



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:46 PM UTC

PDB ID : 2BXD / pdb_00002bxid
Title : Human serum albumin complexed with warfarin
Authors : Ghuman, J.; Zunszain, P.A.; Petitpas, I.; Bhattacharya, A.A.; Curry, S.
Deposited on : 2005-07-26
Resolution : 3.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

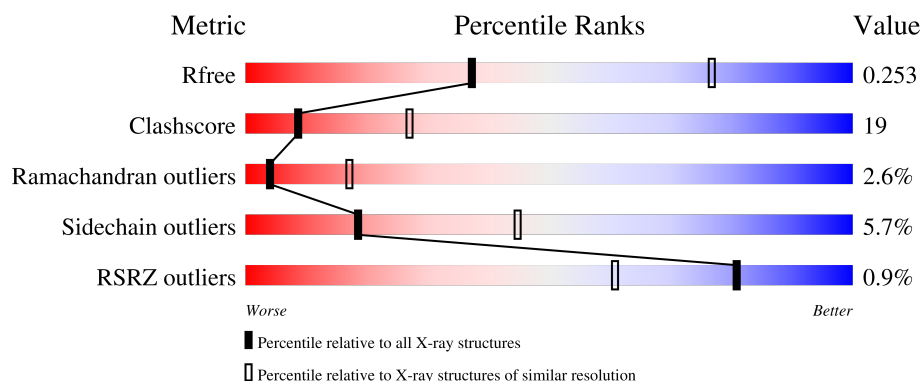
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

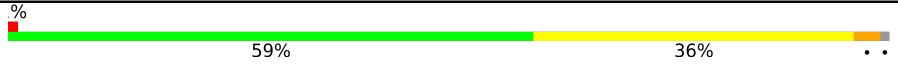
The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	585	
1	B	585	

2 Entry composition [i](#)

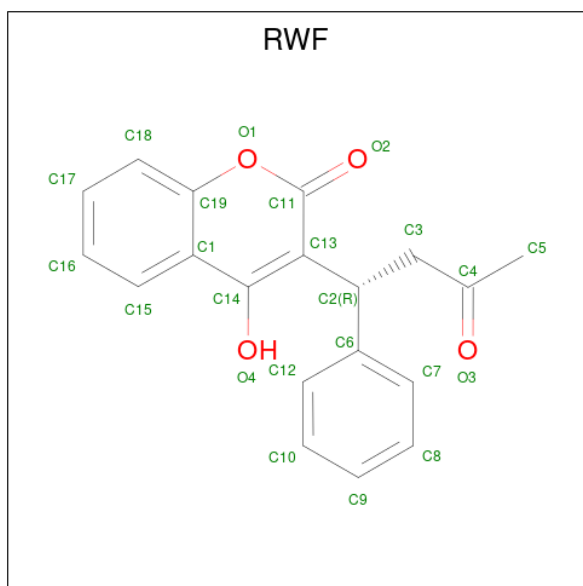
There are 2 unique types of molecules in this entry. The entry contains 8632 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

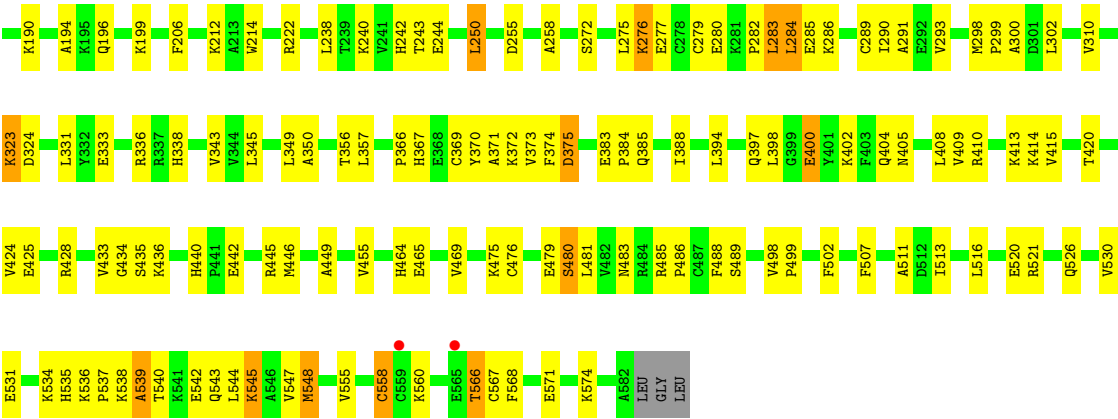
- Molecule 1 is a protein called SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4323	2727	725	830	41			
1	B	578	Total	C	N	O	S	0	0	0
			4263	2684	719	820	40			

- Molecule 2 is R-WARFARIN (CCD ID: RWF) (formula: $C_{19}H_{16}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	19	4		
2	B	1	Total	C	O	0	0
			23	19	4		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.02Å 55.36Å 119.59Å 81.14° 90.53° 64.79°	Depositor
Resolution (Å)	49.32 – 3.05 49.32 – 3.05	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.32-3.05) 97.7 (49.32-3.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.07Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.259 0.206 , 0.253	Depositor DCC
R_{free} test set	1129 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	70.8	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 77.1	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	0.94	EDS
Total number of atoms	8632	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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, 0.333 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: RWF

