



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:34 am BST

PDB ID : 2R7S
Title : Crystal Structure of Rotavirus SA11 VP1 / RNA (UGUGCC) complex
Authors : Lu, X.; Harrison, S.C.; Tao, Y.J.; Patton, J.T.; Nibert, M.L.
Deposited on : 2007-09-10
Resolution : 3.24 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

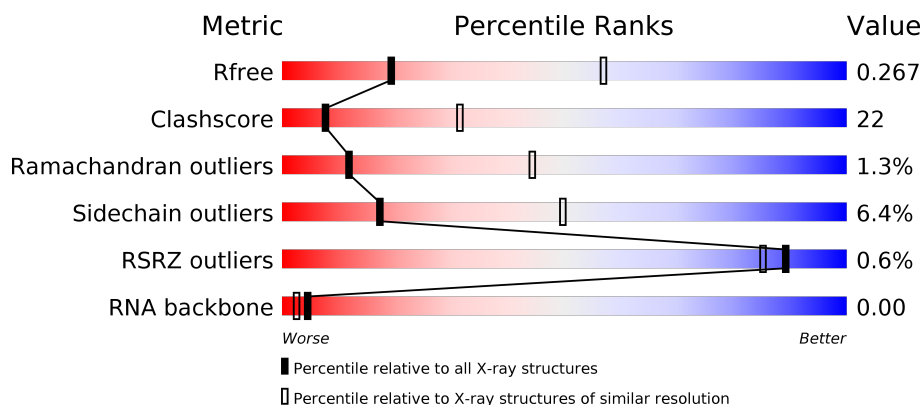
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)
RNA backbone	3102	1034 (3.58-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	6	<div> <div>33%</div> <div>17% 83%</div> </div>
2	A	1095	<div> <div>54% 40%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	X	1201	-	X	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8827 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.

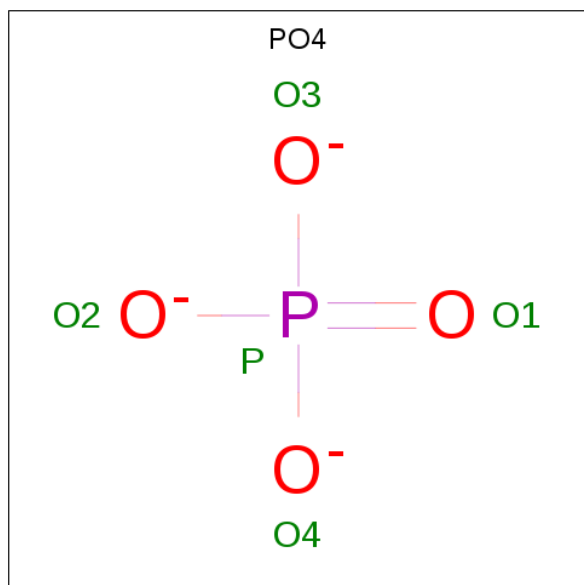
- Molecule 1 is a RNA chain called RNA (5'-R(*UP*GP*UP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	6	Total	C	N	O	P	0	0	0
			123	56	20	42	5			

- 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			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	X	1	Total	O	P	0	0
			5	4	1		

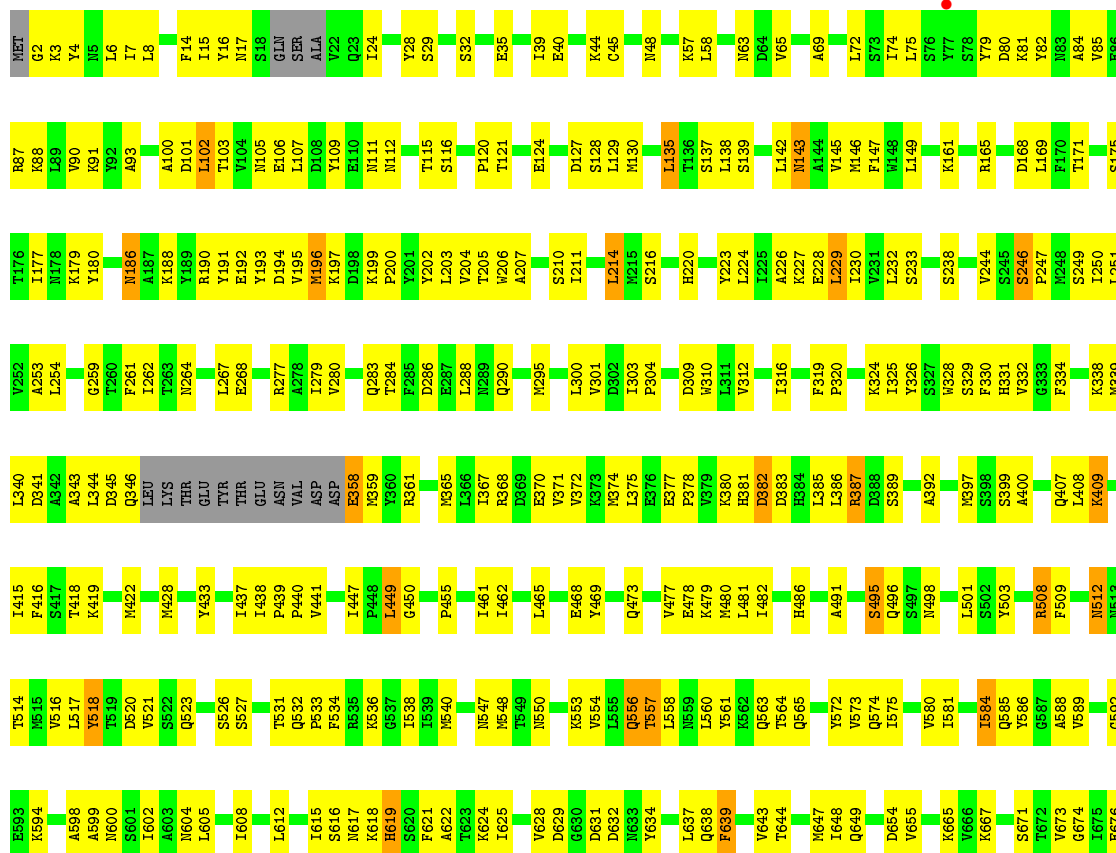
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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*CP*C)-3')



