



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:37 PM GMT

PDB ID : 4YVF
Title : Structure of S-adenosyl-L-homocysteine hydrolase
Authors : Akiko, K.
Deposited on : 2015-03-20
Resolution : 2.70 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-20026982
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-20026982

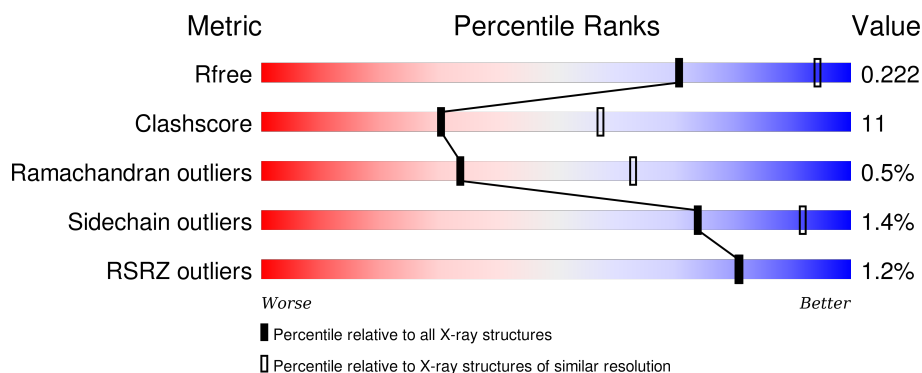
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	432	 2% 72% 26% ..
1	B	432	 72% 27% .

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
3	XFA	A	502	-	-	-	X

2 Entry composition [i](#)

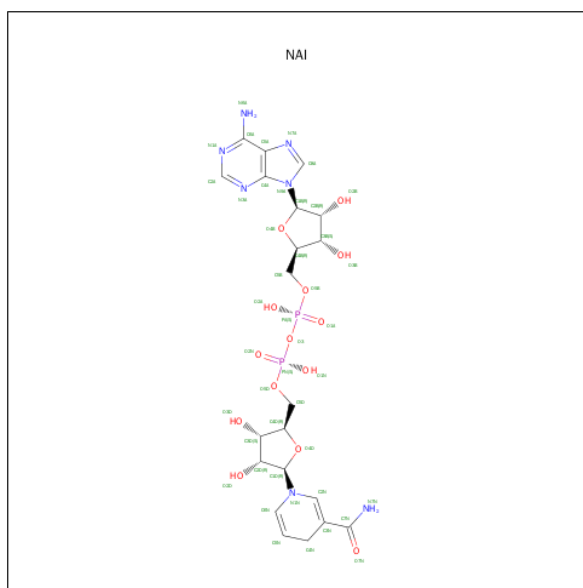
There are 4 unique types of molecules in this entry. The entry contains 7052 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosylhomocysteinase.

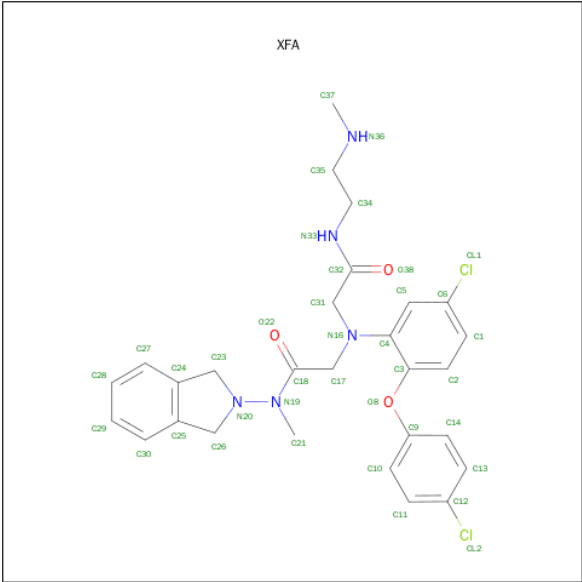
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3322	2108	570	619	25			
1	B	429	Total	C	N	O	S	0	0	0
			3322	2108	570	619	25			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 2-{[5-chloro-2-(4-chlorophenoxy)phenyl][2-{[2-(methylamino)ethyl]amino}-2-oxoethyl]amino}-N-(1,3-dihydro-2H-isoindol-2-yl)-N-methylacetamide (three-letter code: XFA) (formula: C₂₈H₃₁Cl₂N₅O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			38	28	2	5	3		
3	B	1	Total	C	Cl	N	O	0	0
			38	28	2	5	3		

