Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:55 PM GMT

PDB ID	:	1D5J
Title	:	CRYSTAL STRUCTURE OF MMP3 COMPLEXED WITH A THIAZEPINE BASED INHIBITOR.
Authors	:	Almstead, N.G.; Bradley, R.S.; Pikul, S.; De, B.; Natchus, M.G.
Deposited on	:	1999-10-07
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

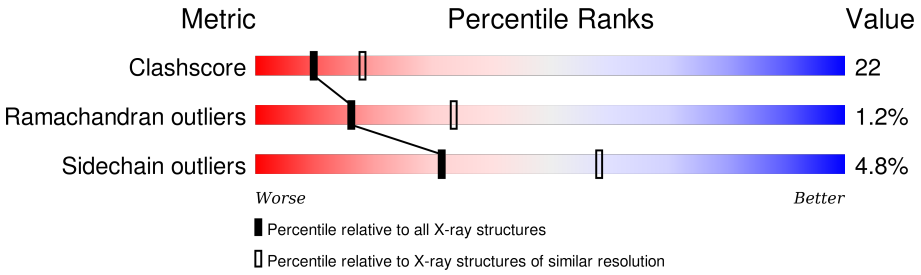
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	173	67% 25%
1	B	173	54% 36% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2869 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 STROMELYSIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1346	865	224	255	2			
1	B	173	Total	C	N	O	S	1	0	0
			1376	882	228	264	2			

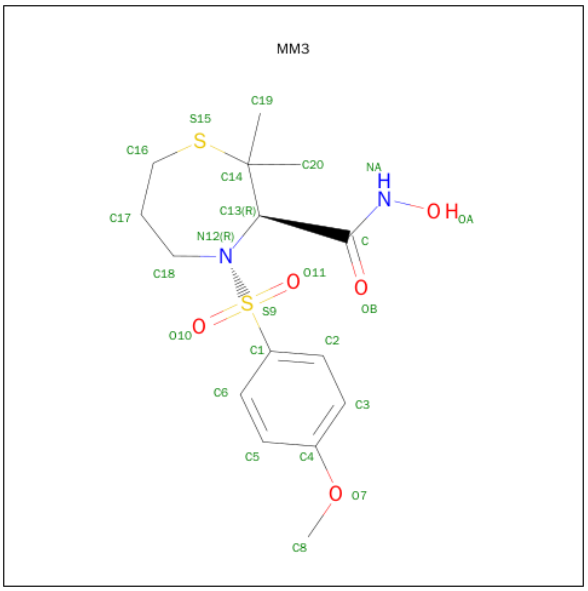
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		

- Molecule 4 is N-HYDROXY-4-[(4-METHOXYLPHENYL)SULFONYL]-2,2-DIMETHYL-HEXAHYDRO-1,4-THIAZEPINE-3(S)-CARBOXAMIDE (three-letter code: MM3) (formula: $C_{15}H_{22}N_2O_5S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			24	15	2	5	2		
4	B	1	Total	C	N	O	S	0	0
			24	15	2	5	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		
5	B	40	Total	O	0	0
			40	40		

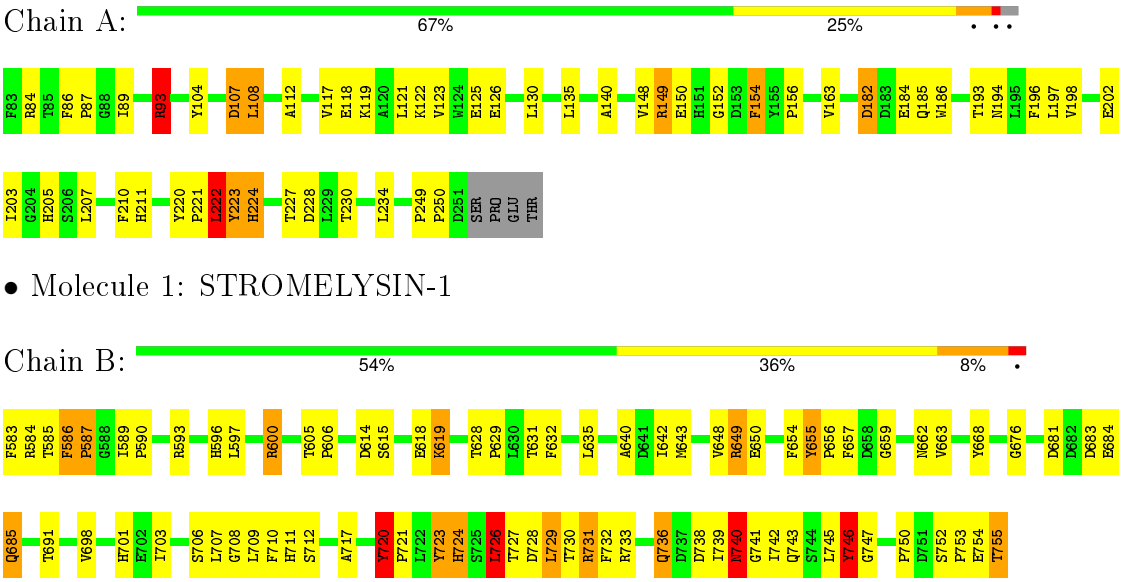
3 Residue-property plots (i)