- Molecule 2: RNA-dependent RNA polymerase



I1052	I1053	L1054	F1055	C1056	N1057	Y1058	P1059	K1060	S1061	E1062	M1063	I1064	M1067	M1071	S1078	E1088	P1090	H1S	H1S	H1S	H1S	H1S	H1S	H1S																									
I951	H954	E957	I958	Q959	I962	S964	I967	P968	D971	A972	Y975	V976	Y981	D984	K985	I988	L989	E990	S991	Y992	V993	S998	C1003	Y1004	Q1005	L1006	F1007	D1008	L1017	I1018	R1019	F1022	K1023	G1024	K1025	I1026	P1027	A1028	V1029	I1032	A1037	G1049							
Q853	L861	Q862	K863	P864	V865	T866	K868	S869	I874	N875	R879	D880	I881	K882	P883	F884	F885	T886	D889	L892	P893	I894	Q895	Y896	Q897	K898	F899	N900	P901	T902	L903	Y909	S916	R917	T918	E922	K927	S928	L929	I930	S931	R932	L933	I934	Y939	E945			
N760	S761	K764	V765	I772	T777	T778	E781	V782	Y783	I784	Q785	R786	A787	F788	R789	S790	L791	I798	A804	S805	S806	T807	F808	K809	N810	Y811	L820	F821	S822	K823	N824	N825	S828	R829	Q830	P831	A832	K836	Y842	A843	P844	I845	S846	L847	E848	K849	R850	R851	A852
I677	R680	Y681	G684	I687	F688	F689	R690	A691	G692	I693	N694	L695	R701	Q702	Q703	D708	Q709	A710	A711	I712	L713	Y714	S715	N716	Y717	I718	V719	N720	R721	L722	R723	Q724	F725	R729	L733	T734	M737	I744	L748	R749	L750	S753	E754	R755	V756	L757	T758	T759	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.12Å 112.66Å 144.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.24 40.92 – 3.20	Depositor EDS
% Data completeness (in resolution range)	82.2 (30.00-3.24) 85.2 (40.92-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.283 0.205 , 0.267	Depositor DCC
R_{free} test set	1693 reflections (7.89%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8827	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.48	0/136	1.65	10/210 (4.8%)
2	A	0.44	0/8870	0.60	2/11989 (0.0%)
All	All	0.44	0/9006	0.63	12/12199 (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	1	0

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1105	C	C2'-C3'-O3'	8.04	127.18	109.50
2	A	824	ASN	N-CA-C	8.02	132.65	111.00
1	X	1101	U	C2'-C3'-O3'	7.46	125.91	109.50
1	X	1103	U	C2'-C3'-O3'	7.44	125.88	109.50
2	A	825	ASN	N-CA-C	6.40	128.27	111.00
1	X	1102	G	C4'-C3'-C2'	5.78	108.38	102.60
1	X	1102	G	C2'-C3'-O3'	5.74	122.89	113.70
1	X	1105	C	C4'-C3'-C2'	5.47	108.07	102.60
1	X	1103	U	C4'-C3'-C2'	5.34	107.94	102.60
1	X	1104	G	C2'-C3'-O3'	5.12	121.89	113.70
1	X	1105	C	C4'-C3'-O3'	5.11	123.21	113.00
1	X	1104	G	C4'-C3'-C2'	5.04	107.64	102.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	X	1105	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	123	0	66	12	0
2	A	8699	0	8793	381	0
3	X	5	0	0	4	0
All	All	8827	0	8859	388	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 22.

