



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2016 – 08:23 PM EDT

PDB ID : 5DPL
Title : The structure of PKMT2 from Rickettsia typhi in complex with AdoHcy
Authors : Noinaj, N.; Abeykoon, A.; He, Y.; Yang, D.C.; Buchanan, S.K.
Deposited on : 2015-09-12
Resolution : 3.20 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

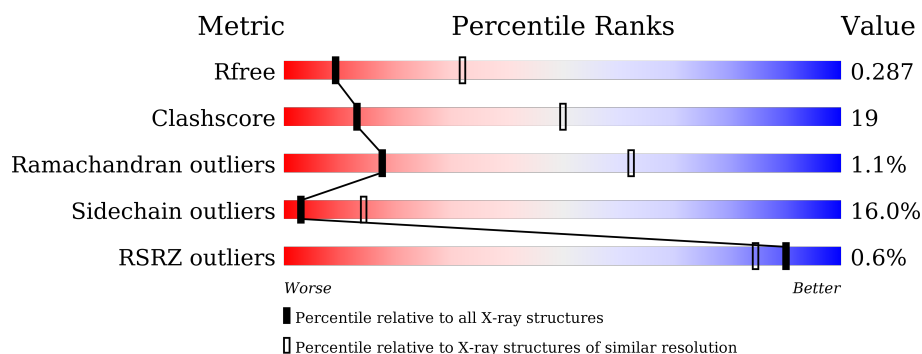
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	535	<div> <div></div> <div>53% 37% 6% . .</div> </div>
1	B	535	<div> <div></div> <div>53% 35% 7% . .</div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8077 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.

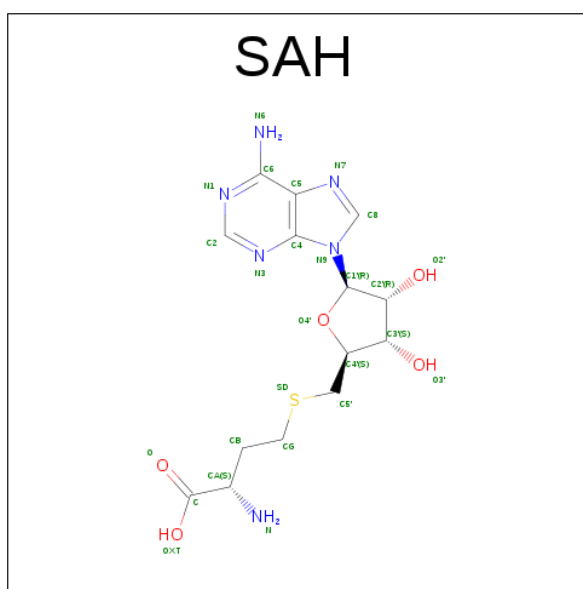
- Molecule 1 is a protein called protein lysine methyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	1	0
			4055	2615	659	768	13			
1	B	512	Total	C	N	O	S	0	1	0
			3970	2566	643	749	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q68XQ5
B	0	GLY	-	expression tag	UNP Q68XQ5

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



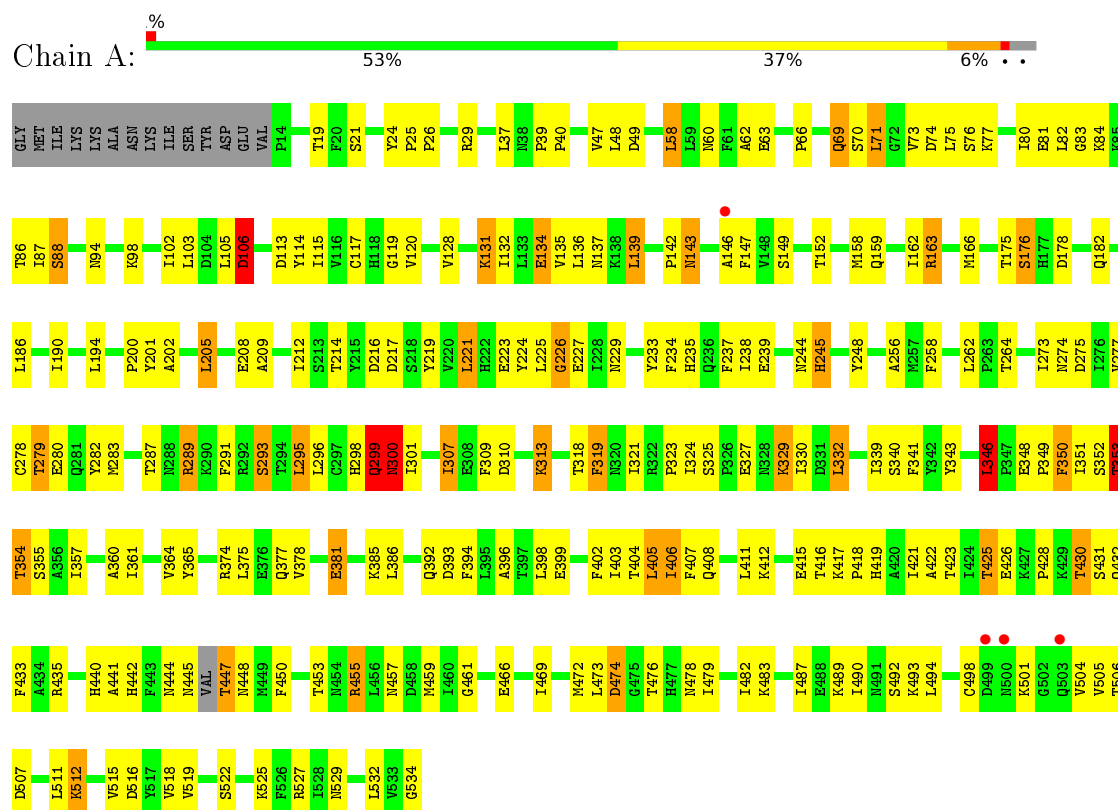
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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 ($\text{RSRZ} > 2$). 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: protein lysine methyltransferase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.35Å 91.03Å 105.83Å 90.00° 112.30° 90.00°	Depositor
Resolution (Å)	48.95 – 3.20 48.96 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.95-3.20) 93.5 (48.96-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10_2142: ???)	Depositor
R, R_{free}	0.244 , 0.280 0.249 , 0.287	Depositor DCC
R_{free} test set	1912 reflections (8.35%)	DCC
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , -13.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.107 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8077	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH

