WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2017 – 10:17 PM EDT

PDB ID	:	3MWW
Title	:	Crystal structure of HCV NS5B polymerase
Authors	:	Coulombe, R.
Deposited on	:	unknown
Resolution	:	2.80 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

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 2.80 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	Percentile Ranks	Value
Rfree		0.277
Clashscore		18
Ramachandran outliers		2.3%
Sidechain outliers		2.8%
RSRZ outliers		4.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
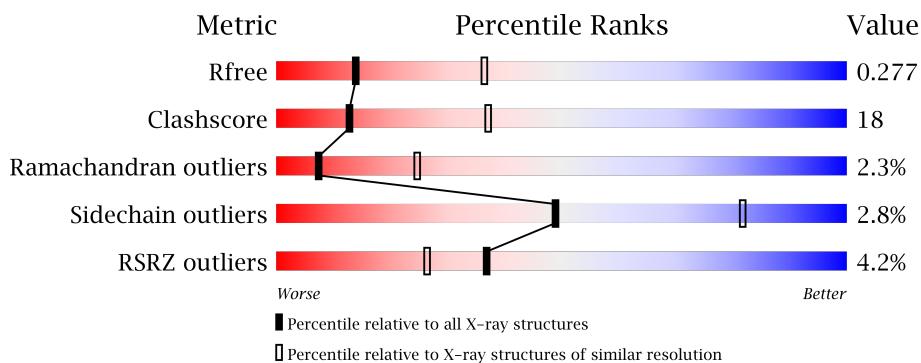
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	576	.% 69% 27% · ·
1	B	576	7% 56% 34% · 6%
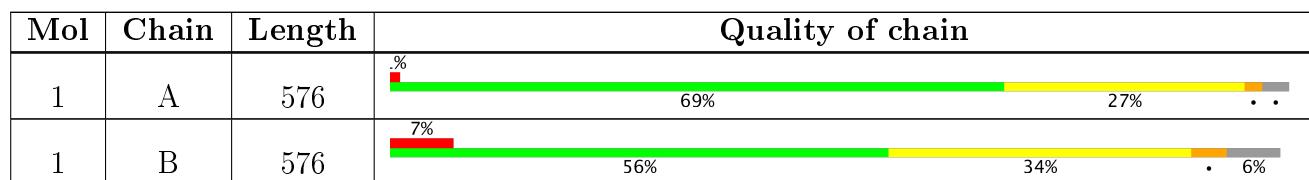
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	578	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8683 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4358	2745	770	811	32			
1	B	541	Total	C	N	O	S	0	0	0
			4210	2652	741	785	32			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	EXPRESSION TAG	UNP O92972
A	572	HIS	-	EXPRESSION TAG	UNP O92972
A	573	HIS	-	EXPRESSION TAG	UNP O92972
A	574	HIS	-	EXPRESSION TAG	UNP O92972
A	575	HIS	-	EXPRESSION TAG	UNP O92972
A	576	HIS	-	EXPRESSION TAG	UNP O92972
B	571	HIS	-	EXPRESSION TAG	UNP O92972
B	572	HIS	-	EXPRESSION TAG	UNP O92972
B	573	HIS	-	EXPRESSION TAG	UNP O92972
B	574	HIS	-	EXPRESSION TAG	UNP O92972
B	575	HIS	-	EXPRESSION TAG	UNP O92972
B	576	HIS	-	EXPRESSION TAG	UNP O92972

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
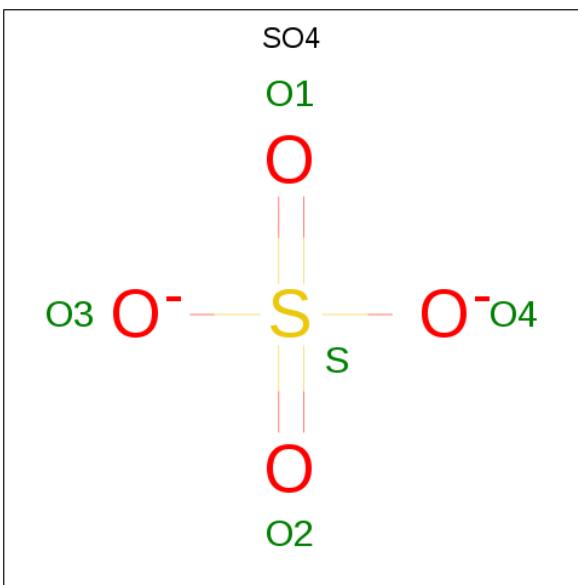
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is 1-[2-(4-carboxypiperidin-1-yl)-2-oxoethyl]-3-cyclohexyl-2-furan-3-yl-1H-indole-6-carboxylic acid (three-letter code: BIW) (formula: $C_{27}H_{30}N_2O_6$).
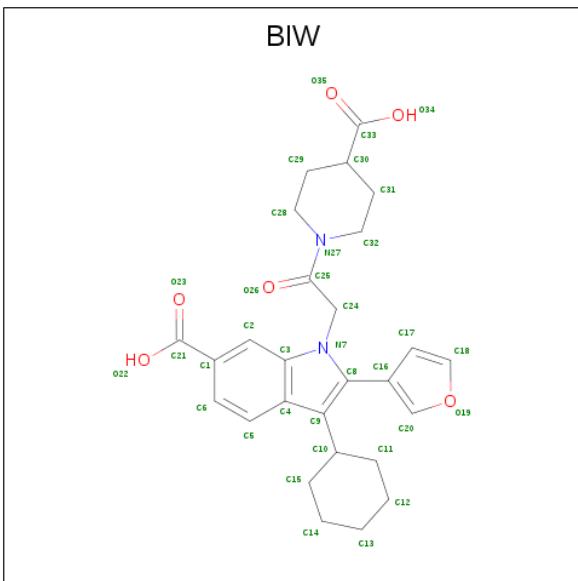
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 35	C 27	N 2	O 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total 43	O 43	0	0
4	B	22	Total 22	O 22	0	0