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/4408	1.04	23/5999 (0.4%)
1	B	0.49	0/4343	0.98	15/5911 (0.3%)
All	All	0.51	0/8751	1.01	38/11910 (0.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	GLN	OE1-CD-NE2	-9.88	112.72	122.60
1	A	34	CYS	CA-C-N	9.64	129.72	119.89
1	A	34	CYS	C-N-CA	9.64	129.72	119.89
1	A	98	ARG	N-CA-C	-8.12	102.40	111.82
1	A	415	VAL	CA-C-N	8.08	127.80	119.56
1	A	415	VAL	C-N-CA	8.08	127.80	119.56
1	B	49	PHE	N-CA-C	-7.44	103.60	114.39
1	B	415	VAL	CA-C-N	6.72	126.40	119.82
1	B	415	VAL	C-N-CA	6.72	126.40	119.82
1	A	417	GLN	CG-CD-NE2	6.64	126.36	116.40
1	A	564	LYS	N-CA-C	-6.63	101.75	110.43
1	B	168	CYS	N-CA-C	6.59	119.02	111.11
1	B	436	LYS	N-CA-C	6.50	118.36	111.28
1	A	204	GLN	N-CA-C	6.32	117.96	111.14
1	A	400	GLU	N-CA-C	6.31	117.82	111.07
1	B	338	HIS	N-CA-C	6.21	119.86	108.94
1	B	250	LEU	N-CA-C	6.19	118.82	111.33
1	A	483	ASN	N-CA-C	6.18	120.95	113.17
1	A	360	CYS	N-CA-C	6.17	117.67	111.07
1	A	250	LEU	N-CA-C	6.09	118.69	111.33
1	A	479	GLU	N-CA-C	5.81	118.11	111.02
1	A	522	GLN	N-CA-C	-5.81	104.30	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	GLU	N-CA-C	5.65	119.43	112.03
1	A	105	HIS	N-CA-C	5.63	119.85	112.92
1	B	539	ALA	N-CA-C	-5.58	102.27	110.52
1	A	76	THR	N-CA-C	-5.56	106.16	113.17
1	B	34	CYS	CA-C-N	5.50	125.40	119.85
1	B	34	CYS	C-N-CA	5.50	125.40	119.85
1	B	440	HIS	N-CA-C	5.40	117.84	110.01
1	A	146	HIS	CA-C-N	5.31	126.47	119.84
1	A	146	HIS	C-N-CA	5.31	126.47	119.84
1	B	400	GLU	N-CA-C	5.27	116.71	111.07
1	A	262	LYS	N-CA-C	-5.15	105.35	110.97
1	A	64	LYS	N-CA-C	5.15	117.47	109.60
1	B	21	ALA	N-CA-C	-5.09	105.19	111.40
1	B	83	THR	N-CA-C	-5.08	107.03	113.43
1	A	552	ALA	N-CA-C	-5.01	105.71	111.07
1	B	243	THR	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4323	0	3976	166	0
1	B	4263	0	3894	145	0
2	A	23	0	15	4	0
2	B	23	0	15	5	0
All	All	8632	0	7900	311	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 19.

