



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 09:38 PM EDT

PDB ID : 3IVA / pdb_00003iva
Title : Structure of the B12-dependent Methionine Synthase (MetH) C-terminal half with AdoHcy bound
Authors : Pattridge, K.A.; Koutmos, M.; Smith, J.L.
Deposited on : 2009-08-31
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

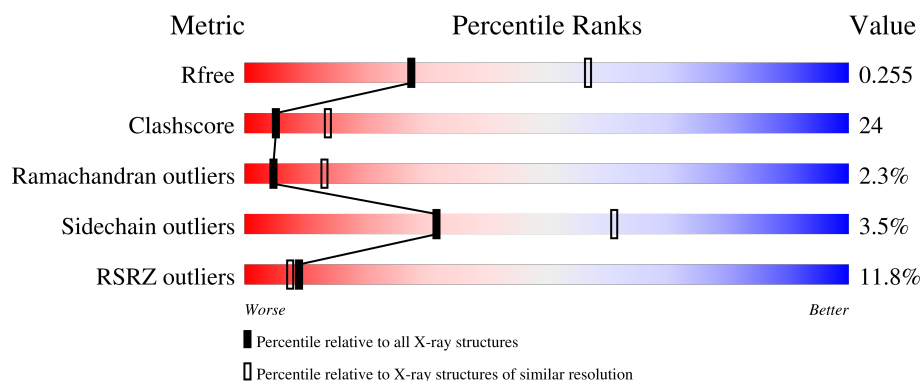
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	579	

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	B12	A	1301	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4722 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.

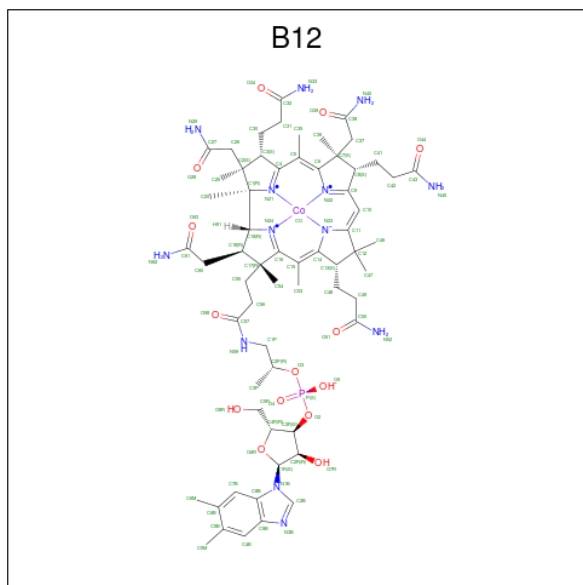
- Molecule 1 is a protein called Methionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	576	4563	2886	788	870	19	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

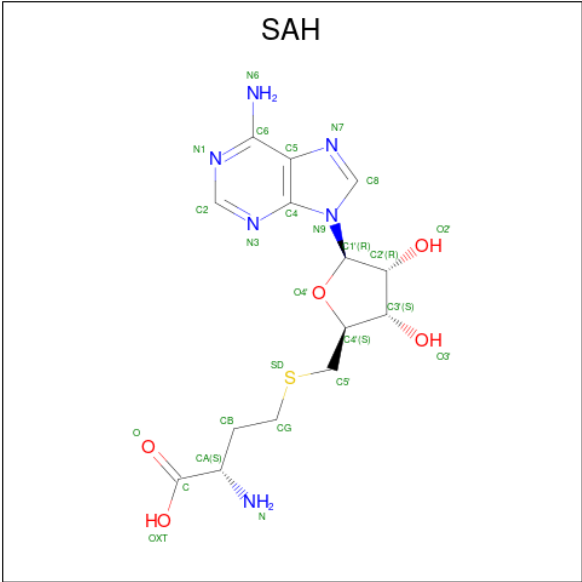
Chain	Residue	Modelled	Actual	Comment	Reference
A	690	CYS	ILE	engineered mutation	UNP P13009
A	743	CYS	GLY	engineered mutation	UNP P13009

- Molecule 2 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



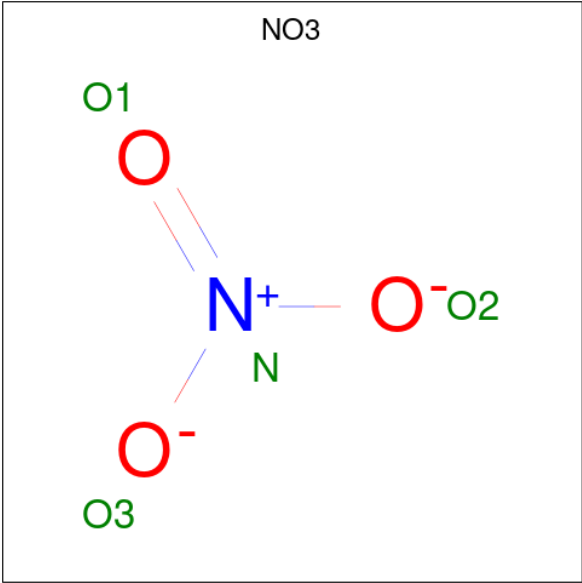
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Co	N	O	P		
2	A	1	91	62	1	13	14	1	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 4 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		
4	A	1	Total	N	O	0	0
			4	1	3		
4	A	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Methionine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.01Å 107.01Å 141.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.32 – 2.70 45.32 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.32-2.70) 99.9 (45.32-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.246 , 0.300 0.246 , 0.255	Depositor DCC
R_{free} test set	1119 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4722	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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, B12, NO3