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 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: Genome polyprotein
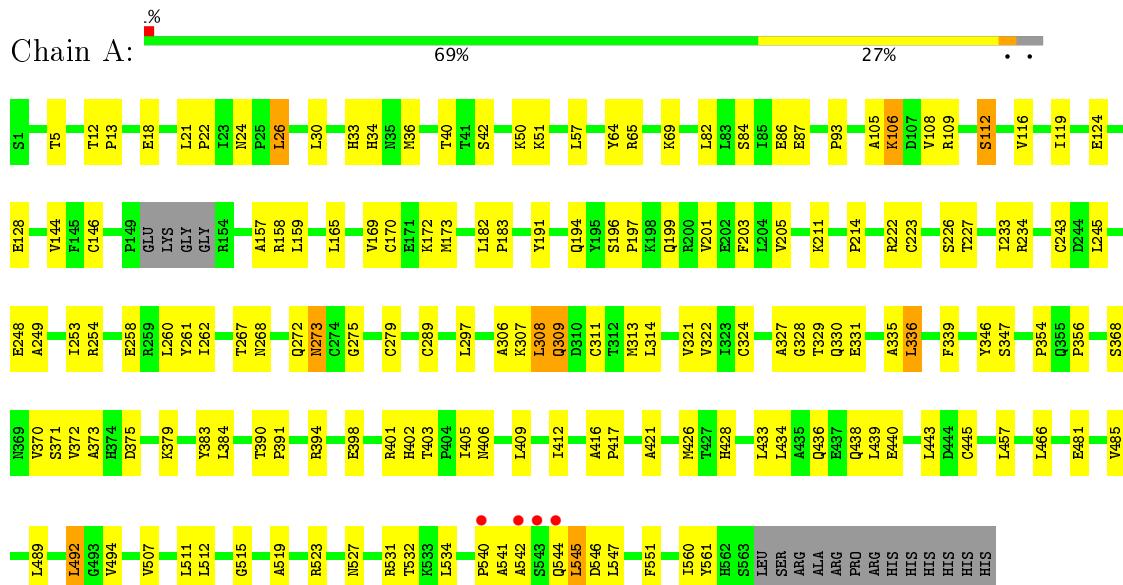
• Molecule 1: Genome polyprotein
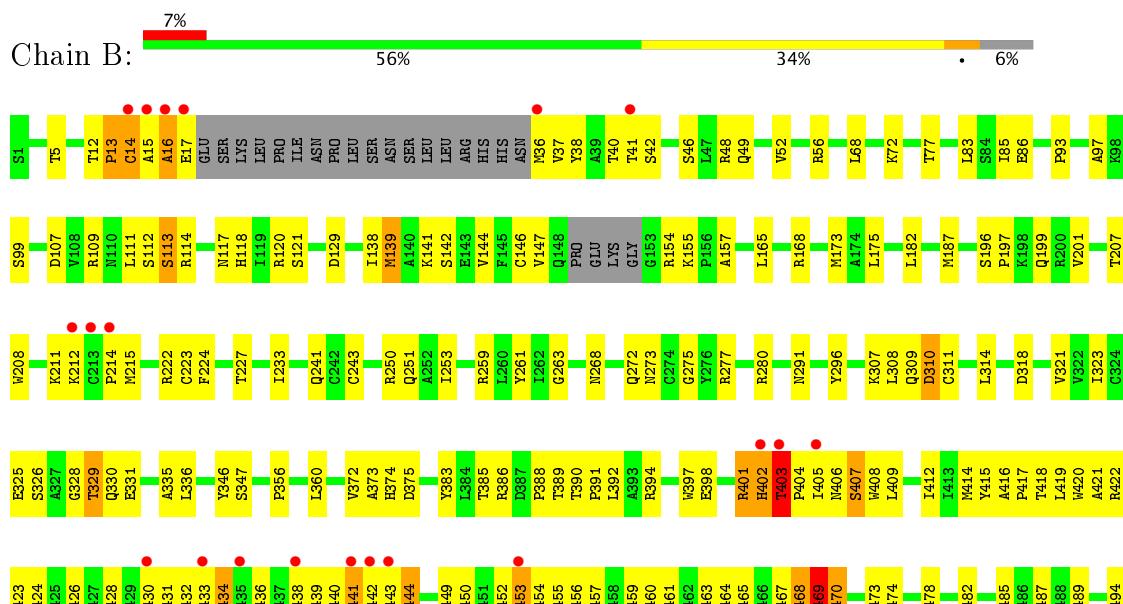
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.12Å 106.55Å 133.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 44.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-2.80) 98.3 (44.77-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.281 0.217 , 0.277	Depositor DCC
R_{free} test set	3704 reflections (10.01%)	DCC
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8683	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BIW, SO4

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	0.40	0/4453	0.64	0/6044
1	B	0.38	0/4299	0.67	3/5831 (0.1%)
All	All	0.39	0/8752	0.66	3/11875 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	403	THR	N-CA-C	10.67	139.81	111.00
1	B	404	PRO	N-CA-C	-7.53	92.53	112.10
1	B	402	HIS	N-CA-C	5.43	125.66	111.00

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	4358	0	4371	119	0
1	B	4210	0	4218	202	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0
3	B	35	0	28	1	0
4	A	43	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	22	0	0	0	0
All	All	8683	0	8617	318	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 18.

