



Full wwPDB X-ray Structure Validation Report

May 27, 2020 – 03:33 am BST

PDB ID : 2R7R
Title : Crystal Structure of Rotavirus SA11 VP1/RNA (UGUGACC) complex
Authors : Lu, X.; Harrison, S.C.; Tao, Y.J.; Patton, J.T.; Nibert, M.L.
Deposited on : 2007-09-09
Resolution : 2.60 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
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

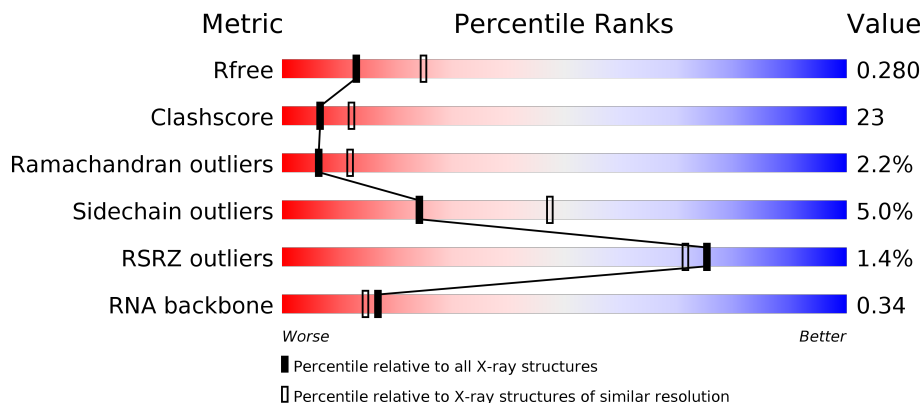
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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	7	
2	A	1095	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8844 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*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	7	145	66	25	48	6	0	0	0

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

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

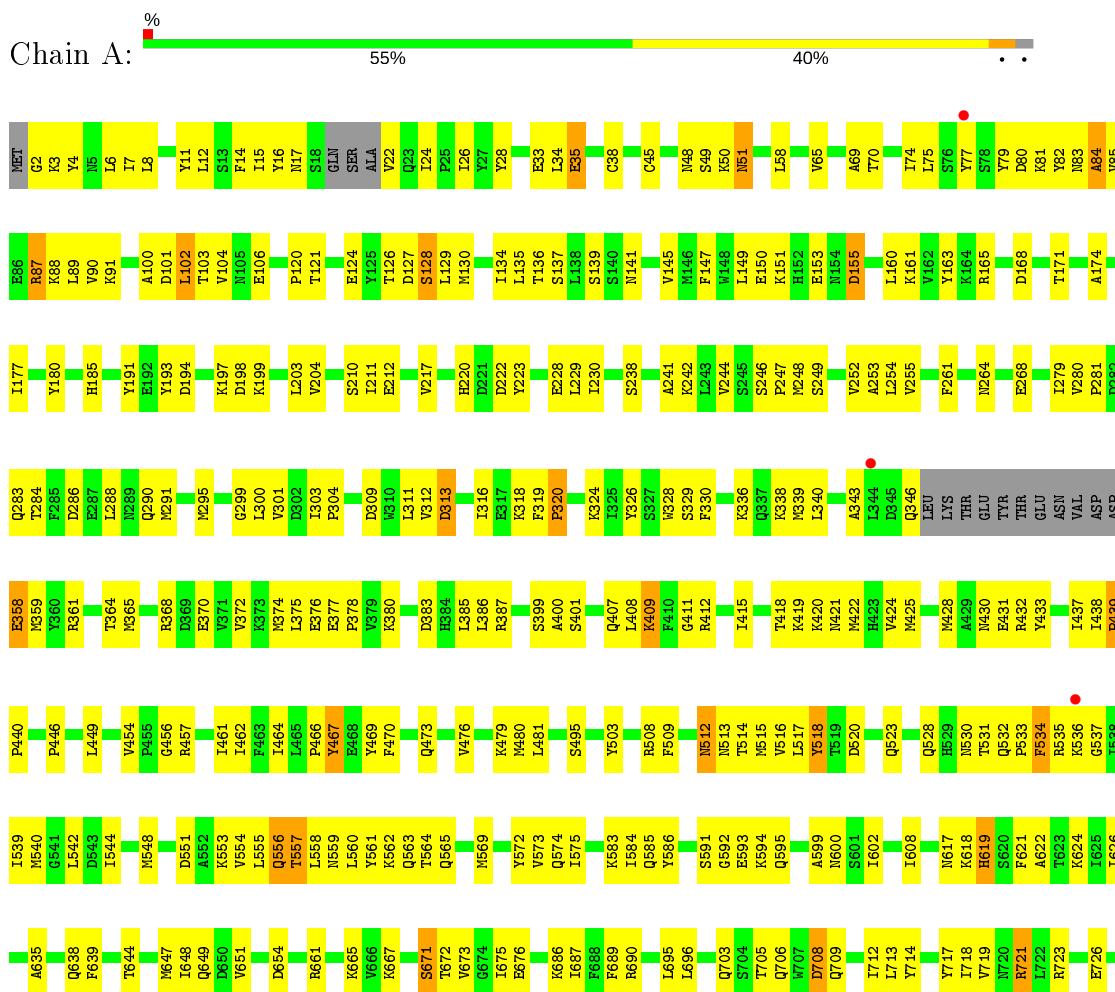
3 Residue-property plots [i](#)