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	0.38	0/4662	0.92	17/6325 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1027	HIS	N-CA-C	8.36	122.02	111.24
1	A	1085	LYS	N-CA-C	-8.27	101.51	111.69
1	A	1170	ALA	N-CA-C	-6.24	100.75	110.42
1	A	1041	TYR	N-CA-C	5.85	118.75	110.50
1	A	1003	PRO	N-CA-C	-5.76	102.15	111.19
1	A	707	LEU	N-CA-C	-5.66	105.02	111.07
1	A	897	LYS	N-CA-C	-5.59	105.08	112.24
1	A	1113	GLY	N-CA-C	5.56	123.70	114.48
1	A	855	VAL	N-CA-C	5.38	115.65	108.11
1	A	1157	VAL	N-CA-C	5.29	115.74	110.23
1	A	1142	CYS	CA-C-N	5.16	124.77	119.05
1	A	1142	CYS	C-N-CA	5.16	124.77	119.05
1	A	673	GLU	N-CA-C	5.12	117.53	111.33
1	A	901	THR	CA-C-N	5.08	125.62	120.38
1	A	901	THR	C-N-CA	5.08	125.62	120.38
1	A	947	TRP	N-CA-C	5.03	118.68	112.54
1	A	902	PRO	N-CA-C	5.01	116.81	110.70

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	4563	0	4478	227	0
2	A	91	0	73	1	0
3	A	26	0	19	0	0
4	A	16	0	0	0	0
5	A	26	0	0	0	0
All	All	4722	0	4570	227	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 24.

