



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 04:29 AM EDT

PDB ID : 1K7Y  
Title : E. coli MetH C-terminal fragment (649-1227)  
Authors : Bandarian, V.; Patridge, K.A.; Lennon, B.W.; Huddler, D.P.; Matthews, R.G.; Ludwig, M.L.  
Deposited on : 2001-10-22  
Resolution : 3.00 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

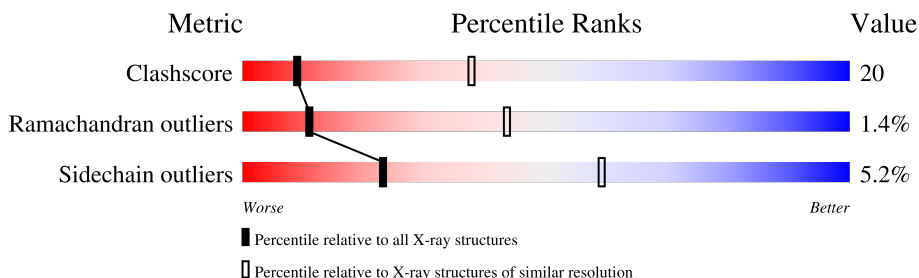
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	577	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4749 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	577	4566	2888	787	874	17	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	759	GLY	HIS	engineered mutation	UNP P13009

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



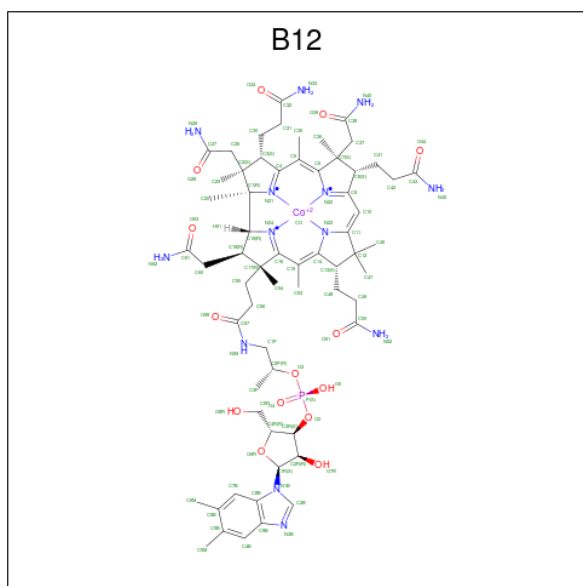
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



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

- Molecule 4 is water.

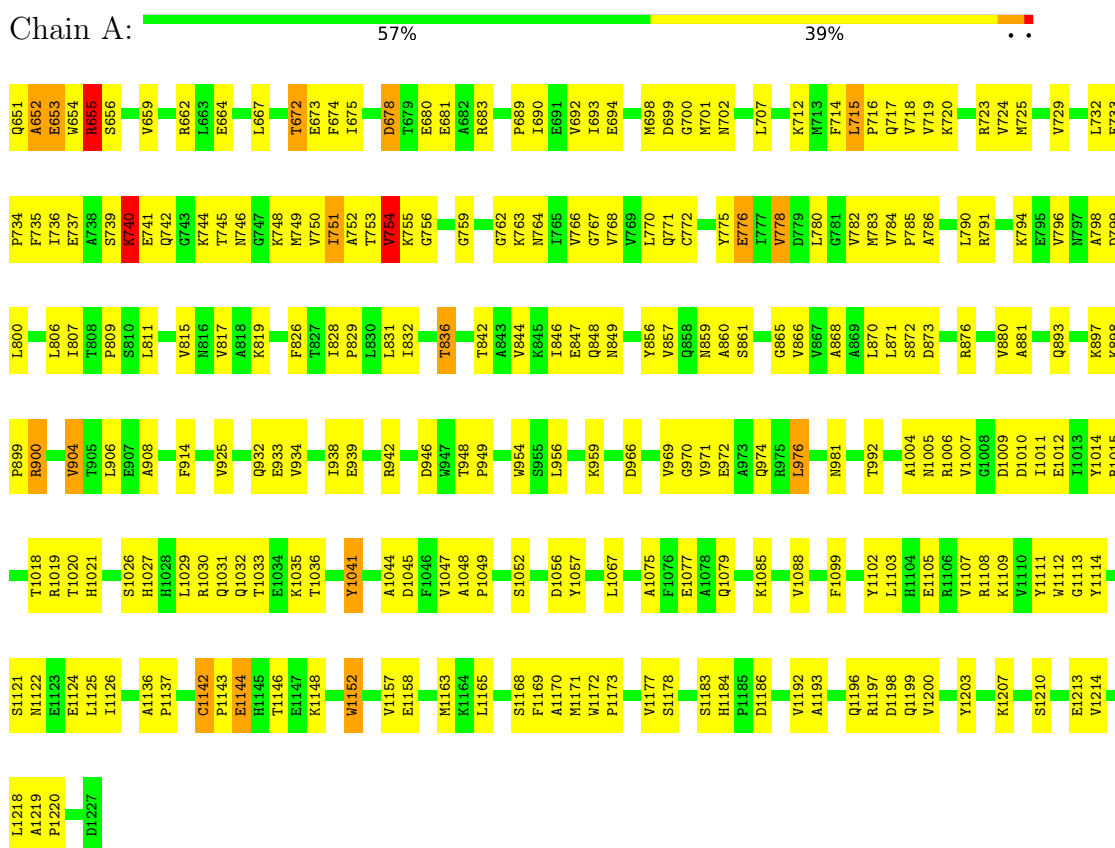
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		

