

Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 03:57 pm GMT

PDB ID	:	2XW1
Title	:	Human serum albumin complexed with dansyl-L-norvaline
Authors	:	Ryan, A.J.; Curry, S.
Deposited on	:	2010-10-28
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.50 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	130704	4661 (2.50-2.50)		
Clashscore	141614	5346 (2.50-2.50)		
Ramachandran outliers	138981	5231 (2.50-2.50)		
Sidechain outliers	138945	5233 (2.50-2.50)		
RSRZ outliers	127900	4559 (2.50-2.50)		

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 <=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	А	585	3% 67%	29%	• •		
1	В	585	3% 67%	28%	•••		



2XW1

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8540 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	А	569	Total 4296	C 2710	N 726	O 820	S 40	0	0	0
1	В	566	Total 4169	C 2626	N 707	O 796	S 40	0	0	0

• Molecule 2 is DANSYL-L-NORVALINE (three-letter code: 9NV) (formula: $C_{17}H_{22}N_2O_4S$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
9	Λ	1	Total	С	Ν	0	S	0	0
		1	22	17	2	2	1	0	0
0	Р	1	Total	С	Ν	0	S	0	0
	L	22	17	2	2	1	0	0	

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	19	Total O 19 19	0	0
3	В	12	Total O 12 12	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: SERUM ALBUMIN



D563 K444 K445 K333 E666 R445 R333 E665 R446 R333 E665 R446 R333 E665 R447 V325 E664 R446 R333 E665 R447 V325 E664 R449 R334 K579 R499 R337 A582 R494 R334 A582 R494 R334 A582 R494 R347 A582 R494 R349 A582 R494 R349 A583 R494 R344 A583 R494 R349 A584 R496 R346 K504 R504 R347 K504 R504 R377 K504 R504 R377 K504 R504 R377 K506 R394 R371 K506 R536 R343 K506 R536 R3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	55.18Å 55.39Å 119.91Å	Depositor
a, b, c, α , β , γ	81.17° 91.76° 64.74°	Depositor
Bosolution (Å)	35.29 - 2.50	Depositor
	49.23 - 2.50	EDS
% Data completeness	90.9 (35.29-2.50)	Depositor
(in resolution range)	91.0(49.23-2.50)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.81 (at 2.51 \text{\AA})$	Xtriage
Refinement program	$CNS \ 1.2$	Depositor
R R.	0.225 , 0.256	Depositor
II, II, <i>free</i>	0.221 , 0.250	DCC
R_{free} test set	2081 reflections $(4.78%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	56.5	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.28 , 57.2	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8540	wwPDB-VP
Average B, all atoms $(Å^2)$	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.14% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: $9\mathrm{NV}$

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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.40	0/4378	0.61	0/5945	
1	В	0.40	0/4249	0.59	0/5785	
All	All	0.40	0/8627	0.60	0/11730	

There are no bond length outliers.

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	А	4296	0	4011	132	0
1	В	4169	0	3777	135	0
2	А	22	0	21	2	0
2	В	22	0	21	3	0
3	А	19	0	0	2	0
3	В	12	0	0	0	0
All	All	8540	0	7830	267	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 16.