All (227) 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:983:MET:HE1	1:A:1088:VAL:HA	1.41	0.99
1:A:657:TRP:HB3	1:A:661:LYS:HE2	1.52	0.90
1:A:950:PHE:HZ	1:A:1087:MET:HE1	1.36	0.87
1:A:819:LYS:O	1:A:823:ARG:HG2	1.77	0.84
1:A:692:VAL:HG23	1:A:693:ILE:HD12	1.61	0.82
1:A:983:MET:HE2	1:A:1091:LEU:CD2	2.09	0.82
1:A:987:LEU:HD13	1:A:992:THR:HG23	1.61	0.81
1:A:950:PHE:CZ	1:A:1087:MET:HE1	2.16	0.80
1:A:1194:GLN:HA	1:A:1221:ASN:O	1.82	0.80
1:A:1120:LEU:HB3	1:A:1124:GLU:HB3	1.66	0.77
1:A:799:ASP:C	1:A:800:LEU:HD12	2.09	0.77
1:A:938:ILE:O	1:A:942:ARG:HG3	1.86	0.76
1:A:1144:GLU:OE1	1:A:1146:THR:HB	1.86	0.75
1:A:1163:MET:HE3	1:A:1176:SER:HB2	1.67	0.75
1:A:660:ASN:HB3	1:A:696:PRO:HB3	1.67	0.74
1:A:750:VAL:HA	1:A:778:VAL:HG23	1.70	0.74
1:A:805:GLY:O	1:A:836:THR:HG22	1.88	0.73
1:A:983:MET:HE1	1:A:1088:VAL:CA	2.17	0.72
1:A:983:MET:HE2	1:A:1091:LEU:HD23	1.70	0.71
1:A:1084:ASN:HA	1:A:1087:MET:HB3	1.73	0.70
1:A:753:THR:HB	1:A:782:VAL:HA	1.74	0.69
1:A:858:GLN:HB2	1:A:862:ARG:HD2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1219:ALA:HB3	1:A:1220:PRO:HD3	1.73	0.69
1:A:888:GLU:O	1:A:892:ILE:HG12	1.93	0.69
1:A:748:LYS:HE3	1:A:776:GLU:OE2	1.93	0.69
1:A:750:VAL:HG22	1:A:778:VAL:HG21	1.75	0.69
1:A:983:MET:HE2	1:A:1091:LEU:HD22	1.75	0.69
1:A:1211:VAL:O	1:A:1215:GLU:HG3	1.93	0.68
1:A:967:GLU:CD	1:A:967:GLU:H	2.02	0.68
1:A:750:VAL:HA	1:A:778:VAL:CG2	2.23	0.67
1:A:730:ALA:O	1:A:733:GLU:HG2	1.94	0.67
1:A:754:VAL:HG13	1:A:813:GLU:HG2	1.75	0.67
1:A:1150:THR:O	1:A:1154:LEU:HD13	1.95	0.66
1:A:726:LYS:HG2	1:A:1080:HIS:HB3	1.77	0.65
1:A:758:VAL:HG11	1:A:1171:MET:O	1.96	0.65
1:A:983:MET:O	1:A:987:LEU:HD23	1.96	0.65
1:A:703:VAL:O	1:A:707:LEU:HB2	1.96	0.65
1:A:832:ILE:HD11	1:A:842:THR:OG1	1.97	0.64
1:A:1152:TRP:HA	1:A:1157:VAL:HG23	1.78	0.64
1:A:749:MET:HE1	1:A:831:LEU:HD12	1.79	0.64
1:A:948:THR:HB	1:A:949:PRO:HD3	1.80	0.64
1:A:683:ARG:HH21	1:A:735:PHE:HB3	1.64	0.63
1:A:983:MET:CE	1:A:1088:VAL:HA	2.21	0.63
1:A:658:GLU:HB3	1:A:661:LYS:HB2	1.79	0.62
1:A:692:VAL:HG21	1:A:732:LEU:CD1	2.29	0.62
1:A:754:VAL:HG13	1:A:813:GLU:CG	2.29	0.62
1:A:887:TYR:O	1:A:891:ARG:HB2	1.99	0.61
1:A:889:THR:O	1:A:893:GLN:HB2	2.01	0.61
1:A:900:ARG:HD3	1:A:901:THR:N	2.16	0.61
1:A:732:LEU:O	1:A:732:LEU:HD23	2.01	0.61
1:A:745:THR:HA	1:A:774:ASN:ND2	2.16	0.61
1:A:692:VAL:HG21	1:A:732:LEU:HD11	1.82	0.60
1:A:652:ALA:HB3	1:A:655:ARG:HG2	1.83	0.60
1:A:1084:ASN:HA	1:A:1087:MET:CB	2.32	0.59
1:A:745:THR:HA	1:A:774:ASN:HD21	1.67	0.59
1:A:861:SER:O	1:A:864:VAL:HG12	2.02	0.59
1:A:862:ARG:O	1:A:866:VAL:HG23	2.02	0.59
1:A:692:VAL:O	1:A:697:LEU:HB2	2.03	0.59
1:A:790:LEU:O	1:A:794:LYS:HG3	2.03	0.58
1:A:683:ARG:NH2	1:A:735:PHE:HB3	2.19	0.58
1:A:651:GLN:O	1:A:652:ALA:HB2	2.02	0.58
1:A:689:PRO:O	1:A:692:VAL:HG22	2.03	0.58
1:A:900:ARG:HD3	1:A:900:ARG:C	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:PHE:HE2	1:A:976:LEU:CD1	2.17	0.57
1:A:663:LEU:O	1:A:667:LEU:HG	2.04	0.57
1:A:706:ASP:O	1:A:710:GLU:HG3	2.05	0.57
1:A:800:LEU:HD11	1:A:871:LEU:HD13	1.86	0.57
1:A:674:PHE:O	1:A:678:ASP:HB2	2.05	0.57
1:A:901:THR:O	1:A:901:THR:HG23	2.05	0.56
1:A:701:MET:HE3	1:A:725:MET:HB2	1.86	0.56
1:A:950:PHE:CZ	1:A:1087:MET:CE	2.88	0.56
1:A:809:PRO:HB2	1:A:1168:SER:OG	2.05	0.56
1:A:829:PRO:HB3	1:A:870:LEU:HD21	1.87	0.56
1:A:693:ILE:CD1	1:A:732:LEU:HD22	2.35	0.56
1:A:1032:GLN:HE22	1:A:1196:GLN:HB2	1.71	0.56
1:A:1007:VAL:O	1:A:1007:VAL:HG23	2.05	0.55
1:A:1108:ARG:HG2	1:A:1114:TYR:CZ	2.42	0.55
1:A:1133:ILE:HG13	1:A:1135:PRO:HD3	1.88	0.55
1:A:752:ALA:HB2	1:A:780:LEU:HB2	1.89	0.55
1:A:987:LEU:HD12	1:A:993:LEU:HB2	1.88	0.55
1:A:905:THR:HG22	1:A:907:GLU:H	1.71	0.54
1:A:872:SER:O	1:A:876:ARG:HB2	2.07	0.54
1:A:1019:ARG:HH12	1:A:1056:ASP:H	1.54	0.54
1:A:750:VAL:HG22	1:A:778:VAL:CG2	2.37	0.54
1:A:869:ALA:HB1	1:A:875:GLN:HG2	1.90	0.54
1:A:1105:GLU:HG2	1:A:1109:LYS:HD3	1.90	0.54
1:A:1148:LYS:O	1:A:1152:TRP:HD1	1.90	0.54
1:A:904:VAL:HG12	1:A:908:ALA:HB3	1.90	0.53
1:A:693:ILE:O	1:A:698:MET:HG2	2.09	0.53
1:A:732:LEU:O	1:A:736:ILE:HG13	2.09	0.53
1:A:733:GLU:N	1:A:734:PRO:CD	2.72	0.53
1:A:692:VAL:HG23	1:A:693:ILE:CD1	2.36	0.53
1:A:1087:MET:HE3	1:A:1087:MET:HA	1.91	0.52
1:A:1196:GLN:O	1:A:1200:VAL:HG23	2.09	0.52
1:A:749:MET:O	1:A:778:VAL:HG22	2.10	0.52
1:A:1148:LYS:O	1:A:1152:TRP:CD1	2.62	0.52
1:A:667:LEU:HB3	1:A:701:MET:HE2	1.92	0.52
1:A:680:GLU:O	1:A:683:ARG:HG2	2.10	0.52
1:A:1218:LEU:O	1:A:1222:LEU:HD13	2.10	0.52
1:A:776:GLU:C	1:A:777:ILE:HD12	2.35	0.52
1:A:1011:ILE:HB	1:A:1026:SER:HB3	1.93	0.51
1:A:950:PHE:HE2	1:A:976:LEU:HD13	1.75	0.51
1:A:1010:ASP:OD2	1:A:1206:ARG:HD2	2.11	0.51
1:A:1010:ASP:OD1	1:A:1027:HIS:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:ALA:HB1	1:A:691:GLU:HB2	1.93	0.51
1:A:1032:GLN:NE2	1:A:1196:GLN:HB2	2.26	0.51
1:A:1144:GLU:CD	1:A:1146:THR:HB	2.34	0.51
1:A:880:VAL:HG23	1:A:881:ALA:N	2.26	0.51
1:A:715:LEU:HB3	1:A:716:PRO:HD3	1.93	0.50
1:A:652:ALA:O	1:A:653:GLU:HB3	2.11	0.50
1:A:1152:TRP:CE3	1:A:1157:VAL:HB	2.45	0.50
1:A:926:ALA:HB1	1:A:1001:LEU:HD13	1.92	0.50
1:A:904:VAL:CG1	1:A:908:ALA:HB3	2.42	0.50
