



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:32 AM GMT

PDB ID : 3IV9  
Title : Structure of the B12-dependent Methionine Synthase (MetH) C-terminal half  
in a "His-On" conformation  
Authors : Pattridge, K.A.; Koutmos, M.; Smith, J.L.  
Deposited on : 2009-08-31  
Resolution : 3.25 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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

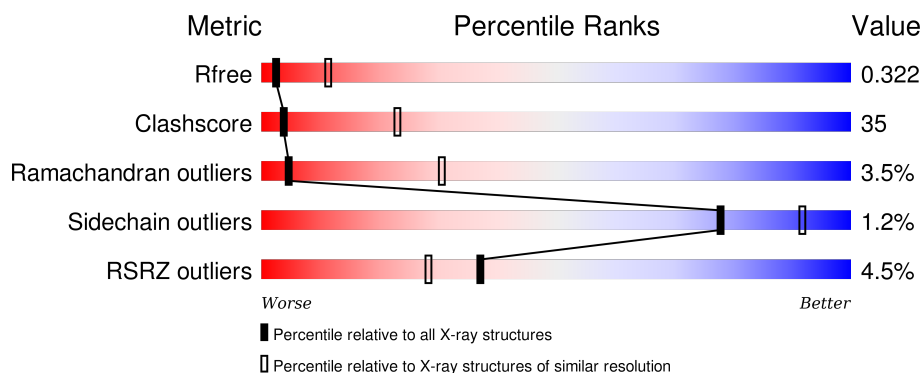
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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  $\geq 3$ , 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	579	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4685 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.

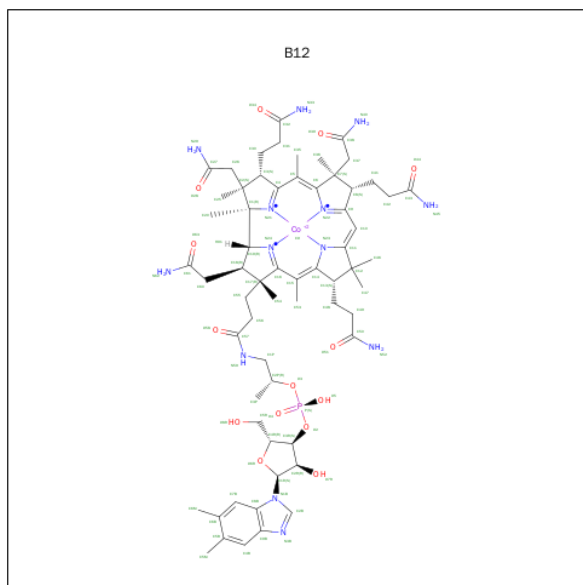
- Molecule 1 is a protein called Methionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	577	4572	2890	789	874	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	UNP P13009
A	743	CYS	GLY	ENGINEERED	UNP P13009

- Molecule 2 is COBALAMIN (three-letter code: 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

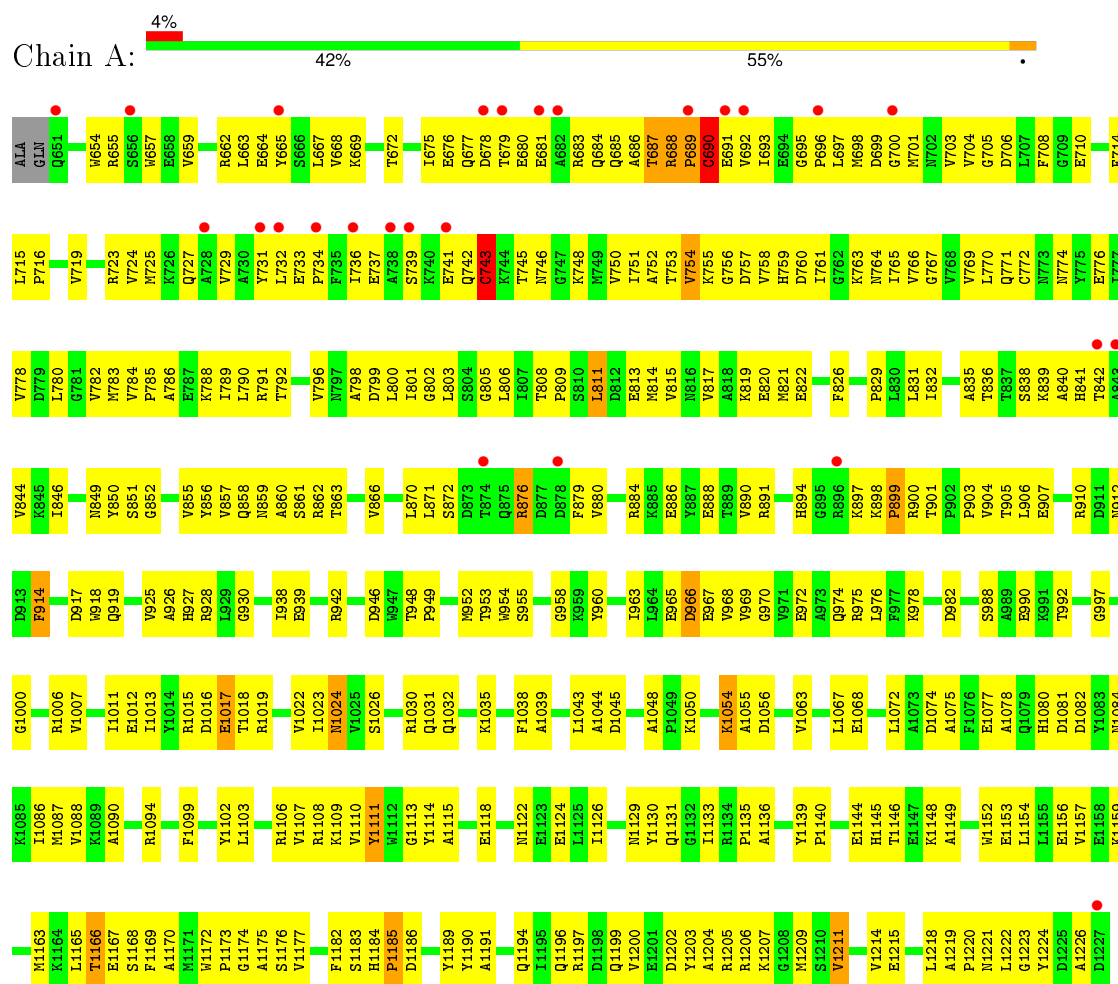
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		

### 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 ( $RSRZ > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	107.55Å 107.55Å 144.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.10 – 3.25 48.10 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.10-3.25) 99.2 (48.10-3.25)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 3.25Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.282 , 0.321 0.276 , 0.322	Depositor DCC
$R_{free}$ test set	693 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	109.8	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 69.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 13846 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4685	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.26	0/4671	0.49	0/6336