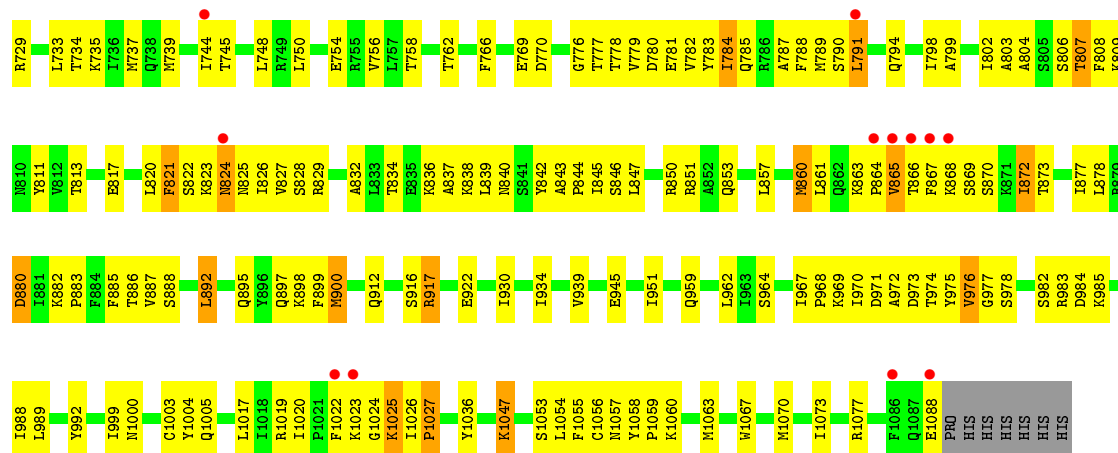
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($RSRZ > 2$). 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*CP*C)-3')



- Molecule 2: RNA-dependent RNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.35Å 112.75Å 143.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 40.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.5 (50.00-2.60) 84.5 (40.59-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.61Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.287 0.232 , 0.280	Depositor DCC
R_{free} test set	3030 reflections (7.88%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtrriage
Anisotropy	0.351	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8844	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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](#)

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	0.53	0/161	0.91	0/249
2	A	0.46	1/8870 (0.0%)	0.63	0/11989
All	All	0.46	1/9031 (0.0%)	0.64	0/12238

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	CYS	CB-SG	-5.97	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	145	0	77	16	0
2	A	8699	0	8793	405	0
All	All	8844	0	8870	414	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 23.

