Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:05 AM GMT

PDB ID	:	3D5M
Title	:	Crystal structure of HCV NS5B polymerase with a novel pyridazinone inhibitor
Authors	:	Zhao, Q.; Showalter, R.E.; Han, Q.; Kissinger, C.R.
Deposited on	:	2008-05-16
Resolution	:	2.20 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
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 ⓘ

The following experimental techniques were used to determine the structure:
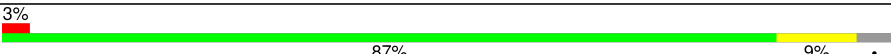*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.
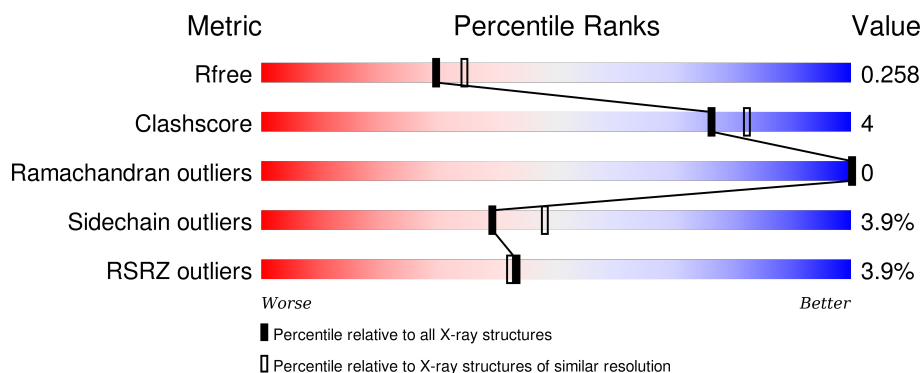
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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.

Mol	Chain	Length	Quality of chain
1	A	578	4% / 86% / 10%
1	B	578	3% / 87% / 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9072 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4345	2742	766	806	31			
1	B	557	Total	C	N	O	S	0	0	0
			4334	2735	764	804	31			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	544	GLN	ARG	ENGINEERED	UNP P26663
A	571	LEU	-	EXPRESSION TAG	UNP P26663
A	572	GLU	-	EXPRESSION TAG	UNP P26663
A	573	HIS	-	EXPRESSION TAG	UNP P26663
A	574	HIS	-	EXPRESSION TAG	UNP P26663
A	575	HIS	-	EXPRESSION TAG	UNP P26663
A	576	HIS	-	EXPRESSION TAG	UNP P26663
A	577	HIS	-	EXPRESSION TAG	UNP P26663
A	578	HIS	-	EXPRESSION TAG	UNP P26663
B	544	GLN	ARG	ENGINEERED	UNP P26663
B	571	LEU	-	EXPRESSION TAG	UNP P26663
B	572	GLU	-	EXPRESSION TAG	UNP P26663
B	573	HIS	-	EXPRESSION TAG	UNP P26663
B	574	HIS	-	EXPRESSION TAG	UNP P26663
B	575	HIS	-	EXPRESSION TAG	UNP P26663
B	576	HIS	-	EXPRESSION TAG	UNP P26663
B	577	HIS	-	EXPRESSION TAG	UNP P26663
B	578	HIS	-	EXPRESSION TAG	UNP P26663

- Molecule 2 is N-({3-[(5S)-5-TERT-BUTYL-1-(3-CHLORO-4-FLUOROBENZYL)-4-HY DROXY-2-OXO-2,5-DIHYDRO-1H-PYRROL-3-YL]-1,1-DIOXIDO-1,2-BENZISOTHI AZOL-7-YL}METHYL)METHANESULFONAMIDE (three-letter code: 4MS) (formula: $C_{24}H_{25}ClFN_3O_6S_2$).
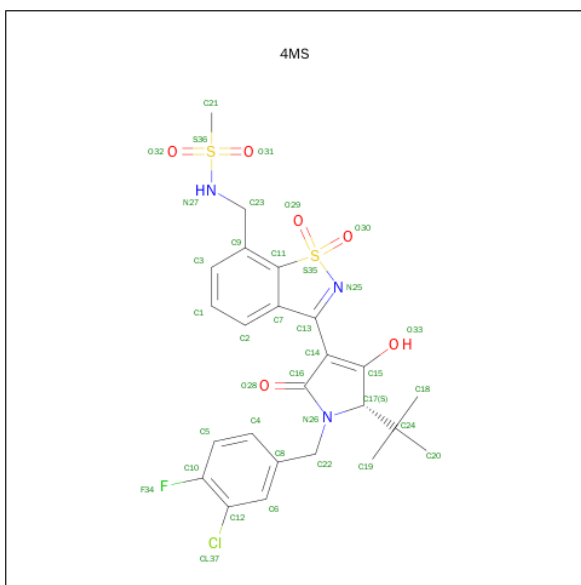
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			37	24	1	1	3	6	2		
2	B	1	Total	C	Cl	F	N	O	S	0	0
			37	24	1	1	3	6	2		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	158	Total	O	0	0
			158	158		
3	B	161	Total	O	0	0
			161	161		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