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	0.32	0/4145	0.62	3/5643 (0.1%)
1	B	0.32	0/4059	0.63	2/5530 (0.0%)
All	All	0.32	0/8204	0.63	5/11173 (0.0%)

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	6
1	B	0	5
All	All	0	11

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	LEU	CA-CB-CG	7.28	132.05	115.30
1	B	118	HIS	C-N-CA	-6.63	108.38	122.30
1	B	180	LEU	CA-CB-CG	6.23	129.63	115.30
1	A	205	LEU	CA-CB-CG	5.06	126.95	115.30
1	A	353	THR	C-N-CA	5.02	134.25	121.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	176	SER	Peptide
1	A	226	GLY	Peptide
1	A	299	GLN	Peptide
1	A	501	LYS	Peptide
1	A	505	VAL	Peptide
1	B	107	GLU	Peptide
1	B	119	GLY	Peptide
1	B	196	ASN	Peptide
1	B	346	LEU	Peptide
1	B	506	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4055	0	3881	151	0
1	B	3970	0	3781	151	0
2	A	26	0	19	2	0
2	B	26	0	19	2	0
All	All	8077	0	7700	300	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (300) 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:320:ASN:HA	1:B:369:ILE:HD11	1.36	1.03
1:A:435:ARG:NH1	1:A:473:LEU:O	2.01	0.92
1:B:186:LEU:O	1:B:189:PHE:HB3	1.68	0.92
1:B:393:ASP:OD1	1:B:393:ASP:N	2.05	0.89
1:A:421:ILE:HG22	1:A:423:THR:H	1.42	0.84
1:A:432:GLN:OE1	1:A:435:ARG:NH2	2.12	0.83
1:B:207:ASP:O	1:B:211:LEU:HB2	1.78	0.82
1:A:441:ALA:HB1	1:A:442:HIS:HA	1.61	0.81
1:B:435:ARG:NH1	1:B:473:LEU:O	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:THR:OG1	1:A:448:ASN:N	2.12	0.80
1:A:234:PHE:O	1:A:237:PHE:N	2.15	0.78
1:A:354:THR:HG23	1:A:355:SER:H	1.46	0.78
1:A:422:ALA:O	1:A:527:ARG:NH1	2.17	0.78
1:B:103:LEU:HD11	1:B:128:VAL:HG22	1.67	0.76
1:A:421:ILE:HD12	1:A:534:GLY:HA2	1.69	0.75
1:B:40:PRO:HG3	1:B:113:ASP:HB3	1.69	0.74
1:A:353:THR:HA	1:A:354:THR:HG22	1.69	0.74
1:B:189:PHE:O	1:B:193:SER:N	2.15	0.74
1:B:68:SER:O	1:B:94:ASN:ND2	2.20	0.74
1:A:283:MET:O	1:A:287:THR:OG1	2.05	0.73
1:A:299:GLN:O	1:A:301:ILE:N	2.12	0.73
1:B:422:ALA:O	1:B:527:ARG:NE	2.21	0.73
1:A:103:LEU:HD11	1:A:128:VAL:HG22	1.71	0.72
1:A:343:TYR:HB2	1:A:350:PHE:HD2	1.54	0.71
1:A:60:ASN:ND2	1:A:457:ASN:OD1	2.23	0.71
1:A:307:ILE:HG21	1:A:407:PHE:HZ	1.56	0.70
1:B:316:TYR:HB3	1:B:372:PRO:HB2	1.72	0.70
1:B:312:LEU:HD23	1:B:403:ILE:HD12	1.73	0.70
1:B:29:ARG:NH2	1:B:40:PRO:O	2.24	0.70
1:B:242:GLN:C	1:B:244:ASN:H	1.95	0.69
1:B:23:THR:HG21	1:B:57:ASN:HD21	1.58	0.69
1:B:199:THR:OG1	1:B:199:THR:O	2.09	0.69
1:B:524:GLU:OE1	1:B:527:ARG:NH1	2.25	0.69
1:B:371:ASN:HB3	1:B:422:ALA:HB2	1.75	0.68
1:A:48:LEU:HD23	1:A:115:ILE:HD12	1.76	0.68
1:A:69:GLN:NE2	1:A:94:ASN:O	2.26	0.67
1:A:49:ASP:HB2	1:A:58:LEU:HD11	1.76	0.67
1:B:307:ILE:HG12	1:B:407:PHE:HZ	1.58	0.67
1:A:256:ALA:HB1	1:A:289:ARG:HH12	1.60	0.67
1:B:102:ILE:O	1:B:131:LYS:NZ	2.29	0.66
1:B:283:MET:O	1:B:287:THR:OG1	2.12	0.66
1:A:178:ASP:O	1:A:182:GLN:HG2	1.96	0.65
1:A:62:ALA:HB1	1:A:94:ASN:HB2	1.78	0.65
1:A:163:ARG:NH2	1:A:226:GLY:O	2.31	0.64