All (318) 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:B:13:PRO:HB3	1:B:17:GLU:HB2	1.35	1.05
1:B:523:ARG:HG3	1:B:534:LEU:HD23	1.44	0.99
1:B:536:LEU:HD12	1:B:536:LEU:H	1.29	0.95
1:B:434:LEU:HD23	1:B:434:LEU:H	1.37	0.89
1:B:464:GLU:O	1:B:468:GLY:HA2	1.75	0.85
1:B:457:LEU:HD13	1:B:517:ARG:HG2	1.55	0.84
1:B:434:LEU:HD22	1:B:511:LEU:HD21	1.59	0.83
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.64	0.80
1:B:46:SER:HA	1:B:49:GLN:HE21	1.47	0.78
1:B:441:LYS:HD3	1:B:443:LEU:HD21	1.65	0.77
1:B:508:ARG:HH12	1:B:530:VAL:HG21	1.49	0.77
1:B:405:ILE:HG13	1:B:443:LEU:HD13	1.66	0.76
1:B:470:SER:O	1:B:474:LEU:HG	1.87	0.75
1:B:13:PRO:CB	1:B:17:GLU:HB2	2.16	0.73
1:A:523:ARG:HG3	1:A:534:LEU:HD12	1.71	0.72
1:B:465:ARG:HD3	1:B:547:LEU:HD22	1.70	0.72
1:B:461:GLN:HB3	1:B:541:ALA:O	1.89	0.72
1:B:514:GLN:HB3	1:B:518:ALA:HB3	1.74	0.69
1:B:118:HIS:O	1:B:121:SER:HB3	1.92	0.69
1:B:421:ALA:O	1:B:426:MET:HG3	1.94	0.68
1:B:457:LEU:HD13	1:B:517:ARG:CG	2.25	0.66
1:B:196:SER:OG	1:B:199:GLN:HG3	1.95	0.66
1:B:129:ASP:HB3	1:B:259:ARG:NH1	2.11	0.66
1:B:424:ILE:HD13	1:B:489:LEU:HD21	1.77	0.66
1:B:336:LEU:CD2	1:B:356:PRO:HD3	2.25	0.66
1:A:313:MET:HG3	1:A:322:VAL:HG22	1.78	0.65
1:B:452:TYR:OH	1:B:550:TRP:HA	1.97	0.65
1:A:233:ILE:HD13	1:A:261:TYR:O	1.97	0.65
1:B:346:TYR:O	1:B:347:SER:HB3	1.97	0.65
1:B:517:ARG:CD	1:B:517:ARG:H	2.09	0.65
1:B:418:THR:O	1:B:422:ARG:HG3	1.97	0.65
1:B:465:ARG:HH11	1:B:545:LEU:HB2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ILE:HG22	1:B:455:GLU:N	2.12	0.64
1:A:254:ARG:HG2	1:B:251:GLN:NE2	2.13	0.63
1:B:46:SER:HA	1:B:49:GLN:NE2	2.14	0.63
1:B:508:ARG:NH1	1:B:530:VAL:HG11	2.13	0.63
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.63	0.63
1:B:401:ARG:HG3	1:B:402:HIS:H	1.63	0.63
1:A:69:LYS:HD2	1:B:77:THR:HA	1.81	0.63
1:B:423:MET:HA	1:B:528:TRP:CZ2	2.34	0.63
1:A:306:ALA:O	1:A:307:LYS:HB2	1.99	0.62
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.81	0.62
1:B:508:ARG:HH12	1:B:530:VAL:CG2	2.12	0.62
1:B:15:ALA:O	1:B:16:ALA:CB	2.47	0.62
1:B:40:THR:HB	1:B:157:ALA:HB2	1.81	0.62
1:B:433:LEU:HD13	1:B:439:LEU:HD23	1.82	0.62
1:B:372:VAL:HG12	1:B:373:ALA:H	1.65	0.61
1:A:308:LEU:CD1	1:A:335:ALA:HB1	2.30	0.61
1:B:15:ALA:O	1:B:16:ALA:HB3	2.00	0.61
1:B:444:ASP:HA	1:B:453:SER:HA	1.83	0.61
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.81	0.60
1:B:478:SER:O	1:B:482:ILE:HG13	2.00	0.60
1:B:215:MET:HB2	1:B:326:SER:HB2	1.82	0.60
1:A:439:LEU:O	1:A:457:LEU:HG	2.02	0.60
1:A:406:ASN:ND2	1:A:443:LEU:HB3	2.17	0.60
1:B:336:LEU:HD22	1:B:356:PRO:HD3	1.84	0.60
1:B:187:MET:HG2	1:B:296:TYR:CD2	2.37	0.59
1:B:372:VAL:HG12	1:B:373:ALA:N	2.17	0.59
1:A:440:GLU:HG2	1:A:457:LEU:HD12	1.84	0.59
1:B:452:TYR:O	1:B:453:SER:HB2	2.03	0.59
1:A:196:SER:OG	1:A:199:GLN:HG3	2.03	0.59
1:B:38:TYR:OH	1:B:155:LYS:HG2	2.03	0.59
1:A:201:VAL:HG22	1:A:384:LEU:HD13	1.85	0.58
1:B:469:LEU:HD23	1:B:469:LEU:H	1.67	0.58
1:B:423:MET:HG2	1:B:528:TRP:CH2	2.38	0.58
1:A:390:THR:HB	1:A:391:PRO:HD3	1.85	0.58
1:B:405:ILE:O	1:B:405:ILE:HG22	2.04	0.58
1:A:182:LEU:HD12	1:A:243:CYS:SG	2.44	0.58
1:B:449:GLY:HA3	1:B:556:SER:HA	1.87	0.57
1:B:36:MET:O	1:B:146:CYS:HA	2.06	0.56
1:B:141:LYS:HG2	1:B:142:SER:N	2.19	0.56
1:B:147:VAL:HG11	1:B:154:ARG:HH21	1.71	0.56
1:B:459:LEU:HB2	1:B:460:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG21	1:A:165:LEU:HD21	1.87	0.55
1:B:503:ARG:O	1:B:507:VAL:HG23	2.07	0.55
1:A:203:PHE:CE2	1:A:314:LEU:HD13	2.41	0.55