All (267) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:135:LEU:HD11	1:B:162:LYS:HG3	1.13	1.13
1:A:152:PRO:HB2	1:A:257:ARG:HH11	1.12	1.08
1:B:57:GLU:HG3	1:B:58:SER:H	1.28	0.95
1:A:61:ASN:HD22	1:A:64:LYS:HE3	1.28	0.94
1:B:557:LYS:HG3	1:B:558:CYS:N	1.82	0.91
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.35	0.88
1:A:66:LEU:O	1:A:70:PHE:HD1	1.57	0.88
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.56	0.87
1:A:152:PRO:HB2	1:A:257:ARG:NH1	1.88	0.87
1:A:545:LYS:HD2	1:A:545:LYS:C	1.95	0.85
1:B:120:VAL:HG21	1:B:175:ALA:HA	1.59	0.84
1:B:319:TYR:CE1	1:B:323:LYS:HG3	2.13	0.83
1:A:424:VAL:O	1:A:428:ARG:HG3	1.78	0.82
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.61	0.82
1:A:135:LEU:HD11	1:A:162:LYS:HG3	1.62	0.80
1:A:133:THR:O	1:A:137:LYS:HG3	1.82	0.80
1:B:557:LYS:HG3	1:B:558:CYS:H	1.45	0.80
1:B:39:HIS:O	1:B:43:VAL:HG23	1.82	0.78
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.63	0.78
1:B:117:ARG:NH2	1:B:182:LEU:HB3	2.01	0.76
1:B:95:GLU:OE1	1:B:99:ASN:HB2	1.87	0.75
1:B:110:PRO:HB2	1:B:112:LEU:CD2	2.16	0.75
1:A:95:GLU:CB	1:A:96:PRO:HD3	2.16	0.75
1:A:276:LYS:HG3	3:A:2007:HOH:O	1.84	0.75
1:B:557:LYS:HD3	1:B:571:GLU:CB	2.16	0.74
1:B:424:VAL:O	1:B:428:ARG:HG3	1.87	0.74
1:B:345:LEU:HD22	1:B:446:MET:HE1	1.69	0.73
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.70	0.72
1:B:43:VAL:O	1:B:46:VAL:HG23	1.90	0.72
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.70	0.72
1:B:42:LEU:O	1:B:46:VAL:HG22	1.90	0.72
1:B:265:CYS:O	1:B:268:GLN:HG3	1.89	0.72
1:B:110:PRO:HB2	1:B:112:LEU:HD22	1.69	0.72
1:B:66:LEU:O	1:B:70:PHE:HD1	1.71	0.72
1:B:378:LYS:HB2	1:B:379:PRO:HD3	1.74	0.69
1:B:364:ALA:O	1:B:366:PRO:HD3	1.92	0.69
1:A:218:ARG:NH2	1:A:222:ARG:HH21	1.90	0.69
1:A:513:ILE:HG13	1:A:514:CYS:N	2.06	0.68
1:B:127:PHE:O	1:B:131:GLU:HB3	1.93	0.68
1:B:557:LYS:NZ	1:B:567:CYS:SG	2.65	0.68
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.34	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.59	0.67
1:A:225:LYS:HG2	1:A:299:PRO:HG3	1.76	0.67
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.29	0.67
1:A:545:LYS:HD2	1:A:546:ALA:N	2.10	0.67
1:A:531:GLU:O	1:A:535:HIS:ND1	2.23	0.67
1:B:325:VAL:O	1:B:329:MET:HG3	1.94	0.67
1:A:240:LYS:O	1:A:244:GLU:HG3	1.95	0.66
1:B:483:ASN:O	1:B:486:PRO:HD2	1.94	0.66
1:B:483:ASN:C	1:B:486:PRO:HD2	2.17	0.65
1:A:169:CYS:HA	1:A:174:LYS:HD3	1.79	0.65
1:B:25:ILE:O	1:B:29:GLN:HG3	1.96	0.65
1:B:117:ARG:HH22	1:B:182:LEU:HB3	1.62	0.65