1:A:66:PRO:O	1:A:94:ASN:ND2	2.26	0.64
1:B:477:HIS:HB3	1:B:481:ASP:HB3	1.79	0.64
1:B:146:ALA:O	1:B:295:LEU:HA	1.98	0.64
1:B:256:ALA:HB1	1:B:289:ARG:HH12	1.63	0.63
1:B:483:LYS:O	1:B:487:ILE:HG12	1.98	0.63
1:B:428:PRO:HB2	1:B:473:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:TYR:HE1	1:B:168:PHE:HD2	1.46	0.63
1:A:310:ASP:HA	1:A:313:LYS:HD2	1.81	0.62
1:B:437:GLN:OE1	1:B:453:THR:OG1	2.17	0.62
1:A:483:LYS:HD3	1:A:516:ASP:HA	1.82	0.62
1:B:159:GLN:OE1	1:B:224:TYR:OH	2.06	0.62
1:A:223:GLU:OE2	1:A:229:ASN:ND2	2.32	0.62
1:A:343:TYR:HB2	1:A:350:PHE:CD2	2.34	0.62
1:A:117:CYS:SG	1:A:120:VAL:HG22	2.39	0.62
1:B:183:ALA:O	1:B:186:LEU:HB3	2.00	0.62
1:B:398:LEU:O	1:B:402:PHE:HB2	1.99	0.62
1:B:402:PHE:O	1:B:405:LEU:N	2.32	0.62
1:B:235:HIS:O	1:B:239:GLU:CB	2.48	0.61
1:A:106:ASP:OD1	1:A:106:ASP:N	2.33	0.61
1:B:259:ILE:HG12	1:B:260:GLY:H	1.66	0.61
1:A:364:VAL:HG12	1:A:385:LYS:HD3	1.82	0.61
1:A:343:TYR:O	1:A:346:LEU:HD13	2.01	0.60
1:B:59:LEU:HD21	1:B:87:ILE:HG12	1.82	0.60
1:A:447:THR:HG1	1:A:448:ASN:H	1.50	0.60
1:B:108:SER:CB	1:B:109:TYR:HA	2.31	0.60
1:B:450:PHE:HB2	1:B:462:ILE:HG23	1.81	0.60
1:A:299:GLN:C	1:A:301:ILE:H	2.03	0.59
1:B:120:VAL:HG12	2:B:601:SAH:H5'2	1.84	0.59
1:A:29:ARG:HG3	1:A:39:PRO:HB2	1.84	0.59
1:A:69:GLN:HE21	1:A:69:GLN:HA	1.66	0.59
1:A:323:PRO:HA	1:A:341:PHE:HD1	1.68	0.59
1:A:115:ILE:HG23	1:A:146:ALA:HA	1.85	0.59
1:B:40:PRO:CG	1:B:113:ASP:HB3	2.32	0.59
1:A:307:ILE:HG21	1:A:407:PHE:CZ	2.38	0.58
1:B:390:ARG:HB3	1:B:393:ASP:OD1	2.03	0.58
1:A:450:PHE:O	1:A:461:GLY:HA2	2.03	0.58
1:A:19:THR:H	1:A:459:MET:HE1	1.69	0.58
1:A:354:THR:CG2	1:A:355:SER:H	2.15	0.58
1:B:235:HIS:O	1:B:239:GLU:HB3	2.04	0.57
1:A:209:ALA:HA	1:A:212:ILE:HD12	1.86	0.57
1:A:324:ILE:HG13	1:A:325:SER:N	2.19	0.57
1:A:402:PHE:O	1:A:405:LEU:N	2.36	0.57
1:A:353:THR:HG22	1:A:354:THR:HG22	1.86	0.57
1:A:415:GLU:O	1:A:416:THR:OG1	2.20	0.57
1:B:430:THR:HG22	1:B:431:SER:H	1.68	0.57
1:A:159:GLN:NE2	1:A:208:GLU:OE2	2.38	0.57
1:A:354:THR:HG23	1:A:355:SER:N	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:GLU:HG2	1:A:522:SER:HB3	1.87	0.57
1:A:194:LEU:HD11	1:B:286:ILE:HG23	1.87	0.57
1:A:235:HIS:O	1:A:239:GLU:CB	2.52	0.57
1:B:338:ASN:OD1	1:B:352:SER:HB3	2.04	0.56
1:A:142:PRO:HA	1:A:298:HIS:ND1	2.21	0.56
1:B:487:ILE:O	1:B:491:ASN:HB2	2.05	0.56
1:A:386:LEU:HD12	1:A:386:LEU:O	2.06	0.56
1:A:318:THR:HG23	1:A:412:LYS:HB2	1.86	0.56
1:B:466:GLU:HG2	1:B:522:SER:HB3	1.88	0.55
1:A:396:ALA:O	1:A:399:GLU:N	2.40	0.55
1:B:348:GLU:HB3	1:B:349:PRO:HD2	1.86	0.55
1:B:515:VAL:HA	1:B:518:VAL:HG12	1.88	0.55
1:A:146:ALA:O	1:A:295:LEU:HA	2.07	0.55
1:A:525:LYS:O	1:A:529:ASN:ND2	2.33	0.55
1:B:480:ASP:OD1	1:B:481:ASP:N	2.41	0.54
1:B:430:THR:HG23	1:B:531:LEU:O	2.06	0.54
1:A:324:ILE:HG21	1:A:340:SER:HB2	1.89	0.54
1:A:77:LYS:O	1:A:81:GLU:HG2	2.08	0.54
1:B:478:ASN:ND2	1:B:480:ASP:OD1	2.41	0.54
1:B:115:ILE:HG13	1:B:146:ALA:HA	1.90	0.53