All (414) 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	1.07
2:A:865:VAL:HG22	2:A:866:THR:H	1.22	1.02
2:A:385:LEU:HD23	2:A:479:LYS:HE2	1.38	1.01
2:A:101:ASP:OD1	2:A:103:THR:HG22	1.66	0.96
2:A:556:GLN:HE21	2:A:556:GLN:HA	1.29	0.94
2:A:866:THR:HG22	2:A:867:PHE:H	1.34	0.91
1:X:1105:A:H5'	2:A:400:ALA:HB1	1.57	0.87
2:A:503:TYR:HB2	2:A:687:ILE:HD13	1.57	0.85
2:A:824:ASN:ND2	2:A:827:VAL:HB	1.92	0.85
2:A:24:ILE:HB	2:A:75:LEU:HB2	1.58	0.84
2:A:945:GLU:HG2	2:A:992:TYR:HE1	1.44	0.82
2:A:87:ARG:O	2:A:90:VAL:HG22	1.79	0.81
2:A:283:GLN:OE1	2:A:649:GLN:HG3	1.79	0.81
2:A:892:LEU:HD22	2:A:1017:LEU:HD11	1.64	0.80
2:A:254:LEU:HD23	2:A:280:VAL:HG21	1.65	0.78
2:A:161:LYS:O	2:A:165:ARG:HG3	1.85	0.77
2:A:386:LEU:O	2:A:557:THR:HG21	1.85	0.77
2:A:84:ALA:HB1	2:A:88:LYS:NZ	2.01	0.76
2:A:573:VAL:HG12	2:A:575:ILE:HG13	1.68	0.74
2:A:248:MET:O	2:A:248:MET:HE3	1.87	0.74
2:A:438:ILE:HD12	2:A:563:GLN:HB3	1.69	0.74
2:A:865:VAL:HG22	2:A:866:THR:N	2.00	0.74
2:A:708:ASP:O	2:A:712:ILE:HG13	1.88	0.74
2:A:820:LEU:HD23	2:A:820:LEU:H	1.53	0.73
2:A:667:LYS:O	2:A:667:LYS:HG3	1.89	0.73
2:A:446:PRO:HG2	2:A:583:LYS:HD3	1.70	0.72
2:A:622:ALA:HB3	2:A:638:GLN:HB3	1.71	0.72
2:A:866:THR:HG22	2:A:867:PHE:N	2.05	0.71
2:A:286:ASP:O	2:A:290:GLN:HG3	1.90	0.71
2:A:824:ASN:HD21	2:A:827:VAL:HB	1.56	0.71
2:A:885:PHE:CE1	2:A:1056:CYS:HB2	2.24	0.71
2:A:461:ILE:HD11	2:A:586:TYR:CZ	2.26	0.71
2:A:618:LYS:HD2	2:A:654:ASP:OD2	1.90	0.70
2:A:1059:PRO:O	2:A:1063:MET:HG3	1.93	0.69
2:A:777:THR:HG21	2:A:882:LYS:HE3	1.72	0.69
2:A:102:LEU:H	2:A:102:LEU:HD22	1.55	0.69
2:A:135:LEU:HD22	2:A:709:GLN:NE2	2.08	0.69
2:A:1019:ARG:HD2	2:A:1053:SER:OG	1.92	0.68
2:A:343:ALA:O	2:A:346:GLN:HG3	1.93	0.68
2:A:253:ALA:HB1	2:A:671:SER:HB2	1.76	0.68
2:A:80:ASP:O	2:A:81:LYS:HG3	1.94	0.68
1:X:1105:A:H5'	2:A:400:ALA:CB	2.22	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:50:LYS:O	2:A:50:LYS:HG2	1.94	0.68
2:A:217:VAL:HG13	2:A:222:ASP:HB2	1.74	0.68
2:A:553:LYS:O	2:A:557:THR:HG22	1.94	0.68
2:A:975:TYR:O	2:A:977:GLY:N	2.27	0.67
2:A:558:LEU:HD23	2:A:558:LEU:O	1.94	0.67
2:A:804:ALA:HA	2:A:809:LYS:HE3	1.74	0.67
2:A:377:GLU:HB2	2:A:378:PRO:HD3	1.77	0.67
2:A:778:THR:O	2:A:782:VAL:HG23	1.95	0.67
2:A:865:VAL:CG2	2:A:866:THR:H	2.04	0.66
2:A:473:GLN:HG2	2:A:561:TYR:CE1	2.30	0.66
2:A:385:LEU:HD23	2:A:479:LYS:CE	2.21	0.66
2:A:1023:LYS:O	2:A:1060:LYS:HG2	1.95	0.66
2:A:120:PRO:HD2	2:A:124:GLU:OE2	1.96	0.66
2:A:419:LYS:HB2	2:A:422:MET:HG3	1.78	0.66
1:X:1104:G:H5'	2:A:401:SER:HB2	1.78	0.65
2:A:823:LYS:HE3	2:A:825:ASN:HD22	1.62	0.65
2:A:882:LYS:HB3	2:A:883:PRO:HD3	1.78	0.65
2:A:177:ILE:HD13	2:A:203:LEU:HD11	1.78	0.64
2:A:324:LYS:O	2:A:328:TRP:HD1	1.81	0.64
2:A:520:ASP:CB	2:A:667:LYS:HG2	2.21	0.64
2:A:528:GLN:O	2:A:531:THR:HG22	1.97	0.63
2:A:644:THR:OG1	2:A:647:MET:HG3	1.99	0.63
2:A:264:ASN:HD21	2:A:268:GLU:HG3	1.62	0.63
2:A:886:THR:OG1	2:A:1055:PHE:HB3	1.98	0.63
2:A:744:ILE:HD13	2:A:748:LEU:HD22	1.80	0.63
2:A:3:LYS:HA	2:A:6:LEU:HD23	1.80	0.62
2:A:820:LEU:HB2	2:A:964:SER:O	1.98	0.62
2:A:84:ALA:HB1	2:A:88:LYS:HZ2	1.64	0.62
2:A:346:GLN:HG2	2:A:586:TYR:CE1	2.35	0.62
2:A:823:LYS:HE3	2:A:825:ASN:ND2	2.15	0.62
2:A:312:VAL:HG23	2:A:313:ASP:OD2	2.00	0.62
2:A:789:MET:HE1	2:A:873:THR:HG21	1.80	0.62
2:A:976:VAL:O	2:A:976:VAL:HG12	2.00	0.62
2:A:851:ARG:HH11	2:A:851:ARG:HG2	1.63	0.62
2:A:309:ASP:O	2:A:312:VAL:HG22	2.00	0.61
2:A:193:TYR:CE2	2:A:197:LYS:HD2	2.36	0.61
2:A:824:ASN:OD1	2:A:828:SER:HB2	2.00	0.61
2:A:608:ILE:HD13	2:A:626:ILE:HG23	1.83	0.61
2:A:945:GLU:HG2	2:A:992:TYR:CE1	2.33	0.61
2:A:972:ALA:O	2:A:976:VAL:HG23	2.01	0.61