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	4572	0	4482	324	0
2	A	91	0	74	6	0
3	A	22	0	0	0	0
All	All	4685	0	4556	324	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 35.

All (324) 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:753:THR:HB	1:A:782:VAL:HA	1.40	1.00

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:ILE:HD11	1:A:1044:ALA:HA	1.43	0.99
1:A:844:VAL:HG22	1:A:891:ARG:HG2	1.46	0.98
1:A:948:THR:HB	1:A:949:PRO:HD3	1.47	0.96
1:A:693:ILE:HA	1:A:697:LEU:HD22	1.50	0.92
1:A:752:ALA:HB1	1:A:784:VAL:HG11	1.54	0.89
1:A:832:ILE:HD12	1:A:842:THR:HG23	1.52	0.89
1:A:729:VAL:O	1:A:733:GLU:HG3	1.73	0.87
1:A:752:ALA:HB2	1:A:780:LEU:HB2	1.65	0.79
1:A:900:ARG:HG3	1:A:901:THR:HG23	1.63	0.79
1:A:756:GLY:H	1:A:783:MET:HA	1.48	0.78
1:A:1019:ARG:HH21	1:A:1055:ALA:HB1	1.49	0.78
1:A:784:VAL:HG23	1:A:788:LYS:HD3	1.63	0.78
1:A:1219:ALA:HB3	1:A:1220:PRO:HD3	1.65	0.78
1:A:857:VAL:HB	2:A:1301:B12:HM61	1.66	0.77
1:A:1067:LEU:HA	1:A:1173:PRO:HG2	1.67	0.77
1:A:780:LEU:HD22	1:A:788:LYS:HE2	1.67	0.77
1:A:938:ILE:O	1:A:942:ARG:HG3	1.83	0.77
1:A:897:LYS:HD3	1:A:900:ARG:HH21	1.48	0.76
1:A:655:ARG:NH2	1:A:662:ARG:HH21	1.82	0.76
1:A:857:VAL:HG13	1:A:862:ARG:HB3	1.68	0.76
1:A:755:LYS:HD2	1:A:785:PRO:HA	1.68	0.76
1:A:815:VAL:HG22	1:A:846:ILE:HG12	1.68	0.75
1:A:659:VAL:HG21	1:A:681:GLU:HB2	1.68	0.74
1:A:1048:ALA:HB3	1:A:1056:ASP:HB2	1.68	0.74
1:A:766:VAL:HG22	1:A:860:ALA:HB2	1.71	0.72
1:A:688:ARG:HB3	1:A:688:ARG:NH1	2.05	0.71
1:A:760:ASP:HB3	1:A:782:VAL:CG1	2.20	0.71
1:A:733:GLU:HB2	1:A:734:PRO:HD3	1.73	0.71
1:A:733:GLU:O	1:A:737:GLU:HG3	1.90	0.70
1:A:800:LEU:HD11	1:A:871:LEU:HD21	1.73	0.70
1:A:1019:ARG:NH2	1:A:1055:ALA:HB1	2.07	0.69
1:A:906:LEU:HD21	1:A:910:ARG:NH2	2.06	0.69
1:A:806:LEU:O	1:A:836:THR:HG21	1.93	0.69
1:A:1032:GLN:HE22	1:A:1196:GLN:HB2	1.58	0.69
1:A:821:MET:HA	1:A:826:PHE:HD2	1.57	0.68
1:A:832:ILE:HD12	1:A:842:THR:CG2	2.25	0.67
1:A:688:ARG:H	1:A:688:ARG:HD2	1.59	0.67