1:A:737:GLU:C	1:A:739:SER:H	2.20	0.50
1:A:759:HIS:CB	1:A:806:LEU:HD22	2.42	0.50
1:A:950:PHE:CE2	1:A:976:LEU:CD1	2.94	0.50
1:A:760:ASP:HB2	1:A:763:LYS:HE3	1.94	0.50
1:A:778:VAL:HG23	1:A:778:VAL:O	2.12	0.50
1:A:857:VAL:HG23	1:A:862:ARG:HG3	1.95	0.49
1:A:987:LEU:HD13	1:A:992:THR:CG2	2.36	0.49
1:A:737:GLU:HG3	1:A:738:ALA:N	2.28	0.49
1:A:750:VAL:HG21	1:A:793:ALA:HA	1.95	0.49
1:A:1013:ILE:CD1	1:A:1154:LEU:HD21	2.42	0.49
1:A:1172:TRP:HA	1:A:1173:PRO:C	2.37	0.49
1:A:857:VAL:CG2	1:A:862:ARG:HG3	2.42	0.49
1:A:960:TYR:CD1	1:A:961:PRO:HA	2.48	0.48
1:A:1107:VAL:HA	1:A:1111:TYR:HB2	1.95	0.48
1:A:1152:TRP:HZ3	1:A:1163:MET:O	1.97	0.48
1:A:888:GLU:C	1:A:890:VAL:H	2.21	0.48
1:A:1081:ASP:CG	1:A:1084:ASN:OD1	2.57	0.48
1:A:748:LYS:NZ	1:A:796:VAL:HB	2.29	0.47
1:A:906:LEU:HD22	1:A:1199:GLN:HA	1.95	0.47
1:A:978:LYS:HE3	1:A:982:ASP:OD1	2.14	0.47
1:A:950:PHE:CE2	1:A:976:LEU:HD11	2.49	0.47
1:A:912:ASN:O	1:A:1039:ALA:HB1	2.14	0.47
1:A:950:PHE:HZ	1:A:1087:MET:CE	2.15	0.47
1:A:946:ASP:O	1:A:949:PRO:HD2	2.14	0.47
1:A:1149:ALA:O	1:A:1153:GLU:HG3	2.15	0.47
1:A:1152:TRP:CE2	1:A:1165:LEU:HD13	2.49	0.47
1:A:753:THR:HG22	1:A:757:ASP:HB3	1.97	0.47
1:A:780:LEU:HD11	1:A:792:THR:HG21	1.95	0.47
1:A:869:ALA:HB1	1:A:875:GLN:CG	2.45	0.47
1:A:888:GLU:C	1:A:890:VAL:N	2.73	0.47
1:A:896:ARG:HG3	1:A:897:LYS:HG3	1.96	0.47
1:A:767:GLY:O	1:A:771:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:VAL:O	1:A:797:ASN:C	2.57	0.47
1:A:1108:ARG:HG2	1:A:1114:TYR:OH	2.15	0.47
1:A:1140:PRO:HB3	1:A:1191:ALA:HB2	1.96	0.46
1:A:904:VAL:HG21	1:A:1034:GLU:HA	1.97	0.46
1:A:921:TYR:CE2	1:A:923:PRO:HG3	2.50	0.46
1:A:652:ALA:HB3	1:A:655:ARG:CG	2.45	0.46
1:A:676:GLU:HB2	1:A:677:GLN:NE2	2.31	0.46
1:A:792:THR:O	1:A:796:VAL:HG22	2.16	0.46
1:A:877:ASP:O	1:A:880:VAL:HG22	2.14	0.46
1:A:1198:ASP:OD1	1:A:1199:GLN:N	2.48	0.46
1:A:739:SER:C	1:A:740:LYS:HG2	2.40	0.46
1:A:950:PHE:HB2	1:A:1094:ARG:HD2	1.97	0.46
1:A:733:GLU:CG	1:A:734:PRO:HD3	2.46	0.46
1:A:898:LYS:HA	1:A:899:PRO:HD3	1.83	0.46
1:A:1200:VAL:HG13	1:A:1214:VAL:HG23	1.97	0.46
1:A:657:TRP:HB3	1:A:661:LYS:CE	2.34	0.45
1:A:683:ARG:NH2	1:A:689:PRO:HG3	2.31	0.45
1:A:1005:ASN:OD1	1:A:1019:ARG:NH1	2.45	0.45
1:A:880:VAL:O	1:A:884:ARG:HG3	2.17	0.45
1:A:1013:ILE:HD13	1:A:1154:LEU:HD21	1.98	0.45
1:A:953:THR:HG23	2:A:1301:B12:H3P3	1.99	0.45
1:A:987:LEU:HA	1:A:992:THR:CG2	2.47	0.45
1:A:692:VAL:HG23	1:A:693:ILE:N	2.32	0.45
1:A:733:GLU:HG2	1:A:734:PRO:HD3	1.99	0.45
1:A:719:VAL:CG2	1:A:1083:TYR:HD1	2.31	0.44
1:A:1144:GLU:HG3	1:A:1203:TYR:OH	2.18	0.44
1:A:904:VAL:HG12	1:A:905:THR:N	2.31	0.44
1:A:651:GLN:NE2	1:A:651:GLN:N	2.66	0.44
1:A:651:GLN:O	1:A:652:ALA:CB	2.66	0.44
1:A:1099:PHE:HD1	1:A:1099:PHE:O	2.00	0.44
1:A:740:LYS:O	1:A:741:GLU:HB2	2.18	0.44
1:A:848:GLN:NE2	1:A:891:ARG:HD3	2.33	0.44
1:A:1194:GLN:HG3	1:A:1222:LEU:O	2.18	0.43
1:A:719:VAL:HG23	1:A:1083:TYR:HD1	1.83	0.43
1:A:742:GLN:HE21	1:A:742:GLN:N	2.16	0.43
1:A:847:GLU:OE2	1:A:891:ARG:NH2	2.51	0.43
1:A:1009:ASP:HB2	1:A:1206:ARG:HH12	1.83	0.43
1:A:799:ASP:O	1:A:800:LEU:HD12	2.18	0.43
1:A:986:LYS:O	1:A:990:GLU:HG3	2.18	0.43
1:A:720:LYS:HE3	1:A:1083:TYR:CZ	2.53	0.43
1:A:1134:ARG:HA	1:A:1180:TRP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:PRO:HB3	1:A:1191:ALA:CB	2.48	0.42
1:A:1184:HIS:ND1	1:A:1185:PRO:HD2	2.34	0.42
1:A:1078:ALA:C	1:A:1080:HIS:H	2.28	0.42
1:A:1200:VAL:HG21	1:A:1224:TYR:OH	2.19	0.42
1:A:716:PRO:O	1:A:719:VAL:HG22	2.20	0.42
1:A:1103:LEU:O	1:A:1107:VAL:HG23	2.19	0.42
1:A:858:GLN:CD	1:A:858:GLN:H	2.27	0.42
1:A:1194:GLN:NE2	1:A:1220:PRO:O	2.52	0.42
1:A:764:ASN:O	1:A:768:VAL:HG23	2.20	0.42
1:A:1193:ALA:O	1:A:1221:ASN:HB3	2.19	0.42
1:A:898:LYS:HE3	1:A:900:ARG:HH21	1.84	0.42
1:A:876:ARG:NH2	1:A:877:ASP:OD1	2.53	0.42
1:A:1091:LEU:HD12	1:A:1091:LEU:HA	1.82	0.42
1:A:1068:GLU:OE1	1:A:1068:GLU:N	2.51	0.42
1:A:733:GLU:O	1:A:737:GLU:HG2	2.20	0.42
1:A:999:VAL:HG22	1:A:1000:GLY:N	2.34	0.42
1:A:987:LEU:HD12	1:A:993:LEU:CB	2.50	0.41
1:A:754:VAL:CG1	1:A:813:GLU:HB3	2.49	0.41
1:A:1067:LEU:HD11	1:A:1161:THR:O	2.20	0.41
1:A:894:HIS:O	1:A:895:GLY:C	2.63	0.41
1:A:930:GLY:O	1:A:1000:GLY:HA2	2.19	0.41
1:A:811:LEU:HD13	1:A:841:HIS:CD2	2.56	0.41
1:A:700:GLY:O	1:A:703:VAL:HB	2.21	0.41
1:A:716:PRO:HG3	1:A:954:TRP:HB3	2.03	0.41
1:A:856:TYR:CE2	1:A:858:GLN:NE2	2.89	0.41
1:A:675:ILE:O	1:A:679:THR:HG22	2.21	0.41
1:A:1183:SER:O	1:A:1184:HIS:C	2.64	0.41
1:A:760:ASP:HB3	1:A:782:VAL:CG1	2.51	0.40
1:A:914:PHE:CE2	1:A:916:PHE:HB2	2.56	0.40
1:A:919:GLN:HA	1:A:1054:LYS:NZ	2.36	0.40
1:A:925:VAL:HA	1:A:1057:TYR:CE2	2.55	0.40
1:A:687:THR:N	1:A:691:GLU:OE1	2.49	0.40
1:A:1074:ASP:O	1:A:1077:GLU:HB3	2.21	0.40
1:A:699:ASP:O	1:A:703:VAL:HG23	2.20	0.40
1:A:714:PHE:O	1:A:718:VAL:HG23	2.21	0.40
1:A:693:ILE:HD11	1:A:732:LEU:HD22	2.03	0.40
1:A:900:ARG:O	1:A:901:THR:HB	2.21	0.40
1:A:1152:TRP:CZ3	1:A:1163:MET:O	2.74	0.40
1:A:821:MET:HE2	1:A:850:TYR:CZ	2.56	0.40
1:A:902:PRO:HA	1:A:903:PRO:HD3	1.87	0.40
1:A:1048:ALA:HA	1:A:1049:PRO:HD3	1.92	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	574/579 (99%)	523 (91%)	38 (7%)	13 (2%)	5	13