All (388) 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:X:1106:C:H3'	3:X:1201:PO4:P	1.80	1.22
2:A:503:TYR:HB2	2:A:687:ILE:HD13	1.43	1.00
2:A:385:LEU:HD23	2:A:479:LYS:HE2	1.46	0.94
2:A:865:VAL:HG22	2:A:866:THR:H	1.38	0.88
2:A:8:LEU:HD23	2:A:74:ILE:HD12	1.59	0.84
2:A:186:ASN:ND2	2:A:190:ARG:H	1.76	0.82
2:A:509:PHE:CD2	2:A:624:LYS:HB3	2.16	0.81
2:A:885:PHE:CE1	2:A:1056:CYS:HB2	2.17	0.80
2:A:930:ILE:HG22	2:A:984:ASP:OD2	1.82	0.80
2:A:4:TYR:HD1	2:A:733:LEU:HD13	1.46	0.79
2:A:886:THR:OG1	2:A:1055:PHE:HB3	1.83	0.79
2:A:820:LEU:HD23	2:A:820:LEU:H	1.48	0.79
2:A:250:ILE:HG21	2:A:288:LEU:HB2	1.63	0.78
2:A:734:THR:HA	2:A:737:MET:HE2	1.64	0.78
2:A:368:ARG:O	2:A:372:VAL:HG23	1.82	0.78
2:A:254:LEU:HD23	2:A:280:VAL:HG21	1.67	0.77
2:A:177:ILE:HD13	2:A:203:LEU:HD11	1.69	0.75
2:A:644:THR:OG1	2:A:647:MET:HG3	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:101:ASP:OD1	2:A:103:THR:HG22	1.88	0.74
2:A:503:TYR:CB	2:A:687:ILE:HD13	2.16	0.73
2:A:473:GLN:HG2	2:A:561:TYR:CE1	2.24	0.73
2:A:1018:ILE:HD12	2:A:1037:ALA:HB1	1.71	0.72
2:A:882:LYS:HB3	2:A:883:PRO:HD3	1.72	0.72
2:A:556:GLN:HE21	2:A:556:GLN:HA	1.55	0.71
2:A:375:LEU:C	2:A:378:PRO:HD2	2.10	0.71
2:A:781:GLU:O	2:A:785:GLN:HG3	1.89	0.71
2:A:180:TYR:HB3	2:A:199:LYS:HG3	1.73	0.71
2:A:553:LYS:O	2:A:557:THR:HG22	1.91	0.70
2:A:598:ALA:O	2:A:602:ILE:HG13	1.92	0.70
2:A:283:GLN:OE1	2:A:649:GLN:HG3	1.91	0.70
2:A:116:SER:HB3	2:A:197:LYS:HG3	1.72	0.70
2:A:186:ASN:HD21	2:A:190:ARG:H	1.37	0.70
2:A:777:THR:HG21	2:A:882:LYS:HE3	1.74	0.69
2:A:478:GLU:O	2:A:482:ILE:HD12	1.91	0.69
2:A:262:ILE:HD12	2:A:508:ARG:HD2	1.74	0.69
2:A:729:ARG:HG2	2:A:729:ARG:HH11	1.58	0.69
2:A:756:VAL:HG13	2:A:788:PHE:CZ	2.28	0.68
2:A:2:GLY:HA2	2:A:754:GLU:OE2	1.94	0.68
2:A:24:ILE:HD12	2:A:45:CYS:HB3	1.75	0.68
2:A:532:GLN:HB3	2:A:533:PRO:HD3	1.76	0.68
2:A:386:LEU:O	2:A:557:THR:HG21	1.94	0.67
2:A:142:LEU:HD23	2:A:211:ILE:HD11	1.77	0.67
2:A:223:TYR:HD2	2:A:224:LEU:HD23	1.59	0.67
2:A:1059:PRO:O	2:A:1063:MET:HG3	1.95	0.66
2:A:717:TYR:OH	2:A:729:ARG:HD2	1.94	0.66
2:A:387:ARG:HH11	2:A:387:ARG:HB3	1.60	0.66
2:A:477:VAL:O	2:A:481:LEU:HG	1.94	0.66
2:A:264:ASN:HD21	2:A:268:GLU:HG3	1.61	0.66
2:A:787:ALA:O	2:A:790:SER:HB3	1.96	0.66
2:A:778:THR:O	2:A:782:VAL:HG23	1.96	0.66
2:A:972:ALA:O	2:A:976:VAL:HG23	1.96	0.66
2:A:449:LEU:HD22	2:A:573:VAL:HG11	1.78	0.65
2:A:6:LEU:H	2:A:6:LEU:HD22	1.61	0.65
2:A:1017:LEU:HD22	2:A:1052:ILE:O	1.97	0.64
2:A:72:LEU:HD23	2:A:861:LEU:O	1.97	0.64
2:A:264:ASN:HD21	2:A:268:GLU:CG	2.10	0.64
2:A:370:GLU:O	2:A:374:MET:HG3	1.97	0.64
1:X:1106:C:C3'	3:X:1201:PO4:P	2.73	0.64
1:X:1104:G:H2'	1:X:1104:G:N3	2.13	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:330:PHE:CE1	2:A:690:ARG:CZ	2.81	0.64
2:A:24:ILE:HB	2:A:75:LEU:HB2	1.78	0.64
2:A:865:VAL:HG22	2:A:866:THR:N	2.10	0.64
2:A:930:ILE:O	2:A:934:ILE:HG13	1.97	0.63
2:A:324:LYS:O	2:A:328:TRP:HD1	1.80	0.63
2:A:438:ILE:HD11	2:A:560:LEU:HD22	1.81	0.63
1:X:1105:C:O2	2:A:592:GLY:HA2	1.98	0.63
2:A:824:ASN:CG	2:A:828:SER:HB2	2.20	0.62
2:A:744:ILE:HB	2:A:748:LEU:HB3	1.82	0.62
2:A:622:ALA:HB3	2:A:638:GLN:HB3	1.81	0.62
2:A:734:THR:HA	2:A:737:MET:CE	2.29	0.62
2:A:1003:CYS:SG	2:A:1007:PHE:CZ	2.92	0.62
2:A:286:ASP:O	2:A:290:GLN:HG3	1.98	0.62
2:A:503:TYR:CG	2:A:687:ILE:HD13	2.34	0.62
2:A:247:PRO:O	2:A:251:LEU:HG	1.99	0.62
2:A:340:LEU:O	2:A:344:LEU:HB2	2.00	0.62
2:A:3:LYS:O	2:A:7:ILE:HG12	2.01	0.61
2:A:784:ILE:HG13	2:A:788:PHE:CE2	2.35	0.61
2:A:407:GLN:O	2:A:408:LEU:HD23	2.00	0.61
2:A:536:LYS:O	2:A:540:MET:HG3	2.01	0.61
2:A:968:PRO:HG2	2:A:971:ASP:HB2	1.83	0.61
2:A:843:ALA:HB3	2:A:844:PRO:HD3	1.83	0.60
2:A:381:HIS:O	2:A:382:ASP:HB2	2.02	0.60
2:A:309:ASP:O	2:A:312:VAL:HG22	2.02	0.60
2:A:146:MET:HA	2:A:149:LEU:HD12	1.83	0.60
2:A:279:ILE:HG22	2:A:648:ILE:HD12	1.82	0.60
2:A:3:LYS:HA	2:A:6:LEU:HD23	1.83	0.60
2:A:842:TYR:CE2	2:A:844:PRO:HB2	2.37	0.59
2:A:192:GLU:O	2:A:196:MET:HB2	2.02	0.59
2:A:385:LEU:HD23	2:A:479:LYS:CE	2.27	0.59
2:A:367:ILE:O	2:A:371:VAL:HG23	2.03	0.59
2:A:984:ASP:O	2:A:988:ILE:HG12	2.03	0.59
2:A:85:VAL:HG22	2:A:143:ASN:HD21	1.68	0.58
2:A:168:ASP:O	2:A:171:THR:HB	2.02	0.58
2:A:449:LEU:HD22	2:A:573:VAL:CG1	2.33	0.58
2:A:503:TYR:HB2	2:A:687:ILE:CD1	2.27	0.58
2:A:534:PHE:CZ	2:A:599:ALA:HB1	2.39	0.58