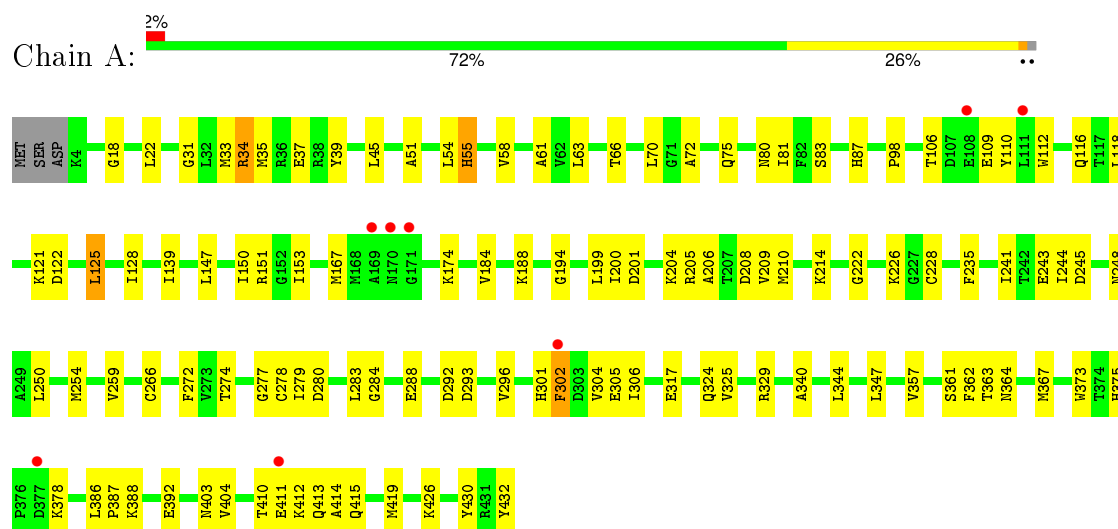
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	130	Total	O	0	0
			130	130		

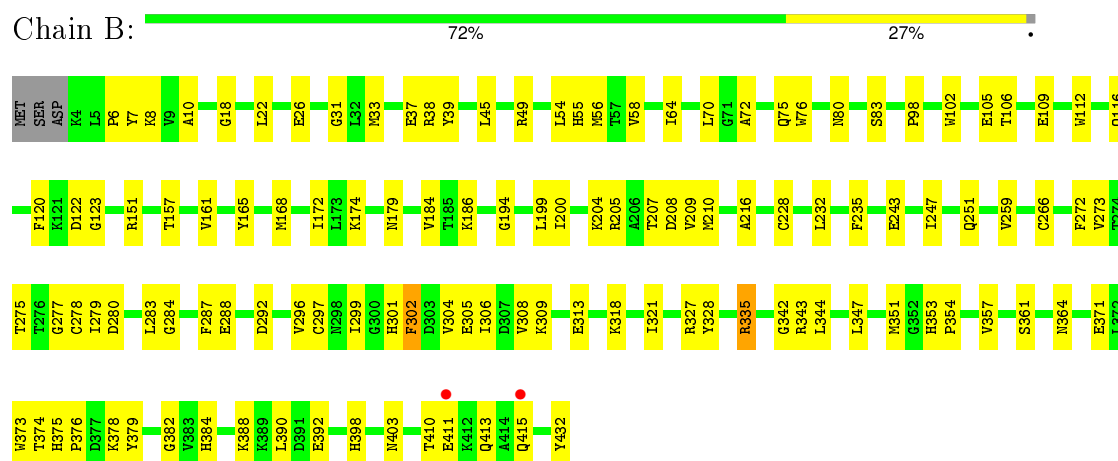
3 Residue-property plots

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: Adenosylhomocysteinase



• Molecule 1: Adenosylhomocysteinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	91.53Å 134.15Å 185.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.81 – 2.70 47.81 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.81-2.70) 99.1 (47.81-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.84 (at 2.69Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.199 , 0.239 0.182 , 0.222	Depositor DCC
R_{free} test set	1565 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 31605 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7052	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 35.54 % 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 5.7398e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: XFA, NAI