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	652	ALA
1	A	743	CYS
1	A	797	ASN
1	A	898	LYS
1	A	901	THR
1	A	754	VAL
1	A	1144	GLU
1	A	740	LYS
1	A	848	GLN
1	A	899	PRO
1	A	1028	HIS
1	A	1079	GLN
1	A	741	GLU

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	482/484 (100%)	465 (96%)	17 (4%)	32	61

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	651	GLN
1	A	663	LEU
1	A	672	THR
1	A	732	LEU
1	A	740	LYS
1	A	742	GLN
1	A	808	THR
1	A	877	ASP
1	A	964	LEU
1	A	967	GLU
1	A	1084	ASN
1	A	1091	LEU
1	A	1095	LEU
1	A	1140	PRO
1	A	1144	GLU
1	A	1188	LYS
1	A	1222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	651	GLN
1	A	727	GLN
1	A	742	GLN
1	A	774	ASN
1	A	848	GLN
1	A	893	GLN
1	A	912	ASN
1	A	1040	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	B12	A	1301	-	94,101,101	2.69	41 (43%)	149,166,166	2.63	57 (38%)
4	NO3	A	1306	-	1,3,3	0.38	0	0,3,3	-	-
4	NO3	A	1304	-	1,3,3	0.37	0	0,3,3	-	-
3	SAH	A	1401	-	27,28,28	1.02	3 (11%)	36,40,40	1.90	9 (25%)
4	NO3	A	1305	-	1,3,3	0.35	0	0,3,3	-	-
4	NO3	A	1303	-	1,3,3	0.33	0	0,3,3	-	-