2:A:329:SER:O	2:A:332:VAL:HG22	2.04	0.57
2:A:191:TYR:CE2	2:A:204:VAL:HG11	2.38	0.57
2:A:165:ARG:HD3	2:A:223:TYR:CB	2.33	0.57
2:A:161:LYS:O	2:A:165:ARG:HG3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:210:SER:OG	2:A:230:ILE:HG23	2.04	0.57
2:A:180:TYR:CD1	2:A:200:PRO:HD3	2.40	0.57
2:A:361:ARG:O	2:A:365:MET:HG2	2.05	0.57
2:A:295:MET:O	2:A:300:LEU:HB2	2.05	0.57
2:A:580:VAL:HG12	2:A:581:ILE:N	2.20	0.56
2:A:438:ILE:HD12	2:A:563:GLN:HB3	1.86	0.56
2:A:438:ILE:CD1	2:A:560:LEU:HD22	2.35	0.56
2:A:967:ILE:HD12	2:A:967:ILE:N	2.20	0.56
2:A:115:THR:HB	2:A:197:LYS:HA	1.86	0.56
2:A:681:TYR:CZ	2:A:688:PHE:HB3	2.41	0.56
2:A:226:ALA:O	2:A:230:ILE:HG13	2.05	0.56
2:A:520:ASP:HB3	2:A:667:LYS:CG	2.36	0.56
2:A:180:TYR:CE1	2:A:200:PRO:HD3	2.41	0.56
1:X:1106:C:O3'	2:A:594:LYS:HA	2.06	0.56
2:A:4:TYR:CD1	2:A:733:LEU:HD13	2.36	0.56
2:A:165:ARG:HE	2:A:220:HIS:HA	1.71	0.56
2:A:832:ALA:O	2:A:836:LYS:HG3	2.05	0.56
2:A:264:ASN:ND2	2:A:268:GLU:HG3	2.21	0.55
2:A:989:LEU:O	2:A:993:VAL:HG23	2.05	0.55
2:A:85:VAL:HG22	2:A:143:ASN:ND2	2.21	0.55
2:A:343:ALA:O	2:A:346:GLN:HG3	2.07	0.55
2:A:303:ILE:HG23	2:A:325:ILE:HD13	1.88	0.55
2:A:744:ILE:HD11	2:A:750:LEU:HB2	1.88	0.55
2:A:319:PHE:N	2:A:320:PRO:CD	2.70	0.55
2:A:251:LEU:HD22	2:A:310:TRP:CZ3	2.43	0.54
2:A:951:ILE:HG12	2:A:985:LYS:HA	1.87	0.54
2:A:109:TYR:CE1	2:A:338:LYS:HG3	2.43	0.54
2:A:1026:ILE:HG23	2:A:1029:VAL:HB	1.87	0.54
2:A:14:PHE:CE2	2:A:147:PHE:HB2	2.42	0.54
2:A:719:VAL:CG1	2:A:723:ARG:HD2	2.36	0.54
2:A:798:ILE:HG13	2:A:848:GLU:OE1	2.07	0.54
2:A:534:PHE:HZ	2:A:599:ALA:HB1	1.73	0.53
2:A:632:ASP:OD2	2:A:677:ILE:HB	2.08	0.53
2:A:729:ARG:NH1	2:A:729:ARG:HG2	2.23	0.53
2:A:1024:GLY:O	2:A:1025:LYS:HB3	2.08	0.53
2:A:87:ARG:O	2:A:90:VAL:HG22	2.08	0.53
2:A:65:VAL:O	2:A:69:ALA:HB3	2.09	0.53
2:A:381:HIS:O	2:A:382:ASP:CB	2.57	0.53
2:A:532:GLN:CB	2:A:533:PRO:HD3	2.39	0.53
2:A:618:LYS:HD2	2:A:654:ASP:OD2	2.09	0.53
2:A:409:LYS:HB2	2:A:409:LYS:NZ	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:439:PRO:HD3	2:A:468:GLU:HG2	1.91	0.52
2:A:72:LEU:HD21	2:A:861:LEU:HA	1.89	0.52
2:A:863:LYS:O	2:A:863:LYS:HG3	2.10	0.52
2:A:165:ARG:NE	2:A:220:HIS:HA	2.24	0.52
2:A:945:GLU:HG2	2:A:992:TYR:HE1	1.74	0.52
2:A:169:LEU:HD21	2:A:227:LYS:HB2	1.92	0.52
2:A:909:TYR:CE2	2:A:1049:GLY:O	2.63	0.52
1:X:1106:C:H3'	3:X:1201:PO4:O2	2.09	0.52
2:A:138:LEU:HD22	2:A:204:VAL:HG13	1.91	0.52
2:A:573:VAL:HG12	2:A:575:ILE:HG13	1.90	0.52
2:A:188:LYS:O	2:A:190:ARG:HG3	2.10	0.51
2:A:865:VAL:CG2	2:A:866:THR:H	2.18	0.51
2:A:825:ASN:HA	2:A:828:SER:HB3	1.90	0.51
2:A:324:LYS:HG3	2:A:328:TRP:CD1	2.45	0.51
2:A:760:ASN:HA	2:A:764:LYS:HD2	1.91	0.51
2:A:822:SER:OG	2:A:823:LYS:N	2.42	0.51
2:A:922:GLU:OE2	2:A:991:SER:OG	2.24	0.51
2:A:473:GLN:O	2:A:477:VAL:HG23	2.10	0.51
2:A:383:ASP:O	2:A:387:ARG:HG3	2.10	0.51
2:A:711:ALA:HA	2:A:765:VAL:HG13	1.93	0.51
2:A:781:GLU:O	2:A:784:ILE:HG22	2.10	0.51
2:A:900:MET:HE2	2:A:903:LEU:HG	1.93	0.51
2:A:135:LEU:HD22	2:A:709:GLN:NE2	2.26	0.51
2:A:288:LEU:O	2:A:288:LEU:HD12	2.11	0.51
2:A:8:LEU:CD2	2:A:74:ILE:HD12	2.34	0.51
2:A:1058:TYR:HD2	2:A:1063:MET:HG2	1.76	0.50
2:A:428:MET:HE2	2:A:811:TYR:HD1	1.76	0.50
2:A:6:LEU:HD22	2:A:6:LEU:N	2.24	0.50
2:A:616:SER:O	2:A:617:ASN:C	2.48	0.50
2:A:758:THR:O	2:A:764:LYS:HE3	2.11	0.50
2:A:375:LEU:O	2:A:378:PRO:HD2	2.10	0.50
2:A:437:ILE:O	2:A:439:PRO:HD3	2.11	0.50
2:A:503:TYR:CD1	2:A:687:ILE:HD13	2.46	0.50
2:A:755:ARG:HD2	2:A:781:GLU:HG2	1.94	0.50
2:A:928:SER:O	2:A:932:ARG:HG3	2.11	0.50
2:A:223:TYR:CD2	2:A:224:LEU:HD23	2.44	0.50
2:A:316:ILE:HD13	2:A:684:GLY:HA3	1.94	0.50
2:A:193:TYR:OH	2:A:197:LYS:HD2	2.12	0.50
2:A:165:ARG:HD3	2:A:223:TYR:HB2	1.92	0.50
2:A:520:ASP:HB3	2:A:667:LYS:HG3	1.93	0.50
2:A:1023:LYS:O	2:A:1060:LYS:HG2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:VAL:HG21	2:A:139:SER:OG	2.11	0.50
2:A:673:VAL:HG23	2:A:674:GLY:N	2.27	0.50
2:A:301:VAL:C	2:A:304:PRO:HD2	2.31	0.50
2:A:721:ARG:HH11	2:A:721:ARG:CG	2.25	0.50
2:A:791:LEU:HD23	2:A:791:LEU:H	1.76	0.49
2:A:1023:LYS:HB3	2:A:1060:LYS:HG2	1.95	0.49
2:A:449:LEU:CD2	2:A:573:VAL:HG11	2.42	0.49
2:A:575:ILE:HD12	2:A:584:ILE:HG12	1.93	0.49
2:A:28:TYR:HE1	2:A:783:TYR:HD2	1.61	0.49
2:A:1018:ILE:HD12	2:A:1037:ALA:CB	2.40	0.49
1:X:1105:C:C4	2:A:462:ILE:HD13	2.47	0.49
2:A:229:LEU:O	2:A:233:SER:HB3	2.13	0.49