### 3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

- Molecule 1: methionine synthase



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.72Å 109.72Å 148.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00	Depositor
% Data completeness (in resolution range)	98.0 (15.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

## 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: SO4, B12

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	0.41	0/4664	0.61	0/6326

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 [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	4566	0	4484	187	0
2	A	50	0	0	0	0
3	A	91	0	75	6	0
4	A	42	0	0	2	0
All	All	4749	0	4559	187	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 20.

All (187) 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:752:ALA:HB1	1:A:784:VAL:HG11	1.40	1.01
1:A:655:ARG:HH11	1:A:655:ARG:HB3	1.39	0.88
1:A:1178:SER:H	3:A:1248:B12:H402	1.20	0.88
1:A:946:ASP:HB2	1:A:1126:ILE:HD11	1.53	0.87
1:A:1031:GLN:HE22	1:A:1041:TYR:HD2	1.29	0.80
1:A:946:ASP:HB2	1:A:1126:ILE:CD1	2.12	0.79
1:A:1031:GLN:NE2	1:A:1041:TYR:HD2	1.82	0.78
1:A:1219:ALA:HB3	1:A:1220:PRO:HD3	1.67	0.77
1:A:906:LEU:HD22	1:A:1199:GLN:HA	1.67	0.76
1:A:904:VAL:HG13	1:A:908:ALA:HB3	1.69	0.74
1:A:859:ASN:ND2	1:A:861:SER:HB3	2.03	0.74
1:A:956:LEU:HG	1:A:969:VAL:HG21	1.71	0.73
1:A:942:ARG:HH21	1:A:981:ASN:HD22	1.38	0.72
1:A:1032:GLN:NE2	1:A:1196:GLN:HB2	2.06	0.71
1:A:1032:GLN:HE22	1:A:1196:GLN:HB2	1.57	0.69
1:A:1011:ILE:HD11	1:A:1044:ALA:HA	1.75	0.69
1:A:751:ILE:HD12	1:A:763:LYS:HG3	1.73	0.68
1:A:971:VAL:HA	1:A:974:GLN:NE2	2.08	0.68
1:A:1018:THR:OG1	1:A:1020:THR:HG23	1.94	0.67
1:A:807:ILE:HG13	1:A:809:PRO:HD2	1.76	0.67
1:A:1152:TRP:CZ2	1:A:1157:VAL:HG11	2.31	0.66
1:A:1049:PRO:HG2	1:A:1052:SER:HB3	1.78	0.65
1:A:956:LEU:HG	1:A:969:VAL:CG2	2.28	0.64
1:A:699:ASP:HA	1:A:702:ASN:HD22	1.64	0.63
1:A:800:LEU:HD12	1:A:831:LEU:HD13	1.79	0.63
1:A:914:PHE:HB3	1:A:1045:ASP:HB3	1.80	0.63
1:A:740:LYS:HD3	1:A:740:LYS:H	1.65	0.62
1:A:1210:SER:OG	1:A:1213:GLU:HB2	2.00	0.61
1:A:694:GLU:HA	1:A:698:MET:HB2	1.81	0.61
1:A:1184:HIS:CD2	1:A:1186:ASP:HB2	2.36	0.60
1:A:842:THR:HG21	1:A:856:TYR:HB2	1.83	0.60
1:A:764:ASN:O	1:A:768:VAL:HG23	2.01	0.60
1:A:857:VAL:HG22	1:A:866:VAL:HG21	1.84	0.59
1:A:1077:GLU:HG2	1:A:1085:LYS:HD3	1.82	0.59