1:B:390:THR:HB	1:B:391:PRO:HD3	1.88	0.55
1:A:433:LEU:HB3	1:A:439:LEU:HD23	1.89	0.55
1:A:5:THR:O	1:A:275:GLY:HA3	2.06	0.55
1:A:542:ALA:O	1:A:545:LEU:HB2	2.07	0.55
1:B:465:ARG:CD	1:B:547:LEU:HD22	2.37	0.55
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.37	0.54
1:B:505:ARG:NH2	1:B:530:VAL:HG12	2.22	0.54
1:B:93:PRO:HG3	1:B:561:TYR:HB2	1.89	0.54
1:A:21:LEU:HD23	1:A:34:HIS:HA	1.89	0.54
1:A:268:ASN:HD21	1:A:272:GLN:HB2	1.72	0.54
1:B:147:VAL:CG1	1:B:154:ARG:HH21	2.21	0.54
1:B:222:ARG:HG2	1:B:222:ARG:HH11	1.73	0.54
1:B:450:ALA:HB2	1:B:555:TYR:HD2	1.73	0.54
1:B:212:LYS:HB2	1:B:325:GLU:OE2	2.07	0.54
1:A:51:LYS:HG3	1:A:222:ARG:NH2	2.22	0.53
1:B:308:LEU:HB2	1:B:311:CYS:SG	2.47	0.53
1:B:401:ARG:CG	1:B:402:HIS:H	2.21	0.53
1:B:454:ILE:HD11	1:B:550:TRP:CH2	2.44	0.53
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.91	0.53
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.72	0.53
1:B:401:ARG:HG3	1:B:402:HIS:N	2.22	0.53
1:A:248:GLU:HG3	4:A:616:HOH:O	2.07	0.53
1:A:368:SER:HB3	1:A:384:LEU:HG	1.90	0.53
1:B:109:ARG:HH11	1:B:109:ARG:HG2	1.73	0.53
1:B:464:GLU:O	1:B:468:GLY:CA	2.52	0.52
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.91	0.52
1:B:423:MET:HG2	1:B:528:TRP:CZ3	2.45	0.52
1:B:13:PRO:HG3	1:B:42:SER:OG	2.10	0.52
1:B:532:THR:O	1:B:533:LYS:HB2	2.08	0.52
1:A:327:ALA:HB3	1:A:331:GLU:HB2	1.91	0.52
1:B:434:LEU:HD23	1:B:434:LEU:N	2.17	0.52
1:B:330:GLN:N	1:B:330:GLN:OE1	2.39	0.52
1:B:459:LEU:O	1:B:463:ILE:HG13	2.10	0.52
1:A:336:LEU:HD21	1:A:354:PRO:HB2	1.91	0.52
1:B:454:ILE:HG22	1:B:455:GLU:H	1.75	0.51
1:A:273:ASN:HD22	1:A:273:ASN:C	2.12	0.51
1:A:561:TYR:CD1	1:A:561:TYR:O	2.64	0.51
1:B:175:LEU:HD21	1:B:253:ILE:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:THR:O	1:B:275:GLY:HA3	2.10	0.51
1:B:457:LEU:HD13	1:B:517:ARG:CB	2.40	0.51
1:B:268:ASN:ND2	1:B:272:GLN:HB2	2.25	0.51
1:A:268:ASN:ND2	1:A:272:GLN:HB2	2.26	0.51
1:A:36:MET:O	1:A:146:CYS:HA	2.09	0.51
1:B:430:PHE:HD2	1:B:511:LEU:HD11	1.75	0.51
1:A:33:HIS:HB2	1:A:492:LEU:O	2.10	0.51
1:A:82:LEU:HD12	1:A:173:MET:O	2.10	0.51
1:B:187:MET:HE2	1:B:296:TYR:CD2	2.46	0.50
1:B:86:GLU:HG3	1:B:111:LEU:HD11	1.92	0.50
1:B:309:GLN:HA	1:B:309:GLN:OE1	2.12	0.50
1:B:207:THR:HG22	1:B:323:ILE:HG21	1.92	0.50
1:B:469:LEU:N	1:B:469:LEU:HD23	2.26	0.50
1:B:547:LEU:HA	1:B:550:TRP:NE1	2.27	0.50
1:B:83:LEU:HB2	1:B:173:MET:HA	1.94	0.50
1:B:456:PRO:O	1:B:459:LEU:HG	2.12	0.50
1:A:331:GLU:H	1:A:331:GLU:CD	2.15	0.50
1:A:183:PRO:HD2	4:A:586:HOH:O	2.12	0.50
1:A:346:TYR:O	1:A:347:SER:HB3	2.10	0.50
1:B:107:ASP:HB3	1:B:112:SER:OG	2.12	0.49
1:B:457:LEU:O	1:B:460:PRO:HD2	2.12	0.49
1:B:419:LEU:HD23	1:B:485:VAL:HG21	1.95	0.49
1:A:545:LEU:HD13	1:A:547:LEU:HD11	1.93	0.49
1:A:267:THR:HG23	1:A:272:GLN:O	2.12	0.49
1:A:546:ASP:C	1:A:547:LEU:HD12	2.32	0.49
1:A:434:LEU:HD21	1:A:511:LEU:HD23	1.94	0.49
1:B:512:LEU:HD12	1:B:519:ALA:HA	1.94	0.49
1:B:547:LEU:HA	1:B:550:TRP:HE1	1.77	0.49
1:A:106:LYS:HA	1:A:106:LYS:CE	2.43	0.49
1:A:64:TYR:CZ	1:A:297:LEU:HD21	2.47	0.49
1:B:336:LEU:HD23	1:B:356:PRO:HD3	1.93	0.49
1:A:223:CYS:O	1:A:227:THR:HG23	2.13	0.49
1:B:208:TRP:NE1	1:B:214:PRO:HG3	2.28	0.49
1:B:441:LYS:CD	1:B:443:LEU:HD21	2.38	0.48
1:B:37:VAL:HG21	3:B:577:BIW:H18	1.93	0.48
1:A:106:LYS:HA	1:A:106:LYS:HE2	1.94	0.48
1:A:375:ASP:OD2	1:A:379:LYS:HE2	2.13	0.48
1:B:415:TYR:O	1:B:418:THR:HG23	2.13	0.48
1:A:308:LEU:HB3	1:A:311:CYS:SG	2.54	0.48
1:A:30:LEU:O	1:A:494:VAL:HG22	2.14	0.48
1:A:254:ARG:HG2	1:B:251:GLN:HE22	1.79	0.48