2:A:520:ASP:HB3	2:A:667:LYS:CD	2.43	0.49
2:A:734:THR:CA	2:A:737:MET:HE2	2.38	0.49
2:A:190:ARG:HG2	2:A:701:ARG:NH2	2.28	0.49
2:A:847:LEU:HD23	2:A:850:ARG:CZ	2.43	0.49
2:A:1003:CYS:SG	2:A:1007:PHE:HZ	2.33	0.49
2:A:15:ILE:HG22	2:A:16:TYR:CD1	2.48	0.49
2:A:211:ILE:HA	2:A:214:LEU:HD23	1.95	0.49
2:A:428:MET:HG2	2:A:433:TYR:HB2	1.94	0.49
2:A:340:LEU:HD11	2:A:344:LEU:HD13	1.95	0.49
2:A:820:LEU:HD11	2:A:824:ASN:ND2	2.28	0.49
2:A:824:ASN:ND2	2:A:828:SER:HB2	2.28	0.49
2:A:894:ILE:O	2:A:894:ILE:HG13	2.13	0.49
2:A:228:GLU:O	2:A:232:LEU:HB2	2.13	0.48
2:A:639:PHE:CD2	2:A:639:PHE:N	2.80	0.48
2:A:107:LEU:HD23	2:A:107:LEU:N	2.27	0.48
2:A:695:LEU:HG	2:A:713:LEU:CD1	2.42	0.48
2:A:721:ARG:HG3	2:A:721:ARG:HH11	1.78	0.48
2:A:477:VAL:HA	2:A:480:MET:CE	2.42	0.48
2:A:249:SER:HB3	2:A:676:GLU:OE1	2.14	0.48
2:A:450:GLY:O	2:A:462:ILE:N	2.45	0.48
2:A:605:LEU:HA	2:A:608:ILE:HG22	1.96	0.48
2:A:338:LYS:HB2	2:A:341:ASP:OD2	2.14	0.48
2:A:820:LEU:HB2	2:A:964:SER:O	2.14	0.48
2:A:612:LEU:HD23	2:A:615:ILE:HD11	1.96	0.48
2:A:380:LYS:NZ	2:A:548:MET:CE	2.77	0.48
1:X:1105:C:H5"	1:X:1105:C:C6	2.49	0.48
2:A:917:ARG:NH1	2:A:1005:GLN:HA	2.28	0.47
2:A:392:ALA:HB2	2:A:939:VAL:HG21	1.95	0.47
2:A:491:ALA:HB3	2:A:629:ASP:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:334:PHE:CD2	2:A:455:PRO:HD3	2.49	0.47
2:A:538:ILE:HD12	2:A:565:GLN:NE2	2.30	0.47
2:A:441:VAL:HB	2:A:447:ILE:HD11	1.95	0.47
2:A:643:VAL:HA	2:A:647:MET:SD	2.54	0.47
2:A:129:LEU:O	2:A:202:TYR:HE1	1.98	0.47
2:A:556:GLN:NE2	2:A:556:GLN:HA	2.26	0.47
2:A:193:TYR:CZ	2:A:197:LYS:HD2	2.50	0.47
2:A:866:THR:HG22	2:A:867:PHE:N	2.29	0.47
2:A:324:LYS:O	2:A:328:TRP:CD1	2.66	0.47
2:A:523:GLN:HB2	2:A:665:LYS:O	2.15	0.47
2:A:326:TYR:CZ	2:A:690:ARG:NH1	2.83	0.47
2:A:186:ASN:C	2:A:186:ASN:HD22	2.17	0.46
2:A:695:LEU:HG	2:A:713:LEU:HD12	1.96	0.46
2:A:100:ALA:O	2:A:102:LEU:HD22	2.16	0.46
2:A:267:LEU:HD22	2:A:501:LEU:HD11	1.97	0.46
2:A:261:PHE:CD2	2:A:899:PHE:HB3	2.49	0.46
2:A:916:SER:O	2:A:1008:ASP:HB2	2.14	0.46
2:A:761:SER:O	2:A:1078:SER:HB3	2.15	0.46
2:A:791:LEU:HD23	2:A:791:LEU:N	2.30	0.46
2:A:846:SER:O	2:A:850:ARG:HG3	2.14	0.46
2:A:882:LYS:CB	2:A:883:PRO:HD3	2.43	0.46
2:A:316:ILE:HG13	2:A:316:ILE:O	2.16	0.46
2:A:477:VAL:HA	2:A:480:MET:HE2	1.97	0.46
2:A:1067:TRP:HE1	2:A:1071:TRP:HE1	1.62	0.46
2:A:897:GLN:N	2:A:897:GLN:OE1	2.35	0.46
2:A:1059:PRO:HB2	2:A:1062:GLU:HB2	1.97	0.46
2:A:264:ASN:C	2:A:264:ASN:OD1	2.54	0.46
2:A:804:ALA:HA	2:A:809:LYS:HE3	1.98	0.46
2:A:387:ARG:NH1	2:A:387:ARG:HB3	2.29	0.45
2:A:84:ALA:HB1	2:A:88:LYS:NZ	2.31	0.45
2:A:127:ASP:O	2:A:129:LEU:N	2.50	0.45
2:A:35:GLU:O	2:A:39:ILE:HG13	2.16	0.45
2:A:719:VAL:HG12	2:A:723:ARG:HD2	1.99	0.45
2:A:244:VAL:HA	2:A:295:MET:HE3	1.99	0.45
2:A:619:HIS:ND1	2:A:619:HIS:N	2.64	0.45
2:A:246:SER:N	2:A:247:PRO:CD	2.80	0.45
2:A:495:SER:OG	2:A:496:GLN:N	2.49	0.45
2:A:967:ILE:CD1	2:A:967:ILE:N	2.80	0.45
2:A:1019:ARG:HD2	2:A:1053:SER:OG	2.17	0.44
2:A:145:VAL:HG21	2:A:211:ILE:HG23	1.99	0.44
2:A:532:GLN:HB3	2:A:533:PRO:CD	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:616:SER:C	2:A:618:LYS:N	2.70	0.44
2:A:303:ILE:HB	2:A:304:PRO:HD3	2.00	0.44
2:A:691:ALA:HB2	2:A:723:ARG:CB	2.47	0.44
2:A:976:VAL:HG12	2:A:976:VAL:O	2.17	0.44
2:A:853:GLN:HA	2:A:853:GLN:HE21	1.81	0.44
2:A:687:ILE:HG23	2:A:900:MET:HG3	1.99	0.44
2:A:886:THR:HG1	2:A:1055:PHE:HB3	1.79	0.44
2:A:15:ILE:HG22	2:A:16:TYR:CE1	2.52	0.44
2:A:358:GLU:HG3	2:A:359:MET:N	2.32	0.44
2:A:80:ASP:O	2:A:81:LYS:HG3	2.17	0.44
2:A:1064:ILE:HD12	2:A:1064:ILE:HA	1.87	0.44
2:A:389:SER:OG	2:A:557:THR:HB	2.18	0.44
2:A:621:PHE:CE1	2:A:637:LEU:HD22	2.52	0.44
2:A:703:GLN:N	2:A:703:GLN:CD	2.71	0.44
2:A:338:LYS:O	2:A:341:ASP:N	2.51	0.44
2:A:560:LEU:O	2:A:564:THR:HG23	2.17	0.44
2:A:612:LEU:O	2:A:615:ILE:HG12	2.18	0.44
2:A:6:LEU:CD2	2:A:6:LEU:H	2.30	0.44
1:X:1106:C:H3'	3:X:1201:PO4:O3	2.17	0.44
2:A:251:LEU:HD22	2:A:310:TRP:HZ3	1.82	0.44
2:A:572:TYR:CE1	2:A:585:GLN:HB2	2.53	0.44
2:A:703:GLN:H	2:A:703:GLN:CD	2.20	0.44
2:A:733:LEU:O	2:A:737:MET:HG3	2.18	0.44
2:A:899:PHE:C	2:A:901:PRO:HD3	2.37	0.44
1:X:1105:C:O5'	2:A:400:ALA:HB1	2.18	0.44
2:A:554:VAL:O	2:A:557:THR:HG23	2.17	0.44
2:A:120:PRO:HD2	2:A:124:GLU:OE2	2.17	0.43
2:A:138:LEU:O	2:A:138:LEU:HD12	2.18	0.43