All (311) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:CYS:SG	1:A:568:PHE:N	2.31	1.03
1:A:67:HIS:HB3	1:A:98:ARG:HH21	1.26	0.98
1:A:94:GLN:O	1:A:98:ARG:HB3	1.70	0.91
1:A:551:PHE:HA	1:A:554:PHE:HD1	1.37	0.86
1:A:551:PHE:HA	1:A:554:PHE:CD1	2.10	0.86
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.59	0.84
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.60	0.83
1:B:39:HIS:O	1:B:43:VAL:HG23	1.81	0.81
1:A:257:ARG:HG3	2:A:2001:RWF:H16	1.62	0.81
1:B:567:CYS:SG	1:B:568:PHE:N	2.53	0.81
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.63	0.79
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.65	0.79
1:B:544:LEU:O	1:B:548:MET:HB2	1.82	0.79
1:A:67:HIS:CB	1:A:98:ARG:HH21	1.95	0.78
1:B:206:PHE:CD2	1:B:481:LEU:HD22	2.18	0.78
1:A:424:VAL:O	1:A:428:ARG:HG3	1.83	0.78
1:A:115:LEU:HD22	1:A:145:ARG:NH1	2.00	0.76
1:B:485:ARG:NH2	1:B:486:PRO:HG3	2.01	0.76
1:A:87:MET:HE1	1:A:105:HIS:HB3	1.67	0.75
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.70	0.74
1:B:424:VAL:O	1:B:428:ARG:HG3	1.88	0.74
1:B:206:PHE:CE2	1:B:481:LEU:HD13	2.21	0.74
1:A:23:VAL:HG13	1:A:70:PHE:HE2	1.54	0.73
1:A:61:ASN:HD22	1:A:64:LYS:HE3	1.54	0.72
1:A:23:VAL:O	1:A:27:PHE:HD1	1.73	0.72
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.55	0.72
1:B:81:ARG:HE	1:B:88:ALA:HB3	1.53	0.71
1:B:194:ALA:HB1	1:B:455:VAL:HG13	1.72	0.71
1:A:225:LYS:HG2	1:A:299:PRO:HG3	1.72	0.71
1:A:497:TYR:CE2	1:A:537:PRO:HG3	2.25	0.71
1:A:414:LYS:O	1:A:472:ARG:NH1	2.24	0.71
1:B:194:ALA:HB1	1:B:455:VAL:CG1	2.20	0.70
1:B:537:PRO:C	1:B:539:ALA:H	1.99	0.70
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.74	0.69
1:A:564:LYS:C	1:A:566:THR:H	2.00	0.69
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.76	0.68
1:A:199:LYS:HG2	1:A:211:PHE:HE1	1.60	0.67
1:A:497:TYR:HE2	1:A:537:PRO:HG3	1.57	0.67
1:A:98:ARG:CZ	1:A:99:ASN:HB2	2.25	0.66
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.77	0.66
1:B:57:GLU:OE1	1:B:57:GLU:HA	1.96	0.66
1:B:511:ALA:C	1:B:513:ILE:H	2.04	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD22	1:A:145:ARG:HH12	1.58	0.66
1:A:206:PHE:CE2	1:A:481:LEU:HD13	2.30	0.65
1:A:564:LYS:O	1:A:566:THR:N	2.26	0.65
1:B:48:GLU:O	1:B:48:GLU:HG2	1.95	0.65
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.78	0.65
1:A:117:ARG:HB2	1:A:123:MET:CE	2.27	0.65
1:B:545:LYS:HE3	1:B:545:LYS:HA	1.80	0.64
1:A:512:ASP:O	1:A:515:THR:HG22	1.97	0.64
1:B:483:ASN:O	1:B:486:PRO:HD2	1.97	0.64
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.62	0.63
1:A:98:ARG:NH1	1:A:99:ASN:H	1.95	0.63
1:B:42:LEU:O	1:B:46:VAL:HG23	1.97	0.63
1:A:420:THR:HG23	1:A:530:VAL:HG11	1.81	0.62
1:B:81:ARG:NE	1:B:88:ALA:HB3	2.15	0.62
1:A:87:MET:HE1	1:A:105:HIS:CB	2.30	0.62
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.81	0.62
1:A:98:ARG:NH2	1:A:99:ASN:HB2	2.15	0.61
1:B:367:HIS:O	1:B:371:ALA:HB2	2.01	0.61
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.40	0.61
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.66	0.61
1:B:540:THR:O	1:B:544:LEU:HG	2.01	0.61
1:A:376:GLU:O	1:A:379:PRO:HD2	2.01	0.61
1:A:557:LYS:HG2	1:A:558:CYS:N	2.15	0.61
1:A:310:VAL:O	1:A:370:TYR:HE1	1.84	0.61
1:A:49:PHE:HD2	1:A:49:PHE:O	1.83	0.60
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.83	0.60
1:B:279:CYS:HA	1:B:286:LYS:HD2	1.84	0.60
1:B:290:ILE:O	1:B:293:VAL:HG12	2.01	0.60
1:A:257:ARG:HG3	2:A:2001:RWF:C16	2.32	0.59
1:B:372:LYS:O	1:B:375:ASP:HB2	2.01	0.59
1:B:373:VAL:HG13	1:B:374:PHE:N	2.16	0.59
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.85	0.59
1:A:117:ARG:HB2	1:A:123:MET:HE3	1.84	0.59
1:A:551:PHE:CA	1:A:554:PHE:HD1	2.12	0.59
1:B:36:PHE:O	1:B:40:VAL:HG23	2.03	0.59
1:B:544:LEU:O	1:B:548:MET:N	2.34	0.59
1:A:283:LEU:HG	1:A:284:LEU:HD23	1.84	0.58
1:A:279:CYS:HA	1:A:286:LYS:CD	2.33	0.58
1:B:483:ASN:C	1:B:486:PRO:HD2	2.29	0.58
1:B:499:PRO:HB3	1:B:535:HIS:O	2.04	0.58
1:A:168:CYS:SG	1:A:177:CYS:C	2.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.85	0.57
1:B:186:ARG:O	1:B:190:LYS:HG3	2.03	0.57
1:B:409:VAL:O	1:B:413:LYS:HG3	2.03	0.57
1:A:38:ASP:O	1:A:42:LEU:HG	2.05	0.57
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.87	0.57
1:A:372:LYS:O	1:A:375:ASP:HB2	2.04	0.57
1:A:49:PHE:CE2	1:A:53:CYS:SG	2.98	0.56
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.40	0.56
1:A:420:THR:HG23	1:A:530:VAL:CG1	2.35	0.56
1:B:52:THR:HA	1:B:56:ASP:OD2	2.05	0.56
1:B:571:GLU:HA	1:B:574:LYS:HB3	1.86	0.56
1:B:61:ASN:HB3	1:B:64:LYS:HD2	1.87	0.55
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.07	0.55
1:B:98:ARG:O	1:B:101:CYS:HB3	2.06	0.55
1:B:420:THR:HG23	1:B:530:VAL:HG11	1.88	0.55
1:A:550:ASP:HB3	1:A:554:PHE:HE1	1.71	0.54
1:A:387:LEU:HD22	1:A:485:ARG:NH1	2.21	0.54
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.88	0.54
1:B:276:LYS:HG3	1:B:277:GLU:N	2.22	0.54
1:A:420:THR:O	1:A:424:VAL:HG23	2.06	0.54
1:A:49:PHE:C	1:A:49:PHE:CD2	2.85	0.54
1:B:464:HIS:CE1	1:B:469:VAL:H	2.25	0.54
1:A:464:HIS:CE1	1:A:469:VAL:H	2.26	0.54
1:B:511:ALA:C	1:B:513:ILE:N	2.63	0.54
1:B:25:ILE:O	1:B:29:GLN:HG3	2.07	0.53
1:A:348:ARG:HG3	1:A:482:VAL:HG12	1.89	0.53
1:B:400:GLU:O	1:B:404:GLN:HG3	2.07	0.53
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.90	0.53
1:B:480:SER:OG	1:B:483:ASN:HB2	2.08	0.53
1:B:29:GLN:HG2	1:B:143:ALA:O	2.08	0.53
1:A:139:LEU:HD21	1:A:158:ALA:HB2	1.90	0.53
1:B:405:ASN:O	1:B:409:VAL:HG23	2.08	0.53
1:B:103:LEU:C	1:B:105:HIS:H	2.17	0.53
1:B:394:LEU:O	1:B:397:GLN:HG2	2.08	0.53
1:A:279:CYS:HA	1:A:286:LYS:HD2	1.92	0.52
1:A:540:THR:O	1:A:544:LEU:HG	2.09	0.52
1:B:537:PRO:C	1:B:539:ALA:N	2.64	0.52
1:A:178:LEU:O	1:A:179:LEU:C	2.52	0.52
1:A:370:TYR:CD1	1:A:370:TYR:C	2.88	0.52
1:A:323:LYS:HG3	1:A:324:ASP:N	2.25	0.52
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ASN:O	1:A:409:VAL:HG23	2.10	0.51
1:A:578:ALA:O	1:A:581:ALA:HB3	2.10	0.51
1:B:50:ALA:O	1:B:54:VAL:HG23	2.11	0.51
1:B:81:ARG:HE	1:B:88:ALA:CB	2.23	0.51
1:A:117:ARG:HB2	1:A:123:MET:HE1	1.93	0.51
1:A:67:HIS:O	1:A:68:THR:C	2.52	0.51
1:A:281:LYS:HB2	1:A:282:PRO:CD	2.41	0.51
1:A:395:PHE:CD1	1:A:434:GLY:HA3	2.46	0.51
1:A:434:GLY:O	1:A:438:CYS:HB2	2.11	0.51
1:B:32:GLN:NE2	1:B:110:PRO:HG3	2.26	0.51
1:A:6:GLU:O	1:A:9:HIS:HB3	2.10	0.51
1:B:516:LEU:O	1:B:521:ARG:NH2	2.41	0.51
1:A:517:SER:O	1:A:521:ARG:HG3	2.10	0.51
1:A:49:PHE:HD2	1:A:49:PHE:C	2.19	0.51
1:B:23:VAL:O	1:B:27:PHE:HD1	1.94	0.51
1:A:485:ARG:HB3	1:A:486:PRO:CD	2.39	0.50
1:B:139:LEU:HD21	1:B:158:ALA:HB2	1.93	0.50
1:B:168:CYS:SG	1:B:177:CYS:C	2.95	0.50
1:A:282:PRO:HB2	1:A:285:GLU:OE1	2.11	0.50
1:B:291:ALA:HB1	2:B:2001:RWF:H3C1	1.93	0.50
1:B:14:LEU:HD13	1:B:22:LEU:HD12	1.92	0.50
1:B:536:LYS:O	1:B:539:ALA:HB3	2.12	0.50
1:A:325:VAL:HG12	1:A:329:MET:HE2	1.93	0.50
1:A:525:LYS:O	1:A:528:ALA:HB3	2.12	0.50
1:B:442:GLU:HA	1:B:445:ARG:HD2	1.94	0.50
1:B:242:HIS:HE2	2:B:2001:RWF:H12	1.77	0.50
1:B:370:TYR:CD1	1:B:370:TYR:C	2.89	0.50
1:B:333:GLU:OE1	1:B:336:ARG:HD3	2.12	0.50
1:B:37:GLU:CD	1:B:37:GLU:H	2.20	0.50
1:A:290:ILE:O	1:A:293:VAL:HG12	2.12	0.49