1:B:284:ASP:OD1	1:B:292:ARG:NH2	2.27	0.53
1:A:430:THR:OG1	1:A:431:SER:N	2.41	0.53
1:A:186:LEU:O	1:A:190:ILE:HG12	2.08	0.53
1:B:142:PRO:HA	1:B:298:HIS:ND1	2.24	0.53
1:B:361:ILE:O	1:B:364:VAL:HG12	2.09	0.53
1:A:83:GLY:HA2	1:A:86:THR:HG22	1.91	0.53
1:B:137:ASN:ND2	1:B:244:ASN:O	2.41	0.53
1:A:398:LEU:O	1:A:402:PHE:HB2	2.10	0.52
1:B:350:PHE:CD1	1:B:351:ILE:HG13	2.44	0.52
1:B:355:SER:OG	1:B:357:ILE:HG22	2.09	0.52
1:B:392:GLN:N	1:B:392:GLN:OE1	2.35	0.52
1:A:445:ASN:HA	1:A:448:ASN:O	2.08	0.52
1:B:304:ASN:HD21	1:B:306:LYS:HE3	1.74	0.52
1:B:313:LYS:HA	1:B:375:LEU:HB3	1.92	0.52
1:A:120:VAL:HG12	2:A:601:SAH:H5'2	1.91	0.52
1:B:107:GLU:HA	1:B:108:SER:O	2.10	0.52
1:A:392:GLN:N	1:A:392:GLN:OE1	2.37	0.52
1:B:518:VAL:O	1:B:522:SER:OG	2.19	0.51
1:B:118:HIS:O	1:B:120:VAL:N	2.43	0.51
1:A:478:ASN:O	1:A:482:ILE:HG12	2.10	0.51
1:A:212:ILE:HG12	1:A:224:TYR:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ASP:O	1:A:221:LEU:HB2	2.10	0.51
1:B:132:ILE:O	1:B:135:VAL:HG22	2.10	0.51
1:B:259:ILE:HG12	1:B:260:GLY:N	2.25	0.51
1:A:346:LEU:HD23	1:A:348:GLU:HB2	1.91	0.51
1:B:274:ASN:ND2	1:B:274:ASN:O	2.44	0.51
1:B:499:ASP:H	1:B:504:VAL:CB	2.23	0.51
1:A:479:ILE:HG12	1:A:483:LYS:HE2	1.93	0.50
1:A:421:ILE:N	1:A:532:LEU:O	2.44	0.50
1:A:512:LYS:O	1:A:515:VAL:HG12	2.10	0.50
1:B:238:ILE:HG21	1:B:248:TYR:HB2	1.93	0.50
1:A:102:ILE:HG21	1:A:132:ILE:HD13	1.92	0.50
1:B:405:LEU:HB3	1:B:411:LEU:HD13	1.94	0.50
1:B:425:THR:HG21	1:B:534:GLY:O	2.12	0.50
1:A:136:LEU:HD23	1:A:146:ALA:HB1	1.93	0.49
1:B:131:LYS:O	1:B:135:VAL:HG13	2.12	0.49
1:B:325:SER:O	1:B:363:TYR:OH	2.24	0.49
1:A:426:GLU:O	1:A:426:GLU:HG2	2.12	0.49
1:A:428:PRO:HB2	1:A:473:LEU:HD13	1.94	0.49
1:A:137:ASN:HD21	1:A:245:HIS:HB2	1.78	0.49
1:B:469:ILE:HG23	1:B:482:ILE:HD13	1.94	0.49
1:B:103:LEU:HA	1:B:131:LYS:HZ2	1.76	0.49
1:B:406:ILE:HG22	1:B:411:LEU:HD22	1.93	0.49
1:A:319:PHE:CE2	1:A:321:ILE:HD11	2.48	0.49
1:B:320:ASN:OD1	1:B:344:GLU:HG2	2.12	0.49
1:B:465:HIS:O	1:B:469:ILE:HG13	2.13	0.49
1:B:152:THR:HA	1:B:232:THR:O	2.13	0.49
1:B:321:ILE:HA	1:B:342:TYR:O	2.13	0.49
1:B:351:ILE:HG22	1:B:352:SER:H	1.78	0.48
1:A:403:ILE:HA	1:A:406:ILE:HG23	1.95	0.48
1:A:235:HIS:O	1:A:239:GLU:HB2	2.12	0.48
1:B:345:ASN:O	1:B:346:LEU:HB2	2.12	0.48
1:B:482:ILE:HG13	1:B:483:LYS:N	2.29	0.48
1:B:242:GLN:C	1:B:244:ASN:N	2.65	0.48
1:B:74:ASP:OD1	1:B:75:LEU:N	2.45	0.48
1:A:469:ILE:HD11	1:A:519:VAL:HG22	1.96	0.48
1:B:340:SER:OG	1:B:352:SER:OG	2.29	0.48
1:A:339:ILE:HD13	1:A:341:PHE:CE2	2.47	0.48
1:B:204:PHE:C	1:B:206:ARG:H	2.16	0.48
1:B:347:PRO:HB2	1:B:348:GLU:HA	1.95	0.48
1:A:235:HIS:O	1:A:239:GLU:HB3	2.12	0.48
1:A:245:HIS:HA	1:A:299:GLN:NE2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:ND2	1:A:244:ASN:O	2.47	0.47
1:B:479:ILE:O	1:B:483:LYS:HG3	2.14	0.47
1:B:48:LEU:HA	1:B:71:LEU:O	2.15	0.47
1:B:179:LYS:H	1:B:180:LEU:HA	1.79	0.47
1:A:63:GLU:OE1	1:A:433:PHE:HB2	2.15	0.47