1:A:942:ARG:NH2	1:A:981:ASN:HD22	1.99	0.59
1:A:689:PRO:O	1:A:692:VAL:HG22	2.02	0.59
1:A:759:GLY:HA3	1:A:806:LEU:HD22	1.84	0.59
1:A:667:LEU:HD22	1:A:724:VAL:HB	1.84	0.58
1:A:1184:HIS:NE2	1:A:1186:ASP:HB2	2.19	0.57
1:A:750:VAL:HA	1:A:778:VAL:HG13	1.88	0.56
1:A:766:VAL:HG21	3:A:1248:B12:C8B	2.35	0.56
1:A:737:GLU:HA	1:A:742:GLN:OE1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:TRP:CG	1:A:976:LEU:HD11	2.40	0.56
1:A:866:VAL:HG12	1:A:870:LEU:HD22	1.87	0.56
1:A:745:THR:HG22	1:A:746:ASN:N	2.21	0.56
1:A:655:ARG:HB3	1:A:655:ARG:NH1	2.17	0.56
1:A:1033:THR:O	1:A:1035:LYS:HG2	2.07	0.55
1:A:811:LEU:O	1:A:815:VAL:HG23	2.07	0.55
1:A:719:VAL:HG11	1:A:954:TRP:HZ3	1.71	0.55
1:A:1075:ALA:O	1:A:1079:GLN:HG2	2.06	0.55
1:A:1112:TRP:CZ2	1:A:1183:SER:HB3	2.42	0.55
1:A:1203:TYR:CE2	1:A:1207:LYS:HG3	2.42	0.55
1:A:662:ARG:HB3	1:A:678:ASP:OD2	2.07	0.54
1:A:672:THR:HG23	1:A:724:VAL:HG22	1.88	0.54
1:A:938:ILE:O	1:A:942:ARG:HG3	2.07	0.54
1:A:970:GLY:O	1:A:974:GLN:HG3	2.08	0.54
1:A:753:THR:HB	1:A:782:VAL:HA	1.90	0.54
1:A:1077:GLU:HG2	1:A:1085:LYS:CD	2.37	0.54
1:A:925:VAL:HG13	1:A:1057:TYR:OH	2.08	0.54
1:A:1107:VAL:HA	1:A:1111:TYR:HB2	1.90	0.54
1:A:725:MET:O	1:A:729:VAL:HG23	2.08	0.53
1:A:1121:SER:OG	1:A:1124:GLU:HG3	2.07	0.53
1:A:807:ILE:CG1	1:A:809:PRO:HD2	2.38	0.53
1:A:811:LEU:HD21	1:A:836:THR:HB	1.90	0.53
1:A:732:LEU:HB3	1:A:736:ILE:HG13	1.89	0.53
1:A:754:VAL:HG13	1:A:755:LYS:N	2.23	0.52
1:A:1152:TRP:CD1	1:A:1157:VAL:HB	2.44	0.52
1:A:715:LEU:HB3	1:A:716:PRO:HD3	1.91	0.51
1:A:946:ASP:O	1:A:949:PRO:HD2	2.10	0.51
1:A:664:GLU:HG3	1:A:700:GLY:CA	2.40	0.51
1:A:767:GLY:O	1:A:771:GLN:HG3	2.11	0.51
1:A:872:SER:O	1:A:876:ARG:HB2	2.09	0.51
1:A:750:VAL:HG22	1:A:778:VAL:CG1	2.40	0.51
1:A:898:LYS:HG3	1:A:900:ARG:HD3	1.92	0.51
1:A:898:LYS:O	1:A:900:ARG:N	2.44	0.50
1:A:707:LEU:HD22	1:A:712:LYS:HD3	1.94	0.50
1:A:740:LYS:HD3	1:A:740:LYS:N	2.26	0.50
1:A:762:GLY:O	1:A:766:VAL:HG23	2.12	0.50
1:A:1006:ARG:HG2	1:A:1007:VAL:N	2.27	0.50
1:A:733:GLU:HB2	1:A:734:PRO:CD	2.42	0.49
1:A:737:GLU:C	1:A:739:SER:H	2.15	0.49
1:A:1144:GLU:OE2	1:A:1207:LYS:HE2	2.12	0.49
1:A:1157:VAL:CG1	1:A:1163:MET:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:THR:HB	1:A:949:PRO:HD3	1.93	0.49
1:A:651:GLN:O	1:A:652:ALA:HB2	2.13	0.49
1:A:842:THR:HG22	1:A:842:THR:O	2.12	0.49