1:B:116:VAL:O	1:B:118:PRO:HD3	1.98	0.64
1:B:345:LEU:HD22	1:B:446:MET:CE	2.27	0.64
1:A:120:VAL:HG11	1:A:174:LYS:HB2	1.80	0.63
1:A:513:ILE:CD1	1:A:555:VAL:HG13	2.29	0.63
1:B:57:GLU:CG	1:B:58:SER:H	2.08	0.62
1:A:510:HIS:HA	1:A:568:PHE:CB	2.29	0.62
1:A:152:PRO:CB	1:A:257:ARG:HH11	2.00	0.62
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.65	0.62
1:A:209:ARG:HG2	1:A:209:ARG:NH1	2.12	0.62
1:A:433:VAL:HG22	1:A:452:TYR:CD2	2.35	0.62
1:A:483:ASN:O	1:A:486:PRO:HD2	1.99	0.62
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.83	0.61
1:B:42:LEU:O	1:B:46:VAL:CG2	2.47	0.61
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.40	0.61
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.64	0.61
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.83	0.61
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.35	0.61
1:A:61:ASN:ND2	1:A:64:LYS:HE3	2.09	0.61
1:A:209:ARG:HH11	1:A:209:ARG:CG	2.13	0.61
1:B:552:ALA:O	1:B:555:VAL:HG12	2.02	0.60
1:B:135:LEU:CD1	1:B:162:LYS:HG3	2.08	0.60
1:A:483:ASN:C	1:A:486:PRO:HD2	2.22	0.60
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.84	0.60
1:A:325:VAL:O	1:A:329:MET:HG3	2.02	0.59
1:B:557:LYS:NZ	1:B:571:GLU:CB	2.65	0.59
1:A:513:ILE:HD11	1:A:555:VAL:HG13	1.83	0.59
1:B:503:ASN:ND2	1:B:506:THR:OG1	2.36	0.59
1:B:222:ARG:C	1:B:224:PRO:HD3	2.24	0.58
1:B:262:LYS:O	1:B:266:GLU:HG3	2.04	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:400:GLU:O	1:A:404:GLN:HG3	2.04	0.58
1:A:545:LYS:C	1:A:545:LYS:CD	2.71	0.58
1:B:400:GLU:O	1:B:404:GLN:HG3	2.03	0.58
1:B:32:GLN:NE2	1:B:147:PRO:HG3	2.19	0.58
1:B:410:ARG:HH11	1:B:410:ARG:HG2	1.68	0.58
1:A:513:ILE:CG1	1:A:514:CYS:N	2.67	0.58
1:B:410:ARG:HD3	2:B:2001:9NV:HG2C	1.86	0.58
1:B:57:GLU:HG3	1:B:58:SER:N	2.11	0.57
1:B:391:ASN:HB3	2:B:2001:9NV:H222	1.85	0.57
1:B:499:PRO:HB3	1:B:535:HIS:O	2.03	0.57
1:A:388:ILE:HD13	2:A:2001:9NV:H19	1.87	0.57
1:B:444:LYS:O	1:B:447:PRO:HD2	2.05	0.57
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.87	0.57
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.40	0.57
1:B:71:GLY:HA3	1:B:98:ARG:NH2	2.20	0.57
1:A:107:ASP:O	1:A:110:PRO:HD3	2.06	0.56
1:A:222:ARG:O	1:A:224:PRO:HD3	2.05	0.56
1:B:311:GLU:O	1:B:367:HIS:NE2	2.32	0.56
1:B:367:HIS:O	1:B:371:ALA:HB2	2.05	0.56
1:A:529:LEU:O	1:A:533:VAL:HG23	2.06	0.55
1:A:536:LYS:CG	1:A:539:ALA:HB2	2.37	0.55
1:A:510:HIS:O	1:A:513:ILE:HG23	2.06	0.55
1:B:20:LYS:CE	1:B:44:ASN:OD1	2.56	0.54
1:A:222:ARG:C	1:A:224:PRO:HD3	2.28	0.54
1:A:5:SER:HA	1:A:62:CYS:O	2.08	0.53