1:A:102:ILE:HA	1:A:105:LEU:HD12	1.97	0.47
1:A:131:LYS:HA	1:A:134:GLU:CD	2.36	0.47
1:B:419:HIS:O	1:B:455:ARG:HG3	2.15	0.47
1:B:188:LYS:O	1:B:192:ASP:HB2	2.15	0.46
1:A:74:ASP:OD1	2:A:601:SAH:O2'	2.22	0.46
1:A:87:ILE:HG13	1:A:88:SER:N	2.30	0.46
1:B:123:TRP:CE3	1:B:229:ASN:HB3	2.49	0.46
1:B:59:LEU:HD23	1:B:95:VAL:HG11	1.96	0.46
1:B:105:LEU:HG	1:B:139:LEU:HD11	1.97	0.46
1:A:273:ILE:HG13	1:A:273:ILE:H	1.51	0.46
1:A:309:PHE:O	1:A:313:LYS:HG3	2.16	0.46
1:B:235:HIS:O	1:B:239:GLU:HB2	2.14	0.46
1:A:48:LEU:HD13	1:A:71:LEU:HD23	1.98	0.46
1:A:47:VAL:HG22	1:A:70:SER:HB3	1.98	0.46
1:B:389:TYR:HD1	1:B:389:TYR:N	2.14	0.46
1:B:389:TYR:CD1	1:B:389:TYR:N	2.84	0.46
1:A:162:ILE:O	1:A:166:MET:HG3	2.16	0.46
1:A:275:ASP:O	1:A:279:THR:OG1	2.34	0.46
1:B:527:ARG:HA	1:B:532:LEU:HD12	1.97	0.46
1:A:147:PHE:CZ	1:A:293:SER:HB3	2.51	0.46
1:A:361:ILE:O	1:A:364:VAL:HG22	2.16	0.45
1:B:472:MET:HB2	1:B:472:MET:HE2	1.54	0.45
1:A:25:PRO:HB2	1:A:26:PRO:HD3	1.98	0.45
1:B:375:LEU:HD11	1:B:398:LEU:HD11	1.98	0.45
1:A:69:GLN:HG3	1:A:70:SER:N	2.32	0.45
1:B:436:TYR:O	1:B:439:LYS:HB2	2.16	0.45
1:A:419:HIS:O	1:A:455:ARG:HG3	2.17	0.45
1:A:40:PRO:HG2	1:A:113:ASP:HB3	1.99	0.45
1:A:507:ASP:O	1:A:511:LEU:HB2	2.15	0.45
1:A:69:GLN:HG3	1:A:70:SER:H	1.80	0.45
1:B:270:LEU:O	1:B:273:ILE:HG22	2.17	0.45
1:B:338:ASN:HA	1:B:354:THR:H	1.82	0.45
1:A:300:ASN:N	1:A:300:ASN:OD1	2.50	0.45
1:B:163:ARG:O	1:B:167:MET:CB	2.65	0.45
1:B:108:SER:HB3	1:B:109:TYR:CD1	2.51	0.45
1:B:157:ASN:O	1:B:161:THR:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:SER:OG	1:B:493:LYS:N	2.50	0.44
1:B:330:ILE:HA	1:B:330:ILE:HD12	1.66	0.44
1:A:152:THR:HG23	1:A:289:ARG:O	2.18	0.44
1:A:374:ARG:O	1:A:378:VAL:HG23	2.18	0.44
1:A:377:GLN:NE2	1:A:381:GLU:OE2	2.50	0.44
1:B:167:MET:HG3	1:B:167:MET:O	2.17	0.44
1:A:472:MET:HE3	1:A:482:ILE:HD13	1.99	0.44
1:A:143:ASN:OD1	1:A:143:ASN:N	2.35	0.44
1:B:479:ILE:HG12	1:B:483:LYS:HE3	1.98	0.44
1:A:238:ILE:HD12	1:A:248:TYR:HB2	1.99	0.44
1:B:159:GLN:HG2	1:B:159:GLN:H	1.65	0.44
1:B:25:PRO:HB2	1:B:26:PRO:HD3	1.99	0.44
1:B:369:ILE:HD12	1:B:369:ILE:HA	1.45	0.44
1:B:425:THR:O	1:B:426:GLU:HG2	2.18	0.44
1:A:425:THR:O	1:A:426:GLU:HB3	2.18	0.43
1:B:482:ILE:HG13	1:B:483:LYS:H	1.83	0.43
1:A:29:ARG:HD2	1:A:114:TYR:OH	2.18	0.43
1:B:221:LEU:O	1:B:225:LEU:HB2	2.18	0.43
1:B:80:ILE:HG13	1:B:99:ALA:HB2	1.99	0.43
1:A:360:ALA:O	1:A:364:VAL:HG13	2.18	0.43
1:A:490:ILE:HG21	1:A:511:LEU:HD21	1.99	0.43
1:B:305:ARG:O	1:B:307:ILE:HD12	2.18	0.43
1:A:321:ILE:HG23	1:A:341:PHE:HB3	2.01	0.43
1:A:398:LEU:HA	1:A:402:PHE:HD2	1.84	0.43
1:B:135:VAL:O	1:B:139:LEU:HB2	2.18	0.43
1:A:489:LYS:O	1:A:494:LEU:HA	2.18	0.43
1:B:102:ILE:HG13	2:B:601:SAH:N1	2.33	0.43
1:A:80:ILE:HG22	1:A:84:LYS:HE3	1.99	0.43
1:B:135:VAL:HB	1:B:139:LEU:HD12	1.99	0.43
1:A:398:LEU:HA	1:A:402:PHE:CD2	2.54	0.43
1:B:179:LYS:CB	1:B:182:GLN:H	2.31	0.43
1:A:135:VAL:HG13	1:A:139:LEU:CD1	2.49	0.42