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	0.31	0/3386	0.59	0/4582
1	B	0.31	0/3386	0.59	0/4582
All	All	0.31	0/6772	0.59	0/9164

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3322	0	3339	76	0
1	B	3322	0	3339	74	0
2	A	44	0	27	1	0
2	B	44	0	27	1	0
3	A	38	0	31	1	0
3	B	38	0	31	1	0
4	A	114	0	0	3	0
4	B	130	0	0	2	0
All	All	7052	0	6794	150	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 11.

All (150) 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:22:LEU:HD23	1:A:58:VAL:HG13	1.39	1.02
1:A:317:GLU:HB2	1:A:329:ARG:HB3	1.56	0.88
1:A:39:TYR:HB2	1:A:70:LEU:HD22	1.56	0.87
1:B:49:ARG:HH21	1:B:122:ASP:HB2	1.39	0.87
1:B:151:ARG:HD3	1:B:376:PRO:HG3	1.59	0.82
1:B:279:ILE:HG22	1:B:304:VAL:HB	1.60	0.82
1:B:22:LEU:HD23	1:B:58:VAL:HG13	1.67	0.77
1:A:118:LEU:HD22	1:A:139:ILE:HD11	1.68	0.76
1:B:106:THR:OG1	1:B:109:GLU:HG3	1.88	0.73
1:A:33:MET:O	1:A:37:GLU:HG3	1.87	0.72
1:A:375:HIS:HB3	1:A:378:LYS:HD3	1.71	0.71
1:A:284:GLY:O	1:A:288:GLU:HG3	1.93	0.69
1:A:317:GLU:HB2	1:A:329:ARG:CB	2.23	0.69
1:A:45:LEU:HB3	1:A:72:ALA:HB2	1.73	0.69
1:A:34:ARG:HH11	1:A:34:ARG:HA	1.58	0.69
1:A:426:LYS:HE3	4:A:616:HOH:O	1.92	0.68
1:B:321:ILE:HD11	1:B:327:ARG:HB2	1.75	0.66
1:B:45:LEU:HB3	1:B:72:ALA:HB2	1.78	0.64
1:A:128:ILE:HB	1:A:153:ILE:HG12	1.80	0.64
1:B:277:GLY:HA2	1:B:301:HIS:HB2	1.79	0.63
1:A:278:CYS:O	1:A:305:GLU:HG2	2.00	0.61
1:B:75:GLN:HG2	1:B:98:PRO:HB2	1.82	0.61
1:A:147:LEU:HD13	1:A:174:LYS:HB2	1.82	0.61
1:B:388:LYS:O	1:B:392:GLU:HG3	2.01	0.60
1:B:33:MET:O	1:B:37:GLU:HG3	2.01	0.60
1:B:309:LYS:O	1:B:313:GLU:HG3	2.00	0.60
1:A:51:ALA:HB3	1:A:125:LEU:HD23	1.84	0.60
1:B:49:ARG:NH2	1:B:122:ASP:HB2	2.15	0.59
1:B:199:LEU:HD22	1:B:228:CYS:SG	2.43	0.58
1:B:157:THR:O	1:B:161:VAL:HG23	2.04	0.58
1:A:361:SER:O	1:A:364:ASN:HB2	2.02	0.58
1:A:386:LEU:HD12	1:A:387:PRO:HD2	1.86	0.58
1:A:279:ILE:HG22	1:A:304:VAL:HB	1.86	0.57
1:B:284:GLY:O	1:B:288:GLU:HG3	2.04	0.57
1:B:22:LEU:O	1:B:26:GLU:HG3	2.03	0.57
1:A:39:TYR:HB2	1:A:70:LEU:CD2	2.32	0.57
1:B:194:GLY:HA2	1:B:357:VAL:HG21	1.85	0.57
1:B:375:HIS:HB3	1:B:378:LYS:HD3	1.87	0.57
1:A:363:THR:O	1:A:367:MET:HG2	2.04	0.56
1:A:75:GLN:HG2	1:A:98:PRO:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:VAL:HG21	1:B:432:TYR:CE1	2.40	0.56
1:A:118:LEU:CD2	1:A:139:ILE:HD11	2.35	0.56
1:A:18:GLY:HA3	1:A:87:HIS:O	2.06	0.56
1:B:80:ASN:HB3	1:B:83:SER:OG	2.06	0.56
1:A:412:LYS:HE2	1:B:279:ILE:HD12	1.89	0.55