1:B:240:LYS:HE2	1:B:244:GLU:OE2	2.13	0.49
1:B:420:THR:O	1:B:424:VAL:HG23	2.11	0.49
1:A:199:LYS:NZ	2:A:2001:RWF:H5C3	2.28	0.49
1:B:542:GLU:O	1:B:543:GLN:C	2.53	0.49
1:B:51:LYS:C	1:B:53:CYS:H	2.21	0.49
1:A:417:GLN:H	1:A:417:GLN:CD	2.19	0.49
1:A:564:LYS:C	1:A:566:THR:N	2.65	0.49
1:A:23:VAL:HG13	1:A:27:PHE:HE1	1.78	0.49
1:A:430:LEU:O	1:A:433:VAL:HG12	2.12	0.49
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.95	0.49
1:B:498:VAL:O	1:B:499:PRO:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:PRO:O	1:A:367:HIS:C	2.56	0.48
1:A:49:PHE:HE2	1:A:62:CYS:SG	2.36	0.48
1:A:572:GLY:O	1:A:576:VAL:HG23	2.13	0.48
1:B:141:GLU:O	1:B:144:ARG:HG2	2.11	0.48
1:B:151:ALA:CB	1:B:152:PRO:HD3	2.40	0.48
1:B:285:GLU:O	1:B:289:CYS:HB2	2.14	0.48
1:A:279:CYS:HA	1:A:286:LYS:HD3	1.95	0.48
1:A:179:LEU:CB	1:A:180:PRO:HD3	2.42	0.48
1:A:551:PHE:O	1:A:555:VAL:HG23	2.13	0.48
1:B:398:LEU:O	1:B:402:LYS:HB2	2.14	0.48
1:B:279:CYS:HA	1:B:286:LYS:CD	2.43	0.47
1:A:151:ALA:CB	1:A:152:PRO:HD3	2.39	0.47
1:A:310:VAL:HG23	1:A:311:GLU:N	2.28	0.47
1:A:394:LEU:HG	1:A:398:LEU:HD11	1.96	0.47
1:A:417:GLN:CD	1:A:417:GLN:N	2.73	0.47
1:B:38:ASP:O	1:B:42:LEU:HG	2.14	0.47
1:B:282:PRO:O	1:B:283:LEU:C	2.57	0.47
1:A:94:GLN:O	1:A:98:ARG:HD3	2.15	0.47
1:B:558:CYS:C	1:B:560:LYS:H	2.23	0.47
1:A:110:PRO:C	1:A:112:LEU:H	2.22	0.47
1:A:392:CYS:O	1:A:396:GLU:HG3	2.15	0.47
1:B:19:PHE:CD2	1:B:19:PHE:C	2.92	0.47
1:B:345:LEU:O	1:B:349:LEU:HG	2.14	0.47
1:B:178:LEU:O	1:B:179:LEU:C	2.58	0.47
1:A:42:LEU:O	1:A:46:VAL:HG23	2.15	0.46
1:B:276:LYS:HE3	1:B:280:GLU:OE2	2.15	0.46
1:B:283:LEU:HG	1:B:284:LEU:N	2.29	0.46
1:A:156:PHE:CE2	1:A:160:ARG:HD2	2.51	0.46
1:A:98:ARG:NH1	1:A:99:ASN:HB2	2.30	0.46
1:A:27:PHE:CD2	1:A:74:LEU:HD21	2.51	0.46
1:B:333:GLU:O	1:B:336:ARG:HG2	2.15	0.46
1:A:394:LEU:HG	1:A:398:LEU:CD1	2.46	0.46
1:B:78:ALA:C	1:B:80:LEU:N	2.74	0.46
1:B:141:GLU:O	1:B:145:ARG:HG3	2.16	0.46
1:B:168:CYS:SG	1:B:178:LEU:N	2.89	0.46
1:A:32:GLN:HG2	1:A:144:ARG:O	2.16	0.45
1:A:78:ALA:C	1:A:80:LEU:N	2.74	0.45
1:A:306:ALA:HA	1:A:310:VAL:HG22	1.97	0.45
1:A:420:THR:HB	1:A:421:PRO:HD3	1.98	0.45
1:A:499:PRO:HG3	1:A:537:PRO:HG2	1.97	0.45
1:B:199:LYS:HD3	2:B:2001:RWF:H10	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:VAL:CG1	1:B:374:PHE:N	2.78	0.45
1:A:151:ALA:O	1:A:154:LEU:N	2.49	0.45
1:B:78:ALA:C	1:B:80:LEU:H	2.23	0.45
1:B:214:TRP:NE1	1:B:343:VAL:HG11	2.31	0.45
1:B:410:ARG:O	1:B:414:LYS:HG3	2.17	0.45
1:A:298:MET:HE3	1:A:298:MET:HB2	1.79	0.45
1:A:563:ASP:C	1:A:564:LYS:O	2.57	0.45
1:A:214:TRP:NE1	1:A:343:VAL:HG11	2.32	0.45
1:A:553:ALA:O	1:A:556:GLU:HG2	2.17	0.45
1:A:311:GLU:O	1:A:312:SER:C	2.59	0.45
1:B:23:VAL:O	1:B:27:PHE:CD1	2.70	0.45
1:B:81:ARG:HG2	1:B:88:ALA:HB3	1.99	0.45
1:B:54:VAL:HG12	1:B:55:ALA:N	2.32	0.45
1:B:310:VAL:HG21	1:B:374:PHE:CE1	2.51	0.45
1:B:531:GLU:OE1	1:B:531:GLU:HA	2.17	0.45
1:B:81:ARG:HA	1:B:84:TYR:O	2.17	0.45
1:B:323:LYS:HG3	1:B:324:ASP:N	2.31	0.45
1:A:23:VAL:CG1	1:A:27:PHE:CE1	3.00	0.44
1:A:137:LYS:O	1:A:141:GLU:HG2	2.18	0.44
1:B:196:GLN:NE2	1:B:196:GLN:HA	2.32	0.44
1:A:78:ALA:C	1:A:80:LEU:H	2.26	0.44
1:B:139:LEU:O	1:B:140:TYR:C	2.60	0.44
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.76	0.44
1:A:138:TYR:O	1:A:139:LEU:C	2.60	0.44
1:A:198:LEU:HA	1:A:458:ASN:ND2	2.33	0.44
1:A:98:ARG:HG2	1:A:99:ASN:N	2.31	0.44
1:A:327:LEU:O	1:A:328:GLY:C	2.58	0.44
1:B:366:PRO:O	1:B:369:CYS:N	2.50	0.44
1:A:492:GLU:HA	1:A:492:GLU:OE1	2.16	0.44
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.40	0.44
1:A:342:SER:HA	1:A:447:PRO:HA	2.00	0.44
1:A:411:TYR:O	1:A:414:LYS:HB2	2.17	0.44
1:B:507:PHE:N	1:B:507:PHE:CD1	2.85	0.44
1:B:425:GLU:OE1	1:B:425:GLU:HA	2.17	0.43
1:A:110:PRO:HB2	1:A:112:LEU:HG	2.00	0.43
1:B:214:TRP:CE2	1:B:343:VAL:HG11	2.53	0.43
1:B:530:VAL:HG12	1:B:534:LYS:HD2	2.01	0.43
1:A:81:ARG:CB	1:A:85:GLY:HA2	2.47	0.43
1:B:85:GLY:C	1:B:87:MET:H	2.26	0.43
1:B:408:LEU:HD21	1:B:424:VAL:HA	2.00	0.43
1:A:550:ASP:O	1:A:553:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:CG1	1:A:27:PHE:HE1	2.32	0.43
1:A:252:GLU:H	1:A:252:GLU:CD	2.17	0.43
1:A:502:PHE:CE1	1:A:504:ALA:HA	2.53	0.43
1:B:127:PHE:O	1:B:131:GLU:HB3	2.18	0.43
1:B:475:LYS:O	1:B:479:GLU:HB2	2.19	0.43
1:A:74:LEU:C	1:A:76:THR:H	2.26	0.43
1:A:280:GLU:HA	1:A:280:GLU:OE1	2.18	0.43
1:A:331:LEU:HD13	1:A:350:ALA:HB2	2.00	0.43
1:A:376:GLU:C	1:A:379:PRO:HD2	2.44	0.43
1:B:356:THR:O	1:B:357:LEU:C	2.61	0.43
1:A:310:VAL:CG2	1:A:311:GLU:N	2.82	0.42
1:A:536:LYS:N	1:A:537:PRO:CD	2.82	0.42
1:A:153:GLU:O	1:A:157:PHE:HD1	2.02	0.42
1:B:385:GLN:HG3	1:B:446:MET:HE2	2.01	0.42
1:B:388:ILE:HD12	1:B:449:ALA:HB3	2.00	0.42
1:A:127:PHE:HB2	1:A:134:PHE:CE2	2.55	0.42
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.92	0.42
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.86	0.42
1:B:57:GLU:O	1:B:58:SER:C	2.61	0.42
1:B:255:ASP:O	1:B:258:ALA:N	2.51	0.42
1:A:366:PRO:O	1:A:369:CYS:HB3	2.19	0.42
1:B:30:TYR:CE1	1:B:103:LEU:HD23	2.52	0.42
1:B:153:GLU:O	1:B:157:PHE:HD1	2.02	0.42
1:B:242:HIS:NE2	2:B:2001:RWF:H12	2.34	0.42
1:A:388:ILE:HD12	1:A:449:ALA:CB	2.50	0.42
1:B:17:GLU:O	1:B:18:ASN:C	2.63	0.42
1:A:345:LEU:O	1:A:349:LEU:HG	2.20	0.42
1:B:76:THR:O	1:B:77:VAL:HG13	2.19	0.42
1:A:507:PHE:CD1	1:A:507:PHE:N	2.87	0.42
1:A:511:ALA:O	1:A:512:ASP:C	2.63	0.42
1:A:168:CYS:SG	1:A:177:CYS:O	2.78	0.41
1:B:10:ARG:NH1	1:B:255:ASP:OD2	2.52	0.41
1:B:199:LYS:HD3	2:B:2001:RWF:C10	2.50	0.41
1:B:384:PRO:O	1:B:388:ILE:HG12	2.19	0.41
1:A:384:PRO:O	1:A:388:ILE:HG12	2.20	0.41
1:A:464:HIS:HE1	1:A:470:SER:H	1.68	0.41
1:B:331:LEU:HD13	1:B:350:ALA:HB2	2.02	0.41
1:A:99:ASN:O	1:A:100:GLU:C	2.64	0.41
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.88	0.41
1:A:72:ASP:O	1:A:76:THR:HG23	2.20	0.41
1:B:275:LEU:O	1:B:276:LYS:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:MET:O	1:A:90:CYS:HB2	2.21	0.41
1:A:224:PRO:HD2	1:A:296:ASP:HB3	2.01	0.41
1:B:298:MET:O	1:B:299:PRO:C	2.64	0.41
1:A:441:PRO:O	1:A:442:GLU:C	2.63	0.41
1:B:24:LEU:HD13	1:B:43:VAL:HG21	2.02	0.41
1:B:70:PHE:N	1:B:70:PHE:CD1	2.89	0.41
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.96	0.41
1:B:536:LYS:O	1:B:539:ALA:CB	2.69	0.41
1:B:272:SER:HB3	1:B:275:LEU:HG	2.03	0.41
1:B:433:VAL:HG13	1:B:434:GLY:N	2.35	0.41
1:A:34:CYS:HA	1:A:35:PRO:HD3	1.74	0.41
1:A:282:PRO:O	1:A:283:LEU:C	2.64	0.41
1:B:15:GLY:O	1:B:19:PHE:HB3	2.20	0.41
1:B:32:GLN:HG2	1:B:144:ARG:O	2.20	0.41
1:A:49:PHE:HE2	1:A:53:CYS:SG	2.43	0.40
1:A:257:ARG:CG	2:A:2001:RWF:H16	2.43	0.40
1:B:81:ARG:HG2	1:B:88:ALA:CB	2.50	0.40
1:B:516:LEU:HD22	1:B:520:GLU:CB	2.51	0.40
1:B:476:CYS:HB3	1:B:488:PHE:CE2	2.56	0.40
1:A:19:PHE:CD1	1:A:19:PHE:C	3.00	0.40
1:A:433:VAL:HG23	1:A:452:TYR:HD2	1.86	0.40
1:A:458:ASN:O	1:A:462:VAL:HG22	2.21	0.40
1:B:286:LYS:O	1:B:290:ILE:HG13	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	
1	A	576/585 (98%)	496 (86%)	64 (11%)	16 (3%)	4	16
1	B	576/585 (98%)	499 (87%)	63 (11%)	14 (2%)	4	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1152/1170 (98%)	995 (86%)	127 (11%)	30 (3%)	4 17