1:B:66:LEU:O	1:B:70:PHE:CD1	2.57	0.53
1:B:168:CYS:SG	1:B:177:CYS:C	2.86	0.53
1:A:66:LEU:HB3	1:A:70:PHE:CE1	2.43	0.53
1:A:319:TYR:CE1	1:A:323:LYS:HG3	2.44	0.53
1:A:72:ASP:O	1:A:76:THR:HG23	2.08	0.53
1:B:120:VAL:HG21	1:B:175:ALA:CA	2.34	0.53
1:B:557:LYS:HZ2	1:B:571:GLU:CB	2.22	0.53
1:B:563:ASP:CG	1:B:567:CYS:HB2	2.29	0.53
1:A:95:GLU:CB	1:A:96:PRO:CD	2.86	0.53
1:A:161:TYR:CZ	1:A:165:PHE:HE2	2.27	0.53
1:B:9:HIS:CD2	1:B:13:ASP:OD2	2.62	0.53
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.90	0.53
1:A:305:LEU:HD13	1:A:334:TYR:CD2	2.44	0.53
1:B:36:PHE:CZ	1:B:40:VAL:HG21	2.44	0.52
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.90	0.52
1:A:66:LEU:O	1:A:70:PHE:CD1	2.49	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:90:CYS:O	1:B:98:ARG:HG3	2.10	0.52
1:B:543:GLN:O	1:B:546:ALA:HB3	2.10	0.52
1:B:36:PHE:O	1:B:40:VAL:HG23	2.10	0.51
1:B:561:ALA:HB3	1:B:563:ASP:OD1	2.09	0.51
1:A:46:VAL:HG22	1:A:73:LYS:HG3	1.92	0.51
1:A:30:TYR:HE1	1:A:103:LEU:HD23	1.75	0.51
1:A:286:LYS:O	1:A:290:ILE:HG13	2.10	0.51
1:B:398:LEU:HB3	1:B:402:LYS:HB2	1.94	0.50
1:A:14:LEU:HD13	1:A:22:LEU:HD12	1.93	0.50
1:B:179:LEU:N	1:B:180:PRO:HD2	2.27	0.50
1:A:39:HIS:O	1:A:43:VAL:HG23	2.11	0.50
1:A:107:ASP:OD2	1:A:110:PRO:HA	2.12	0.50
1:B:223:PHE:CD1	1:B:272:SER:HB2	2.46	0.50
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.42	0.50
1:B:30:TYR:CE1	1:B:103:LEU:HD23	2.46	0.50
1:A:145:ARG:HG3	1:A:145:ARG:HH11	1.76	0.50
1:B:263:TYR:CD1	1:B:263:TYR:C	2.84	0.50
1:B:498:VAL:O	1:B:498:VAL:HG23	2.11	0.50
1:A:150:TYR:CE2	1:A:257:ARG:CZ	2.95	0.50
1:B:557:LYS:HE2	1:B:567:CYS:SG	2.52	0.49
1:A:42:LEU:O	1:A:46:VAL:HG23	2.12	0.49
1:B:107:ASP:HB3	1:B:110:PRO:HG3	1.94	0.49
1:B:545:LYS:HA	1:B:548:MET:HB2	1.92	0.49
1:A:135:LEU:HD11	1:A:162:LYS:CG	2.37	0.49
1:A:247:HIS:O	1:A:247:HIS:ND1	2.46	0.49
1:A:513:ILE:HD11	1:A:559:CYS:SG	2.53	0.49
1:B:502:PHE:CZ	1:B:504:ALA:HA	2.48	0.49
1:B:57:GLU:O	1:B:58:SER:C	2.51	0.49
1:A:567:CYS:O	1:A:571:GLU:N	2.43	0.48
1:A:511:ALA:O	1:A:514:CYS:SG	2.72	0.48
1:B:10:ARG:O	1:B:14:LEU:HD23	2.13	0.48
1:B:410:ARG:HG2	1:B:410:ARG:NH1	2.28	0.48
1:A:388:ILE:HD13	2:A:2001:9NV:C19	2.43	0.48
1:B:152:PRO:HB2	1:B:257:ARG:HH11	1.79	0.48
1:B:50:ALA:O	1:B:54:VAL:HG23	2.14	0.48
1:B:99:ASN:HA	1:B:102:PHE:HD2	1.78	0.48
1:A:420:THR:HG23	1:A:530:VAL:HG11	1.95	0.47
1:B:9:HIS:HD2	1:B:13:ASP:OD2	1.97	0.47
1:B:117:ARG:HG3	1:B:117:ARG:O	2.15	0.47
1:A:290:ILE:O	1:A:293:VAL:HG22	2.15	0.47
1:A:512:ASP:O	1:A:515:THR:HG22	2.15	0.47