1:A:355:SER:OG	1:A:357:ILE:HG22	2.19	0.42
1:B:425:THR:C	1:B:427:LYS:H	2.22	0.42
1:A:354:THR:CG2	1:A:355:SER:N	2.80	0.42
1:A:425:THR:OG1	1:A:534:GLY:O	2.18	0.42
1:B:152:THR:N	1:B:290:LYS:O	2.34	0.42
1:B:63:GLU:OE1	1:B:433:PHE:HB2	2.19	0.42
1:A:417:LYS:HG3	1:A:418:PRO:HD2	2.02	0.42
1:B:437:GLN:OE1	1:B:453:THR:N	2.51	0.42
1:A:327:GLU:OE1	1:A:385:LYS:NZ	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:HA	1:A:98:LYS:O	2.18	0.42
1:B:23:THR:OG1	1:B:116:VAL:HG11	2.20	0.42
1:B:404:THR:O	1:B:408:GLN:HG3	2.19	0.42
1:A:340:SER:HB3	1:A:349:PRO:HB3	2.02	0.42
1:B:47:VAL:HA	1:B:114:TYR:O	2.19	0.42
1:A:175:THR:HA	1:A:176:SER:CB	2.49	0.42
1:A:332:LEU:HA	1:A:332:LEU:HD12	1.65	0.42
1:A:444:ASN:H	1:A:447:THR:HG23	1.83	0.42
1:A:21:SER:HA	1:A:457:ASN:HB3	2.02	0.42
1:B:532:LEU:HA	1:B:532:LEU:HD23	1.94	0.42
1:B:238:ILE:HG13	1:B:238:ILE:H	1.43	0.42
1:B:465:HIS:CE1	1:B:466:GLU:HG3	2.55	0.42
1:A:128:VAL:O	1:A:132:ILE:HG12	2.20	0.42
1:A:472:MET:HE1	1:A:482:ILE:HA	2.02	0.41
1:B:105:LEU:HD13	1:B:105:LEU:HA	1.91	0.41
1:B:364:VAL:HG22	1:B:368:ASN:ND2	2.34	0.41
1:A:492:SER:O	1:A:494:LEU:N	2.53	0.41
1:B:203:ASN:OD1	1:B:204:PHE:N	2.53	0.41
1:A:518:VAL:O	1:A:522:SER:OG	2.27	0.41
1:B:307:ILE:HG12	1:B:407:PHE:CZ	2.46	0.41
1:B:487:ILE:HD12	1:B:511:LEU:CD1	2.51	0.41
1:A:62:ALA:HB1	1:A:94:ASN:CB	2.46	0.41
1:B:119:GLY:N	1:B:149:SER:OG	2.53	0.41
1:A:404:THR:O	1:A:408:GLN:HG3	2.19	0.41
1:B:321:ILE:HG22	1:B:342:TYR:O	2.20	0.41
1:A:194:LEU:HD21	1:A:202:ALA:HB1	2.03	0.41
1:B:221:LEU:HA	1:B:225:LEU:HD12	2.02	0.41
1:A:329:LYS:HD2	1:A:329:LYS:N	2.35	0.41
1:A:474:ASP:OD1	1:A:476:THR:OG1	2.30	0.41
1:A:352:SER:O	1:A:353:THR:HG23	2.21	0.41
1:B:163:ARG:O	1:B:167:MET:HB3	2.21	0.41
1:B:183:ALA:O	1:B:186:LEU:CB	2.67	0.41
1:A:483:LYS:O	1:A:487:ILE:HG13	2.21	0.40
1:A:357:ILE:HG13	1:A:394:PHE:CE1	2.56	0.40
1:B:200:PRO:HG2	1:B:201:TYR:H	1.87	0.40
1:B:20:PHE:HB2	1:B:23:THR:HG22	2.03	0.40
1:A:280:GLU:O	1:A:283:MET:HB2	2.21	0.40
1:A:307:ILE:HD13	1:A:407:PHE:CE2	2.56	0.40
1:A:318:THR:CG2	1:A:412:LYS:HB2	2.50	0.40
1:B:128:VAL:O	1:B:132:ILE:HG13	2.21	0.40
1:B:187:LEU:HD11	1:B:212:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ILE:HD11	1:B:337:GLU:OE2	2.22	0.40
1:B:518:VAL:HA	1:B:521:VAL:HG22	2.04	0.40
1:A:119:GLY:N	1:A:149:SER:OG	2.42	0.40
1:B:130:ASP:OD1	1:B:130:ASP:N	2.54	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	517/535 (97%)	445 (86%)	67 (13%)	5 (1%)	19	65
1	B	507/535 (95%)	443 (87%)	58 (11%)	6 (1%)	16	60
All	All	1024/1070 (96%)	888 (87%)	125 (12%)	11 (1%)	17	62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	504	VAL
1	B	505	VAL
1	A	299	GLN
1	B	200	PRO
1	A	493	LYS
1	B	198	THR
1	B	504	VAL
1	B	400	GLN
1	A	200	PRO
1	B	346	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/484 (88%)	358 (84%)	68 (16%)	3	14
1	B	414/484 (86%)	348 (84%)	66 (16%)	3	14
All	All	840/968 (87%)	706 (84%)	134 (16%)	3	14