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	B12	A	1301	-	2/2/36/38	16/56/223/223	0/3/11/11
3	SAH	A	1401	-	-	0/15/31/31	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	B12	C7B-C6B	8.54	1.51	1.39
2	A	1301	B12	C7B-C8B	7.62	1.52	1.39
2	A	1301	B12	C8B-C9B	6.52	1.50	1.40
2	A	1301	B12	C3-C4	5.40	1.65	1.51
2	A	1301	B12	C6-C5	4.89	1.50	1.36
2	A	1301	B12	C1-C19	-4.87	1.44	1.55
2	A	1301	B12	C60-C18	4.74	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	B12	C14-N23	4.48	1.41	1.35
2	A	1301	B12	C4B-C5B	4.31	1.45	1.39
2	A	1301	B12	C54-C17	4.24	1.61	1.54
2	A	1301	B12	C36-C7	4.23	1.61	1.54
2	A	1301	B12	C55-C56	4.11	1.62	1.53
2	A	1301	B12	C25-C2	4.09	1.62	1.54
2	A	1301	B12	C12-C11	3.96	1.59	1.52
2	A	1301	B12	C48-C13	3.67	1.62	1.54
2	A	1301	B12	C4B-C9B	3.36	1.45	1.40
2	A	1301	B12	C7-C6	3.27	1.62	1.54
2	A	1301	B12	C6B-C5B	3.24	1.48	1.40
2	A	1301	B12	C13-C14	3.15	1.58	1.52
2	A	1301	B12	C43-N45	-3.04	1.22	1.32
3	A	1401	SAH	C5-N7	-3.02	1.33	1.39
2	A	1301	B12	O6R-C4R	2.96	1.51	1.45
2	A	1301	B12	C61-N62	-2.95	1.23	1.32
2	A	1301	B12	C30-C31	-2.92	1.44	1.52
2	A	1301	B12	C55-C17	2.90	1.61	1.54
2	A	1301	B12	O6R-C1R	2.85	1.48	1.42
2	A	1301	B12	C38-N40	-2.82	1.23	1.32
2	A	1301	B12	C32-N33	-2.79	1.23	1.32
2	A	1301	B12	C1-C2	2.79	1.65	1.58
2	A	1301	B12	C17-C16	2.75	1.61	1.54
2	A	1301	B12	C27-N29	-2.74	1.23	1.32
2	A	1301	B12	O8R-C5R	-2.72	1.31	1.42
2	A	1301	B12	C53-C15	2.66	1.56	1.50
2	A	1301	B12	O3-C2P	-2.55	1.39	1.45
2	A	1301	B12	C37-C7	2.52	1.64	1.56
2	A	1301	B12	O58-C57	2.52	1.28	1.23
2	A	1301	B12	C50-N52	-2.51	1.24	1.32
2	A	1301	B12	C30-C3	2.32	1.59	1.54
3	A	1401	SAH	C8-N9	-2.26	1.33	1.37
2	A	1301	B12	C18-C19	2.21	1.58	1.53
2	A	1301	B12	C48-C49	2.14	1.59	1.52
2	A	1301	B12	C20-C1	2.11	1.57	1.53
3	A	1401	SAH	C4-N9	-2.05	1.33	1.37
2	A	1301	B12	O2-C3R	2.04	1.51	1.44

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	B12	C30-C3-C4	8.84	130.39	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	B12	C19-N24-C16	7.68	115.68	107.29
2	A	1301	B12	C48-C13-C14	7.20	126.39	108.51
2	A	1301	B12	C3-C4-N21	-6.74	103.61	111.98
2	A	1301	B12	C1-C19-C18	6.48	132.42	121.90
2	A	1301	B12	C9B-C8B-N1B	-5.75	102.76	105.30
2	A	1301	B12	C2-C3-C4	5.55	107.89	101.64
3	A	1401	SAH	C5-C4-N3	-5.37	119.32	126.72
2	A	1301	B12	C1-C19-N24	5.37	112.22	106.25
2	A	1301	B12	C9-N22-C6	5.29	111.64	105.28
2	A	1301	B12	C2-C26-C27	5.24	129.75	115.19
2	A	1301	B12	C17-C18-C19	5.03	109.99	102.36
2	A	1301	B12	C7-C6-C5	4.93	135.78	128.07
2	A	1301	B12	C48-C13-C12	4.53	129.47	116.52
2	A	1301	B12	C49-C48-C13	4.51	127.44	114.65
2	A	1301	B12	C41-C8-C7	4.45	126.44	114.19
3	A	1401	SAH	N3-C2-N1	-4.45	121.84	128.58
2	A	1301	B12	C3-C4-C5	4.10	130.69	123.82
2	A	1301	B12	O3-C2P-C1P	-4.02	98.99	106.94
2	A	1301	B12	C17-C16-N24	-3.92	105.18	111.17
2	A	1301	B12	O6R-C4R-C5R	3.90	117.47	109.22
2	A	1301	B12	C56-C55-C17	3.89	123.09	115.58
2	A	1301	B12	C2-C1-C19	3.89	124.66	118.61
2	A	1301	B12	C31-C30-C3	3.84	125.53	114.65
2	A	1301	B12	C41-C8-C9	-3.74	104.66	111.19
2	A	1301	B12	C20-C1-N21	-3.73	104.10	110.26
3	A	1401	SAH	N3-C4-N9	3.72	133.50	127.17
2	A	1301	B12	O34-C32-C31	-3.71	109.83	121.04
3	A	1401	SAH	C2-N3-C4	3.56	120.54	111.83
2	A	1301	B12	C31-C32-N33	3.55	127.89	116.49
2	A	1301	B12	C7-C37-C38	3.49	124.60	114.28
2	A	1301	B12	O6R-C1R-N1B	3.47	114.76	108.09
2	A	1301	B12	C55-C17-C16	-3.44	109.86	116.59
2	A	1301	B12	C2R-C1R-N1B	3.37	121.68	113.30
2	A	1301	B12	O58-C57-N59	3.33	129.56	123.03
2	A	1301	B12	C56-C57-N59	-3.32	110.30	116.34
2	A	1301	B12	C5M-C5B-C4B	-3.17	113.98	119.57
2	A	1301	B12	C60-C18-C19	3.15	122.78	114.59
2	A	1301	B12	C9-C10-C11	3.14	130.45	125.97
2	A	1301	B12	C3R-C2R-C1R	2.98	106.45	99.89
2	A	1301	B12	C7B-C8B-N1B	2.94	137.21	131.39
3	A	1401	SAH	N9-C8-N7	-2.94	109.77	113.94
2	A	1301	B12	C20-C1-C19	-2.90	106.56	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1401	SAH	C4-C5-N7	-2.79	107.39	110.58
2	A	1301	B12	C1R-N1B-C2B	-2.78	120.94	127.09
2	A	1301	B12	C25-C2-C26	-2.74	104.30	109.74
3	A	1401	SAH	C5-N7-C8	2.74	107.75	103.45
2	A	1301	B12	C17-C16-C15	2.70	130.53	126.26
3	A	1401	SAH	C2'-C3'-C4'	-2.68	97.43	102.61
2	A	1301	B12	C13-C14-N23	-2.66	105.49	109.09
2	A	1301	B12	O7R-C2R-C3R	2.53	118.26	111.19
2	A	1301	B12	C18-C17-C16	2.50	103.70	100.69
2	A	1301	B12	C7-C6-N22	-2.41	103.54	107.94
2	A	1301	B12	O2-P-O3	-2.41	96.14	102.87
2	A	1301	B12	C48-C49-C50	2.41	120.73	112.55
2	A	1301	B12	C30-C31-C32	-2.32	104.66	112.55
2	A	1301	B12	C26-C2-C3	-2.27	103.47	107.42
2	A	1301	B12	C13-C14-C15	2.26	127.76	124.32
2	A	1301	B12	C47-C12-C46	-2.26	105.66	109.41
2	A	1301	B12	C16-C15-C14	-2.18	117.94	121.26
2	A	1301	B12	C49-C50-N52	2.16	123.41	116.49
2	A	1301	B12	C25-C2-C3	2.16	118.39	112.91
2	A	1301	B12	C5-C6-N22	-2.12	120.68	123.88
3	A	1401	SAH	C4-N9-C8	2.07	107.91	105.74
2	A	1301	B12	C7B-C8B-C9B	-2.06	120.01	122.47
2	A	1301	B12	C4B-C5B-C6B	2.05	122.69	119.69