1:A:790:LEU:O	1:A:791:ARG:C	2.51	0.49
1:A:865:GLY:O	1:A:868:ALA:HB3	2.12	0.49
1:A:1144:GLU:HG3	1:A:1203:TYR:OH	2.12	0.49
1:A:799:ASP:HB3	1:A:871:LEU:HD21	1.94	0.49
1:A:1109:LYS:O	1:A:1113:GLY:HA2	2.13	0.48
1:A:714:PHE:HD2	1:A:972:GLU:HG3	1.78	0.48
1:A:1142:CYS:HB2	4:A:328:HOH:O	2.13	0.48
1:A:1048:ALA:HB3	1:A:1056:ASP:HB2	1.96	0.48
1:A:1014:TYR:CD2	1:A:1019:ARG:HG2	2.48	0.48
1:A:659:VAL:HG21	1:A:681:GLU:HB3	1.96	0.48
1:A:859:ASN:HD21	1:A:861:SER:HB3	1.76	0.48
1:A:672:THR:C	1:A:673:GLU:HG3	2.34	0.47
1:A:749:MET:CE	1:A:831:LEU:HD22	2.45	0.47
1:A:753:THR:O	1:A:784:VAL:HG12	2.14	0.47
1:A:1067:LEU:HA	1:A:1173:PRO:HG2	1.96	0.47
1:A:1144:GLU:HG3	1:A:1203:TYR:CE2	2.49	0.47
1:A:714:PHE:O	1:A:718:VAL:HG23	2.14	0.47
1:A:786:ALA:HB2	1:A:817:VAL:HG22	1.96	0.47
1:A:1009:ASP:OD1	1:A:1030:ARG:NH2	2.40	0.47
1:A:719:VAL:HG23	1:A:768:VAL:HG11	1.97	0.47
1:A:1015:ARG:NH2	1:A:1021:HIS:CD2	2.83	0.47
1:A:1144:GLU:HG3	1:A:1203:TYR:CZ	2.50	0.47
1:A:1171:MET:N	3:A:1248:B12:O44	2.44	0.47
1:A:729:VAL:O	1:A:732:LEU:N	2.47	0.47
1:A:752:ALA:HB2	1:A:780:LEU:HB2	1.97	0.46
1:A:859:ASN:HD22	1:A:861:SER:HB3	1.78	0.46
1:A:1157:VAL:HG12	1:A:1163:MET:HB2	1.98	0.46
1:A:756:GLY:O	1:A:1168:SER:HB3	2.16	0.46
1:A:720:LYS:HG2	1:A:723:ARG:HH21	1.81	0.46
1:A:1011:ILE:HD12	1:A:1047:VAL:HG21	1.97	0.46
1:A:680:GLU:O	1:A:683:ARG:HB3	2.15	0.46
1:A:748:LYS:NZ	1:A:796:VAL:HG22	2.30	0.46
1:A:828:ILE:HB	1:A:829:PRO:HD2	1.97	0.46
1:A:897:LYS:HA	1:A:900:ARG:HH21	1.81	0.46
1:A:689:PRO:HG2	1:A:735:PHE:O	2.16	0.45
1:A:654:TRP:C	1:A:656:SER:H	2.18	0.45
1:A:948:THR:HG23	1:A:959:LYS:HA	1.98	0.45
1:A:770:LEU:O	1:A:775:TYR:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:HIS:CD2	1:A:1186:ASP:H	2.34	0.45
1:A:1108:ARG:HG2	1:A:1114:TYR:OH	2.17	0.45
1:A:701:MET:HE1	1:A:772:CYS:HB3	1.99	0.45
1:A:1146:THR:HG22	1:A:1169:PHE:CE2	2.53	0.44
1:A:880:VAL:HG23	1:A:881:ALA:N	2.32	0.44
1:A:672:THR:O	1:A:673:GLU:HG3	2.17	0.44
1:A:954:TRP:CD1	1:A:976:LEU:HD11	2.53	0.44
1:A:819:LYS:HG3	1:A:849:ASN:HB3	2.00	0.44
1:A:1007:VAL:HG23	1:A:1007:VAL:O	2.18	0.44
1:A:860:ALA:H	3:A:1248:B12:H5R1	1.81	0.44
1:A:1178:SER:N	3:A:1248:B12:H402	2.01	0.44
1:A:1010:ASP:OD2	1:A:1027:HIS:ND1	2.51	0.44
1:A:1165:LEU:HA	1:A:1170:ALA:O	2.18	0.44
1:A:748:LYS:HE2	1:A:776:GLU:OE1	2.16	0.44
1:A:716:PRO:O	1:A:720:LYS:HB2	2.17	0.44