1:A:888:GLU:HA	1:A:891:ARG:NH1	2.10	0.67
1:A:835:ALA:HB2	2:A:1301:B12:O5	1.96	0.66
1:A:663:LEU:HD23	1:A:696:PRO:HB2	1.76	0.66
1:A:860:ALA:H	2:A:1301:B12:H5R1	1.60	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:HIS:CE1	1:A:1186:ASP:HB2	2.31	0.66
1:A:714:PHE:HD2	1:A:972:GLU:HG3	1.60	0.65
1:A:832:ILE:HD13	1:A:846:ILE:HD12	1.78	0.65
1:A:1109:LYS:O	1:A:1113:GLY:HA2	1.95	0.65
1:A:891:ARG:HB2	1:A:891:ARG:HH11	1.61	0.65
1:A:739:SER:O	1:A:741:GLU:HG3	1.97	0.65
1:A:958:GLY:HA3	1:A:963:ILE:HD12	1.79	0.65
1:A:745:THR:HA	1:A:774:ASN:HD21	1.62	0.64
1:A:1148:LYS:O	1:A:1152:TRP:HD1	1.81	0.64
1:A:1196:GLN:OE1	1:A:1223:GLY:HA3	1.97	0.64
1:A:1023:ILE:O	1:A:1024:ASN:HB2	1.97	0.64
1:A:692:VAL:HG12	1:A:697:LEU:HD13	1.79	0.63
1:A:897:LYS:HD3	1:A:900:ARG:NH2	2.14	0.63
1:A:757:ASP:O	1:A:783:MET:HG3	1.99	0.63
1:A:799:ASP:C	1:A:800:LEU:HD12	2.19	0.63
1:A:765:ILE:O	1:A:769:VAL:HG23	1.99	0.63
1:A:754:VAL:HG21	1:A:814:MET:HG2	1.81	0.62
1:A:758:VAL:HG21	1:A:1174:GLY:HA2	1.81	0.62
1:A:748:LYS:HD3	1:A:796:VAL:HG12	1.80	0.62
1:A:1068:GLU:OE1	1:A:1068:GLU:N	2.33	0.61
1:A:688:ARG:HH11	1:A:688:ARG:HB3	1.66	0.61
1:A:692:VAL:HG12	1:A:697:LEU:CD1	2.32	0.60
1:A:1032:GLN:NE2	1:A:1196:GLN:HB2	2.17	0.60
1:A:745:THR:HA	1:A:774:ASN:ND2	2.15	0.60
1:A:870:LEU:O	1:A:876:ARG:HG3	2.00	0.60
1:A:1194:GLN:HA	1:A:1221:ASN:O	2.01	0.60
1:A:912:ASN:OD1	1:A:1039:ALA:HA	2.03	0.59
1:A:917:ASP:OD2	1:A:919:GLN:HB2	2.03	0.59
1:A:754:VAL:CG1	1:A:813:GLU:HB3	2.33	0.59
1:A:672:THR:O	1:A:675:ILE:HG22	2.02	0.59
1:A:1204:ALA:HB1	1:A:1209:MET:O	2.03	0.59
1:A:654:TRP:O	1:A:662:ARG:HG2	2.03	0.59
1:A:659:VAL:CG2	1:A:678:ASP:HA	2.33	0.58
1:A:748:LYS:CD	1:A:796:VAL:HG12	2.33	0.58
1:A:788:LYS:HA	1:A:791:ARG:HD3	1.85	0.58
1:A:960:TYR:HA	1:A:963:ILE:HG22	1.86	0.58
1:A:716:PRO:HG3	1:A:954:TRP:HB3	1.86	0.58
1:A:1094:ARG:NE	1:A:1094:ARG:HA	2.19	0.58
1:A:696:PRO:HA	1:A:699:ASP:HB2	1.86	0.58
1:A:866:VAL:HG13	1:A:879:PHE:CZ	2.39	0.58