2:A:878:LEU:HD22	2:A:1036:TYR:HD1	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:199:LYS:HD2	2:A:199:LYS:H	1.65	0.60
2:A:180:TYR:HB3	2:A:199:LYS:HG3	1.82	0.60
2:A:821:PHE:CD2	2:A:821:PHE:N	2.68	0.60
2:A:556:GLN:HE21	2:A:556:GLN:CA	2.05	0.60
2:A:217:VAL:HG13	2:A:222:ASP:CB	2.32	0.60
1:X:1106:C:H2'	1:X:1107:C:O4'	2.02	0.60
2:A:135:LEU:HD22	2:A:709:GLN:HE21	1.67	0.59
2:A:719:VAL:HG12	2:A:723:ARG:HD2	1.84	0.59
2:A:85:VAL:HG21	2:A:139:SER:OG	2.03	0.59
2:A:165:ARG:HE	2:A:220:HIS:HA	1.66	0.59
2:A:516:VAL:HG21	2:A:675:ILE:CG2	2.33	0.59
2:A:1024:GLY:O	2:A:1025:LYS:CB	2.50	0.59
2:A:191:TYR:CE2	2:A:204:VAL:HG11	2.37	0.59
1:X:1105:A:C5'	2:A:400:ALA:HB1	2.29	0.59
2:A:984:ASP:O	2:A:988:ILE:HG12	2.03	0.59
2:A:318:LYS:HB2	2:A:318:LYS:NZ	2.18	0.58
2:A:518:TYR:HD2	2:A:518:TYR:H	1.48	0.58
2:A:1000:ASN:O	2:A:1005:GLN:HB3	2.03	0.58
2:A:212:GLU:HB2	2:A:696:LEU:HD12	1.85	0.58
2:A:798:ILE:O	2:A:802:ILE:HG22	2.02	0.58
2:A:385:LEU:CD2	2:A:479:LYS:HE2	2.25	0.58
2:A:279:ILE:HG22	2:A:648:ILE:HD12	1.84	0.58
2:A:312:VAL:HG23	2:A:313:ASP:N	2.19	0.57
2:A:255:VAL:HG11	2:A:316:ILE:HB	1.84	0.57
2:A:83:ASN:O	2:A:85:VAL:N	2.35	0.57
2:A:313:ASP:N	2:A:313:ASP:OD2	2.36	0.57
2:A:261:PHE:HD2	2:A:899:PHE:HB3	1.69	0.57
2:A:542:LEU:HD11	2:A:561:TYR:HD2	1.70	0.57
2:A:129:LEU:HD22	2:A:336:LYS:O	2.05	0.57
2:A:12:LEU:HD22	2:A:16:TYR:HE2	1.70	0.56
2:A:368:ARG:O	2:A:372:VAL:HG23	2.05	0.56
2:A:897:GLN:N	2:A:897:GLN:OE1	2.38	0.56
1:X:1103:U:O2'	1:X:1104:G:H5''	2.05	0.56
2:A:4:TYR:HD1	2:A:733:LEU:HD22	1.71	0.56
2:A:781:GLU:O	2:A:785:GLN:HG3	2.05	0.56
2:A:744:ILE:HD11	2:A:750:LEU:HB2	1.88	0.56
2:A:820:LEU:HD13	2:A:824:ASN:ND2	2.20	0.56
2:A:22:VAL:HG22	2:A:77:TYR:HB2	1.87	0.56
2:A:530:ASN:O	2:A:533:PRO:HD2	2.06	0.55
2:A:473:GLN:HE21	2:A:594:LYS:HB3	1.71	0.55
2:A:821:PHE:N	2:A:821:PHE:HD2	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:165:ARG:NE	2:A:220:HIS:HA	2.20	0.55
2:A:565:GLN:O	2:A:569:MET:HG2	2.07	0.55
2:A:428:MET:HE1	2:A:811:TYR:HD1	1.71	0.55
2:A:261:PHE:CD2	2:A:899:PHE:HB3	2.42	0.55
2:A:617:ASN:N	2:A:617:ASN:HD22	2.04	0.55
2:A:784:ILE:HG23	2:A:788:PHE:CE2	2.41	0.55
2:A:407:GLN:O	2:A:408:LEU:HD23	2.07	0.55
2:A:102:LEU:N	2:A:102:LEU:HD22	2.22	0.54
2:A:866:THR:CG2	2:A:867:PHE:H	2.13	0.54
1:X:1103:U:O2'	1:X:1104:G:P	2.65	0.54
2:A:301:VAL:C	2:A:304:PRO:HD2	2.27	0.54
2:A:428:MET:CE	2:A:811:TYR:HD1	2.20	0.54
2:A:281:PRO:HG2	2:A:284:THR:OG1	2.07	0.54
2:A:8:LEU:HD13	2:A:737:MET:HG2	1.90	0.54
2:A:687:ILE:HG23	2:A:900:MET:HG3	1.90	0.54
2:A:967:ILE:HD12	2:A:967:ILE:N	2.22	0.54
2:A:872:ILE:HG22	2:A:1073:ILE:HA	1.87	0.54
2:A:210:SER:OG	2:A:230:ILE:HG23	2.07	0.54
2:A:364:THR:HG23	2:A:537:GLY:CA	2.37	0.54
2:A:295:MET:O	2:A:300:LEU:HB2	2.08	0.54
2:A:762:THR:HA	2:A:1077:ARG:O	2.08	0.53
2:A:470:PHE:HE1	2:A:594:LYS:HD3	1.73	0.53
2:A:6:LEU:HD22	2:A:6:LEU:N	2.24	0.53
2:A:887:VAL:HG22	2:A:1054:LEU:HD11	1.91	0.53
2:A:464:ILE:HG22	2:A:464:ILE:O	2.09	0.53
2:A:824:ASN:HB3	2:A:828:SER:HB2	1.91	0.53
2:A:837:ALA:O	2:A:840:ASN:ND2	2.41	0.53
2:A:851:ARG:NH1	2:A:851:ARG:HG2	2.24	0.53
2:A:968:PRO:HG2	2:A:971:ASP:OD2	2.08	0.52
2:A:516:VAL:HG21	2:A:675:ILE:HG21	1.91	0.52
2:A:141:ASN:O	2:A:145:VAL:HG23	2.10	0.52
2:A:514:THR:HG22	2:A:638:GLN:HA	1.91	0.52
2:A:361:ARG:O	2:A:365:MET:HG2	2.09	0.52
2:A:137:SER:HB2	2:A:185:HIS:CD2	2.44	0.52
2:A:301:VAL:O	2:A:304:PRO:HD2	2.09	0.52
2:A:420:LYS:O	2:A:424:VAL:HG23	2.10	0.52
2:A:90:VAL:HG23	2:A:91:LYS:N	2.25	0.52
2:A:975:TYR:C	2:A:977:GLY:H	2.13	0.52
2:A:419:LYS:HB2	2:A:422:MET:CG	2.39	0.52
2:A:150:GLU:O	2:A:153:GLU:HB2	2.10	0.52
2:A:518:TYR:N	2:A:518:TYR:CD2	2.78	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:647:MET:O	2:A:651:VAL:HG23	2.10	0.51