1:A:39:TYR:CB	1:A:70:LEU:HD22	2.33	0.55
1:B:112:TRP:O	1:B:116:GLN:HG2	2.08	0.54
1:A:222:GLY:O	1:A:226:LYS:HG3	2.08	0.54
1:B:280:ASP:HB3	1:B:283:LEU:HD21	1.88	0.54
1:A:31:GLY:O	1:A:35:MET:HG2	2.07	0.53
1:A:426:LYS:HD2	1:A:430:TYR:CE2	2.44	0.53
1:B:54:LEU:O	1:B:55:HIS:C	2.47	0.53
1:B:284:GLY:HA2	1:B:287:PHE:HD2	1.73	0.52
1:A:66:THR:O	1:A:70:LEU:HG	2.10	0.52
1:B:302:PHE:O	1:B:343:ARG:HA	2.10	0.52
1:A:209:VAL:CG2	1:A:214:LYS:HE2	2.39	0.52
1:A:388:LYS:O	1:A:392:GLU:HG3	2.10	0.52
1:B:204:LYS:O	1:B:208:ASP:N	2.41	0.52
1:B:39:TYR:HB2	1:B:70:LEU:HD22	1.91	0.51
1:A:151:ARG:HD2	1:A:373:TRP:CE3	2.46	0.51
1:A:200:ILE:HG21	1:A:235:PHE:CE2	2.45	0.51
1:A:277:GLY:HA2	1:A:301:HIS:HB2	1.93	0.50
1:A:209:VAL:HG22	1:A:214:LYS:HE2	1.94	0.50
1:B:102:TRP:O	1:B:105:GLU:HG3	2.12	0.50
1:B:49:ARG:HG3	1:B:49:ARG:HH11	1.77	0.50
1:B:56:MET:HE1	1:B:76:TRP:CD1	2.47	0.50
1:B:410:THR:OG1	1:B:413:GLN:HG3	2.12	0.50
1:A:245:ASP:CG	1:A:248:ASN:HD22	2.14	0.49
1:B:292:ASP:OD2	1:B:335:ARG:NH1	2.45	0.49
1:B:39:TYR:CB	1:B:70:LEU:HD22	2.42	0.49
2:A:501:NAI:O7N	3:A:502:XFA:H10	2.12	0.49
1:A:121:LYS:HE3	1:A:122:ASP:OD2	2.12	0.49
1:A:22:LEU:HD23	1:A:58:VAL:CG1	2.29	0.49
1:A:106:THR:OG1	1:A:109:GLU:HG3	2.12	0.48
1:A:411:GLU:O	1:A:415:GLN:HG3	2.13	0.48
1:A:188:LYS:NZ	4:A:604:HOH:O	2.45	0.48
1:A:55:HIS:HD1	1:A:83:SER:CB	2.26	0.48
1:A:22:LEU:HD21	1:A:61:ALA:HB3	1.96	0.48
1:B:161:VAL:HG12	1:B:165:TYR:CE2	2.48	0.48
1:B:344:LEU:HD12	1:B:347:LEU:HD12	1.95	0.47
1:A:81:ILE:HG22	1:A:110:TYR:HB2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLY:HA2	1:A:357:VAL:HG21	1.96	0.47
1:B:275:THR:HG22	1:B:299:ILE:CG2	2.44	0.47
1:A:200:ILE:HG12	4:A:641:HOH:O	2.13	0.47
1:B:328:TYR:O	1:B:335:ARG:HA	2.15	0.47
1:A:54:LEU:O	1:A:55:HIS:C	2.53	0.47
1:A:45:LEU:HD12	1:A:70:LEU:HB2	1.97	0.46
1:B:216:ALA:HB1	1:B:232:LEU:HD13	1.97	0.46
1:A:204:LYS:O	1:A:208:ASP:N	2.48	0.46
1:B:120:PHE:HB2	1:B:123:GLY:O	2.15	0.46
1:A:34:ARG:CA	1:A:34:ARG:HH11	2.25	0.46
1:B:18:GLY:O	1:B:22:LEU:HG	2.15	0.46
1:A:184:VAL:HG21	1:A:432:TYR:CE1	2.51	0.46
1:B:379:TYR:HD2	1:B:384:HIS:CD2	2.33	0.46
1:B:247:ILE:O	1:B:251:GLN:HG3	2.16	0.45
1:B:38:ARG:O	1:B:38:ARG:HG2	2.15	0.45
1:B:411:GLU:O	1:B:415:GLN:HG3	2.16	0.45
1:B:361:SER:O	1:B:364:ASN:HB2	2.16	0.45
1:A:301:HIS:O	1:A:302:PHE:C	2.55	0.45
1:B:205:ARG:HH12	1:B:351:MET:HG2	1.81	0.45
1:A:404:VAL:HG13	1:B:259:VAL:HB	1.99	0.44