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:THR:HG22	1:A:532:THR:O	2.14	0.48
1:B:241:GLN:OE1	1:B:250:ARG:HG3	2.13	0.48
1:B:408:TRP:CG	1:B:409:LEU:N	2.82	0.48
1:B:465:ARG:NH1	1:B:545:LEU:O	2.47	0.48
1:B:263:GLY:HA3	1:B:277:ARG:O	2.14	0.47
1:B:428:HIS:O	1:B:431:SER:HB2	2.14	0.47
1:B:454:ILE:CG2	1:B:455:GLU:N	2.77	0.47
1:B:461:GLN:CG	1:B:541:ALA:HB3	2.38	0.47
1:B:508:ARG:NH1	1:B:530:VAL:CG1	2.76	0.47
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.97	0.47
1:B:129:ASP:HB3	1:B:259:ARG:HH12	1.79	0.47
1:A:544:GLN:O	1:A:544:GLN:HG2	2.15	0.47
1:A:201:VAL:O	1:A:205:VAL:HG23	2.14	0.47
1:B:68:LEU:O	1:B:72:LYS:HG3	2.14	0.47
1:B:13:PRO:O	1:B:14:CYS:CB	2.62	0.47
1:B:424:ILE:CD1	1:B:489:LEU:HD21	2.43	0.47
1:B:375:ASP:HA	1:B:473:THR:O	2.15	0.47
1:A:24:ASN:OD1	1:A:26:LEU:HB2	2.15	0.47
1:A:512:LEU:HA	1:A:519:ALA:HA	1.97	0.47
1:A:523:ARG:HG3	1:A:534:LEU:CD1	2.44	0.47
1:B:208:TRP:CE3	1:B:360:LEU:HD13	2.49	0.47
1:B:385:THR:OG1	1:B:386:ARG:N	2.48	0.47
1:B:405:ILE:CG2	1:B:405:ILE:O	2.63	0.47
1:A:40:THR:HB	1:A:157:ALA:HB2	1.96	0.47
1:B:13:PRO:O	1:B:14:CYS:HB3	2.15	0.47
1:B:524:TYR:CE2	1:B:536:LEU:HB3	2.50	0.46
1:A:308:LEU:HD12	1:A:335:ALA:HB1	1.96	0.46
1:B:12:THR:HA	1:B:13:PRO:HD3	1.58	0.46
1:B:388:PRO:O	1:B:392:LEU:HG	2.16	0.46
1:B:454:ILE:HD11	1:B:550:TRP:HH2	1.77	0.46
1:B:38:TYR:CZ	1:B:154:ARG:HG3	2.50	0.46
1:A:128:GLU:HA	4:A:596:HOH:O	2.15	0.46
1:A:308:LEU:HD11	1:A:335:ALA:HB1	1.96	0.46
1:B:328:GLY:O	1:B:329:THR:C	2.54	0.46
1:B:330:GLN:CD	1:B:330:GLN:H	2.14	0.46
1:A:211:LYS:HB2	1:A:214:PRO:HB3	1.98	0.46
1:A:93:PRO:HG3	1:A:561:TYR:HB2	1.97	0.46
1:B:416:ALA:HB3	1:B:417:PRO:HD3	1.98	0.46
1:A:21:LEU:HD12	1:A:22:PRO:HD2	1.97	0.46
1:B:407:SER:OG	1:B:408:TRP:N	2.50	0.46
1:B:388:PRO:HB3	1:B:420:TRP:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:HIS:O	1:B:474:LEU:HA	2.17	0.45
1:A:336:LEU:O	1:A:339:PHE:HB3	2.16	0.45
1:A:485:VAL:O	1:A:489:LEU:HG	2.17	0.45
1:B:109:ARG:HG2	1:B:109:ARG:NH1	2.31	0.45
1:B:222:ARG:NH1	1:B:222:ARG:HG2	2.31	0.45
1:A:416:ALA:N	1:A:417:PRO:CD	2.80	0.45
1:B:14:CYS:O	1:B:14:CYS:SG	2.75	0.45
1:A:330:GLN:HA	1:A:330:GLN:OE1	2.16	0.45
1:A:434:LEU:CD2	1:A:439:LEU:HD11	2.47	0.45
1:B:328:GLY:HA3	1:B:331:GLU:OE1	2.16	0.45
1:A:398:GLU:HG2	1:A:403:THR:OG1	2.17	0.45
1:A:65:ARG:O	1:A:69:LYS:HG2	2.16	0.45
1:B:280:ARG:NE	1:B:291:ASN:OD1	2.46	0.45
1:B:501:ARG:O	1:B:505:ARG:HG3	2.16	0.45