2:A:340:LEU:O	2:A:340:LEU:HD12	2.09	0.51
2:A:470:PHE:CE1	2:A:594:LYS:HD3	2.46	0.51
2:A:744:ILE:HD13	2:A:748:LEU:CD2	2.40	0.51
2:A:520:ASP:HB2	2:A:667:LYS:HE2	1.93	0.51
2:A:776:GLY:HA3	2:A:785:GLN:NE2	2.25	0.51
2:A:823:LYS:HG2	2:A:824:ASN:H	1.74	0.51
2:A:24:ILE:HD12	2:A:45:CYS:HB3	1.91	0.51
2:A:556:GLN:NE2	2:A:556:GLN:HA	2.11	0.51
2:A:242:LYS:O	2:A:246:SER:HB2	2.11	0.51
2:A:312:VAL:HG23	2:A:313:ASP:H	1.76	0.51
2:A:733:LEU:O	2:A:737:MET:HE2	2.11	0.50
2:A:58:LEU:HD22	2:A:58:LEU:N	2.26	0.50
2:A:149:LEU:O	2:A:163:TYR:HE1	1.95	0.50
2:A:437:ILE:O	2:A:439:PRO:HD3	2.11	0.50
2:A:735:LYS:O	2:A:739:MET:HG3	2.11	0.50
2:A:303:ILE:HB	2:A:304:PRO:HD3	1.92	0.50
2:A:33:GLU:HG3	2:A:34:LEU:H	1.76	0.50
2:A:466:PRO:HD2	2:A:469:TYR:CD2	2.47	0.50
2:A:535:ARG:HH11	2:A:565:GLN:HE22	1.60	0.50
2:A:687:ILE:HG22	2:A:899:PHE:O	2.12	0.50
2:A:803:ALA:HA	2:A:808:PHE:CD2	2.46	0.50
2:A:536:LYS:O	2:A:540:MET:HG3	2.12	0.50
2:A:847:LEU:O	2:A:851:ARG:HG3	2.12	0.50
2:A:1020:ILE:O	2:A:1020:ILE:HG22	2.11	0.50
2:A:14:PHE:CE2	2:A:147:PHE:HB2	2.47	0.50
1:X:1105:A:C5	2:A:462:ILE:HD13	2.47	0.50
2:A:288:LEU:HD21	2:A:311:LEU:HD11	1.93	0.49
2:A:370:GLU:HG2	2:A:602:ILE:HG23	1.94	0.49
2:A:842:TYR:CE2	2:A:844:PRO:HB2	2.47	0.49
2:A:319:PHE:N	2:A:320:PRO:CD	2.75	0.49
2:A:428:MET:HG2	2:A:433:TYR:CG	2.47	0.49
2:A:794:GLN:HG2	2:A:853:GLN:OE1	2.12	0.49
2:A:1024:GLY:O	2:A:1025:LYS:HB3	2.11	0.49
2:A:399:SER:HB3	2:A:838:LYS:HB3	1.94	0.49
2:A:126:THR:OG1	2:A:128:SER:HB3	2.12	0.49
2:A:279:ILE:O	2:A:648:ILE:HD12	2.13	0.49
2:A:523:GLN:HB2	2:A:665:LYS:O	2.12	0.49
2:A:185:HIS:H	2:A:185:HIS:CD2	2.31	0.49
2:A:4:TYR:HB3	2:A:754:GLU:OE1	2.13	0.49
2:A:100:ALA:O	2:A:102:LEU:HD22	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:254:LEU:CD2	2:A:280:VAL:HG21	2.40	0.49
2:A:383:ASP:O	2:A:387:ARG:HG3	2.13	0.49
2:A:462:ILE:HG23	2:A:591:SER:O	2.12	0.49
2:A:813:THR:O	2:A:817:GLU:HG3	2.13	0.49
2:A:847:LEU:HD23	2:A:850:ARG:NH1	2.27	0.49
2:A:165:ARG:HD3	2:A:223:TYR:CB	2.43	0.49
2:A:509:PHE:CD2	2:A:624:LYS:HB3	2.47	0.49
2:A:84:ALA:HB1	2:A:88:LYS:HZ1	1.76	0.49
2:A:155:ASP:O	2:A:160:LEU:HD13	2.13	0.49
2:A:161:LYS:O	2:A:165:ARG:NH1	2.45	0.49
2:A:608:ILE:HD11	2:A:635:ALA:HB2	1.95	0.49
2:A:617:ASN:N	2:A:617:ASN:ND2	2.61	0.49
2:A:2:GLY:HA2	2:A:754:GLU:OE2	2.12	0.48
1:X:1103:U:O2'	1:X:1104:G:C5'	2.61	0.48
2:A:358:GLU:OE2	2:A:359:MET:HG2	2.13	0.48
2:A:823:LYS:HG2	2:A:824:ASN:N	2.29	0.48
2:A:428:MET:HG2	2:A:433:TYR:CB	2.43	0.48
2:A:721:ARG:HH11	2:A:721:ARG:CG	2.26	0.48
2:A:959:GLN:NE2	2:A:973:ASP:OD1	2.47	0.48
2:A:744:ILE:HG22	2:A:745:THR:HG23	1.95	0.48
2:A:756:VAL:HG13	2:A:788:PHE:CZ	2.49	0.48
2:A:758:THR:HG22	2:A:766:PHE:O	2.13	0.48
2:A:860:MET:CE	2:A:860:MET:HA	2.44	0.48
2:A:134:ILE:HD13	2:A:136:THR:HG22	1.96	0.48
2:A:438:ILE:CD1	2:A:563:GLN:HB3	2.40	0.47
2:A:826:ILE:O	2:A:829:ARG:HG2	2.13	0.47
2:A:246:SER:N	2:A:247:PRO:CD	2.78	0.47
2:A:843:ALA:HB3	2:A:844:PRO:HD3	1.96	0.47
2:A:887:VAL:HG12	2:A:888:SER:N	2.29	0.47
2:A:917:ARG:NH1	2:A:1004:TYR:O	2.48	0.47
2:A:542:LEU:O	2:A:558:LEU:HD21	2.15	0.47
2:A:90:VAL:HG23	2:A:91:LYS:H	1.80	0.47
2:A:544:ILE:O	2:A:548:MET:HG3	2.14	0.47
2:A:127:ASP:O	2:A:129:LEU:N	2.48	0.47
2:A:145:VAL:HG21	2:A:211:ILE:HG23	1.97	0.47
2:A:534:PHE:CZ	2:A:599:ALA:HB1	2.50	0.47
2:A:539:ILE:HG23	2:A:562:LYS:HE3	1.97	0.47
2:A:330:PHE:CE1	2:A:690:ARG:CZ	2.98	0.47
2:A:791:LEU:HD23	2:A:791:LEU:N	2.30	0.47
2:A:619:HIS:ND1	2:A:619:HIS:N	2.63	0.46
2:A:102:LEU:CD2	2:A:102:LEU:H	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:532:GLN:HG3	2:A:536:LYS:HE3	1.97	0.46