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	300	ALA
1	B	54	VAL
1	B	58	SER
1	B	300	ALA
1	A	150	TYR
1	A	565	GLU
1	B	60	GLU
1	B	85	GLY
1	B	129	ASP
1	B	502	PHE
1	B	566	THR
1	A	502	PHE
1	A	557	LYS
1	A	179	LEU
1	A	545	LYS
1	B	150	TYR
1	B	276	LYS
1	A	58	SER
1	A	129	ASP
1	A	276	LYS
1	A	390	GLN
1	A	465	GLU
1	B	77	VAL
1	B	86	GLU
1	B	465	GLU
1	A	315	VAL
1	A	499	PRO
1	A	180	PRO
1	B	179	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	434/511 (85%)	410 (94%)	24 (6%)	19	46
1	B	419/511 (82%)	394 (94%)	25 (6%)	17	43
All	All	853/1022 (84%)	804 (94%)	49 (6%)	18	45

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	79	THR
1	A	83	THR
1	A	98	ARG
1	A	109	ASN
1	A	179	LEU
1	A	212	LYS
1	A	236	THR
1	A	245	CYS
1	A	252	GLU
1	A	268	GLN
1	A	284	LEU
1	A	323	LYS
1	A	329	MET
1	A	375	ASP
1	A	419	SER
1	A	435	SER
1	A	467	THR
1	A	471	ASP
1	A	475	LYS
1	A	486	PRO
1	A	493	VAL
1	A	498	VAL
1	A	550	ASP
1	B	52	THR
1	B	56	ASP
1	B	57	GLU
1	B	58	SER
1	B	68	THR
1	B	82	GLU
1	B	83	THR
1	B	105	HIS
1	B	179	LEU