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:39:HIS:CD2	1:B:140:TYR:HE1	2.33	0.47	
1:B:281:LYS:CG	1:B:285:GLU:OE2	2.63	0.47	
1:B:39:HIS:HD2	1:B:140:TYR:HE1	1.62	0.47	
1:A:370:TYR:HD1	1:A:370:TYR:O	1.98	0.47	
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.97	0.46	
1:A:451:ASP:OD1	1:A:452:TYR:N	2.48	0.46	
1:B:27:PHE:HE1	1:B:70:PHE:HD2	1.62	0.46	
1:B:98:ARG:O	1:B:101:CYS:HB3	2.15	0.46	
1:A:161:TYR:CE2	1:A:165:PHE:CE2	3.04	0.46	
1:A:555:VAL:O	1:A:559:CYS:HB2	2.16	0.46	
1:B:240:LYS:O	1:B:244:GLU:HG3	2.15	0.46	
1:A:46:VAL:CG2	1:A:73:LYS:HG3	2.45	0.46	
1:B:503:ASN:OD1	1:B:503:ASN:N	2.49	0.46	
1:A:39:HIS:HD2	1:A:140:TYR:CE1	2.34	0.46	
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.16	0.45	
1:A:61:ASN:HB3	1:A:64:LYS:HD2	1.98	0.45	
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.42	0.45	
1:A:289:CYS:O	1:A:293:VAL:HG13	2.17	0.45	
1:A:21:ALA:HB1	1:A:155:LEU:HD21	1.98	0.45	
1:A:521:ARG:O	1:A:524:LYS:N	2.48	0.45	
1:B:519:LYS:O	1:B:523:ILE:HG13	2.17	0.45	
1:B:337:ARG:HG3	1:B:337:ARG:HH11	1.80	0.45	
1:B:441:PRO:O	1:B:443:ALA:N	2.49	0.45	
1:B:116:VAL:O	1:B:116:VAL:HG13	2.17	0.45	
1:B:222:ARG:HA	1:B:295:ASN:OD1	2.16	0.45	
1:B:348:ARG:HG3	1:B:482:VAL:CG1	2.47	0.45	
1:B:388:ILE:HD12	1:B:449:ALA:CB	2.47	0.45	
1:B:311:GLU:O	1:B:312:SER:C	2.55	0.45	
1:A:35:PRO:HG2	1:A:38:ASP:OD2	2.15	0.45	
1:B:100:GLU:HG2	1:B:103:LEU:HD12	1.99	0.45	
1:B:535:HIS:C	1:B:537:PRO:HD3	2.36	0.45	
1:A:209:ARG:NH1	1:A:209:ARG:CG	2.74	0.44	
1:B:237:ASP:HB3	1:B:260:LEU:HD12	1.99	0.44	
1:B:237:ASP:CB	1:B:260:LEU:HD12	2.46	0.44	
1:B:557:LYS:CE	1:B:567:CYS:SG	3.05	0.44	
1:A:545:LYS:O	1:A:549:ASP:OD1	2.35	0.44	
1:A:7:VAL:HG23	3:A:2002:HOH:O	2.16	0.44	
1:A:278:CYS:O	1:A:281:LYS:HG2	2.17	0.44	
1:A:410:ARG:O	1:A:414:LYS:HG3	2.17	0.44	
1:B:446:MET:HB3	1:B:447:PRO:HD3	1.97	0.44	
1:B:95:GLU:OE2	1:B:98:ARG:HB3	2.18	0.44	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:38:ASP:O	1:A:42:LEU:HG	2.18	0.44
1:A:161:TYR:CE2	1:A:165:PHE:HE2	2.36	0.44
1:A:31:LEU:HD12	1:A:74:LEU:HD22	1.99	0.44
1:A:513:ILE:HD12	1:A:555:VAL:HG13	1.97	0.44
1:A:549:ASP:O	1:A:552:ALA:HB3	2.17	0.43
1:B:151:ALA:HB3	1:B:152:PRO:CD	2.40	0.43
1:A:25:ILE:HD13	1:A:154:LEU:HD23	2.00	0.43
1:A:425:GLU:HA	1:A:425:GLU:OE1	2.17	0.43
1:A:36:PHE:O	1:A:40:VAL:HG23	2.19	0.43
1:A:296:ASP:OD1	1:A:297:GLU:N	2.51	0.43
1:B:530:VAL:O	1:B:534:LYS:HG3	2.18	0.43
1:A:168:CYS:SG	1:A:177:CYS:C	2.97	0.43
1:A:303:PRO:O	1:A:337:ARG:NH1	2.52	0.43
1:A:426:VAL:O	1:A:430:LEU:HG	2.18	0.43
1:B:384:PRO:O	1:B:388:ILE:HG12	2.19	0.43
1:B:27:PHE:HE1	1:B:70:PHE:CD2	2.35	0.43
1:B:290:ILE:O	1:B:293:VAL:HG12	2.18	0.43
1:B:218:ARG:NH2	1:B:222:ARG:HH21	2.17	0.42
1:B:387:LEU:CD2	1:B:485:ARG:NH1	2.82	0.42
1:A:249:ASP:HB3	1:A:252:GLU:CG	2.49	0.42
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.50	0.42
1:B:409:VAL:O	1:B:413:LYS:HG3	2.19	0.42
1:B:485:ARG:HB3	1:B:486:PRO:HD3	2.01	0.42
1:A:145:ARG:HG3	1:A:145:ARG:NH1	2.34	0.42
1:A:39:HIS:HD2	1:A:140:TYR:HE1	1.66	0.42
1:B:373:VAL:HG13	1:B:374:PHE:CD1	2.50	0.42
1:A:501:GLU:OE1	1:A:501:GLU:HA	2.18	0.42
1:A:56:ASP:O	1:A:58:SER:N	2.47	0.42
1:B:212:LYS:O	1:B:216:VAL:HG23	2.20	0.42
1:B:222:ARG:O	1:B:224:PRO:HD3	2.20	0.42
1:A:281:LYS:HB2	1:A:282:PRO:CD	2.37	0.42
1:B:20:LYS:NZ	1:B:44:ASN:OD1	2.53	0.42
1:B:35:PRO:HD2	1:B:38:ASP:OD2	2.20	0.42
1:A:305:LEU:HD21	1:A:333:GLU:HB3	2.01	0.41
1:A:408:LEU:HD21	1:A:424:VAL:HA	2.01	0.41
1:A:507:PHE:CD1	1:A:507:PHE:N	2.87	0.41
1:B:57:GLU:CG	1:B:58:SER:N	2.78	0.41
1:B:414:LYS:HE3	1:B:488:PHE:O	2.21	0.41
1:A:464:HIS:CE1	1:A:469:VAL:H	2.37	0.41
1:A:493:VAL:HG21	1:A:538:LYS:NZ	2.36	0.41
1:A:56:ASP:C	1:A:58:SER:H	2.23	0.41