1:A:1152:TRP:CE2	1:A:1157:VAL:HG11	2.52	0.43
1:A:966:ASP:O	1:A:970:GLY:HA3	2.18	0.43
1:A:1011:ILE:HB	1:A:1026:SER:HB3	1.99	0.43
1:A:1172:TRP:HA	1:A:1173:PRO:C	2.39	0.43
1:A:1152:TRP:NE1	1:A:1157:VAL:HB	2.34	0.43
1:A:784:VAL:HA	1:A:785:PRO:HD3	1.85	0.43
1:A:1004:ALA:HA	1:A:1012:GLU:O	2.19	0.43
1:A:1122:ASN:HA	1:A:1125:LEU:HD12	2.00	0.43
1:A:750:VAL:HG22	1:A:778:VAL:HG13	2.01	0.43
1:A:1007:VAL:HG11	1:A:1012:GLU:OE2	2.19	0.42
1:A:701:MET:O	1:A:701:MET:HE3	2.20	0.42
1:A:846:ILE:O	1:A:849:ASN:HB2	2.20	0.42
1:A:652:ALA:O	1:A:653:GLU:HB3	2.19	0.42
1:A:655:ARG:HH11	1:A:655:ARG:CB	2.22	0.42
1:A:745:THR:HG22	1:A:746:ASN:H	1.84	0.42
1:A:699:ASP:HA	1:A:702:ASN:ND2	2.32	0.42
1:A:1137:PRO:HB2	1:A:1148:LYS:HG3	2.02	0.42
1:A:717:GLN:O	1:A:720:LYS:N	2.52	0.41
1:A:675:ILE:HD12	1:A:724:VAL:HG13	2.00	0.41
1:A:740:LYS:HB2	1:A:741:GLU:H	1.62	0.41
1:A:1143:PRO:HB2	1:A:1218:LEU:CD2	2.50	0.41
1:A:1198:ASP:OD2	1:A:1198:ASP:N	2.51	0.41
1:A:664:GLU:HG3	1:A:700:GLY:HA2	2.01	0.41
1:A:847:GLU:C	1:A:849:ASN:H	2.24	0.41
1:A:1029:LEU:HD11	1:A:1218:LEU:HD11	2.01	0.41
1:A:800:LEU:HD23	1:A:800:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:GLN:HG2	1:A:933:GLU:N	2.35	0.41
1:A:1102:TYR:O	1:A:1105:GLU:HB3	2.21	0.41
1:A:1136:ALA:HA	1:A:1137:PRO:HD3	1.96	0.41
1:A:1005:ASN:OD1	1:A:1019:ARG:NH1	2.53	0.41
1:A:782:VAL:O	1:A:783:MET:C	2.58	0.41
1:A:751:ILE:HG23	1:A:763:LYS:HD2	2.02	0.41
1:A:790:LEU:HD13	1:A:826:PHE:CE2	2.56	0.41
1:A:715:LEU:HD22	1:A:715:LEU:HA	1.91	0.41
1:A:750:VAL:HG23	1:A:798:ALA:HB2	2.02	0.41
1:A:849:ASN:HD22	1:A:849:ASN:HA	1.69	0.41
1:A:1200:VAL:HG13	1:A:1214:VAL:CG2	2.51	0.41
1:A:690:ILE:O	1:A:693:ILE:HB	2.21	0.41
1:A:934:VAL:HG21	1:A:1103:LEU:HD11	2.03	0.41
1:A:876:ARG:NH1	1:A:876:ARG:HG2	2.37	0.40
1:A:1158:GLU:HA	1:A:1163:MET:O	2.22	0.40
1:A:674:PHE:O	1:A:678:ASP:HB2	2.21	0.40
1:A:794:LYS:HE2	4:A:307:HOH:O	2.21	0.40
1:A:844:VAL:O	1:A:844:VAL:HG12	2.21	0.40
1:A:1085:LYS:O	1:A:1088:VAL:HG12	2.21	0.40
1:A:749:MET:HE1	1:A:831:LEU:HD22	2.02	0.40
1:A:1192:VAL:O	1:A:1193:ALA:HB3	2.21	0.40
1:A:1177:VAL:HA	3:A:1248:B12:N40	2.37	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	575/577 (100%)	507 (88%)	60 (10%)	8 (1%)	11	43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	652	ALA
1	A	740	LYS
1	A	754	VAL
1	A	653	GLU
1	A	1041	TYR
1	A	655	ARG
1	A	848	GLN
1	A	899	PRO