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1301	B12	C3
2	A	1301	B12	C13

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	B12	C42-C41-C8-C7
2	A	1301	B12	C42-C41-C8-C9
2	A	1301	B12	C2P-O3-P-O5
2	A	1301	B12	C2P-O3-P-O2
2	A	1301	B12	C3-C30-C31-C32
2	A	1301	B12	C12-C13-C48-C49
2	A	1301	B12	C14-C13-C48-C49
2	A	1301	B12	C2-C3-C30-C31
2	A	1301	B12	C30-C31-C32-O34

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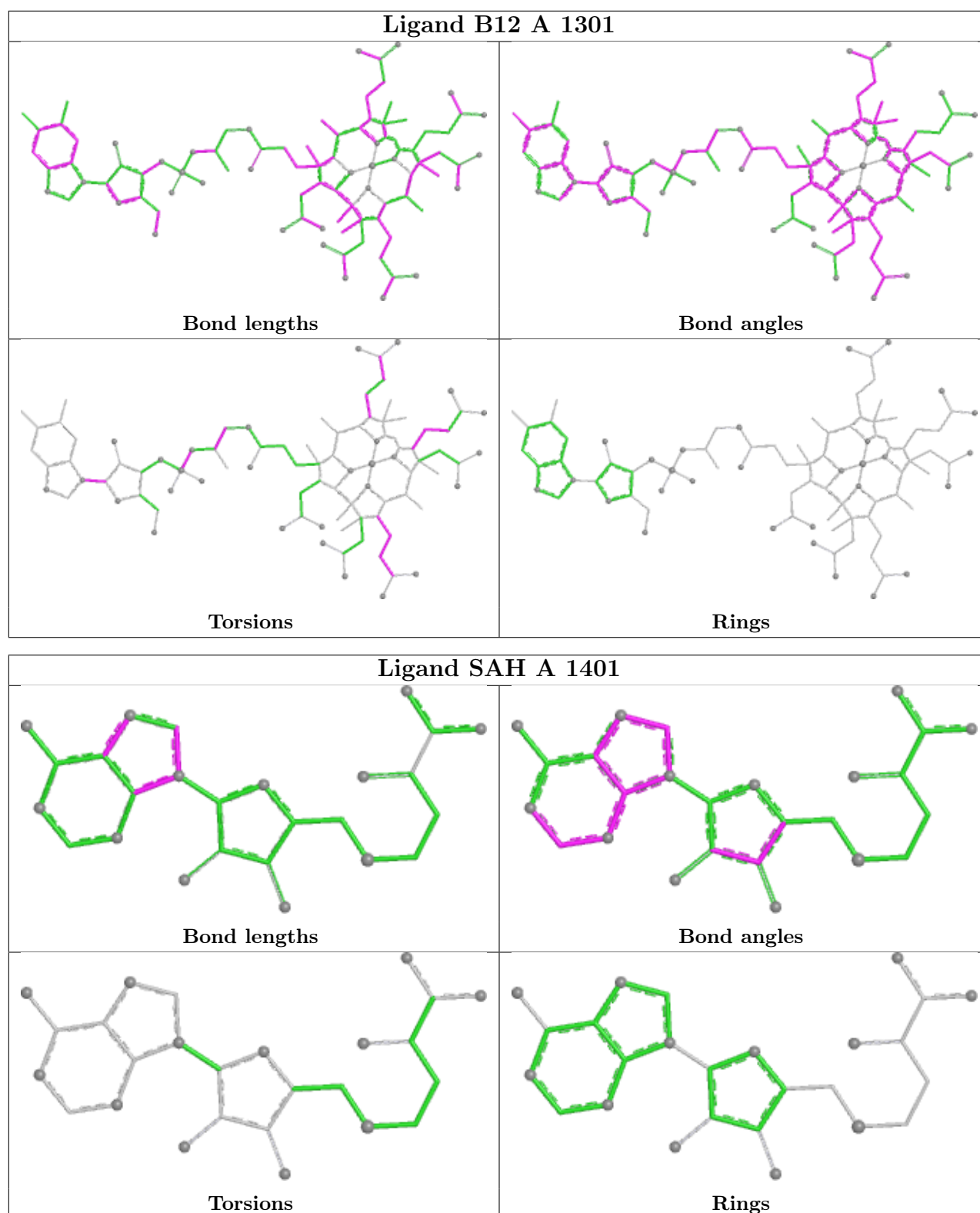
Mol	Chain	Res	Type	Atoms
2	A	1301	B12	N59-C1P-C2P-O3
2	A	1301	B12	C30-C31-C32-N33
2	A	1301	B12	C2R-C1R-N1B-C8B
2	A	1301	B12	O6R-C1R-N1B-C8B
2	A	1301	B12	C8-C41-C42-C43
2	A	1301	B12	C2P-O3-P-O4
2	A	1301	B12	C48-C49-C50-N52

