884:PHE:CD2	2:A:1058:TYR:CE1	3.06	0.43
2:A:860:MET:HE1	2:A:865:VAL:HG12	2.00	0.43
2:A:409:LYS:HB2	2:A:409:LYS:NZ	2.32	0.43
2:A:531:THR:HB	2:A:589:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:556:GLN:HA	2:A:556:GLN:NE2	2.14	0.43
2:A:551:ASP:HB3	2:A:554:VAL:HB	2.01	0.43
2:A:520:ASP:HB3	2:A:667:LYS:CG	2.25	0.43
2:A:872:ILE:HG22	2:A:1073:ILE:HA	2.01	0.43
2:A:761:SER:O	2:A:1078:SER:HB3	2.19	0.42
2:A:65:VAL:O	2:A:69:ALA:HB3	2.18	0.42
2:A:83:ASN:HB3	2:A:84:ALA:H	1.48	0.42
2:A:330:PHE:CE1	2:A:690:ARG:CZ	3.02	0.42
2:A:719:VAL:HG12	2:A:723:ARG:HD2	2.00	0.42
2:A:257:ILE:O	2:A:275:TYR:HA	2.20	0.42
2:A:232:LEU:HD23	2:A:300:LEU:HG	1.95	0.42
2:A:375:LEU:HB2	2:A:545:LEU:CD1	2.49	0.42
2:A:82:TYR:O	2:A:82:TYR:HD1	2.01	0.42
2:A:900:MET:CE	2:A:903:LEU:HD21	2.50	0.42
2:A:820:LEU:CD1	2:A:824:ASN:ND2	2.82	0.42
2:A:28:TYR:CE1	2:A:784:ILE:HG12	2.54	0.42
2:A:502:SER:HB3	2:A:680:ARG:NH1	2.35	0.42
2:A:623:THR:CG2	2:A:626:ILE:HG13	2.50	0.42
2:A:721:ARG:NH1	2:A:721:ARG:CG	2.79	0.42
2:A:301:VAL:C	2:A:304:PRO:HD2	2.39	0.42
2:A:733:LEU:C	2:A:737:MET:HE3	2.40	0.42
2:A:232:LEU:HD21	2:A:300:LEU:HG	1.97	0.42
2:A:495:SER:OG	2:A:496:GLN:N	2.52	0.42
2:A:821:PHE:N	2:A:821:PHE:HD2	2.17	0.42
2:A:466:PRO:HD2	2:A:469:TYR:CD2	2.55	0.42
2:A:959:GLN:CD	2:A:973:ASP:OD1	2.57	0.42
2:A:803:ALA:HA	2:A:808:PHE:CE2	2.55	0.42
2:A:560:LEU:HA	2:A:560:LEU:HD23	1.76	0.42
2:A:813:THR:O	2:A:817:GLU:HG3	2.20	0.42
2:A:193:TYR:CE2	2:A:197:LYS:HD2	2.55	0.42
2:A:346:GLN:HG2	2:A:586:TYR:CE1	2.55	0.42
2:A:735:LYS:HA	2:A:735:LYS:HD2	1.85	0.42
2:A:410:PHE:O	2:A:412:ARG:N	2.53	0.42
2:A:617:ASN:N	2:A:617:ASN:HD22	2.17	0.42
2:A:1077:ARG:HA	2:A:1077:ARG:HD3	1.86	0.42
2:A:409:LYS:H	2:A:409:LYS:NZ	2.18	0.42
2:A:661:ARG:HA	2:A:661:ARG:HD2	1.81	0.42
2:A:138:LEU:HD22	2:A:204:VAL:HG13	2.01	0.41
2:A:447:ILE:HG22	2:A:448:PRO:O	2.19	0.41
2:A:108:ASP:HB2	2:A:113:LYS:NZ	2.35	0.41
2:A:262:ILE:HD12	2:A:508:ARG:HD2	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:534:PHE:CZ	2:A:599:ALA:HB1	2.56	0.41
2:A:869:SER:C	2:A:871:LYS:H	2.22	0.41
2:A:900:MET:HE1	2:A:903:LEU:HD21	2.03	0.41
2:A:210:SER:OG	2:A:230:ILE:HG23	2.20	0.41
2:A:627:ARG:HH11	2:A:627:ARG:HG2	1.84	0.41
2:A:626:ILE:O	2:A:627:ARG:HG2	2.21	0.41
2:A:612:LEU:HA	2:A:615:ILE:HG12	2.02	0.41
2:A:744:ILE:HD13	2:A:748:LEU:CD2	2.51	0.41
2:A:894:ILE:O	2:A:894:ILE:HG13	2.20	0.41
2:A:847:LEU:O	2:A:851:ARG:HG3	2.21	0.41
2:A:531:THR:HG21	2:A:587:GLY:O	2.20	0.41
2:A:534:PHE:HZ	2:A:599:ALA:HB1	1.86	0.41
1:X:1104:A:H5'	1:X:1105:G:OP1	2.20	0.41
2:A:14:PHE:HD1	2:A:150:GLU:OE1	2.03	0.41
1:X:1105:G:N3	2:A:592:GLY:HA2	2.36	0.41
2:A:199:LYS:HD2	2:A:199:LYS:H	1.85	0.41
2:A:375:LEU:HB2	2:A:545:LEU:HD11	2.02	0.41
2:A:820:LEU:C	2:A:821:PHE:HD2	2.25	0.41
2:A:863:LYS:HA	2:A:864:PRO:HD2	1.84	0.41
2:A:424:VAL:O	2:A:428:MET:HG3	2.21	0.41
2:A:100:ALA:HB1	2:A:112:ASN:HB3	2.03	0.41
2:A:512:ASN:N	2:A:512:ASN:ND2	2.69	0.41
2:A:386:LEU:O	2:A:557:THR:HG21	2.21	0.40
2:A:744:ILE:N	2:A:744:ILE:HD12	2.35	0.40
2:A:453:ASP:HB2	2:A:699:GLU:HG3	2.03	0.40
2:A:173:VAL:O	2:A:177:ILE:HG12	2.21	0.40
2:A:515:MET:HG2	2:A:639:PHE:CE2	2.53	0.40
2:A:944:ILE:HG23	2:A:945:GLU:N	2.35	0.40
2:A:908:GLN:O	2:A:912:GLN:HG3	2.21	0.40
2:A:703:GLN:N	2:A:703:GLN:CD	2.74	0.40
2:A:1023:LYS:NZ	2:A:1057:ASN:HA	2.36	0.40
2:A:358:GLU:OE2	2:A:359:MET:CG	2.69	0.40
2:A:963:ILE:HD11	2:A:969:LYS:HG2	2.02	0.40
2:A:796:SER:HB3	2:A:799:ALA:HB3	2.04	0.40
2:A:344:LEU:O	2:A:345:ASP:C	2.59	0.40
2:A:952:SER:HB3	2:A:1071:TRP:CE3	2.57	0.40
2:A:223:TYR:CD2	2:A:224:LEU:HD23	2.57	0.40
2:A:77:TYR:CE1	2:A:748:LEU:HG	2.56	0.40
2:A:857:LEU:O	2:A:861:LEU:HD13	2.21	0.40
2:A:764:LYS:HD3	2:A:1080:TYR:CD2	2.57	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	
2	A	1067/1095 (97%)	967 (91%)	78 (7%)	22 (2%)	9	37