2:A:695:LEU:HG	2:A:713:LEU:CD1	2.45	0.46
1:X:1101:U:O2'	1:X:1102:G:P	2.73	0.46
2:A:228:GLU:OE1	2:A:303:ILE:HG13	2.15	0.46
2:A:667:LYS:O	2:A:667:LYS:CG	2.60	0.46
2:A:689:PHE:HB2	2:A:723:ARG:HG2	1.97	0.46
2:A:719:VAL:CG1	2:A:723:ARG:HD2	2.46	0.46
2:A:449:LEU:CD2	2:A:573:VAL:HG11	2.45	0.46
2:A:514:THR:O	2:A:672:THR:HG22	2.15	0.46
2:A:721:ARG:HG3	2:A:721:ARG:HH11	1.80	0.46
2:A:820:LEU:C	2:A:821:PHE:HD2	2.18	0.46
2:A:974:THR:HG22	2:A:974:THR:O	2.14	0.46
2:A:375:LEU:C	2:A:378:PRO:HD2	2.36	0.46
2:A:50:LYS:O	2:A:51:ASN:OD1	2.33	0.46
2:A:880:ASP:O	2:A:883:PRO:HD2	2.16	0.46
2:A:145:VAL:CG2	2:A:211:ILE:HG23	2.46	0.46
2:A:449:LEU:HD22	2:A:573:VAL:CG1	2.46	0.46
2:A:516:VAL:N	2:A:671:SER:O	2.48	0.46
2:A:88:LYS:HA	2:A:91:LYS:HE2	1.98	0.46
2:A:473:GLN:NE2	2:A:595:GLN:HG2	2.30	0.46
2:A:512:ASN:C	2:A:512:ASN:HD22	2.19	0.46
2:A:101:ASP:O	2:A:103:THR:N	2.49	0.46
2:A:824:ASN:HB3	2:A:825:ASN:H	1.41	0.46
2:A:824:ASN:CB	2:A:828:SER:HB2	2.46	0.46
2:A:839:LEU:HB3	2:A:845:ILE:HD12	1.96	0.46
2:A:28:TYR:CE2	2:A:70:THR:HB	2.51	0.45
2:A:33:GLU:HG3	2:A:34:LEU:N	2.32	0.45
2:A:703:GLN:N	2:A:703:GLN:CD	2.69	0.45
2:A:83:ASN:HB3	2:A:84:ALA:H	1.52	0.45
2:A:790:SER:HB3	2:A:791:LEU:HD23	1.97	0.45
2:A:22:VAL:CG2	2:A:77:TYR:HB2	2.46	0.45
2:A:244:VAL:CG1	2:A:329:SER:HB3	2.47	0.45
2:A:4:TYR:CD1	2:A:733:LEU:HD22	2.50	0.45
2:A:824:ASN:CG	2:A:828:SER:HB2	2.37	0.45
2:A:135:LEU:HB3	2:A:706:GLN:HG2	1.98	0.45
2:A:249:SER:HB3	2:A:676:GLU:OE1	2.16	0.45
2:A:378:PRO:O	2:A:383:ASP:HB2	2.16	0.45
2:A:982:SER:O	2:A:985:LYS:HB2	2.17	0.45
2:A:661:ARG:O	2:A:661:ARG:HG3	2.17	0.45
2:A:721:ARG:HD2	2:A:726:GLU:HG3	1.98	0.45
2:A:898:LYS:HE2	2:A:912:GLN:NE2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:951:ILE:HG13	2:A:985:LYS:HG2	1.98	0.45
2:A:1023:LYS:HD2	2:A:1058:TYR:O	2.17	0.45
2:A:376:GLU:HG2	2:A:380:LYS:HE2	1.99	0.45
2:A:473:GLN:HE22	2:A:593:GLU:HB3	1.82	0.45
2:A:49:SER:C	2:A:51:ASN:H	2.20	0.44
2:A:665:LYS:HA	2:A:665:LYS:HD3	1.84	0.44
2:A:88:LYS:O	2:A:91:LYS:HG3	2.17	0.44
2:A:168:ASP:OD2	2:A:223:TYR:OH	2.24	0.44
2:A:476:VAL:O	2:A:480:MET:HG3	2.18	0.44
2:A:962:LEU:O	2:A:967:ILE:HD13	2.17	0.44
2:A:198:ASP:HB2	2:A:199:LYS:HD2	2.00	0.44
2:A:11:TYR:O	2:A:14:PHE:HB3	2.18	0.44
2:A:199:LYS:CD	2:A:199:LYS:H	2.29	0.44
2:A:515:MET:HG2	2:A:639:PHE:HE2	1.82	0.44
2:A:551:ASP:HB3	2:A:554:VAL:HB	1.99	0.44
2:A:621:PHE:HA	2:A:638:GLN:O	2.18	0.44
2:A:860:MET:HE2	2:A:860:MET:HA	1.99	0.44
1:X:1102:G:O2'	1:X:1103:U:P	2.75	0.44
2:A:1026:ILE:HD11	2:A:1067:TRP:CG	2.53	0.44
2:A:412:ARG:HG2	2:A:412:ARG:O	2.18	0.44
2:A:534:PHE:HZ	2:A:599:ALA:HB1	1.81	0.44
2:A:930:ILE:O	2:A:934:ILE:HG13	2.16	0.44
2:A:165:ARG:HB3	2:A:223:TYR:HB2	1.98	0.44
2:A:532:GLN:CB	2:A:533:PRO:HD3	2.48	0.44
2:A:857:LEU:O	2:A:861:LEU:HD13	2.17	0.44
2:A:87:ARG:HG2	2:A:87:ARG:H	1.42	0.44
2:A:3:LYS:O	2:A:7:ILE:HG12	2.17	0.44
2:A:421:ASN:O	2:A:425:MET:HG3	2.18	0.44
2:A:556:GLN:NE2	2:A:556:GLN:CA	2.77	0.44
1:X:1103:U:HO2'	1:X:1104:G:P	2.41	0.44
2:A:248:MET:HG2	2:A:326:TYR:CD1	2.53	0.43
2:A:420:LYS:HG2	2:A:467:TYR:HB3	1.99	0.43
2:A:572:TYR:CE1	2:A:585:GLN:HB2	2.53	0.43
2:A:193:TYR:CZ	2:A:197:LYS:HD2	2.53	0.43
2:A:248:MET:HE2	2:A:252:VAL:CG1	2.48	0.43
2:A:834:THR:O	2:A:838:LYS:HG3	2.19	0.43
2:A:1023:LYS:HZ1	2:A:1057:ASN:HA	1.83	0.43
2:A:11:TYR:HA	2:A:147:PHE:CE1	2.54	0.43
2:A:255:VAL:O	2:A:673:VAL:HG21	2.18	0.43
2:A:989:LEU:HD23	2:A:989:LEU:C	2.39	0.43
2:A:555:LEU:O	2:A:559:ASN:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:705:THR:O	2:A:709:GLN:HG3	2.19	0.43
2:A:409:LYS:HB2	2:A:409:LYS:NZ	2.34	0.43
2:A:832:ALA:O	2:A:836:LYS:HG3	2.19	0.43