A + 1	A + 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:464:HIS:CG	1:B:473:VAL:HG11	2.55	0.41
1:B:576:VAL:HA	1:B:579:SER:HB2	2.03	0.41
1:B:61:ASN:HB3	1:B:64:LYS:CD	2.51	0.41
1:B:151:ALA:CB	1:B:152:PRO:HD3	2.41	0.41
1:A:388:ILE:HD12	1:A:449:ALA:CB	2.51	0.41
1:B:263:TYR:HD1	1:B:264:ILE:N	2.19	0.41
1:B:370:TYR:CD1	1:B:370:TYR:C	2.94	0.41
1:A:262:LYS:O	1:A:266:GLU:HG3	2.21	0.41
1:A:279:CYS:HA	1:A:286:LYS:CD	2.51	0.41
1:A:61:ASN:HB3	1:A:64:LYS:CD	2.52	0.40
1:A:100:GLU:OE1	1:A:100:GLU:HA	2.22	0.40
1:A:139:LEU:HD21	1:A:158:ALA:HB2	2.03	0.40
1:A:311:GLU:O	1:A:312:SER:C	2.59	0.40
1:B:27:PHE:CE1	1:B:70:PHE:HD2	2.39	0.40
1:A:543:GLN:O	1:A:547:VAL:HG23	2.22	0.40
1:A:98:ARG:O	1:A:101:CYS:HB3	2.21	0.40
1:A:227:GLU:OE1	1:A:227:GLU:HA	2.21	0.40
1:B:388:ILE:HA	2:B:2001:9NV:H19	2.04	0.40
1:A:41:LYS:HG3	1:A:45:GLU:OE2	2.22	0.40
1:B:14:LEU:HD22	1:B:14:LEU:N	2.37	0.40
1:B:558:CYS:C	1:B:560:LYS:N	2.74	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	А	565/585~(97%)	507 (90%)	44 (8%)	14 (2%)	5 8
1	В	562/585~(96%)	498 (89%)	54 (10%)	10 (2%)	8 14
All	All	1127/1170 (96%)	1005 (89%)	98 (9%)	24 (2%)	7 11