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TYR
1	A	37	LEU
1	A	58	LEU
1	A	69	GLN
1	A	71	LEU
1	A	75	LEU
1	A	76	SER
1	A	82	LEU
1	A	88	SER
1	A	106	ASP
1	A	131	LYS
1	A	134	GLU
1	A	139	LEU
1	A	143	ASN
1	A	158	MET
1	A	163	ARG
1	A	201	TYR
1	A	205	LEU
1	A	214	THR
1	A	216	ASP
1	A	219	TYR
1	A	221	LEU
1	A	225	LEU
1	A	227	GLU
1	A	233	TYR
1	A	245	HIS
1	A	258	PHE

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Mol	Chain	Res	Type
1	A	262	LEU
1	A	264	THR
1	A	274	ASN
1	A	277	VAL
1	A	278	CYS
1	A	279	THR
1	A	289	ARG
1	A	291	PHE
1	A	293	SER
1	A	295	LEU
1	A	296	LEU
1	A	299	GLN
1	A	300	ASN
1	A	307	ILE
1	A	313	LYS
1	A	319	PHE
1	A	329	LYS
1	A	330	ILE
1	A	332	LEU
1	A	346	LEU
1	A	350	PHE
1	A	351	ILE
1	A	353	THR
1	A	354	THR
1	A	365	TYR
1	A	375	LEU
1	A	381	GLU
1	A	393	ASP
1	A	405	LEU
1	A	406	ILE
1	A	411	LEU
1	A	425	THR
1	A	430	THR
1	A	440	HIS
1	A	447	THR
1	A	453	THR
1	A	455	ARG
1	A	474	ASP
1	A	498	CYS
1	A	506	THR
1	A	512	LYS
1	B	24	TYR