2:A:1058:TYR:HA	2:A:1059:PRO:HD3	1.87	0.43
2:A:469:TYR:CD1	2:A:564:THR:HG22	2.53	0.43
2:A:449:LEU:HD21	2:A:573:VAL:HG11	2.01	0.43
2:A:446:PRO:HB2	2:A:574:GLN:CG	2.48	0.43
2:A:89:LEU:HD11	2:A:174:ALA:CB	2.48	0.43
2:A:454:VAL:CG1	2:A:457:ARG:HB3	2.49	0.43
2:A:853:GLN:NE2	2:A:853:GLN:HA	2.34	0.43
2:A:358:GLU:OE2	2:A:359:MET:CG	2.67	0.43
2:A:35:GLU:O	2:A:38:CYS:HB2	2.19	0.43
2:A:734:THR:HA	2:A:737:MET:CE	2.49	0.43
2:A:999:ILE:HA	2:A:999:ILE:HD12	1.88	0.43
2:A:877:ILE:O	2:A:880:ASP:HB2	2.19	0.42
2:A:424:VAL:HG22	2:A:467:TYR:CD2	2.54	0.42
2:A:481:LEU:HD23	2:A:481:LEU:HA	1.86	0.42
2:A:532:GLN:HB3	2:A:533:PRO:HD3	2.01	0.42
2:A:1047:LYS:NZ	2:A:1047:LYS:HB2	2.34	0.42
2:A:989:LEU:HD11	2:A:1070:MET:HE3	2.02	0.42
2:A:241:ALA:HB3	2:A:456:GLY:HA2	2.00	0.42
2:A:794:GLN:HG2	2:A:853:GLN:CD	2.40	0.42
2:A:779:VAL:HG23	2:A:780:ASP:N	2.34	0.42
2:A:24:ILE:HG22	2:A:26:ILE:HD11	2.01	0.42
2:A:430:ASN:C	2:A:432:ARG:H	2.23	0.42
2:A:721:ARG:NH1	2:A:721:ARG:CG	2.83	0.42
2:A:744:ILE:CD1	2:A:748:LEU:HD22	2.48	0.42
2:A:161:LYS:HG2	2:A:165:ARG:CZ	2.50	0.42
2:A:512:ASN:HD22	2:A:513:ASN:N	2.18	0.42
2:A:1023:LYS:NZ	2:A:1057:ASN:HA	2.34	0.42
2:A:165:ARG:HD3	2:A:223:TYR:HB2	2.01	0.42
2:A:283:GLN:OE1	2:A:649:GLN:CG	2.59	0.42
2:A:8:LEU:HD23	2:A:74:ILE:HD12	2.02	0.42
2:A:617:ASN:ND2	2:A:617:ASN:H	2.18	0.41
2:A:244:VAL:HG12	2:A:329:SER:HB3	2.01	0.41
2:A:28:TYR:HA	2:A:35:GLU:OE2	2.20	0.41
2:A:370:GLU:O	2:A:374:MET:HG3	2.20	0.41
2:A:438:ILE:HD11	2:A:560:LEU:HB3	2.01	0.41
2:A:806:SER:O	2:A:808:PHE:N	2.53	0.41
1:X:1103:U:O2'	1:X:1104:G:O5'	2.39	0.41
1:X:1107:C:OP1	2:A:594:LYS:NZ	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:65:VAL:O	2:A:69:ALA:HB3	2.19	0.41
2:A:983:ARG:O	2:A:984:ASP:C	2.59	0.41
2:A:799:ALA:HB2	2:A:845:ILE:HD13	2.03	0.41
2:A:101:ASP:O	2:A:104:VAL:HG13	2.21	0.41
2:A:324:LYS:O	2:A:328:TRP:CD1	2.66	0.41
2:A:863:LYS:O	2:A:863:LYS:HG3	2.21	0.41
2:A:969:LYS:O	2:A:970:ILE:C	2.59	0.41
1:X:1101:U:O2'	1:X:1102:G:OP1	2.35	0.41
2:A:319:PHE:N	2:A:320:PRO:HD2	2.36	0.41
2:A:473:GLN:HE22	2:A:595:GLN:H	1.67	0.41
2:A:744:ILE:CG1	2:A:748:LEU:HD22	2.51	0.41
2:A:803:ALA:HA	2:A:808:PHE:CE2	2.56	0.41
2:A:8:LEU:HA	2:A:737:MET:SD	2.61	0.41
2:A:147:PHE:O	2:A:151:LYS:HG2	2.21	0.41
2:A:291:MET:O	2:A:295:MET:HG3	2.21	0.41
2:A:338:LYS:O	2:A:339:MET:C	2.59	0.41
2:A:376:GLU:CG	2:A:380:LYS:HE2	2.51	0.41
2:A:449:LEU:HD13	2:A:573:VAL:HG13	2.03	0.41
2:A:842:TYR:CZ	2:A:844:PRO:HG2	2.56	0.41
2:A:769:GLU:HG2	2:A:1047:LYS:NZ	2.36	0.41
2:A:15:ILE:HG22	2:A:16:TYR:CD1	2.55	0.41
2:A:430:ASN:O	2:A:432:ARG:N	2.54	0.41
2:A:703:GLN:H	2:A:703:GLN:CD	2.24	0.41
2:A:866:THR:O	2:A:867:PHE:HB2	2.21	0.41
2:A:199:LYS:HD2	2:A:199:LYS:N	2.32	0.40
2:A:299:GLY:O	2:A:301:VAL:HG23	2.21	0.40
2:A:714:TYR:O	2:A:717:TYR:HB3	2.21	0.40
2:A:769:GLU:HG2	2:A:1047:LYS:HZ2	1.85	0.40
2:A:824:ASN:O	2:A:825:ASN:HB2	2.21	0.40
2:A:846:SER:OG	2:A:850:ARG:NH2	2.54	0.40
2:A:439:PRO:HA	2:A:440:PRO:HD3	1.85	0.40
2:A:253:ALA:CB	2:A:671:SER:HB2	2.47	0.40
2:A:729:ARG:HE	2:A:770:ASP:CG	2.23	0.40
2:A:780:ASP:O	2:A:783:TYR:HB3	2.21	0.40
2:A:1000:ASN:C	2:A:1005:GLN:HB3	2.40	0.40
2:A:168:ASP:O	2:A:171:THR:N	2.48	0.40
2:A:126:THR:HG23	2:A:126:THR:O	2.22	0.40
1:X:1105:A:C6	2:A:462:ILE:HD13	2.56	0.40
2:A:467:TYR:C	2:A:467:TYR:CD1	2.95	0.40
2:A:686:LYS:HD2	2:A:899:PHE:HA	2.02	0.40
2:A:714:TYR:CZ	2:A:718:ILE:HD11	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:787:ALA:O	2:A:790:SER:HB3	2.21	0.40
2:A:860:MET:HE1	2:A:865:VAL:HG12	2.03	0.40
2:A:409:LYS:HB2	2:A:409:LYS:HZ3	1.87	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%)	949 (89%)	95 (9%)	23 (2%)	6 12