Mol	Chain Res		Type
1	А	59	ALA
1	А	95	GLU
1	А	300	ALA
1	В	54	VAL
1	В	57	GLU
1	В	300	ALA
1	В	565	GLU
1	А	58	SER
1	А	315	VAL
1	А	546	ALA
1	А	557	LYS
1	В	58	SER
1	В	442	GLU
1	А	57	GLU
1	А	60	GLU
1	А	562	ASP
1	В	312	SER
1	А	312	SER
1	В	60	GLU
1	В	118	PRO
1	В	283	LEU
1	А	307	ALA
1	A	96	PRO
1	A	303	PRO

All (24) Ramachandran outliers are listed below:

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		
1	А	437/511~(86%)	422~(97%)	15 (3%)	37 63		
1	В	404/511 (79%)	393~(97%)	11 (3%)	44 71		
All	All	841/1022 (82%)	815(97%)	26 (3%)	40 67		

All (26) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	99	ASN
1	А	104	GLN
1	А	109	ASN
1	А	114	ARG
1	А	117	ARG
1	А	186	ARG
1	А	245	CYS
1	А	252	GLU
1	А	262	LYS
1	А	442	GLU
1	А	452	TYR
1	А	467	THR
1	А	493	VAL
1	А	545	LYS
1	А	550	ASP
1	В	37	GLU
1	В	46	VAL
1	В	105	HIS
1	В	112	LEU
1	В	245	CYS
1	В	375	ASP
1	В	489	SER
1	В	501	GLU
1	В	503	ASN
1	В	548	MET
1	В	557	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	29	GLN
1	А	39	HIS
1	А	61	ASN
1	А	109	ASN
1	А	318	ASN
1	А	464	HIS
1	А	483	ASN
1	В	9	HIS
1	В	67	HIS
1	В	247	HIS
1	В	464	HIS
1	В	483	ASN
1	В	503	ASN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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).

Mal	Tuno	Chain	Dec	Tink	B	ond leng	gths	B	ond ang	les
WIOI	туре	Unam	nes	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	9NV	А	2001	-	22,23,25	2.20	9 (40%)	29,33,36	1.40	5 (17%)
2	9NV	В	2001	-	22,23,25	2.26	10 (45%)	29,33,36	1.34	2 (6%)

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	9NV	А	2001	-	-	3/18/18/22	0/2/2/2
2	9NV	В	2001	-	-	2/18/18/22	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	2001	9NV	C19-C20	5.35	1.48	1.38