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

Note EDS was not executed.

- Molecule 1: STROMELYSIN-1

Chain A:



- Molecule 1: STROMELYSIN-1

Chain B:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	37.78Å 78.54Å 105.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	92.2 (8.00-2.60)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.237 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2869	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, MM3

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	0.45	0/1390	1.70	16/1899 (0.8%)
1	B	0.47	0/1421	2.61	43/1941 (2.2%)
All	All	0.46	0/2811	2.21	59/3840 (1.5%)

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	A	0	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	733	ARG	NE-CZ-NH2	-34.11	103.25	120.30
1	B	600	ARG	NE-CZ-NH2	-32.55	104.02	120.30
1	A	149	ARG	NE-CZ-NH1	-32.49	104.06	120.30
1	B	733	ARG	NE-CZ-NH1	31.29	135.94	120.30
1	B	600	ARG	NE-CZ-NH1	30.45	135.52	120.30
1	A	149	ARG	NE-CZ-NH2	27.10	133.85	120.30
1	B	731	ARG	NE-CZ-NH2	-26.52	107.04	120.30
1	B	586	PHE	CB-CG-CD2	-25.24	103.13	120.80
1	A	93	ARG	NE-CZ-NH1	-25.16	107.72	120.30
1	B	746	TYR	CB-CG-CD1	-25.05	105.97	121.00
1	B	723	TYR	CB-CG-CD2	-23.00	107.20	121.00
1	B	586	PHE	CB-CG-CD1	22.38	136.46	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	223	TYR	CB-CG-CD2	-21.88	107.87	121.00
1	B	732	PHE	CB-CG-CD2	-21.59	105.69	120.80
1	B	710	PHE	CB-CG-CD1	-21.49	105.75	120.80
1	B	731	ARG	NE-CZ-NH1	20.33	130.47	120.30
1	B	723	TYR	CB-CG-CD1	20.08	133.05	121.00
1	B	655	TYR	CB-CG-CD1	-19.93	109.04	121.00
1	B	746	TYR	CB-CG-CD2	19.27	132.56	121.00
1	A	93	ARG	NE-CZ-NH2	19.08	129.84	120.30
1	B	732	PHE	CB-CG-CD1	18.13	133.49	120.80
1	B	710	PHE	CB-CG-CD2	17.47	133.03	120.80
1	B	720	TYR	CB-CG-CD2	-17.13	110.72	121.00
1	B	655	TYR	CB-CG-CD2	17.06	131.23	121.00
1	A	223	TYR	CB-CG-CD1	15.52	130.31	121.00
1	A	154	PHE	CB-CG-CD2	-14.85	110.41	120.80
1	B	720	TYR	CB-CG-CD1	12.22	128.33	121.00
1	A	224	HIS	CA-CB-CG	-11.38	94.26	113.60
1	B	726	LEU	N-CA-C	-10.54	82.54	111.00
1	A	223	TYR	CA-CB-CG	-9.94	94.52	113.40
1	B	736	GLN	CG-CD-OE1	9.28	140.16	121.60
1	A	154	PHE	CB-CG-CD1	8.69	126.88	120.80
1	B	685	GLN	CG-CD-OE1	8.64	138.88	121.60
1	B	736	GLN	CG-CD-NE2	-8.51	96.29	116.70
1	B	685	GLN	CG-CD-NE2	-8.11	97.23	116.70
1	B	733	ARG	CG-CD-NE	-7.73	95.56	111.80
1	B	685	GLN	CA-CB-CG	-7.42	97.08	113.40
1	A	149	ARG	CG-CD-NE	7.10	126.71	111.80
1	A	93	ARG	CD-NE-CZ	7.00	133.40	123.60
1	B	733	ARG	CA-CB-CG	6.61	127.94	113.40
1	B	585	THR	N-CA-CB	6.34	122.35	110.30
1	B	723	TYR	CA-CB-CG	-6.25	101.52	113.40
1	A	108	LEU	CA-CB-CG	6.20	129.56	115.30
1	B	733	ARG	CB-CG-CD	-6.06	95.84	111.60
1	A	222	LEU	N-CA-C	6.06	127.35	111.00
1	B	600	ARG	CG-CD-NE	6.00	124.41	111.80
1	B	740	ASN	CB-CG-ND2	-5.92	102.50	116.70
1	B	736	GLN	CB-CG-CD	-5.88	96.31	111.60
1	B	754	GLU	CA-CB-CG	5.84	126.25	113.40
1	B	600	ARG	CD-NE-CZ	5.76	131.67	123.60
1	B	600	ARG	CB-CG-CD	5.71	126.45	111.60
1	B	727	THR	N-CA-CB	-5.44	99.95	110.30
1	A	149	ARG	CB-CG-CD	5.42	125.70	111.60
1	A	154	PHE	CA-CB-CG	-5.39	100.97	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	701	HIS	CA-CB-CG	5.35	122.70	113.60
1	B	755	THR	N-CA-C	5.34	125.42	111.00
1	B	600	ARG	CA-CB-CG	5.22	124.88	113.40
1	B	740	ASN	CB-CG-OD1	5.16	131.92	121.60
1	B	740	ASN	CA-CB-CG	5.09	124.60	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	PHE	Sidechain
1	A	223	TYR	Sidechain
1	A	93	ARG	Sidechain
1	B	720	TYR	Sidechain
1	B	746	TYR	Sidechain