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	102	LEU
2	A	106	GLU
2	A	128	SER
2	A	865	VAL
2	A	976	VAL
2	A	978	SER
2	A	1025	LYS
2	A	822	SER
2	A	1027	PRO
2	A	82	TYR
2	A	84	ALA
2	A	870	SER
2	A	592	GLY
2	A	807	THR
2	A	238	SER
2	A	431	GLU
2	A	864	PRO
2	A	51	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	439	PRO
2	A	495	SER
2	A	534	PHE
2	A	869	SER
2	A	411	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%)	926 (95%)	49 (5%)	24 47

All (49) 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	87	ARG
2	A	121	THR
2	A	130	MET
2	A	155	ASP
2	A	194	ASP
2	A	229	LEU
2	A	313	ASP
2	A	320	PRO
2	A	358	GLU
2	A	409	LYS
2	A	415	ILE
2	A	418	THR
2	A	467	TYR
2	A	508	ARG
2	A	512	ASN
2	A	517	LEU
2	A	518	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	556	GLN
2	A	557	THR
2	A	584	ILE
2	A	600	ASN
2	A	619	HIS
2	A	671	SER
2	A	708	ASP
2	A	721	ARG
2	A	784	ILE
2	A	791	LEU
2	A	807	THR
2	A	821	PHE
2	A	824	ASN
2	A	860	MET
2	A	868	LYS
2	A	872	ILE
2	A	880	ASP
2	A	892	LEU
2	A	895	GLN
2	A	900	MET
2	A	916	SER
2	A	917	ARG
2	A	922	GLU
2	A	939	VAL
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 (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	36	ASN
2	A	48	ASN
2	A	63	ASN
2	A	143	ASN
2	A	185	HIS
2	A	289	ASN
2	A	294	ASN
2	A	308	GLN
2	A	473	GLN
2	A	496	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	617	ASN
2	A	646	GLN
2	A	653	ASN
2	A	698	ASN
2	A	709	GLN
2	A	760	ASN
2	A	810	ASN
2	A	824	ASN
2	A	825	ASN
2	A	853	GLN
2	A	895	GLN
2	A	912	GLN
2	A	959	GLN
2	A	1034	HIS
2	A	1043	ASN
2	A	1057	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	7/7 (100%)	4 (57%)	3 (42%)

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	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1101	U
1	X	1102	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1103	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	7/7 (100%)	-0.12	0 100 100	47, 63, 76, 81	0
2	A	1073/1095 (97%)	-0.11	15 (1%) 75 71	16, 51, 80, 122	0
All	All	1080/1102 (98%)	-0.11	15 (1%) 75 71	16, 51, 80, 122	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	867	PHE	4.9
2	A	824	ASN	4.5
2	A	866	THR	4.4
2	A	865	VAL	4.4
2	A	1088	GLU	4.1
2	A	864	PRO	3.6
2	A	77	TYR	2.8
2	A	868	LYS	2.3
2	A	1086	PHE	2.3
2	A	536	LYS	2.2
2	A	1023	LYS	2.1
2	A	1022	PHE	2.1
2	A	344	LEU	2.1
2	A	791	LEU	2.0
2	A	744	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.