1:A:201:ASP:O	1:A:205:ARG:HG3	2.17	0.44
1:A:80:ASN:HB3	1:A:83:SER:OG	2.17	0.44
1:B:278:CYS:O	1:B:305:GLU:HG2	2.17	0.44
1:A:426:LYS:HD2	1:A:430:TYR:CD2	2.51	0.44
1:B:296:VAL:HG12	1:B:306:ILE:HD13	1.99	0.44
2:B:501:NAI:O7N	3:B:502:XFA:H10	2.18	0.43
1:A:324:GLN:OE1	1:A:340:ALA:HA	2.18	0.43
1:A:63:LEU:HD13	1:A:362:PHE:HB3	1.98	0.43
1:A:274:THR:HB	1:A:305:GLU:OE1	2.18	0.43
1:A:125:LEU:N	1:A:125:LEU:HD12	2.34	0.43
1:B:207:THR:O	1:B:208:ASP:HB2	2.18	0.43
1:A:206:ALA:HB1	1:A:325:VAL:HG22	1.99	0.43
1:A:414:ALA:HB1	1:A:419:MET:O	2.19	0.43
1:B:308:VAL:HG21	1:B:342:GLY:HA3	2.01	0.43
1:A:199:LEU:HD22	1:A:228:CYS:SG	2.59	0.43
1:B:31:GLY:HA3	1:B:398:HIS:CE1	2.54	0.43
1:B:186:LYS:C	1:B:186:LYS:HD3	2.39	0.42
1:B:266:CYS:HA	1:B:272:PHE:CE2	2.55	0.42
1:B:273:VAL:HG22	1:B:297:CYS:SG	2.60	0.42
1:B:216:ALA:CB	1:B:232:LEU:HD13	2.49	0.42
1:B:80:ASN:HA	4:B:615:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LYS:HD3	1:B:102:TRP:CZ3	2.55	0.42
1:B:172:ILE:O	1:B:174:LYS:HG2	2.20	0.42
1:A:112:TRP:O	1:A:116:GLN:HG2	2.19	0.42
1:B:22:LEU:CD2	1:B:58:VAL:HG13	2.41	0.42
1:A:250:LEU:O	1:A:254:MET:HG2	2.18	0.42
1:A:125:LEU:HD13	1:A:150:ILE:HG12	2.02	0.42
1:A:244:ILE:HG13	1:A:245:ASP:N	2.34	0.42
1:B:354:PRO:HG3	4:B:674:HOH:O	2.20	0.42
1:B:371:GLU:CG	1:B:390:LEU:HD11	2.50	0.42
1:A:344:LEU:HD12	1:A:347:LEU:HD12	2.01	0.41
1:A:410:THR:OG1	1:A:413:GLN:HG3	2.20	0.41
1:A:280:ASP:HA	1:A:283:LEU:HD21	2.02	0.41
1:A:55:HIS:HB3	1:A:83:SER:HB2	2.01	0.41
1:A:241:ILE:O	1:A:259:VAL:HA	2.20	0.41
1:A:266:CYS:HA	1:A:272:PHE:CE2	2.55	0.41
1:B:279:ILE:HG22	1:B:304:VAL:CB	2.42	0.41
1:A:167:MET:HE2	1:A:167:MET:HB3	1.90	0.41
1:B:209:VAL:HG22	1:B:210:MET:N	2.35	0.41
1:B:200:ILE:HD13	1:B:235:PHE:CD1	2.56	0.41
1:A:296:VAL:HG12	1:A:306:ILE:HD13	2.03	0.41
1:B:353:HIS:HA	1:B:354:PRO:HD3	1.92	0.41
1:B:168:MET:SD	1:B:382:GLY:HA2	2.61	0.41
1:B:374:THR:C	1:B:376:PRO:HD3	2.41	0.40
1:B:6:PRO:O	1:B:7:TYR:HB3	2.22	0.40
1:B:151:ARG:HD2	1:B:373:TRP:HA	2.02	0.40
1:B:56:MET:HE1	1:B:64:ILE:HD11	2.02	0.40
1:A:292:ASP:O	1:A:293:ASP:HB2	2.20	0.40
1:B:344:LEU:HD12	1:B:347:LEU:CD1	2.52	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	427/432 (99%)	407 (95%)	18 (4%)	2 (0%)	34	63
1	B	427/432 (99%)	411 (96%)	14 (3%)	2 (0%)	34	63
All	All	854/864 (99%)	818 (96%)	32 (4%)	4 (0%)	34	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	PHE
1	B	302	PHE
1	B	10	ALA
1	A	55	HIS