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	A	1346	0	1270	57	0
1	B	1376	0	1295	61	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	24	0	21	2	0
4	B	24	0	21	5	0
5	A	49	0	0	1	0
5	B	40	0	0	1	0
All	All	2869	0	2607	119	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 (119) 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:224:HIS:O	1:A:224:HIS:CD2	1.97	1.17
1:A:224:HIS:NE2	1:A:227:THR:HG21	1.67	1.09
1:A:228:ASP:HB2	1:A:230:THR:HG22	1.29	1.09
1:A:224:HIS:CD2	1:A:227:THR:HG23	1.86	1.08
1:A:224:HIS:HD2	1:A:224:HIS:O	1.32	1.02
1:A:224:HIS:NE2	1:A:227:THR:CG2	2.24	1.00
1:A:224:HIS:CD2	1:A:227:THR:CG2	2.56	0.89
1:B:736:GLN:HG3	1:B:740:ASN:OD1	1.77	0.85
1:A:123:VAL:HG13	1:A:234:LEU:HG	1.63	0.81
1:A:220:TYR:C	1:A:222:LEU:H	1.84	0.80
1:A:224:HIS:CE1	1:A:227:THR:HG21	2.18	0.78
1:B:586:PHE:HE1	1:B:709:LEU:O	1.69	0.74
1:B:586:PHE:HD1	1:B:708:GLY:O	1.71	0.72
1:B:589:ILE:HG22	1:B:589:ILE:O	1.87	0.72
1:B:663:VAL:HG13	4:B:901:MM3:H203	1.73	0.71
1:A:118:GLU:O	1:A:122:LYS:HG2	1.92	0.70
1:A:228:ASP:HB2	1:A:230:THR:CG2	2.17	0.70
1:A:108:LEU:HG	1:A:112:ALA:HB3	1.74	0.69
1:A:194:ASN:HD22	1:A:197:LEU:H	1.41	0.69
1:A:224:HIS:C	1:A:224:HIS:CD2	2.57	0.69
1:B:586:PHE:O	1:B:590:PRO:HD2	1.93	0.67
1:B:584:ARG:HD2	1:B:711:HIS:O	1.95	0.67
1:B:615:SER:O	1:B:619:LYS:HD2	1.96	0.66
1:B:663:VAL:HG11	5:B:45:HOH:O	1.95	0.65
1:B:703:ILE:O	1:B:707:LEU:HG	1.96	0.65
1:A:186:TRP:CZ3	1:A:193:THR:HG22	2.31	0.65
1:A:186:TRP:CZ3	1:A:193:THR:CG2	2.80	0.65
1:B:597:LEU:O	1:B:632:PHE:HA	1.96	0.64
1:B:731:ARG:HG3	1:B:731:ARG:O	1.96	0.64
1:B:659:GLY:HA2	1:B:683:ASP:OD2	1.98	0.64
1:B:628:THR:HG21	1:B:742:ILE:HG13	1.80	0.64
1:B:655:TYR:CD1	1:B:655:TYR:N	2.65	0.63
1:A:152:GLY:HA2	1:B:650:GLU:HG3	1.83	0.61
1:A:123:VAL:CG1	1:A:234:LEU:HG	2.28	0.61
1:B:586:PHE:CE1	1:B:709:LEU:O	2.53	0.61
1:A:220:TYR:HD2	1:A:222:LEU:HB2	1.65	0.61
1:B:736:GLN:HA	1:B:739:ILE:HD12	1.83	0.59