1:A:1015:ARG:HB2	1:A:1023:ILE:HG23	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:LEU:HD21	1:A:863:THR:HG22	1.86	0.57
1:A:748:LYS:HD3	1:A:796:VAL:CG1	2.34	0.57
1:A:859:ASN:OD1	1:A:861:SER:HB3	2.02	0.57
1:A:811:LEU:HB3	1:A:841:HIS:NE2	2.19	0.57
1:A:1196:GLN:O	1:A:1200:VAL:HG23	2.05	0.57
1:A:1115:ALA:HB1	1:A:1118:GLU:HB2	1.88	0.56
1:A:948:THR:HB	1:A:949:PRO:CD	2.30	0.56
1:A:748:LYS:HE2	1:A:776:GLU:OE2	2.05	0.56
1:A:1144:GLU:HG3	1:A:1203:TYR:OH	2.05	0.56
1:A:664:GLU:O	1:A:668:VAL:HG23	2.06	0.56
1:A:1152:TRP:HH2	1:A:1163:MET:HB3	1.71	0.56
1:A:683:ARG:NH1	1:A:689:PRO:HG3	2.21	0.56
1:A:903:PRO:HG3	1:A:1196:GLN:NE2	2.21	0.56
1:A:1022:VAL:HG12	1:A:1024:ASN:H	1.71	0.56
1:A:698:MET:HE1	1:A:774:ASN:HB2	1.87	0.56
1:A:872:SER:O	1:A:876:ARG:HB2	2.06	0.56
1:A:723:ARG:HD3	1:A:1081:ASP:OD1	2.06	0.56
1:A:1146:THR:HG22	1:A:1169:PHE:CE2	2.40	0.56
1:A:888:GLU:CD	1:A:891:ARG:HH12	2.09	0.55
1:A:700:GLY:O	1:A:703:VAL:HB	2.07	0.55
1:A:939:GLU:HG2	1:A:988:SER:OG	2.07	0.55
1:A:697:LEU:O	1:A:701:MET:HG2	2.06	0.55
1:A:1152:TRP:HA	1:A:1157:VAL:HG23	1.88	0.55
1:A:790:LEU:HD11	1:A:820:GLU:HB3	1.88	0.55
1:A:1152:TRP:CE3	1:A:1157:VAL:HB	2.42	0.55
1:A:783:MET:SD	1:A:1166:THR:HG21	2.47	0.55
1:A:756:GLY:HA3	1:A:1168:SER:OG	2.06	0.54
1:A:756:GLY:N	1:A:783:MET:HA	2.19	0.54
1:A:949:PRO:HA	1:A:952:MET:HB3	1.88	0.54
1:A:700:GLY:O	1:A:704:VAL:HG23	2.07	0.54
1:A:672:THR:HA	1:A:675:ILE:HB	1.88	0.54
1:A:946:ASP:O	1:A:949:PRO:HD2	2.07	0.54
1:A:808:THR:HG23	1:A:1220:PRO:HG2	1.90	0.54
1:A:790:LEU:CD1	1:A:820:GLU:HB3	2.38	0.54
1:A:891:ARG:HB2	1:A:891:ARG:NH1	2.23	0.54
1:A:714:PHE:CD2	1:A:972:GLU:HG3	2.42	0.54
1:A:698:MET:CE	1:A:774:ASN:HB2	2.38	0.54
1:A:1145:HIS:O	1:A:1148:LYS:HG3	2.08	0.54
1:A:1224:TYR:HE2	1:A:1226:ALA:HB2	1.73	0.54
1:A:1048:ALA:CB	1:A:1056:ASP:HB2	2.38	0.53
1:A:1133:ILE:HG13	1:A:1135:PRO:HD3	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:ASP:O	1:A:1077:GLU:HB3	2.08	0.53
1:A:663:LEU:HD21	1:A:697:LEU:HD12	1.90	0.53
1:A:1122:ASN:O	1:A:1126:ILE:HG12	2.08	0.53