- Molecule 1: RNA-directed RNA polymerase
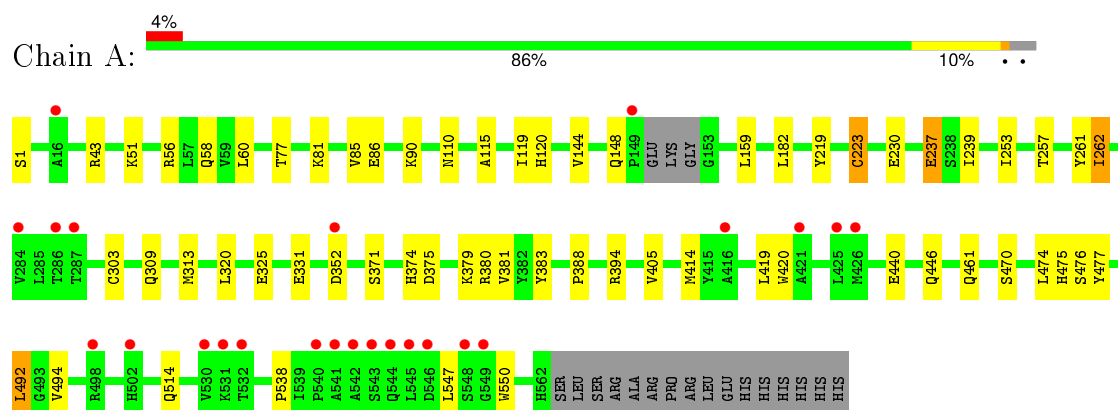
- Molecule 1: RNA-directed RNA polymerase
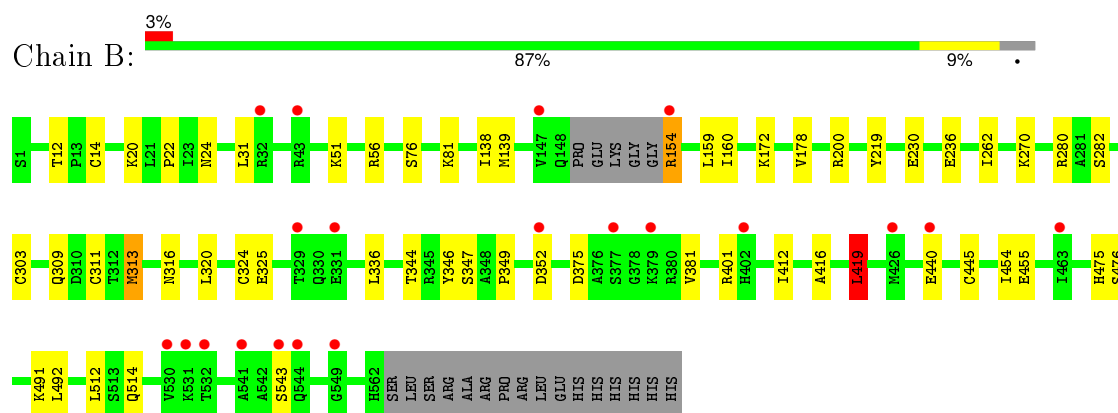
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.30Å 106.77Å 126.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.20 29.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.00-2.20) 99.7 (29.00-2.20)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.261 0.208 , 0.258	Depositor DCC
R_{free} test set	2981 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	4 of 59611 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9072	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.29 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0137e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 4MS

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	0.46	0/4440	0.58	0/6026
1	B	0.46	0/4428	0.57	2/6009 (0.0%)
All	All	0.46	0/8868	0.58	2/12035 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	31	LEU	CA-CB-CG	5.60	128.18	115.30
1	B	419	LEU	CA-CB-CG	5.18	127.22	115.30

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	A	4345	0	4362	29	0
1	B	4334	0	4354	30	0
2	A	37	0	24	6	0
2	B	37	0	24	5	0
3	A	158	0	0	5	0
3	B	161	0	0	5	0
All	All	9072	0	8764	67	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 4.