1:B:723:TYR:CD2	1:B:723:TYR:C	2.75	0.59
1:B:649:ARG:HD3	1:B:657:PHE:O	2.03	0.58
1:A:224:HIS:HE2	1:A:227:THR:HG21	1.63	0.58
1:A:203:ILE:O	1:A:207:LEU:HG	2.04	0.57
1:A:135:LEU:HD12	1:A:140:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:VAL:HG13	4:B:901:MM3:H51	1.89	0.54
1:A:220:TYR:O	1:A:222:LEU:N	2.40	0.54
1:A:122:LYS:O	1:A:126:GLU:HG3	2.08	0.53
1:A:202:GLU:O	1:A:205:HIS:HB2	2.08	0.53
1:A:194:ASN:HD21	1:A:196:PHE:HB3	1.72	0.53
1:B:583:PHE:HA	1:B:712:SER:OG	2.09	0.53
1:B:589:ILE:CG2	1:B:589:ILE:O	2.56	0.52
1:B:728:ASP:C	1:B:730:THR:H	2.11	0.52
1:B:654:PHE:HB2	1:B:655:TYR:CE1	2.43	0.52
1:A:186:TRP:CZ3	1:A:193:THR:HG21	2.43	0.52
1:B:596:HIS:HD2	1:B:631:THR:OG1	1.93	0.51
1:B:635:LEU:HD12	1:B:640:ALA:HB2	1.94	0.50
1:B:614:ASP:O	1:B:618:GLU:HG3	2.11	0.50
1:A:182:ASP:C	1:A:184:GLU:H	2.14	0.50
1:B:755:THR:O	1:B:755:THR:HG23	2.12	0.50
1:B:663:VAL:HG22	4:B:901:MM3:S15	2.52	0.49
1:B:586:PHE:HD1	1:B:708:GLY:C	2.16	0.48
1:B:726:LEU:HD12	1:B:728:ASP:N	2.27	0.48
1:A:220:TYR:CD2	1:A:222:LEU:HB2	2.48	0.48
1:A:210:PHE:CG	1:A:211:HIS:N	2.83	0.47
1:B:668:TYR:O	1:B:706:SER:HA	2.14	0.47
1:B:681:ASP:O	1:B:684:GLU:HG2	2.15	0.47
1:A:108:LEU:HD22	1:A:186:TRP:O	2.15	0.46
1:B:726:LEU:HD11	1:B:729:LEU:HD13	1.97	0.46
1:A:194:ASN:ND2	1:A:197:LEU:H	2.09	0.46
1:A:150:GLU:OE2	1:A:156:PRO:HG3	2.16	0.46
1:A:89:ILE:HG22	1:A:89:ILE:O	2.15	0.46
1:A:220:TYR:HB3	1:A:222:LEU:HB2	1.97	0.46
1:B:717:ALA:HB1	1:B:738:ASP:OD1	2.15	0.46
1:B:587:PRO:O	1:B:590:PRO:HD3	2.17	0.45
1:B:739:ILE:O	1:B:742:ILE:HG22	2.16	0.45
1:A:220:TYR:C	1:A:222:LEU:N	2.59	0.45
4:B:901:MM3:H161	4:B:901:MM3:H192	1.85	0.45
1:A:117:VAL:O	1:A:121:LEU:HG	2.17	0.45
1:B:724:HIS:ND1	1:B:724:HIS:C	2.70	0.45
4:B:901:MM3:H202	4:B:901:MM3:HNA	1.82	0.45
1:A:125:GLU:HG3	1:A:130:LEU:O	2.16	0.45
1:A:148:VAL:HG12	1:A:149:ARG:HG2	1.98	0.45
1:B:655:TYR:HA	1:B:656:PRO:HD2	1.92	0.44