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	2001	9NV	C19-C20	4.97	1.48	1.38
2	А	2001	9NV	C16-C15	3.72	1.50	1.43
2	В	2001	9NV	C18-C19	3.64	1.46	1.38
2	А	2001	9NV	C11-C16	3.63	1.49	1.43
2	В	2001	9NV	C16-C15	3.55	1.50	1.43
2	А	2001	9NV	C18-C19	3.50	1.46	1.38
2	В	2001	9NV	C11-S8	-3.37	1.74	1.77
2	В	2001	9NV	C14-C15	2.82	1.48	1.42
2	А	2001	9NV	C12-C11	2.71	1.40	1.37
2	В	2001	9NV	C11-C16	2.69	1.47	1.43
2	А	2001	9NV	C13-C12	2.62	1.44	1.38
2	В	2001	9NV	C12-C11	2.60	1.40	1.37
2	А	2001	9NV	C20-C15	2.57	1.48	1.42
2	В	2001	9NV	C20-C15	2.55	1.48	1.42
2	А	2001	9NV	C18-C17	2.36	1.42	1.36
2	А	2001	9NV	C14-C15	2.35	1.47	1.42
2	В	2001	9NV	C18-C17	2.34	1.42	1.36
2	В	2001	9NV	C13-C12	2.08	1.43	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	В	2001	9NV	C22-N21-C23	-3.22	105.76	116.12
2	А	2001	9NV	C22-N21-C23	-2.90	106.78	116.12
2	А	2001	9NV	C-CA-CB	-2.58	106.58	111.47
2	А	2001	9NV	CG-CB-CA	2.37	118.02	114.19
2	А	2001	9NV	O10-S8-N	-2.33	102.67	106.88
2	В	2001	9NV	C19-C20-N21	2.32	125.18	121.68
2	А	2001	9NV	C19-C20-N21	2.07	124.81	121.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	2001	9NV	N-CA-CB-CG
2	А	2001	9NV	C-CA-CB-CG
2	В	2001	9NV	N-CA-CB-CG
2	В	2001	9NV	C-CA-CB-CG
2	А	2001	9NV	CA-N-S8-O10

There are no ring outliers.



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	2001	9NV	2	0
2	В	2001	9NV	3	0

2 monomers are involved in 5 short contacts:

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 then 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 similar 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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	569/585~(97%)	0.03	20 (3%) 44 47	35, 71, 147, 158	0
1	В	566/585~(96%)	-0.06	17 (3%) 50 53	34, 72, 141, 161	0
All	All	1135/1170~(97%)	-0.01	37 (3%) 46 50	34, 71, 144, 161	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	509	PHE	7.1
1	В	562	ASP	5.8
1	А	563	ASP	5.3
1	А	504	ALA	5.3
1	А	568	PHE	5.0
1	А	569	ALA	4.9
1	В	509	PHE	3.8
1	А	505	GLU	3.5
1	А	508	THR	3.5
1	В	8	ALA	3.3
1	В	504	ALA	3.1
1	В	7	VAL	2.9
1	А	507	PHE	2.9
1	А	92	ALA	2.9
1	А	555	VAL	2.8
1	А	510	HIS	2.8
1	В	54	VAL	2.7
1	В	128	HIS	2.6
1	В	582	ALA	2.6
1	А	561	ALA	2.5
1	А	558	CYS	2.5
1	А	513	ILE	2.5
1	В	566	THR	2.5
1	А	506	THR	2.4



		1	1 0	
Mol	Chain	Res	Type	RSRZ
1	В	561	ALA	2.4
1	В	52	THR	2.4
1	В	11	PHE	2.4
1	А	582	ALA	2.3
1	А	562	ASP	2.3
1	А	511	ALA	2.3
1	В	56	ASP	2.2
1	А	59	ALA	2.2
1	В	63	ASP	2.2
1	А	559	CYS	2.1
1	В	5	SER	2.1
1	В	577	ALA	2.1
1	В	70	PHE	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 monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	9NV	В	2001	22/24	0.94	0.21	57,61,72,73	0
2	9NV	А	2001	22/24	0.96	0.17	53,57,71,73	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.







6.5 Other polymers (i)

There are no such residues in this entry.