All (67) 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:B:579:4MS:H22A	2:B:579:4MS:H18A	1.64	0.79
2:A:579:4MS:O28	2:A:579:4MS:H2	1.84	0.77
1:A:374:HIS:HA	3:A:735:HOH:O	1.84	0.77
2:A:579:4MS:H18A	2:A:579:4MS:H22A	1.66	0.76
2:B:579:4MS:O28	2:B:579:4MS:H2	1.93	0.68
1:B:200:ARG:HH12	1:B:316:ASN:HD21	1.45	0.63
1:B:138:ILE:HD11	1:B:159:LEU:HD13	1.81	0.63
1:A:375:ASP:O	1:A:475:HIS:HE1	1.80	0.62
1:A:313:MET:HG2	1:A:320:LEU:HD11	1.82	0.61
1:A:223:CYS:SG	3:A:731:HOH:O	2.57	0.59
1:B:475:HIS:HD2	1:B:476:SER:OG	1.86	0.58
1:B:375:ASP:O	1:B:475:HIS:HE1	1.91	0.54
1:B:455:GLU:HB3	3:B:728:HOH:O	2.09	0.53
1:A:470:SER:O	1:A:474:LEU:HD13	2.09	0.53
1:B:313:MET:HG2	1:B:320:LEU:HD11	1.90	0.52
2:B:579:4MS:C18	2:B:579:4MS:H22A	2.38	0.52
1:B:419:LEU:C	1:B:419:LEU:HD12	2.30	0.52
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.92	0.52
1:A:383:TYR:HH	1:A:477:TYR:HD1	1.55	0.52
1:B:236:GLU:OE2	1:B:280:ARG:NH2	2.29	0.51
1:A:86:GLU:O	1:A:90:LYS:HG2	2.10	0.51
1:A:475:HIS:HD2	1:A:476:SER:OG	1.94	0.51
1:B:303:CYS:HB3	1:B:311:CYS:SG	2.50	0.51
1:B:412:ILE:O	1:B:416:ALA:HB2	2.11	0.51
1:B:178:VAL:HG23	3:B:714:HOH:O	2.11	0.50
1:A:379:LYS:C	3:A:735:HOH:O	2.49	0.50
2:B:579:4MS:C16	2:B:579:4MS:H4	2.43	0.49
1:A:538:PRO:HG2	1:B:270:LYS:O	2.13	0.49
1:A:375:ASP:O	1:A:475:HIS:CE1	2.62	0.48
1:B:12:THR:HG21	1:B:270:LYS:HE2	1.94	0.48
1:B:22:PRO:HG2	1:B:401:ARG:HG3	1.95	0.47
1:B:375:ASP:O	1:B:475:HIS:CE1	2.67	0.47
2:A:579:4MS:O28	2:A:579:4MS:C2	2.59	0.46
1:A:309:GLN:HB3	1:A:325:GLU:HB2	1.98	0.46
1:B:154:ARG:NH2	3:B:710:HOH:O	2.48	0.46
1:A:230:GLU:HG3	1:A:262:ILE:HG12	1.97	0.46
2:A:579:4MS:C18	2:A:579:4MS:H22A	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:THR:O	1:B:24:ASN:HB2	2.17	0.45
1:A:1:SER:N	3:A:647:HOH:O	2.49	0.44
1:B:344:THR:HG23	1:B:349:PRO:HB3	1.99	0.44
1:B:230:GLU:HG3	1:B:262:ILE:HG23	1.99	0.44
2:A:579:4MS:C16	2:A:579:4MS:H4	2.48	0.44
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.99	0.44
1:A:547:LEU:O	1:A:550:TRP:HB2	2.18	0.43
1:A:405:VAL:HG21	1:A:446:GLN:HG3	1.99	0.43
1:A:380:ARG:HA	3:A:735:HOH:O	2.18	0.43
1:A:257:THR:HA	1:A:261:TYR:HB2	2.00	0.42
1:B:303:CYS:CB	1:B:311:CYS:HG	2.33	0.42
1:A:144:VAL:HB	1:A:394:ARG:HG2	2.01	0.42
1:A:237:GLU:OE2	1:A:253:ILE:HG22	2.20	0.42
1:A:414:MET:HG3	2:A:579:4MS:H20A	2.02	0.42
1:A:58:GLN:HG2	1:A:60:LEU:HD21	2.01	0.42
1:A:492:LEU:HB3	1:A:494:VAL:HG23	2.01	0.42
1:B:172:LYS:HE2	3:B:642:HOH:O	2.20	0.42
1:B:309:GLN:HB3	1:B:325:GLU:HB2	2.02	0.41
1:B:475:HIS:CD2	1:B:476:SER:OG	2.70	0.41
1:A:85:VAL:HG21	1:A:120:HIS:CE1	2.55	0.41
1:B:139:MET:HB2	1:B:160:ILE:HG23	2.02	0.41
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.61	0.41
1:B:309:GLN:O	1:B:324:CYS:HB2	2.20	0.41
1:B:160:ILE:HD12	1:B:282:SER:OG	2.21	0.41
2:B:579:4MS:O28	2:B:579:4MS:C2	2.66	0.41
1:A:182:LEU:HD21	1:A:239:ILE:HG22	2.03	0.41
1:A:388:PRO:HB3	1:A:420:TRP:CD2	2.56	0.40
1:A:115:ALA:O	1:A:119:ILE:HG12	2.21	0.40
1:B:346:TYR:O	1:B:347:SER:HB3	2.22	0.40
1:B:51:LYS:HE3	3:B:740:HOH:O	2.21	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	555/578 (96%)	542 (98%)	13 (2%)	0	100	100
1	B	553/578 (96%)	545 (99%)	8 (1%)	0	100	100
All	All	1108/1156 (96%)	1087 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	476/493 (97%)	456 (96%)	20 (4%)	36	44
1	B	475/493 (96%)	458 (96%)	17 (4%)	42	52
All	All	951/986 (96%)	914 (96%)	37 (4%)	39	48