### 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	481/481 (100%)	456 (95%)	25 (5%)	23 59

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	655	ARG
1	A	672	THR
1	A	678	ASP
1	A	715	LEU
1	A	740	LYS
1	A	744	LYS
1	A	751	ILE
1	A	754	VAL
1	A	776	GLU
1	A	778	VAL
1	A	832	ILE
1	A	836	THR
1	A	873	ASP
1	A	893	GLN
1	A	900	ARG
1	A	904	VAL
1	A	939	GLU
1	A	976	LEU
1	A	992	THR

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Mol	Chain	Res	Type
1	A	1036	THR
1	A	1099	PHE
1	A	1142	CYS
1	A	1144	GLU
1	A	1152	TRP
1	A	1197	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	660	ASN
1	A	702	ASN
1	A	727	GLN
1	A	764	ASN
1	A	849	ASN
1	A	858	GLN
1	A	859	ASN
1	A	893	GLN
1	A	974	GLN
1	A	981	ASN
1	A	1021	HIS
1	A	1079	GLN
1	A	1084	ASN
1	A	1117	ASN
1	A	1129	ASN
1	A	1145	HIS
1	A	1184	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

11 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	255	-	4,4,4	0.33	0	6,6,6	0.05	0
2	SO4	A	282	-	4,4,4	0.33	0	6,6,6	0.05	0
3	B12	A	1248	-	80,101,101	3.26	44 (55%)	101,166,166	2.50	44 (43%)
2	SO4	A	270	-	4,4,4	0.31	0	6,6,6	0.06	0
2	SO4	A	267	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	A	254	-	4,4,4	0.26	0	6,6,6	0.05	0
2	SO4	A	309	-	4,4,4	0.33	0	6,6,6	0.06	0
2	SO4	A	260	-	4,4,4	0.33	0	6,6,6	0.06	0
2	SO4	A	251	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	A	259	-	4,4,4	0.36	0	6,6,6	0.05	0
2	SO4	A	323	-	4,4,4	0.27	0	6,6,6	0.06	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
3	B12	A	1248	-	-	22/51/223/223	0/3/11/11