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Mol	Chain	Res	Type
1	B	212	LYS
1	B	222	ARG
1	B	283	LEU
1	B	284	LEU
1	B	323	LYS
1	B	375	ASP
1	B	435	SER
1	B	480	SER
1	B	489	SER
1	B	538	LYS
1	B	545	LYS
1	B	547	VAL
1	B	548	MET
1	B	555	VAL
1	B	558	CYS
1	B	566	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	61	ASN
1	A	99	ASN
1	A	109	ASN
1	A	268	GLN
1	A	338	HIS
1	A	385	GLN
1	A	404	GLN
1	A	464	HIS
1	A	483	ASN
1	A	543	GLN
1	B	99	ASN
1	B	111	ASN
1	B	196	GLN
1	B	221	GLN
1	B	338	HIS
1	B	385	GLN
1	B	386	ASN
1	B	464	HIS
1	B	543	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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$
2	RWF	B	2001	-	25,25,25	1.82	7 (28%)	34,35,35	1.18	3 (8%)
2	RWF	A	2001	-	25,25,25	1.58	4 (16%)	34,35,35	1.16	3 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RWF	B	2001	-	-	0/12/12/12	0/3/3/3
2	RWF	A	2001	-	-	0/12/12/12	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	RWF	O3-C4	4.94	1.40	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	RWF	O3-C4	4.90	1.39	1.21
2	B	2001	RWF	C14-C13	2.79	1.41	1.36
2	B	2001	RWF	C15-C1	2.63	1.43	1.39
2	A	2001	RWF	C14-C13	2.49	1.40	1.36
2	B	2001	RWF	C1-C14	2.27	1.49	1.45
2	B	2001	RWF	C7-C6	2.22	1.42	1.39
2	B	2001	RWF	C2-C13	2.17	1.54	1.52
2	A	2001	RWF	C15-C1	2.13	1.43	1.39
2	A	2001	RWF	C2-C13	2.04	1.54	1.52
2	B	2001	RWF	C8-C7	2.02	1.42	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	RWF	C5-C4-C3	3.90	121.95	116.53
2	A	2001	RWF	C5-C4-C3	3.62	121.57	116.53
2	B	2001	RWF	O3-C4-C3	-3.24	116.67	121.74
2	A	2001	RWF	O3-C4-C3	-3.03	116.99	121.74
2	A	2001	RWF	C3-C2-C13	-2.40	109.28	113.25
2	B	2001	RWF	C3-C2-C13	-2.25	109.53	113.25

There are no chirality outliers.

There are no torsion outliers.