1:A:784:VAL:HG13	1:A:789:ILE:HD11	1.91	0.53
1:A:655:ARG:CZ	1:A:662:ARG:HH21	2.22	0.53
1:A:1224:TYR:CE2	1:A:1226:ALA:HB2	2.44	0.53
1:A:1017:GLU:O	1:A:1019:ARG:HG2	2.09	0.52
1:A:1202:ASP:O	1:A:1206:ARG:HG3	2.09	0.52
1:A:752:ALA:CB	1:A:780:LEU:HB2	2.35	0.52
1:A:857:VAL:CG1	1:A:862:ARG:HB3	2.38	0.52
1:A:1144:GLU:OE2	1:A:1146:THR:HG23	2.10	0.52
1:A:757:ASP:OD1	1:A:805:GLY:HA2	2.10	0.52
1:A:888:GLU:HA	1:A:891:ARG:HH12	1.72	0.52
1:A:672:THR:CG2	1:A:724:VAL:HG22	2.40	0.52
1:A:756:GLY:O	1:A:1170:ALA:HB2	2.10	0.52
1:A:820:GLU:OE1	1:A:820:GLU:HA	2.10	0.52
1:A:1197:ARG:NH2	1:A:1211:VAL:HG11	2.24	0.52
1:A:748:LYS:HE2	1:A:776:GLU:CD	2.31	0.52
1:A:1211:VAL:O	1:A:1215:GLU:HG3	2.10	0.52
1:A:1103:LEU:O	1:A:1107:VAL:HG23	2.10	0.52
1:A:725:MET:O	1:A:729:VAL:HG23	2.10	0.51
1:A:750:VAL:HA	1:A:778:VAL:HG13	1.92	0.51
1:A:778:VAL:O	1:A:778:VAL:HG13	2.11	0.51
1:A:1006:ARG:HG2	1:A:1007:VAL:N	2.24	0.51
1:A:801:ILE:HD12	1:A:821:MET:CE	2.41	0.51
1:A:683:ARG:HH11	1:A:683:ARG:HG2	1.75	0.51
1:A:811:LEU:HD13	1:A:841:HIS:CD2	2.46	0.51
1:A:688:ARG:O	1:A:688:ARG:HG2	2.10	0.50
1:A:663:LEU:O	1:A:667:LEU:HD23	2.11	0.50
1:A:858:GLN:O	2:A:1301:B12:H2R	2.11	0.50
1:A:1067:LEU:HD23	1:A:1173:PRO:HD3	1.93	0.50
1:A:659:VAL:HG23	1:A:678:ASP:HA	1.94	0.50
1:A:1204:ALA:HB2	1:A:1214:VAL:HG21	1.93	0.50
1:A:750:VAL:HG23	1:A:798:ALA:HB2	1.93	0.50
1:A:990:GLU:HB3	1:A:992:THR:HG23	1.93	0.50
1:A:914:PHE:HB3	1:A:1045:ASP:HB3	1.93	0.50
1:A:811:LEU:O	1:A:815:VAL:HG23	2.12	0.50
1:A:953:THR:C	1:A:955:SER:H	2.15	0.50
1:A:750:VAL:HG23	1:A:798:ALA:CB	2.42	0.49
1:A:1139:TYR:HB3	1:A:1140:PRO:HD2	1.94	0.49
1:A:1156:GLU:HB3	1:A:1159:LYS:HD2	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:TYR:CE2	1:A:852:GLY:HA3	2.47	0.49
1:A:866:VAL:HG13	1:A:879:PHE:HZ	1.76	0.49
1:A:677:GLN:O	1:A:681:GLU:HG3	2.12	0.49
1:A:821:MET:HA	1:A:826:PHE:CD2	2.41	0.49
1:A:997:GLY:HA3	1:A:1063:VAL:HG12	1.93	0.49
1:A:1016:ASP:OD1	1:A:1018:THR:HG23	2.12	0.49