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1248	B12	C53-C15	11.08	1.74	1.52
3	A	1248	B12	C20-C1	9.67	1.72	1.53
3	A	1248	B12	C5M-C5B	-6.69	1.37	1.51
3	A	1248	B12	C1P-C2P	6.41	1.68	1.51
3	A	1248	B12	CO-N24	5.91	2.03	1.89
3	A	1248	B12	C37-C38	5.37	1.69	1.51
3	A	1248	B12	C4B-C9B	5.33	1.50	1.41
3	A	1248	B12	C7B-C6B	4.81	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1248	B12	O3-C2P	4.80	1.58	1.45
3	A	1248	B12	C35-C5	4.65	1.61	1.52
3	A	1248	B12	C16-C15	4.57	1.58	1.41
3	A	1248	B12	C7B-C8B	4.55	1.49	1.40
3	A	1248	B12	C25-C2	4.53	1.63	1.54
3	A	1248	B12	C6M-C6B	4.52	1.60	1.51
3	A	1248	B12	C1-C19	-4.32	1.45	1.55
3	A	1248	B12	O6R-C4R	-4.27	1.35	1.45
3	A	1248	B12	C2-C3	-4.17	1.51	1.58
3	A	1248	B12	C4B-C5B	4.08	1.48	1.37
3	A	1248	B12	C6B-C5B	3.71	1.50	1.40
3	A	1248	B12	CO-N21	3.57	1.97	1.89
3	A	1248	B12	C6-C5	3.38	1.55	1.41
3	A	1248	B12	C32-N33	-3.33	1.21	1.32
3	A	1248	B12	C43-N45	-3.12	1.22	1.32
3	A	1248	B12	C61-N62	-3.10	1.22	1.32
3	A	1248	B12	O8R-C5R	-3.07	1.29	1.42
3	A	1248	B12	C27-N29	-2.96	1.23	1.32
3	A	1248	B12	C26-C2	2.92	1.62	1.55
3	A	1248	B12	C50-N52	-2.89	1.23	1.32
3	A	1248	B12	C36-C7	2.68	1.60	1.55
3	A	1248	B12	C55-C56	2.66	1.59	1.53
3	A	1248	B12	C42-C43	-2.64	1.40	1.51
3	A	1248	B12	C26-C27	2.61	1.60	1.51
3	A	1248	B12	P-O4	-2.57	1.41	1.50
3	A	1248	B12	C31-C32	-2.39	1.42	1.51
3	A	1248	B12	C14-C15	2.34	1.49	1.40
3	A	1248	B12	C3P-C2P	2.29	1.60	1.51
3	A	1248	B12	P-O5	-2.29	1.44	1.55
3	A	1248	B12	C38-N40	-2.28	1.25	1.32
3	A	1248	B12	C54-C17	2.23	1.59	1.55
3	A	1248	B12	C18-C19	2.21	1.58	1.53
3	A	1248	B12	C8B-C9B	2.21	1.44	1.40
3	A	1248	B12	C37-C7	2.20	1.63	1.56
3	A	1248	B12	C17-C18	-2.16	1.51	1.54
3	A	1248	B12	C60-C18	2.11	1.58	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1248	B12	C56-C55-C17	6.82	128.69	115.50
3	A	1248	B12	C3P-C2P-C1P	6.70	124.39	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1248	B12	C2-C3-C4	5.90	107.86	101.67
3	A	1248	B12	O3-C2P-C3P	5.85	131.30	108.72
3	A	1248	B12	C2-C1-C19	5.51	127.29	118.60
3	A	1248	B12	C41-C8-C7	5.45	128.83	114.08
3	A	1248	B12	C47-C12-C46	-5.16	98.91	109.73
3	A	1248	B12	C17-C18-C19	5.07	110.10	102.37
3	A	1248	B12	C8-C9-N22	-4.18	105.89	111.12
3	A	1248	B12	O58-C57-N59	4.15	130.84	123.01
3	A	1248	B12	O51-C50-N52	3.93	133.22	122.50
3	A	1248	B12	C2P-C1P-N59	-3.88	107.22	112.93
3	A	1248	B12	C54-C17-C55	-3.84	102.92	109.26
3	A	1248	B12	C1-C19-C18	3.77	128.16	121.93
3	A	1248	B12	C42-C43-N45	3.67	127.93	116.51
3	A	1248	B12	C26-C2-C3	-3.65	100.76	107.47
3	A	1248	B12	C16-C15-C14	-3.65	118.58	124.27
3	A	1248	B12	C36-C7-C37	-3.47	104.90	110.83
3	A	1248	B12	C30-C3-C2	3.25	126.02	119.13
3	A	1248	B12	O58-C57-C56	-3.17	116.23	122.02
3	A	1248	B12	C60-C61-N62	-3.03	108.90	116.21
3	A	1248	B12	C2-C26-C27	2.98	123.61	115.22
3	A	1248	B12	O6R-C4R-C5R	-2.88	102.98	109.21
3	A	1248	B12	C6-C5-C4	-2.67	120.11	124.27
3	A	1248	B12	C56-C57-N59	-2.66	111.95	116.42
3	A	1248	B12	C1P-N59-C57	2.63	128.42	122.69
3	A	1248	B12	O63-C61-N62	2.60	129.59	122.50
3	A	1248	B12	C5M-C5B-C4B	-2.42	114.56	120.34
3	A	1248	B12	O44-C43-N45	-2.41	115.93	122.50
3	A	1248	B12	O6R-C1R-C2R	-2.34	103.51	106.93
3	A	1248	B12	O3-C2P-C1P	-2.34	102.25	106.92
3	A	1248	B12	C6M-C6B-C5B	2.34	125.52	120.74
3	A	1248	B12	O7R-C2R-C1R	2.33	119.47	110.85
3	A	1248	B12	O8R-C5R-C4R	-2.29	103.44	111.29
3	A	1248	B12	C55-C17-C16	2.25	117.41	109.92
3	A	1248	B12	C37-C7-C8	2.21	114.29	108.37
3	A	1248	B12	C12-C11-C10	2.19	128.36	124.64
3	A	1248	B12	C1-C19-N24	2.19	108.70	106.24
3	A	1248	B12	C9-C10-C11	-2.15	123.41	130.91
3	A	1248	B12	C7-C37-C38	2.15	120.59	114.20
3	A	1248	B12	C6M-C6B-C7B	-2.13	115.24	120.34
3	A	1248	B12	C5M-C5B-C6B	2.12	125.08	120.74
3	A	1248	B12	C55-C56-C57	2.11	115.83	111.23
3	A	1248	B12	O2-P-O4	2.07	117.25	109.47