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	B12	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	576/579 (99%)	0.67	68 (11%) 9 7	27, 69, 139, 181	2 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1121	SER	5.1
1	A	1226	ALA	4.4
1	A	898	LYS	3.9
1	A	1106	ARG	3.9
1	A	892	ILE	3.8
1	A	899	PRO	3.7
1	A	675	ILE	3.6
1	A	889	THR	3.5
1	A	903	PRO	3.4
1	A	897	LYS	3.3
1	A	901	THR	3.2
1	A	693	ILE	3.2
1	A	745	THR	3.1
1	A	800	LEU	3.0
1	A	887	TYR	2.9
1	A	880	VAL	2.9
1	A	732	LEU	2.9
1	A	860	ALA	2.9
1	A	871	LEU	2.8
1	A	740	LYS	2.8
1	A	896	ARG	2.8
1	A	1193	ALA	2.8
1	A	894	HIS	2.7
1	A	815	VAL	2.7
1	A	678	ASP	2.7
1	A	885	LYS	2.7
1	A	905	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	677	GLN	2.6
1	A	827	THR	2.6
1	A	674	PHE	2.6
1	A	867	VAL	2.6
1	A	734	PRO	2.5
1	A	825	GLY	2.5
1	A	735	PHE	2.5
1	A	893	GLN	2.5
1	A	689	PRO	2.4
1	A	687	THR	2.4
1	A	690	CYS	2.4
1	A	743	CYS	2.4
1	A	729	VAL	2.4
1	A	652	ALA	2.4
1	A	823	ARG	2.4
1	A	1222	LEU	2.4
1	A	1192	VAL	2.4
1	A	881	ALA	2.4
1	A	863	THR	2.3
1	A	794	LYS	2.3
1	A	891	ARG	2.3
1	A	832	ILE	2.3
1	A	884	ARG	2.3
1	A	1223	GLY	2.3
1	A	870	LEU	2.3
1	A	798	ALA	2.2
1	A	738	ALA	2.2
1	A	679	THR	2.2
1	A	848	GLN	2.2
1	A	952	MET	2.2
1	A	671	ILE	2.2
1	A	904	VAL	2.2
1	A	676	GLU	2.1
1	A	888	GLU	2.1
1	A	755	LYS	2.1
1	A	754	VAL	2.1
1	A	895	GLY	2.1
1	A	828	ILE	2.1
1	A	797	ASN	2.1
1	A	1224	TYR	2.1
1	A	879	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

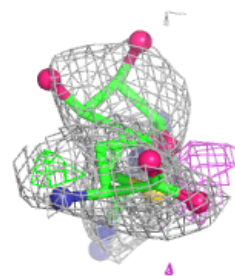
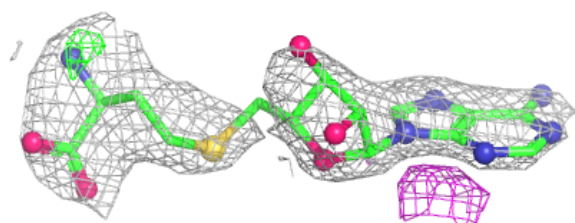
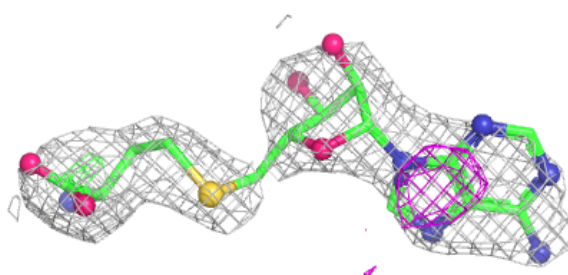
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NO3	A	1306	4/4	0.58	0.11	146,147,147,147	0
4	NO3	A	1303	4/4	0.65	0.20	124,124,125,125	0
4	NO3	A	1305	4/4	0.81	0.16	121,122,122,123	0
3	SAH	A	1401	26/26	0.81	0.23	115,117,118,119	0
4	NO3	A	1304	4/4	0.90	0.15	120,120,120,120	0
2	B12	A	1301	91/91	0.93	0.14	59,81,89,95	0

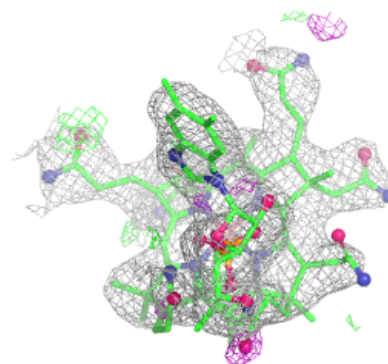
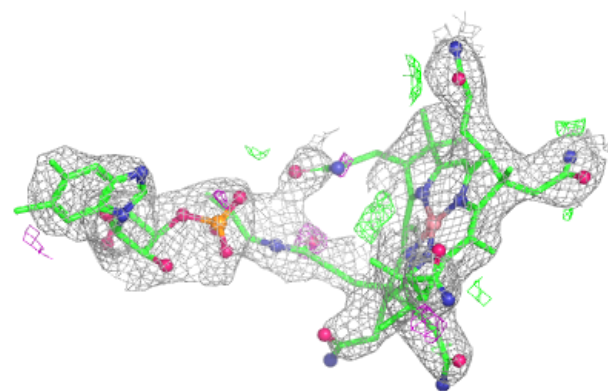
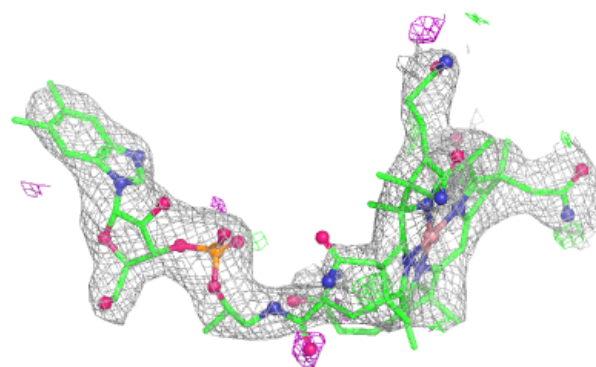
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAH A 1401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around B12 A 1301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.