2:A:625:ILE:O	2:A:625:ILE:HG13	2.16	0.43
2:A:75:LEU:HD23	2:A:75:LEU:HA	1.86	0.43
2:A:439:PRO:HA	2:A:440:PRO:HD3	1.79	0.43
2:A:512:ASN:N	2:A:512:ASN:HD22	2.15	0.43
2:A:521:VAL:HG21	2:A:604:ASN:OD1	2.18	0.43
2:A:750:LEU:HD21	2:A:861:LEU:HB3	2.00	0.43
2:A:853:GLN:CA	2:A:853:GLN:HE21	2.31	0.43
2:A:981:TYR:CZ	2:A:985:LYS:HD2	2.54	0.43
2:A:380:LYS:NZ	2:A:548:MET:HE2	2.33	0.43
2:A:100:ALA:HB1	2:A:112:ASN:HB3	2.00	0.43
2:A:377:GLU:HB2	2:A:378:PRO:HD3	2.01	0.43
2:A:784:ILE:HA	2:A:784:ILE:HD12	1.84	0.43
2:A:498:ASN:HD21	2:A:918:THR:HA	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4:TYR:HB3	2:A:754:GLU:OE1	2.19	0.43
2:A:516:VAL:HG12	2:A:671:SER:O	2.19	0.43
2:A:277:ARG:HH11	2:A:277:ARG:HG2	1.84	0.42
2:A:503:TYR:CD1	2:A:687:ILE:HB	2.53	0.42
2:A:721:ARG:NH1	2:A:721:ARG:CG	2.81	0.42
2:A:843:ALA:O	2:A:847:LEU:HG	2.19	0.42
2:A:882:LYS:O	2:A:884:PHE:N	2.52	0.42
2:A:1017:LEU:HD22	2:A:1053:SER:HA	2.02	0.42
2:A:772:ILE:HG22	2:A:772:ILE:O	2.19	0.42
2:A:842:TYR:HD2	2:A:845:ILE:HG13	1.85	0.42
2:A:186:ASN:C	2:A:186:ASN:ND2	2.72	0.42
2:A:461:ILE:HD11	2:A:586:TYR:CZ	2.54	0.42
2:A:518:TYR:HA	2:A:634:TYR:HB3	2.01	0.42
2:A:58:LEU:HD22	2:A:58:LEU:N	2.34	0.42
2:A:253:ALA:CB	2:A:671:SER:HB2	2.49	0.42
2:A:283:GLN:HG3	2:A:284:THR:N	2.34	0.42
2:A:526:SER:O	2:A:588:ALA:HB1	2.20	0.42
2:A:531:THR:HB	2:A:589:VAL:HG23	2.00	0.42
1:X:1102:G:H3'	1:X:1103:U:C5	2.55	0.42
2:A:143:ASN:HA	2:A:143:ASN:HD22	1.60	0.42
2:A:575:ILE:CD1	2:A:584:ILE:HG12	2.49	0.42
2:A:845:ILE:O	2:A:849:LYS:HG2	2.19	0.42
2:A:853:GLN:HA	2:A:853:GLN:NE2	2.35	0.42
2:A:959:GLN:HG3	2:A:976:VAL:HG21	2.01	0.42
2:A:580:VAL:HG12	2:A:581:ILE:H	1.85	0.42
2:A:867:PHE:CE2	2:A:869:SER:HA	2.55	0.42
2:A:928:SER:OG	2:A:931:SER:HB2	2.20	0.42
2:A:930:ILE:HB	2:A:975:TYR:CZ	2.55	0.42
2:A:1058:TYR:CD2	2:A:1063:MET:HG2	2.54	0.42
2:A:338:LYS:O	2:A:339:MET:C	2.58	0.42
2:A:29:SER:H	2:A:35:GLU:HG2	1.83	0.42
2:A:220:HIS:NE2	2:A:224:LEU:HD21	2.35	0.41
2:A:72:LEU:C	2:A:753:SER:HB3	2.41	0.41
2:A:616:SER:O	2:A:618:LYS:N	2.53	0.41
2:A:330:PHE:CD1	2:A:690:ARG:NE	2.88	0.41
2:A:179:LYS:HD3	2:A:180:TYR:CE2	2.56	0.41
2:A:205:THR:HG23	2:A:206:TRP:N	2.34	0.41
2:A:345:ASP:CG	2:A:346:GLN:N	2.74	0.41
2:A:419:LYS:HB2	2:A:422:MET:HG3	2.02	0.41
2:A:57:LYS:HA	2:A:57:LYS:HD3	1.90	0.41
2:A:514:THR:HG22	2:A:638:GLN:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:40:GLU:O	2:A:44:LYS:HG3	2.20	0.41
2:A:628:VAL:O	2:A:628:VAL:HG13	2.20	0.41
2:A:301:VAL:O	2:A:304:PRO:HD2	2.20	0.41
2:A:554:VAL:O	2:A:558:LEU:HB2	2.20	0.41
2:A:428:MET:CE	2:A:811:TYR:HD1	2.34	0.41
2:A:881:ILE:HD11	2:A:1032:ILE:HG12	2.03	0.41
2:A:244:VAL:HA	2:A:295:MET:CE	2.50	0.41
2:A:331:HIS:CD2	2:A:725:PHE:CE1	3.08	0.41
2:A:441:VAL:HG13	2:A:469:TYR:OH	2.20	0.41
2:A:496:GLN:HE22	2:A:927:LYS:NZ	2.19	0.41
2:A:93:ALA:HB1	2:A:175:SER:HA	2.02	0.41
2:A:105:ASN:HB2	2:A:111:ASN:ND2	2.35	0.41
2:A:1061:SER:O	2:A:1064:ILE:HG22	2.20	0.41
2:A:573:VAL:CG1	2:A:574:GLN:N	2.84	0.41
2:A:829:ARG:HG3	2:A:830:GLY:N	2.35	0.41
2:A:516:VAL:HG22	2:A:517:LEU:N	2.36	0.41
2:A:806:SER:O	2:A:808:PHE:N	2.54	0.41
2:A:863:LYS:HA	2:A:864:PRO:HD2	1.84	0.41
2:A:207:ALA:O	2:A:211:ILE:HG13	2.21	0.41
2:A:415:ILE:HG12	2:A:842:TYR:OH	2.21	0.41
2:A:851:ARG:HH11	2:A:851:ARG:HG2	1.86	0.41
2:A:1058:TYR:HA	2:A:1059:PRO:HD3	1.88	0.41
2:A:195:VAL:HG23	2:A:196:MET:N	2.36	0.41
2:A:532:GLN:HA	2:A:532:GLN:OE1	2.21	0.41
2:A:708:ASP:O	2:A:712:ILE:HG13	2.20	0.41
2:A:693:ILE:CG2	2:A:716:ASN:ND2	2.84	0.41
2:A:874:ILE:HG23	2:A:875:ASN:N	2.36	0.41
2:A:882:LYS:C	2:A:884:PHE:H	2.25	0.41
2:A:954:HIS:O	2:A:957:GLU:N	2.53	0.41
2:A:100:ALA:CB	2:A:112:ASN:HB3	2.51	0.40
2:A:415:ILE:HG23	2:A:416:PHE:N	2.36	0.40
2:A:449:LEU:HD13	2:A:573:VAL:HG13	2.02	0.40
1:X:1101:U:O4	2:A:415:ILE:HG13	2.21	0.40
2:A:711:ALA:CA	2:A:765:VAL:HG13	2.51	0.40
2:A:214:LEU:C	2:A:216:SER:H	2.25	0.40
2:A:916:SER:OG	2:A:1006:LEU:O	2.30	0.40
2:A:438:ILE:HD13	2:A:564:THR:HG22	2.03	0.40
2:A:617:ASN:N	2:A:617:ASN:HD22	2.18	0.40
2:A:616:SER:HA	2:A:619:HIS:O	2.22	0.40
2:A:615:ILE:HG21	2:A:655:VAL:HG22	2.02	0.40
2:A:879:ARG:HG3	2:A:879:ARG:HH11	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:962:LEU:O	2:A:967:ILE:HD13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	1067/1095 (97%)	954 (89%)	99 (9%)	14 (1%)	12 44