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Mol	Chain	Res	Type
1	B	43	GLU
1	B	52	CYS
1	B	58	LEU
1	B	78	THR
1	B	92	ILE
1	B	95	VAL
1	B	100	LEU
1	B	108	SER
1	B	109	TYR
1	B	118	HIS
1	B	124	VAL
1	B	130	ASP
1	B	158	MET
1	B	170	SER
1	B	180	LEU
1	B	186	LEU
1	B	194	LEU
1	B	201	TYR
1	B	207	ASP
1	B	208	GLU
1	B	211	LEU
1	B	212	ILE
1	B	214	THR
1	B	216	ASP
1	B	219	TYR
1	B	238	ILE
1	B	242	GLN
1	B	253	SER
1	B	258	PHE
1	B	278	CYS
1	B	287	THR
1	B	289	ARG
1	B	291	PHE
1	B	295	LEU
1	B	296	LEU
1	B	325	SER
1	B	330	ILE
1	B	332	LEU
1	B	333	ASN
1	B	340	SER
1	B	350	PHE
1	B	351	ILE

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Mol	Chain	Res	Type
1	B	353	THR
1	B	357	ILE
1	B	365	TYR
1	B	369	ILE
1	B	386	LEU
1	B	389	TYR
1	B	393	ASP
1	B	401	HIS
1	B	402	PHE
1	B	405	LEU
1	B	406	ILE
1	B	416	THR
1	B	425	THR
1	B	431	SER
1	B	437	GLN
1	B	439	LYS
1	B	453	THR
1	B	474	ASP
1	B	488	GLU
1	B	495	LEU
1	B	507	ASP
1	B	509	LYS
1	B	513	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	137	ASN

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 [i](#)

There are no carbohydrates 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SAH	A	601	-	22,28,28	1.07	2 (9%)	18,40,40	2.90	3 (16%)
2	SAH	B	601	-	22,28,28	1.07	2 (9%)	18,40,40	2.91	3 (16%)

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	SAH	A	601	-	-	0/7/31/31	0/3/3/3
2	SAH	B	601	-	-	0/7/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	SAH	C2-N1	2.33	1.38	1.33
2	A	601	SAH	C2-N1	2.37	1.38	1.33
2	A	601	SAH	C2-N3	3.62	1.38	1.32
2	B	601	SAH	C2-N3	3.63	1.38	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	SAH	N3-C2-N1	-10.93	120.29	128.87
2	A	601	SAH	N3-C2-N1	-10.79	120.39	128.87
2	B	601	SAH	C5'-SD-CG	-4.32	89.29	102.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	SAH	C5'-SD-CG	-3.69	91.22	102.42
2	B	601	SAH	O4'-C1'-N9	2.44	112.72	108.11
2	A	601	SAH	O4'-C1'-N9	2.90	113.58	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SAH	2	0
2	B	601	SAH	2	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	520/535 (97%)	-0.45	4 (0%) 87 80	33, 68, 101, 126	0
1	B	512/535 (95%)	-0.41	2 (0%) 93 90	44, 77, 105, 121	0
All	All	1032/1070 (96%)	-0.43	6 (0%) 90 84	33, 72, 104, 126	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	ASP	4.6
1	A	503	GLN	2.4
1	A	500	ASN	2.2
1	B	441	ALA	2.2
1	A	146	ALA	2.1
1	B	339	ILE	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(\AA^2)	Q<0.9
2	SAH	A	601	26/26	0.92	0.18	-0.23	66,76,87,113	0
2	SAH	B	601	26/26	0.95	0.13	-1.01	53,67,78,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.