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	51	LYS
1	A	56	ARG
1	A	81	LYS
1	A	110	ASN
1	A	148	GLN
1	A	159	LEU
1	A	223	CYS
1	A	237	GLU
1	A	262	ILE
1	A	303	CYS
1	A	331	GLU
1	A	352	ASP
1	A	371	SER
1	A	381	VAL

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Mol	Chain	Res	Type
1	A	419	LEU
1	A	440	GLU
1	A	461	GLN
1	A	492	LEU
1	A	514	GLN
1	B	14	CYS
1	B	20	LYS
1	B	56	ARG
1	B	76	SER
1	B	81	LYS
1	B	154	ARG
1	B	313	MET
1	B	336	LEU
1	B	352	ASP
1	B	381	VAL
1	B	419	LEU
1	B	440	GLU
1	B	491	LYS
1	B	492	LEU
1	B	512	LEU
1	B	514	GLN
1	B	543	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	110	ASN
1	A	117	ASN
1	A	120	HIS
1	A	251	GLN
1	A	316	ASN
1	A	330	GLN
1	A	446	GLN
1	A	475	HIS
1	B	117	ASN
1	B	120	HIS
1	B	251	GLN
1	B	273	ASN
1	B	316	ASN
1	B	475	HIS

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 carbohydrates 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	4MS	A	579	-	38,40,40	1.07	3 (7%)	49,64,64	2.16	12 (24%)
2	4MS	B	579	-	38,40,40	1.16	3 (7%)	49,64,64	2.21	13 (26%)