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	353/356 (99%)	348 (99%)	5 (1%)	74	92
1	B	353/356 (99%)	348 (99%)	5 (1%)	74	92
All	All	706/712 (99%)	696 (99%)	10 (1%)	74	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	125	LEU
1	A	210	MET
1	A	243	GLU
1	A	403	ASN
1	B	179	ASN
1	B	243	GLU
1	B	318	LYS
1	B	335	ARG
1	B	403	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	248	ASN
1	A	403	ASN
1	A	415	GLN
1	B	403	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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	NAI	A	501	-	41,48,48	1.50	7 (17%)	46,73,73	2.04	6 (13%)
3	XFA	A	502	-	38,41,41	1.70	8 (21%)	46,56,56	1.94	7 (15%)
2	NAI	B	501	-	41,48,48	1.48	7 (17%)	46,73,73	2.05	6 (13%)
3	XFA	B	502	-	38,41,41	1.79	10 (26%)	46,56,56	1.99	6 (13%)

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	NAI	A	501	-	-	0/25/72/72	0/5/5/5
3	XFA	A	502	-	-	0/24/37/37	0/4/4/4
2	NAI	B	501	-	-	0/25/72/72	0/5/5/5
3	XFA	B	502	-	-	0/24/37/37	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAI	C4N-C5N	-3.19	1.42	1.49
2	A	501	NAI	C4N-C5N	-2.89	1.42	1.49
3	B	502	XFA	C17-C18	-2.69	1.48	1.53
3	A	502	XFA	C17-C18	-2.31	1.49	1.53
3	B	502	XFA	C1-C2	2.04	1.42	1.38
3	B	502	XFA	C14-C9	2.07	1.42	1.38
3	A	502	XFA	C5-C4	2.10	1.43	1.39
3	B	502	XFA	C14-C13	2.12	1.43	1.38
3	B	502	XFA	C31-N16	2.20	1.48	1.45
3	A	502	XFA	C1-C2	2.24	1.43	1.38
3	A	502	XFA	C10-C11	2.27	1.43	1.38
2	A	501	NAI	C2A-N3A	2.31	1.36	1.32
3	B	502	XFA	C10-C11	2.32	1.43	1.38
2	B	501	NAI	C2A-N3A	2.34	1.36	1.32
2	B	501	NAI	C2N-C3N	2.45	1.41	1.34
3	B	502	XFA	C5-C4	2.52	1.43	1.39
3	A	502	XFA	C31-N16	2.55	1.48	1.45
2	A	501	NAI	C2N-C3N	2.55	1.41	1.34
3	B	502	XFA	C2-C3	2.64	1.45	1.39
2	B	501	NAI	C6N-N1N	2.76	1.44	1.37
3	A	502	XFA	C2-C3	2.76	1.45	1.39
3	A	502	XFA	C17-N16	2.97	1.48	1.45
2	B	501	NAI	C2N-N1N	3.02	1.42	1.37
2	A	501	NAI	C6N-N1N	3.08	1.45	1.37
3	A	502	XFA	C5-C6	3.12	1.43	1.38
2	A	501	NAI	O4B-C1B	3.13	1.45	1.41
3	B	502	XFA	C5-C6	3.16	1.43	1.38
2	B	501	NAI	O4B-C1B	3.24	1.45	1.41
2	A	501	NAI	C2N-N1N	3.26	1.43	1.37
3	B	502	XFA	C17-N16	3.46	1.49	1.45