1:A:105:ALA:O	1:A:109:ARG:HG3	2.17	0.45
1:A:13:PRO:HG3	1:A:42:SER:OG	2.16	0.45
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.47	0.45
1:B:517:ARG:H	1:B:517:ARG:NE	2.14	0.45
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.56	0.44
1:B:112:SER:O	1:B:113:SER:C	2.55	0.44
1:B:407:SER:O	1:B:408:TRP:C	2.54	0.44
1:A:182:LEU:HD23	1:A:182:LEU:C	2.38	0.44
1:A:57:LEU:HD23	1:A:57:LEU:C	2.38	0.44
1:B:233:ILE:HD13	1:B:261:TYR:O	2.17	0.44
1:A:18:GLU:HB3	1:A:401:ARG:NH2	2.32	0.44
1:B:224:PHE:CD2	1:B:318:ASP:HB2	2.53	0.44
1:B:434:LEU:C	1:B:436:GLN:H	2.20	0.44
1:B:388:PRO:C	1:B:391:PRO:HD2	2.38	0.44
1:B:408:TRP:CD2	1:B:409:LEU:N	2.85	0.44
1:B:508:ARG:HH12	1:B:530:VAL:HG11	1.78	0.44
1:B:506:SER:O	1:B:510:LYS:HG3	2.18	0.44
1:B:13:PRO:HB3	1:B:17:GLU:CB	2.26	0.44
1:A:273:ASN:C	1:A:273:ASN:ND2	2.71	0.44
1:A:372:VAL:HG12	1:A:373:ALA:N	2.32	0.44
1:A:336:LEU:CD1	1:A:356:PRO:HD3	2.48	0.44
1:B:321:VAL:O	1:B:321:VAL:HG13	2.18	0.44
1:B:405:ILE:HG23	1:B:408:TRP:NE1	2.33	0.44
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.83	0.44
1:A:383:TYR:OH	1:A:481:GLU:HG2	2.18	0.44
1:B:514:GLN:HB3	1:B:518:ALA:CB	2.46	0.44
1:B:138:ILE:O	1:B:139:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLU:OE2	1:B:407:SER:OG	2.36	0.43
1:B:432:ILE:HG22	1:B:432:ILE:O	2.18	0.43
1:A:421:ALA:O	1:A:426:MET:HG3	2.17	0.43
1:A:406:ASN:HD22	1:A:443:LEU:HB3	1.83	0.43
1:B:532:THR:O	1:B:533:LYS:CB	2.67	0.43
1:B:97:ALA:O	1:B:168:ARG:NH2	2.48	0.43
1:B:523:ARG:O	1:B:527:ASN:HB2	2.18	0.43
1:B:48:ARG:HD3	1:B:52:VAL:HG13	2.01	0.43
1:B:85:ILE:CD1	1:B:120:ARG:HG2	2.49	0.43
1:A:313:MET:CG	1:A:322:VAL:HG22	2.48	0.43
1:B:113:SER:O	1:B:114:ARG:C	2.56	0.43
1:A:440:GLU:HG2	1:A:457:LEU:CD1	2.46	0.43
1:B:38:TYR:CE2	1:B:154:ARG:HG3	2.52	0.43
1:B:328:GLY:O	1:B:331:GLU:N	2.52	0.43
1:B:412:ILE:O	1:B:416:ALA:N	2.52	0.42
1:A:112:SER:O	1:A:116:VAL:HG23	2.18	0.42
1:B:401:ARG:HE	1:B:401:ARG:HA	1.84	0.42
1:A:545:LEU:HB3	1:A:547:LEU:CD1	2.48	0.42
1:B:56:ARG:HD3	1:B:56:ARG:N	2.34	0.42
1:A:412:ILE:O	1:A:416:ALA:N	2.52	0.42
1:B:155:LYS:HE2	1:B:155:LYS:HB3	1.90	0.42
1:A:523:ARG:CG	1:A:534:LEU:HD12	2.47	0.42
1:B:182:LEU:HD12	1:B:243:CYS:SG	2.59	0.42
1:B:223:CYS:O	1:B:227:THR:HG23	2.18	0.42
1:B:309:GLN:O	1:B:310:ASP:C	2.57	0.42
1:B:426:MET:O	1:B:430:PHE:HB2	2.19	0.42
1:B:530:VAL:C	1:B:532:THR:H	2.22	0.42
1:A:12:THR:HA	1:A:13:PRO:HD3	1.75	0.42
1:A:170:CYS:HA	1:A:173:MET:CE	2.50	0.42