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	382	ASP
2	A	822	SER
2	A	128	SER
2	A	807	THR
2	A	82	TYR
2	A	397	MET
2	A	495	SER
2	A	527	SER
2	A	32	SER
2	A	883	PRO
2	A	1025	LYS
2	A	1027	PRO
2	A	106	GLU
2	A	259	GLY

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	975/996 (98%)	913 (94%)	62 (6%)	17	50

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	17	ASN
2	A	48	ASN
2	A	63	ASN
2	A	79	TYR
2	A	91	LYS
2	A	102	LEU
2	A	121	THR
2	A	130	MET
2	A	135	LEU
2	A	137	SER
2	A	143	ASN
2	A	186	ASN
2	A	194	ASP
2	A	196	MET
2	A	214	LEU
2	A	229	LEU
2	A	238	SER
2	A	246	SER
2	A	358	GLU
2	A	387	ARG
2	A	399	SER
2	A	409	LYS
2	A	418	THR
2	A	449	LEU
2	A	465	LEU
2	A	486	HIS
2	A	508	ARG
2	A	512	ASN
2	A	518	TYR
2	A	547	ASN
2	A	550	ASN
2	A	556	GLN
2	A	557	THR
2	A	584	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	600	ASN
2	A	619	HIS
2	A	631	ASP
2	A	639	PHE
2	A	680	ARG
2	A	715	SER
2	A	717	TYR
2	A	721	ARG
2	A	748	LEU
2	A	791	LEU
2	A	807	THR
2	A	824	ASN
2	A	868	LYS
2	A	889	ASP
2	A	892	LEU
2	A	895	GLN
2	A	902	THR
2	A	916	SER
2	A	917	ARG
2	A	922	GLU
2	A	939	VAL
2	A	981	TYR
2	A	984	ASP
2	A	998	SER
2	A	1003	CYS
2	A	1022	PHE
2	A	1027	PRO
2	A	1088	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	36	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	473	GLN
2	A	496	GLN
2	A	512	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	653	ASN
2	A	760	ASN
2	A	824	ASN
2	A	853	GLN
2	A	895	GLN
2	A	912	GLN
2	A	959	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	6/6 (100%)	4 (66%)	4 (66%)