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	106	GLU
2	A	382	ASP
2	A	822	SER
2	A	865	VAL
2	A	978	SER
2	A	1025	LYS
2	A	82	TYR
2	A	128	SER
2	A	411	GLY
2	A	1027	PRO
2	A	102	LEU
2	A	431	GLU
2	A	760	ASN
2	A	870	SER
2	A	397	MET
2	A	807	THR
2	A	869	SER
2	A	617	ASN
2	A	882	LYS
2	A	1002	GLY
2	A	592	GLY
2	A	864	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	975/996 (98%)	923 (95%)	52 (5%)	28	64

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	17	ASN
2	A	35	GLU
2	A	48	ASN
2	A	79	TYR
2	A	121	THR
2	A	130	MET
2	A	135	LEU
2	A	143	ASN
2	A	186	ASN
2	A	194	ASP
2	A	195	VAL
2	A	229	LEU
2	A	233	SER
2	A	246	SER
2	A	300	LEU
2	A	311	LEU
2	A	313	ASP
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	508	ARG
2	A	512	ASN
2	A	518	TYR
2	A	556	GLN
2	A	600	ASN
2	A	619	HIS
2	A	620	SER
2	A	628	VAL
2	A	671	SER
2	A	680	ARG
2	A	721	ARG
2	A	784	ILE

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Mol	Chain	Res	Type
2	A	791	LEU
2	A	824	ASN
2	A	868	LYS
2	A	888	SER
2	A	892	LEU
2	A	895	GLN
2	A	900	MET
2	A	916	SER
2	A	922	GLU
2	A	939	VAL
2	A	956	ASN
2	A	970	ILE
2	A	1011	SER
2	A	1022	PHE
2	A	1027	PRO
2	A	1047	LYS
2	A	1088	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	36	ASN
2	A	42	HIS
2	A	48	ASN
2	A	63	ASN
2	A	143	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	512	ASN
2	A	528	GLN
2	A	556	GLN
2	A	563	GLN
2	A	565	GLN
2	A	574	GLN
2	A	585	GLN
2	A	617	ASN
2	A	646	GLN
2	A	649	GLN

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Mol	Chain	Res	Type
2	A	653	ASN
2	A	810	ASN
2	A	824	ASN
2	A	853	GLN
2	A	875	ASN
2	A	895	GLN
2	A	912	GLN
2	A	959	GLN
2	A	1034	HIS
2	A	1057	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	5/7 (71%)	4 (80%)	2 (40%)

All (4) RNA backbone outliers are listed below:

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

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1103	A
1	X	1105	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

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	X	5/7 (71%)	0.30	0 100 100	50, 56, 74, 74	0
2	A	1073/1095 (97%)	-0.33	12 (1%) 82 66	11, 46, 78, 120	0
All	All	1078/1102 (97%)	-0.33	12 (1%) 82 66	11, 46, 78, 120	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	824	ASN	4.0
2	A	867	PHE	3.4
2	A	1024	GLY	2.8
2	A	157	ALA	2.8
2	A	868	LYS	2.4
2	A	866	THR	2.4
2	A	82	TYR	2.2
2	A	703	GLN	2.2
2	A	209	SER	2.2
2	A	79	TYR	2.2
2	A	414	THR	2.2
2	A	865	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.