2	B	501	NAI	C6N-C5N	4.16	1.40	1.33
2	A	501	NAI	C6N-C5N	4.42	1.41	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAI	N3A-C2A-N1A	-10.10	120.94	128.87
2	B	501	NAI	N3A-C2A-N1A	-10.04	120.99	128.87
3	B	502	XFA	C5-C4-N16	-3.93	117.01	122.63
3	A	502	XFA	C5-C4-N16	-3.63	117.44	122.63
2	B	501	NAI	C1D-N1N-C2N	-3.20	115.29	120.85
2	A	501	NAI	C1D-N1N-C2N	-3.19	115.30	120.85
2	A	501	NAI	C4N-C5N-C6N	-2.99	117.64	122.58
2	A	501	NAI	C3N-C2N-N1N	-2.95	118.91	123.24
2	B	501	NAI	C4N-C5N-C6N	-2.79	117.97	122.58
2	B	501	NAI	C3N-C2N-N1N	-2.77	119.17	123.24
2	B	501	NAI	C4B-O4B-C1B	-2.48	107.02	109.64
2	A	501	NAI	C4B-O4B-C1B	-2.21	107.31	109.64
3	B	502	XFA	C21-N19-N20	2.12	122.53	116.58
3	A	502	XFA	C31-C32-N33	2.22	121.07	115.88
3	A	502	XFA	C21-N19-N20	2.23	122.85	116.58
3	A	502	XFA	C3-C4-N16	2.53	123.11	119.39
3	B	502	XFA	C3-C4-N16	2.94	123.71	119.39
2	A	501	NAI	C5N-C4N-C3N	4.36	123.70	112.41
2	B	501	NAI	C5N-C4N-C3N	4.38	123.77	112.41
3	A	502	XFA	C3-O8-C9	4.44	129.65	117.83
3	B	502	XFA	C3-O8-C9	4.58	130.03	117.83
3	A	502	XFA	O8-C3-C4	5.04	124.63	117.20
3	B	502	XFA	O8-C3-C4	5.29	125.01	117.20
3	B	502	XFA	C18-C17-N16	8.18	123.34	111.05
3	A	502	XFA	C18-C17-N16	8.36	123.62	111.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAI	1	0
3	A	502	XFA	1	0
2	B	501	NAI	1	0
3	B	502	XFA	1	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 [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	429/432 (99%)	-0.31	8 (1%) 70 70	12, 23, 34, 44	0
1	B	429/432 (99%)	-0.33	2 (0%) 91 93	11, 23, 34, 42	0
All	All	858/864 (99%)	-0.32	10 (1%) 81 81	11, 23, 34, 44	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	ASP	3.5
1	A	169	ALA	3.4
1	A	171	GLY	2.9
1	A	108	GLU	2.8
1	A	302	PHE	2.6
1	B	411	GLU	2.4
1	B	415	GLN	2.4
1	A	411	GLU	2.3
1	A	170	ASN	2.1
1	A	111	LEU	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
3	XFA	A	502	38/38	0.89	0.16	2.51	2,20,27,31	0
3	XFA	B	502	38/38	0.91	0.15	1.59	5,21,23,24	0
2	NAI	A	501	44/44	0.98	0.12	-0.60	11,18,23,24	0
2	NAI	B	501	44/44	0.98	0.12	-0.91	13,18,21,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.