1:A:687:THR:OG1	1:A:688:ARG:HD2	2.12	0.49
1:A:750:VAL:HG22	1:A:778:VAL:CG1	2.43	0.49
1:A:966:ASP:OD1	1:A:968:VAL:HB	2.13	0.49
1:A:684:GLN:C	1:A:686:ALA:H	2.15	0.49
1:A:1013:ILE:HG22	1:A:1023:ILE:HD11	1.95	0.48
1:A:808:THR:HB	1:A:809:PRO:HD3	1.95	0.48
1:A:686:ALA:HB1	1:A:691:GLU:OE1	2.13	0.48
1:A:789:ILE:HD13	1:A:803:LEU:CD2	2.43	0.48
1:A:949:PRO:HB2	1:A:1094:ARG:NH1	2.28	0.48
1:A:675:ILE:HG23	1:A:676:GLU:N	2.28	0.48
1:A:1175:ALA:HA	2:A:1301:B12:H471	1.96	0.48
1:A:680:GLU:HB2	1:A:731:TYR:HE2	1.78	0.48
1:A:758:VAL:O	1:A:782:VAL:HG11	2.14	0.48
1:A:688:ARG:HB2	1:A:741:GLU:OE1	2.14	0.48
1:A:680:GLU:HB2	1:A:731:TYR:CE2	2.49	0.48
1:A:1124:GLU:HB3	1:A:1129:ASN:HB2	1.96	0.48
1:A:1078:ALA:C	1:A:1080:HIS:H	2.16	0.48
1:A:767:GLY:O	1:A:771:GLN:HG3	2.13	0.48
1:A:1015:ARG:HG3	1:A:1015:ARG:HH11	1.79	0.48
1:A:925:VAL:HG12	1:A:926:ALA:N	2.29	0.47
1:A:1011:ILE:HB	1:A:1026:SER:HB3	1.95	0.47
1:A:850:TYR:C	1:A:852:GLY:H	2.18	0.47
1:A:715:LEU:O	1:A:719:VAL:HG23	2.14	0.47
1:A:665:TYR:CZ	1:A:669:LYS:HG3	2.49	0.47
1:A:1218:LEU:O	1:A:1222:LEU:HG	2.15	0.47
1:A:1012:GLU:OE1	1:A:1050:LYS:HD2	2.14	0.47
1:A:978:LYS:HG3	1:A:982:ASP:OD2	2.15	0.47
1:A:891:ARG:HH11	1:A:891:ARG:CB	2.26	0.47
1:A:714:PHE:CZ	1:A:969:VAL:HG12	2.49	0.47
1:A:965:GLU:O	1:A:966:ASP:C	2.53	0.47
1:A:1035:LYS:HB3	1:A:1038:PHE:O	2.14	0.47
1:A:1102:TYR:CZ	1:A:1106:ARG:HD2	2.49	0.47
1:A:1140:PRO:HB2	1:A:1191:ALA:HA	1.97	0.46
1:A:655:ARG:NH2	1:A:662:ARG:NH2	2.59	0.46
1:A:894:HIS:O	1:A:898:LYS:HG3	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:THR:O	1:A:784:VAL:HG12	2.15	0.46
1:A:769:VAL:HG21	1:A:860:ALA:HB1	1.98	0.46
1:A:1152:TRP:HA	1:A:1157:VAL:CG2	2.45	0.46
1:A:884:ARG:HH11	1:A:884:ARG:HG2	1.80	0.46
1:A:692:VAL:O	1:A:697:LEU:HD13	2.16	0.46
1:A:769:VAL:HG11	1:A:860:ALA:O	2.16	0.46
1:A:770:LEU:C	1:A:772:CYS:H	2.17	0.46
1:A:897:LYS:O	1:A:899:PRO:HA	2.16	0.46
1:A:677:GLN:HG3	1:A:678:ASP:N	2.31	0.46
1:A:963:ILE:HG12	1:A:963:ILE:O	2.16	0.46
1:A:1067:LEU:HA	1:A:1173:PRO:CG	2.41	0.46