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.49	0.42
1:A:84:SER:OG	1:A:87:GLU:HG3	2.20	0.42
1:B:144:VAL:HG21	1:B:397:TRP:CG	2.55	0.42
1:B:415:TYR:HB3	1:B:418:THR:CG2	2.49	0.42
1:A:30:LEU:HB2	1:A:428:HIS:CE1	2.55	0.42
1:A:309:GLN:O	1:A:324:CYS:HB2	2.19	0.42
1:B:113:SER:HB2	1:B:117:ASN:ND2	2.35	0.42
1:B:207:THR:O	1:B:211:LYS:HG2	2.20	0.42
1:B:414:MET:O	1:B:467:HIS:HE1	2.03	0.42
1:A:409:LEU:HB3	1:A:445:CYS:HB3	2.02	0.41
1:B:405:ILE:HA	1:B:405:ILE:HD13	1.96	0.41
1:B:438:GLN:C	1:B:440:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:NH1	1:A:258:GLU:OE2	2.53	0.41
1:A:531:ARG:HD3	1:A:531:ARG:HA	1.65	0.41
1:B:187:MET:HE2	1:B:296:TYR:HD2	1.85	0.41
1:B:489:LEU:HD22	1:B:494:VAL:HB	2.02	0.41
1:A:405:ILE:HG22	1:A:406:ASN:N	2.35	0.41
1:B:505:ARG:CZ	1:B:530:VAL:HG12	2.51	0.41
1:B:99:SER:HB2	1:B:165:LEU:HB3	2.02	0.41
1:A:328:GLY:O	1:A:329:THR:C	2.58	0.41
1:B:307:LYS:HB3	1:B:307:LYS:HE2	1.92	0.41
1:B:207:THR:HG22	1:B:323:ILE:CG2	2.51	0.41
1:B:536:LEU:CD1	1:B:536:LEU:H	2.07	0.41
1:A:13:PRO:HG3	1:A:42:SER:CB	2.50	0.41
1:B:401:ARG:CG	1:B:402:HIS:N	2.83	0.41
1:A:507:VAL:O	1:A:511:LEU:HG	2.21	0.41
1:A:191:TYR:O	1:A:194:GLN:HG2	2.20	0.41
1:A:196:SER:O	1:A:197:PRO:C	2.59	0.41
1:A:260:LEU:HA	4:A:580:HOH:O	2.21	0.41
1:B:402:HIS:HB2	1:B:403:THR:H	1.71	0.41
1:A:201:VAL:CG2	1:A:384:LEU:HB2	2.51	0.41
1:A:226:SER:HA	1:A:279:CYS:SG	2.60	0.41
1:B:547:LEU:O	1:B:548:SER:O	2.38	0.41
1:A:233:ILE:CD1	1:A:262:ILE:HA	2.51	0.41
1:A:245:LEU:HD13	1:A:253:ILE:HD12	2.03	0.41
1:B:442:ALA:HB2	1:B:455:GLU:HG2	2.02	0.41
1:B:508:ARG:HH12	1:B:530:VAL:CG1	2.33	0.41
1:B:540:PRO:O	1:B:542:ALA:N	2.53	0.41
1:A:370:VAL:HG12	1:A:371:SER:N	2.35	0.40
1:B:187:MET:HE3	1:B:296:TYR:HB2	2.03	0.40
1:B:454:ILE:CG2	1:B:455:GLU:H	2.33	0.40
1:A:436:GLN:O	1:A:438:GLN:HG3	2.22	0.40
1:A:158:ARG:NH2	2:A:577:SO4:O3	2.55	0.40
1:B:430:PHE:O	1:B:433:LEU:HB2	2.20	0.40
1:A:144:VAL:HB	1:A:394:ARG:HG2	2.04	0.40
1:A:336:LEU:HD12	1:A:356:PRO:HD3	2.04	0.40
1:A:527:ASN:HD21	1:A:534:LEU:H	1.69	0.40
1:B:197:PRO:O	1:B:201:VAL:HG23	2.22	0.40
1:B:308:LEU:CD2	1:B:335:ALA:HB1	2.52	0.40
1:B:465:ARG:HB2	1:B:545:LEU:HD12	2.02	0.40
1:A:124:GLU:OE1	1:A:124:GLU:HA	2.21	0.40
1:B:511:LEU:O	1:B:514:GLN:HB3	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	555/576 (96%)	515 (93%)	38 (7%)	2 (0%)	38	72
1	B	535/576 (93%)	449 (84%)	63 (12%)	23 (4%)	3	10
All	All	1090/1152 (95%)	964 (88%)	101 (9%)	25 (2%)	7	25