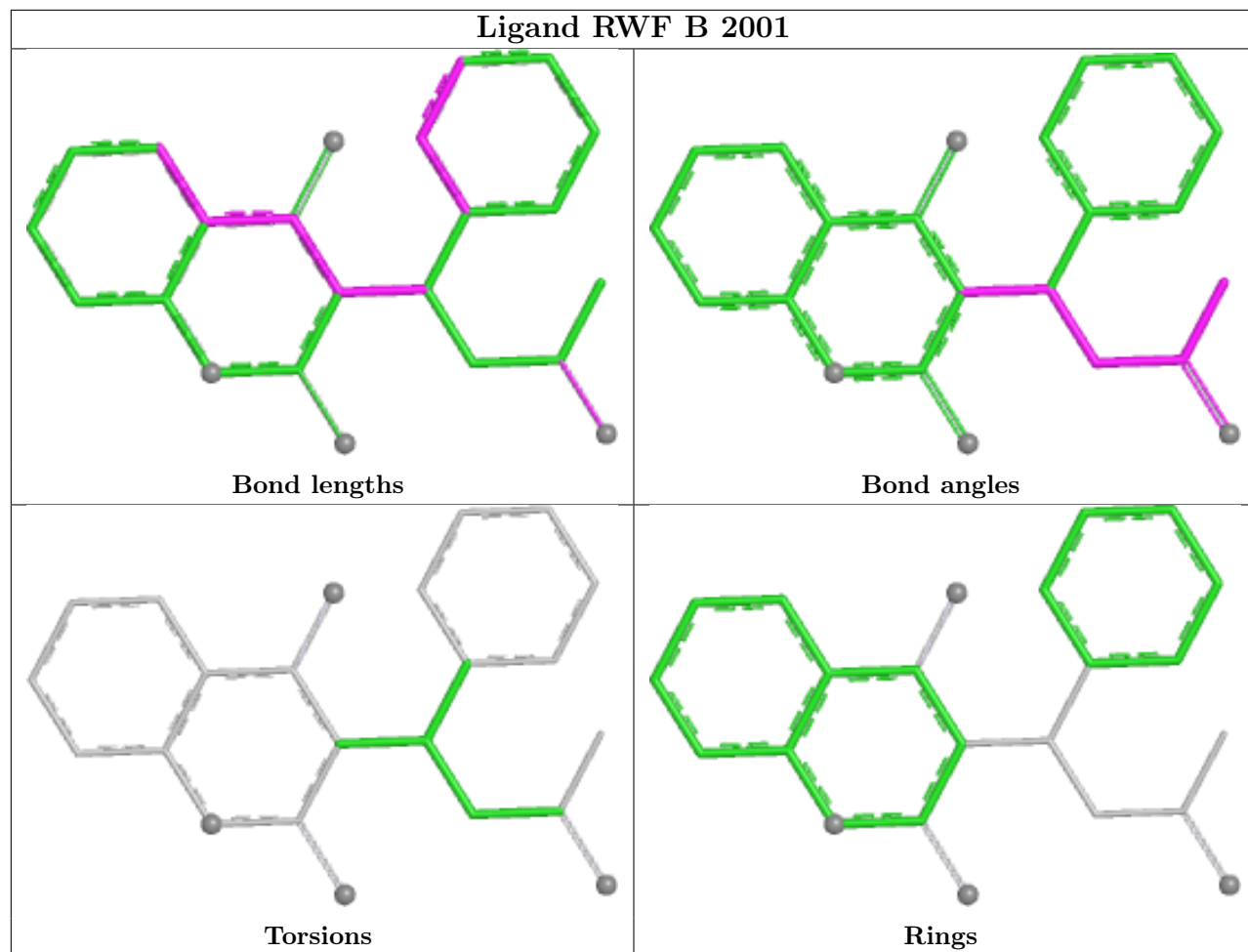
There are no ring outliers.

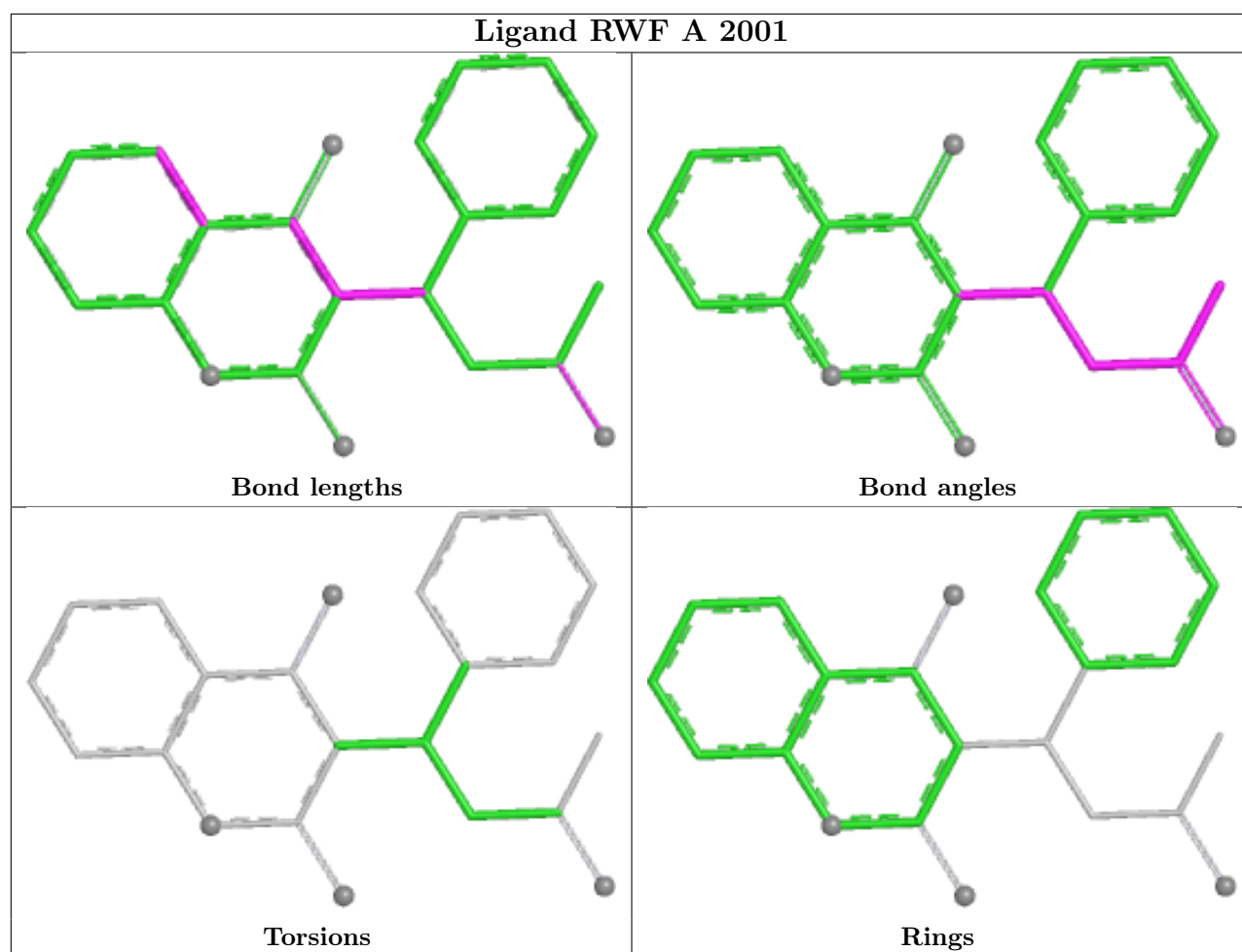
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	RWF	5	0
2	A	2001	RWF	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.