1:A:958:GLY:HA3	1:A:963:ILE:CD1	2.45	0.46
1:A:750:VAL:HG22	1:A:778:VAL:HG11	1.96	0.46
1:A:705:GLY:O	1:A:708:PHE:HB3	2.16	0.46
1:A:761:ILE:HA	1:A:764:ASN:HD22	1.81	0.46
1:A:760:ASP:HB3	1:A:782:VAL:HG13	1.97	0.45
1:A:906:LEU:HD21	1:A:910:ARG:HH21	1.79	0.45
1:A:1194:GLN:HB3	1:A:1223:GLY:HA2	1.99	0.45
1:A:679:THR:O	1:A:683:ARG:HB2	2.16	0.45
1:A:683:ARG:NH1	1:A:683:ARG:HG2	2.31	0.45
1:A:840:ALA:HA	1:A:890:VAL:HG11	1.98	0.45
1:A:1172:TRP:HA	1:A:1173:PRO:C	2.36	0.45
1:A:1084:ASN:HA	1:A:1087:MET:HB3	1.99	0.45
1:A:1043:LEU:N	1:A:1190:TYR:OH	2.49	0.45
1:A:706:ASP:O	1:A:710:GLU:HG3	2.17	0.45
1:A:789:ILE:HD13	1:A:803:LEU:HD22	1.97	0.45
1:A:839:LYS:HD2	1:A:886:GLU:OE1	2.17	0.45
1:A:657:TRP:H	1:A:662:ARG:HD2	1.81	0.45
1:A:1133:ILE:HB	1:A:1189:TYR:CE1	2.52	0.45
1:A:832:ILE:CD1	1:A:842:THR:HG23	2.36	0.45
1:A:672:THR:HG23	1:A:724:VAL:HG22	1.98	0.45
1:A:751:ILE:HA	1:A:802:GLY:O	2.17	0.45
1:A:752:ALA:CB	1:A:784:VAL:HG11	2.38	0.44
1:A:784:VAL:CG2	1:A:788:LYS:HD3	2.42	0.44
1:A:857:VAL:HG22	1:A:866:VAL:HG21	2.00	0.44
1:A:1152:TRP:CD1	1:A:1165:LEU:HD11	2.52	0.44
1:A:930:GLY:O	1:A:1000:GLY:HA2	2.17	0.44
1:A:756:GLY:C	1:A:783:MET:HG2	2.37	0.44
1:A:1172:TRP:CD1	1:A:1173:PRO:HA	2.52	0.44
1:A:792:THR:O	1:A:796:VAL:HG23	2.18	0.44
1:A:736:ILE:O	1:A:736:ILE:HG22	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ALA:HB1	1:A:817:VAL:HG22	1.98	0.44
1:A:689:PRO:O	1:A:690:CYS:HB2	2.17	0.44
1:A:1149:ALA:O	1:A:1153:GLU:HG3	2.17	0.44
1:A:808:THR:HG23	1:A:1220:PRO:CD	2.47	0.43
1:A:1107:VAL:HA	1:A:1111:TYR:HB2	2.00	0.43
1:A:906:LEU:HD22	1:A:1199:GLN:HA	1.99	0.43
1:A:888:GLU:HA	1:A:891:ARG:CZ	2.47	0.43
1:A:928:ARG:HH11	1:A:928:ARG:HG3	1.83	0.43
1:A:1136:ALA:HB3	1:A:1139:TYR:CE2	2.53	0.43
1:A:927:HIS:ND1	1:A:928:ARG:HG2	2.33	0.43
1:A:1108:ARG:HG2	1:A:1114:TYR:OH	2.18	0.43
1:A:803:LEU:HD11	1:A:817:VAL:HG11	2.00	0.43
1:A:688:ARG:HB2	1:A:741:GLU:OE2	2.19	0.43
1:A:1183:SER:O	1:A:1184:HIS:C	2.55	0.43
1:A:1203:TYR:CE2	1:A:1207:LYS:HG3	2.54	0.43