1:B:691:THR:O	1:B:691:THR:CG2	2.66	0.44
1:A:108:LEU:HG	1:A:112:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:THR:HB	1:B:629:PRO:HD2	2.00	0.44
1:B:654:PHE:CD1	1:B:654:PHE:N	2.85	0.43
1:A:194:ASN:ND2	1:A:196:PHE:HB3	2.33	0.43
1:B:707:LEU:HD23	1:B:707:LEU:HA	1.75	0.43
1:B:605:THR:HA	1:B:606:PRO:HD3	1.90	0.43
1:A:198:VAL:O	1:A:202:GLU:HG2	2.20	0.42
1:A:119:LYS:O	1:A:123:VAL:HG23	2.18	0.42
1:B:648:VAL:O	1:B:649:ARG:C	2.56	0.42
1:B:662:ASN:O	1:B:663:VAL:C	2.57	0.42
1:B:596:HIS:CD2	1:B:631:THR:OG1	2.72	0.42
1:B:628:THR:HB	1:B:629:PRO:CD	2.50	0.42
1:A:86:PHE:HB3	1:A:87:PRO:HD2	2.02	0.41
1:A:107:ASP:OD2	1:A:185:GLN:HA	2.20	0.41
1:A:222:LEU:O	1:A:222:LEU:HG	2.19	0.41
1:B:642:ILE:HG23	1:B:676:GLY:O	2.20	0.41
1:B:597:LEU:N	1:B:597:LEU:HD12	2.36	0.41
1:A:222:LEU:HG	1:A:224:HIS:ND1	2.35	0.41
1:B:743:GLN:HG2	1:B:747:GLY:C	2.40	0.41
1:A:224:HIS:HE2	1:A:227:THR:CG2	2.24	0.41
1:B:742:ILE:HD12	1:B:742:ILE:HA	1.90	0.41
1:B:709:LEU:HD21	1:B:741:GLY:C	2.40	0.41
1:A:121:LEU:CD2	1:A:203:ILE:HD13	2.51	0.41
1:A:163:VAL:HG13	4:A:401:MM3:H203	2.02	0.41
1:B:720:TYR:CD1	1:B:721:PRO:HD2	2.55	0.41
1:A:123:VAL:CG1	1:A:234:LEU:CG	2.99	0.41
1:B:649:ARG:HA	1:B:657:PHE:O	2.21	0.41
1:B:681:ASP:HB3	1:B:684:GLU:HG2	2.02	0.41
1:B:728:ASP:C	1:B:730:THR:N	2.73	0.41
1:A:104:TYR:HB3	5:A:405:HOH:O	2.19	0.41
1:B:589:ILE:HD13	1:B:589:ILE:HG21	1.87	0.40
1:A:121:LEU:HD23	1:A:203:ILE:HD13	2.02	0.40
1:A:249:PRO:HA	1:A:250:PRO:HD3	1.86	0.40
1:B:600:ARG:HD3	1:B:643:MET:HE1	2.03	0.40
1:A:198:VAL:HG13	4:A:401:MM3:C5	2.51	0.40
1:B:752:SER:HA	1:B:753:PRO:HD3	1.87	0.40
1:A:86:PHE:HD1	1:A:87:PRO:HD2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	167/173 (96%)	147 (88%)	18 (11%)	2 (1%)	16 33
1	B	171/173 (99%)	149 (87%)	20 (12%)	2 (1%)	16 33
All	All	338/346 (98%)	296 (88%)	38 (11%)	4 (1%)	16 33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	LEU
1	A	221	PRO
1	B	649	ARG
1	B	750	PRO