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	4MS	A	579	-	-	0/17/55/55	0/4/4/4
2	4MS	B	579	-	-	0/17/55/55	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	579	4MS	C23-N27	-3.79	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	579	4MS	C23-N27	-2.81	1.44	1.47
2	B	579	4MS	C11-S35	-2.57	1.74	1.76
2	A	579	4MS	C11-S35	-2.47	1.74	1.76
2	B	579	4MS	C9-C11	-2.27	1.37	1.40
2	A	579	4MS	C16-N26	2.10	1.38	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	579	4MS	C8-C22-N26	-6.26	101.80	113.46
2	A	579	4MS	C8-C22-N26	-5.37	103.46	113.46
2	B	579	4MS	C11-C7-C13	-5.26	107.99	112.70
2	A	579	4MS	C11-C7-C13	-4.84	108.37	112.70
2	B	579	4MS	C11-S35-N25	-4.46	93.89	96.75
2	A	579	4MS	O30-S35-C11	-3.48	107.22	110.95
2	A	579	4MS	C11-S35-N25	-3.47	94.52	96.75
2	B	579	4MS	C12-C6-C8	-3.19	118.30	120.36
2	B	579	4MS	C23-C9-C11	-2.38	119.71	122.20
2	B	579	4MS	C10-C12-CL37	-2.02	118.21	120.06
2	B	579	4MS	O28-C16-C14	-2.01	125.63	130.33
2	A	579	4MS	C18-C24-C17	2.10	113.81	109.89
2	A	579	4MS	O31-S36-N27	2.21	108.90	107.23
2	B	579	4MS	C22-N26-C17	3.16	124.66	121.60
2	B	579	4MS	O31-S36-N27	3.21	109.66	107.23
2	B	579	4MS	C6-C12-C10	3.28	122.63	119.71
2	A	579	4MS	C22-N26-C17	3.50	124.98	121.60
2	A	579	4MS	F34-C10-C12	3.97	122.51	119.01
2	B	579	4MS	O30-S35-O29	4.00	121.85	115.99
2	A	579	4MS	C7-C11-S35	4.22	109.58	106.87
2	A	579	4MS	C13-N25-S35	4.28	111.84	106.34
2	A	579	4MS	O32-S36-N27	4.49	110.64	107.23
2	B	579	4MS	C13-N25-S35	4.53	112.16	106.34
2	A	579	4MS	O30-S35-O29	4.58	122.70	115.99
2	B	579	4MS	C7-C11-S35	5.14	110.17	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	579	4MS	6	0
2	B	579	4MS	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	559/578 (96%)	0.02	24 (4%)	39	38	32, 45, 69, 108	0
1	B	557/578 (96%)	0.01	20 (3%)	46	45	33, 47, 69, 96	0
All	All	1116/1156 (96%)	0.01	44 (3%)	43	42	32, 46, 69, 108	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	541	ALA	5.8
1	A	541	ALA	5.7
1	B	532	THR	5.5
1	B	544	GLN	5.2
1	A	543	SER	5.2
1	A	544	GLN	4.6
1	A	545	LEU	4.3
1	A	542	ALA	4.0
1	A	532	THR	3.9
1	B	531	LYS	3.4
1	A	530	VAL	3.3
1	A	502	HIS	3.1
1	A	546	ASP	3.1
1	A	549	GLY	3.0
1	A	540	PRO	3.0
1	B	463	ILE	2.9
1	B	329	THR	2.9
1	A	421	ALA	2.8
1	A	531	LYS	2.7
1	B	154	ARG	2.7
1	A	425	LEU	2.6
1	A	16	ALA	2.6
1	B	402	HIS	2.6
1	B	331	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	284	VAL	2.4
1	A	548	SER	2.4
1	B	549	GLY	2.4
1	B	147	VAL	2.3
1	A	287	THR	2.3
1	B	352	ASP	2.3
1	A	352	ASP	2.2
1	A	426	MET	2.2
1	A	498	ARG	2.2
1	A	286	THR	2.2
1	B	426	MET	2.1
1	B	43	ARG	2.1
1	B	377	SER	2.1
1	B	440	GLU	2.1
1	B	379	LYS	2.1
1	B	543	SER	2.1
1	B	530	VAL	2.1
1	B	32	ARG	2.0
1	A	416	ALA	2.0
1	A	149	PRO	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 (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	4MS	A	579	37/37	0.94	0.14	0.14	36,42,44,49	0
2	4MS	B	579	37/37	0.96	0.14	0.04	36,40,43,47	0

6.5 Other polymers (i)

There are no such residues in this entry.