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	16	ALA
1	B	113	SER
1	B	406	ASN
1	B	453	SER
1	B	469	LEU
1	B	538	PRO
1	B	540	PRO
1	B	548	SER
1	B	13	PRO
1	B	14	CYS
1	B	407	SER
1	B	468	GLY
1	B	470	SER
1	B	534	LEU
1	B	535	LYS
1	B	541	ALA
1	B	542	ALA
1	A	541	ALA
1	B	441	LYS
1	B	533	LYS
1	A	540	PRO
1	B	310	ASP
1	B	329	THR
1	B	389	THR
1	B	403	THR

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	477/491 (97%)	464 (97%)	13 (3%)	50	83
1	B	458/491 (93%)	445 (97%)	13 (3%)	49	82
All	All	935/982 (95%)	909 (97%)	26 (3%)	49	82

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

Mol	Chain	Res	Type
1	A	26	LEU
1	A	50	LYS
1	A	86	GLU
1	A	106	LYS
1	A	112	SER
1	A	159	LEU
1	A	273	ASN
1	A	308	LEU
1	A	309	GLN
1	A	336	LEU
1	A	402	HIS
1	A	492	LEU
1	A	545	LEU
1	B	41	THR
1	B	139	MET
1	B	273	ASN
1	B	383	TYR
1	B	401	ARG
1	B	434	LEU
1	B	444	ASP
1	B	469	LEU
1	B	487	SER
1	B	517	ARG
1	B	536	LEU
1	B	539	ILE
1	B	546	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	A	309	GLN
1	A	406	ASN
1	A	527	ASN
1	A	544	GLN
1	B	49	GLN
1	B	206	ASN
1	B	251	GLN
1	B	273	ASN
1	B	438	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)

4 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	SO4	A	577	-	4,4,4	0.41	0	6,6,6	0.09	0
2	SO4	A	578	-	4,4,4	0.35	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BIW	B	577	-	26,39,39	1.72	4 (15%)	27,56,56	1.17	2 (7%)
2	SO4	B	578	-	4,4,4	0.42	0	6,6,6	0.11	0

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	SO4	A	577	-	-	0/0/0/0	0/0/0/0
2	SO4	A	578	-	-	0/0/0/0	0/0/0/0
3	BIW	B	577	-	-	0/8/42/42	0/4/5/5
2	SO4	B	578	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	577	BIW	C2-C1	2.40	1.44	1.38
3	B	577	BIW	C5-C6	2.88	1.42	1.36
3	B	577	BIW	C25-N27	4.17	1.44	1.35
3	B	577	BIW	C9-C4	4.82	1.45	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	577	BIW	C16-C8-C9	-2.61	125.35	129.35
3	B	577	BIW	C28-N27-C32	3.16	118.58	112.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	577	SO4	1	0
3	B	577	BIW	1	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	559/576 (97%)	-0.33	4 (0%) 87	83	15, 28, 50, 80	0
1	B	541/576 (93%)	0.16	42 (7%) 14	7	14, 47, 92, 99	0
All	All	1100/1152 (95%)	-0.09	46 (4%) 37	26	14, 34, 87, 99	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	ALA	4.8
1	B	14	CYS	4.6
1	B	563	SER	4.3
1	B	511	LEU	4.2
1	B	535	LYS	3.9
1	B	520	THR	3.6
1	B	15	ALA	3.5
1	B	405	ILE	3.5
1	B	402	HIS	3.5
1	B	453	SER	3.4
1	B	524	TYR	3.3
1	B	403	THR	3.2
1	B	438	GLN	3.2
1	B	515	GLY	3.1
1	B	433	LEU	3.0
1	B	513	SER	3.0
1	B	17	GLU	2.8
1	B	518	ALA	2.8
1	B	561	TYR	2.7
1	B	536	LEU	2.6
1	B	542	ALA	2.6
1	B	537	THR	2.6
1	B	514	GLN	2.5
1	B	442	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	435	ALA	2.4
1	B	523	ARG	2.4
1	B	516	GLY	2.4
1	B	214	PRO	2.3
1	B	519	ALA	2.3
1	B	512	LEU	2.3
1	B	36	MET	2.2
1	B	532	THR	2.2
1	B	548	SER	2.2
1	B	443	LEU	2.2
1	A	542	ALA	2.2
1	B	212	LYS	2.2
1	B	534	LEU	2.2
1	B	430	PHE	2.2
1	B	530	VAL	2.2
1	B	441	LYS	2.2
1	B	41	THR	2.1
1	A	540	PRO	2.1
1	A	544	GLN	2.1
1	A	543	SER	2.1
1	B	544	GLN	2.0
1	B	213	CYS	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	SO4	A	578	5/5	0.95	0.23	2.24	73,73,73,73	0
3	BIW	B	577	35/35	0.85	0.29	1.18	76,81,88,89	0
2	SO4	B	578	5/5	0.90	0.20	0.85	93,93,94,94	0
2	SO4	A	577	5/5	0.94	0.18	0.46	89,89,89,89	0

6.5 Other polymers (i)

There are no such residues in this entry.