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	143/147 (97%)	139 (97%)	4 (3%)	51 78
1	B	147/147 (100%)	137 (93%)	10 (7%)	20 39
All	All	290/294 (99%)	276 (95%)	14 (5%)	31 58

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	93	ARG

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Mol	Chain	Res	Type
1	A	107	ASP
1	A	182	ASP
1	B	587	PRO
1	B	593	ARG
1	B	619	LYS
1	B	685	GLN
1	B	724	HIS
1	B	726	LEU
1	B	729	LEU
1	B	740	ASN
1	B	745	LEU
1	B	746	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	194	ASN
1	B	596	HIS
1	B	736	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	MM3	A	401	2	21,25,25	8.08	12 (57%)	23,37,37	4.56	15 (65%)
4	MM3	B	901	2	21,25,25	8.02	12 (57%)	23,37,37	3.77	13 (56%)

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
4	MM3	A	401	2	-	0/18/38/38	0/1/2/2
4	MM3	B	901	2	-	0/18/38/38	0/1/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	MM3	C14-S15	-3.35	1.80	1.85
4	A	401	MM3	O7-C8	-2.88	1.34	1.42
4	B	901	MM3	O7-C8	-2.76	1.34	1.42
4	A	401	MM3	C1-S9	2.10	1.79	1.76
4	A	401	MM3	C6-C5	3.38	1.44	1.38
4	B	901	MM3	C5-C4	3.45	1.45	1.38
4	B	901	MM3	C3-C2	3.50	1.45	1.38
4	B	901	MM3	C6-C1	3.54	1.44	1.38
4	B	901	MM3	C6-C5	3.62	1.45	1.38
4	A	401	MM3	C6-C1	3.66	1.44	1.38
4	A	401	MM3	C5-C4	3.85	1.46	1.38
4	B	901	MM3	OA-NA	3.92	1.46	1.39
4	B	901	MM3	C3-C4	4.04	1.46	1.38
4	A	401	MM3	C3-C4	4.17	1.47	1.38
4	B	901	MM3	C2-C1	4.21	1.45	1.38
4	A	401	MM3	C3-C2	4.21	1.46	1.38
4	A	401	MM3	C2-C1	4.21	1.45	1.38
4	A	401	MM3	OA-NA	6.68	1.51	1.39
4	A	401	MM3	S9-N12	7.80	1.74	1.63
4	B	901	MM3	S9-N12	8.23	1.75	1.63
4	A	401	MM3	O11-S9	20.05	1.68	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	MM3	O11-S9	21.49	1.70	1.43
4	B	901	MM3	O10-S9	26.42	1.77	1.43
4	A	401	MM3	O10-S9	27.39	1.78	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	401	MM3	C20-C14-C19	-13.09	96.79	111.07
4	A	401	MM3	OA-NA-C	-9.53	106.38	119.86
4	B	901	MM3	O10-S9-C1	-7.80	97.88	108.00
4	B	901	MM3	OA-NA-C	-7.30	109.54	119.86
4	B	901	MM3	O11-S9-O10	-5.64	109.74	119.47
4	A	401	MM3	O11-S9-O10	-5.46	110.05	119.47
4	A	401	MM3	C2-C1-S9	-5.44	113.79	119.79
4	A	401	MM3	C5-C6-C1	-4.59	114.41	119.48
4	B	901	MM3	C6-C1-S9	-4.27	115.08	119.79
4	A	401	MM3	O11-S9-N12	-3.70	99.12	106.97
4	B	901	MM3	C2-C1-S9	-3.65	115.76	119.79
4	B	901	MM3	C3-C2-C1	-3.48	115.63	119.48
4	B	901	MM3	C18-N12-S9	-3.34	106.87	117.79
4	B	901	MM3	C5-C6-C1	-3.18	115.96	119.48
4	A	401	MM3	C2-C3-C4	-2.69	116.35	119.74
4	A	401	MM3	C18-N12-S9	-2.31	110.26	117.79
4	A	401	MM3	C16-C17-C18	-2.10	110.71	115.29
4	A	401	MM3	O10-S9-N12	2.16	111.55	106.97
4	A	401	MM3	C5-C4-C3	2.21	123.79	120.20
4	B	901	MM3	C5-C4-C3	2.56	124.35	120.20
4	A	401	MM3	C8-O7-C4	2.97	124.47	117.51
4	A	401	MM3	O11-S9-C1	3.70	112.81	108.00
4	B	901	MM3	O11-S9-N12	4.10	115.67	106.97
4	B	901	MM3	C20-C14-C19	4.71	116.20	111.07
4	A	401	MM3	C6-C1-C2	5.24	127.42	120.42
4	B	901	MM3	C1-S9-N12	5.31	116.06	107.38
4	B	901	MM3	C6-C1-C2	5.40	127.64	120.42
4	A	401	MM3	C1-S9-N12	5.97	117.13	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	MM3	2	0
4	B	901	MM3	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.