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	A	578/585 (98%)	-0.39	4 (0%) 84 66	25, 65, 147, 166	0
1	B	578/585 (98%)	-0.35	6 (1%) 79 59	25, 70, 150, 168	0
All	All	1156/1170 (98%)	-0.37	10 (0%) 81 61	25, 67, 149, 168	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	GLU	3.4
1	A	83	THR	2.9
1	A	570	GLU	2.8
1	B	84	TYR	2.8
1	A	582	ALA	2.4
1	A	551	PHE	2.2
1	B	87	MET	2.2
1	B	83	THR	2.2
1	B	559	CYS	2.1
1	B	565	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

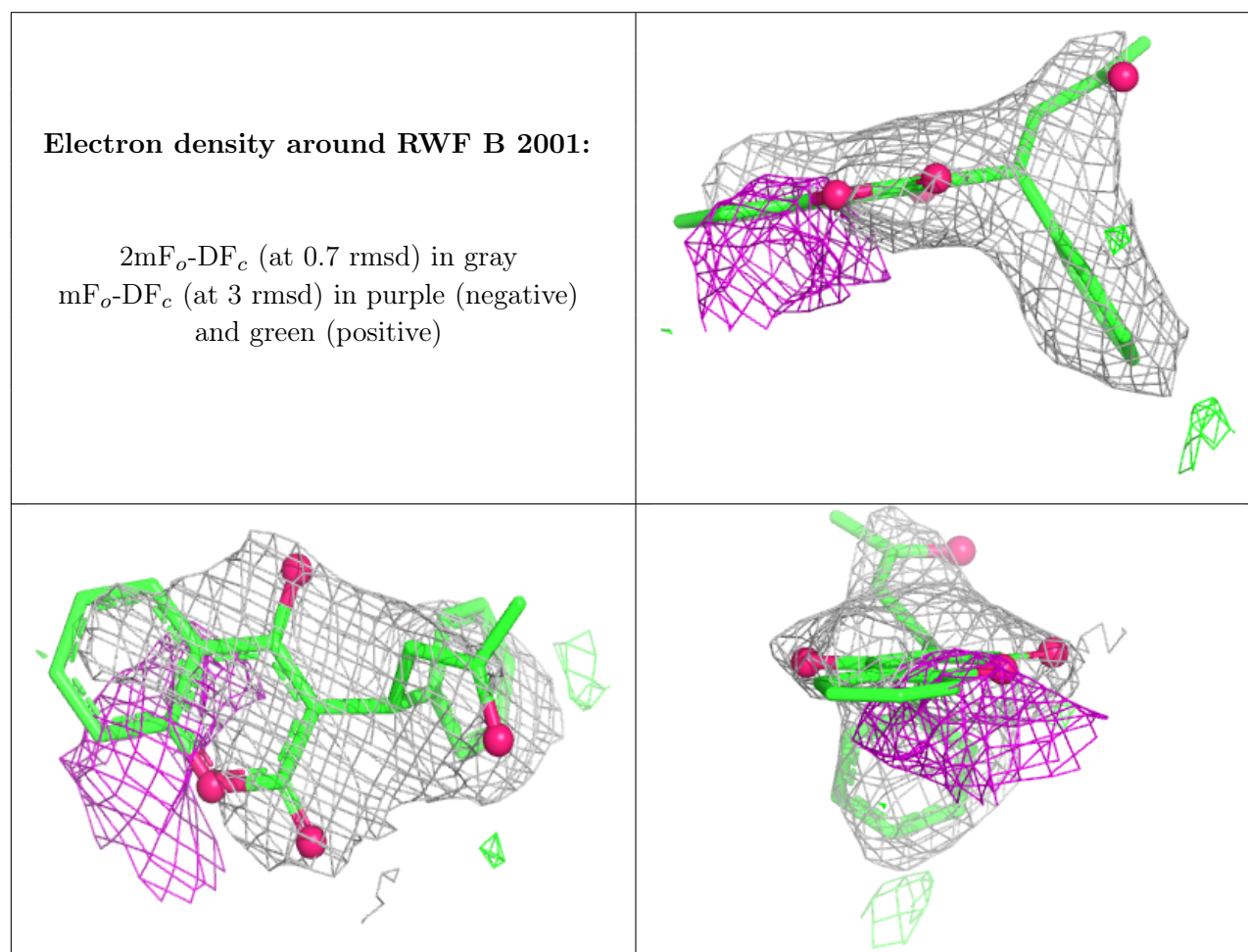
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

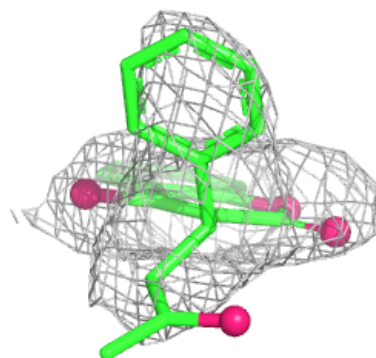
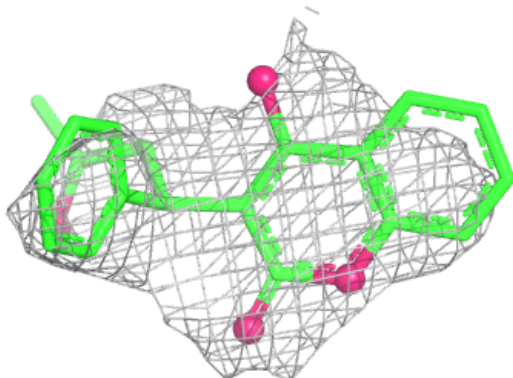
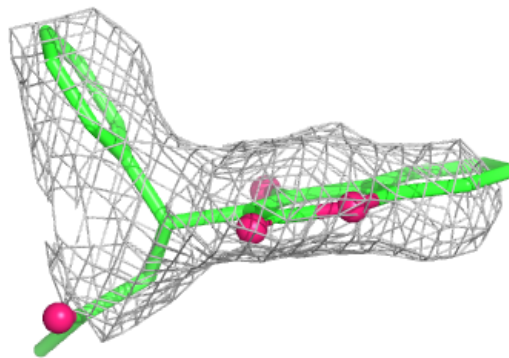
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	RWF	B	2001	23/23	0.78	0.21	107,113,116,116	0
2	RWF	A	2001	23/23	0.88	0.18	111,113,116,117	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around RWF A 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.