All (4) 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	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1101	U
1	X	1102	G
1	X	1103	U
1	X	1104	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	X	1201	-	4,4,4	2.93	3 (75%)	6,6,6	5.60	5 (83%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	1201	PO4	P-O1	3.95	1.60	1.50
3	X	1201	PO4	P-O4	2.92	1.63	1.54
3	X	1201	PO4	P-O3	2.73	1.62	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	1201	PO4	O4-P-O2	-7.73	83.15	107.97
3	X	1201	PO4	O4-P-O1	-7.34	84.02	110.89
3	X	1201	PO4	O4-P-O3	-7.22	84.81	107.97
3	X	1201	PO4	O2-P-O1	3.56	123.94	110.89
3	X	1201	PO4	O3-P-O2	2.75	116.80	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	1201	PO4	4	0

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	6/6 (100%)	0.88	2 (33%) 0 0	52, 92, 118, 120	0
2	A	1073/1095 (97%)	-0.43	4 (0%) 92 90	5, 42, 86, 141	0
All	All	1079/1101 (98%)	-0.42	6 (0%) 89 85	5, 43, 87, 141	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	865	VAL	3.3
2	A	824	ASN	3.0
2	A	1088	GLU	2.6
1	X	1102	G	2.5
2	A	77	TYR	2.2
1	X	1101	U	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
3	PO4	X	1201	5/5	0.94	0.27	69,69,70,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.