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1248	B12	C4-C3-C30-C31
3	A	1248	B12	N59-C1P-C2P-C3P
3	A	1248	B12	N59-C1P-C2P-O3
3	A	1248	B12	C3P-C2P-O3-P
3	A	1248	B12	C8-C41-C42-C43
3	A	1248	B12	C3R-C4R-C5R-O8R
3	A	1248	B12	O6R-C4R-C5R-O8R
3	A	1248	B12	C2P-O3-P-O2
3	A	1248	B12	C17-C55-C56-C57
3	A	1248	B12	C12-C13-C48-C49
3	A	1248	B12	C16-C17-C55-C56
3	A	1248	B12	O58-C57-N59-C1P
3	A	1248	B12	C3R-O2-P-O3
3	A	1248	B12	C18-C17-C55-C56
3	A	1248	B12	C14-C13-C48-C49
3	A	1248	B12	C41-C42-C43-O44
3	A	1248	B12	C41-C42-C43-N45
3	A	1248	B12	C2P-O3-P-O4
3	A	1248	B12	C2P-O3-P-O5
3	A	1248	B12	C17-C18-C60-C61
3	A	1248	B12	C2-C3-C30-C31
3	A	1248	B12	C19-C18-C60-C61

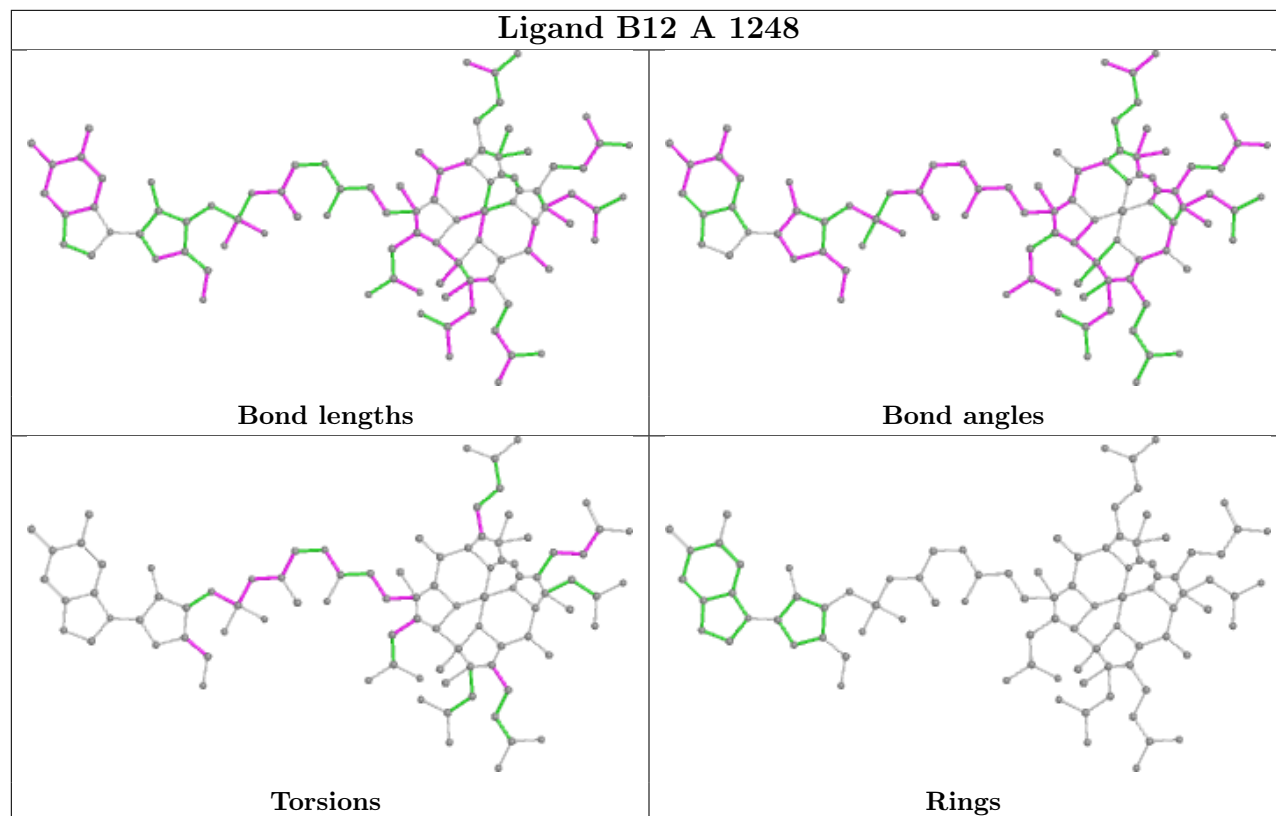
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1248	B12	6	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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.