1:A:1084:ASN:O	1:A:1088:VAL:HG12	2.19	0.43
1:A:1202:ASP:O	1:A:1205:ARG:HB3	2.18	0.43
1:A:691:GLU:O	1:A:695:GLY:N	2.52	0.43
1:A:679:THR:HG22	1:A:732:LEU:HD21	2.00	0.43
1:A:1131:GLN:OE1	1:A:1185:PRO:HB3	2.19	0.43
1:A:754:VAL:CG2	1:A:814:MET:HG2	2.48	0.43
1:A:811:LEU:HB3	1:A:841:HIS:CE1	2.54	0.43
1:A:1177:VAL:HA	2:A:1301:B12:N40	2.34	0.43
1:A:754:VAL:HG21	1:A:814:MET:CG	2.48	0.43
1:A:681:GLU:O	1:A:685:GLN:HG3	2.18	0.43
1:A:904:VAL:O	1:A:1032:GLN:HG2	2.19	0.43
1:A:672:THR:HG22	1:A:724:VAL:HA	2.00	0.43
1:A:1167:GLU:CD	1:A:1167:GLU:N	2.71	0.43
1:A:819:LYS:CG	1:A:849:ASN:HD22	2.32	0.43
1:A:876:ARG:O	1:A:880:VAL:HG23	2.18	0.42
1:A:904:VAL:HG22	1:A:1032:GLN:O	2.19	0.42
1:A:1197:ARG:CZ	1:A:1211:VAL:HG11	2.49	0.42
1:A:829:PRO:CB	1:A:870:LEU:HD21	2.49	0.42
1:A:838:SER:C	1:A:840:ALA:H	2.22	0.42
1:A:742:GLN:C	1:A:743:CYS:SG	2.98	0.42
1:A:1204:ALA:CB	1:A:1214:VAL:HG21	2.49	0.42
1:A:689:PRO:O	1:A:736:ILE:HG12	2.19	0.42
1:A:1082:ASP:O	1:A:1086:ILE:HG13	2.19	0.42
1:A:663:LEU:HD23	1:A:696:PRO:CB	2.45	0.42
1:A:667:LEU:HD11	1:A:725:MET:HB2	2.01	0.42
1:A:714:PHE:CE2	1:A:969:VAL:HG12	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ASN:OD1	1:A:774:ASN:HB3	2.19	0.42
1:A:715:LEU:HB3	1:A:716:PRO:HD3	2.01	0.42
1:A:751:ILE:HG13	1:A:802:GLY:O	2.19	0.42
1:A:1030:ARG:O	1:A:1031:GLN:C	2.57	0.42
1:A:831:LEU:HA	1:A:855:VAL:O	2.19	0.42
1:A:659:VAL:O	1:A:659:VAL:HG22	2.20	0.42
1:A:958:GLY:HA3	1:A:963:ILE:CG1	2.50	0.42
1:A:716:PRO:HB3	1:A:976:LEU:HD13	2.01	0.42
1:A:970:GLY:O	1:A:974:GLN:HG3	2.19	0.42
1:A:1090:ALA:O	1:A:1094:ARG:HG2	2.19	0.41
1:A:752:ALA:HB2	1:A:780:LEU:HD12	2.02	0.41
1:A:699:ASP:O	1:A:703:VAL:HG23	2.20	0.41
1:A:657:TRP:HB2	1:A:662:ARG:HG3	2.01	0.41
1:A:829:PRO:HB3	1:A:870:LEU:HD21	2.02	0.41
1:A:1081:ASP:OD2	1:A:1084:ASN:HB2	2.20	0.41
1:A:822:GLU:HB2	1:A:850:TYR:HA	2.01	0.41
1:A:884:ARG:HG2	1:A:884:ARG:NH1	2.34	0.41
1:A:1043:LEU:O	1:A:1182:PHE:HE2	2.03	0.41
1:A:918:TRP:O	1:A:1054:LYS:HE3	2.19	0.41
1:A:904:VAL:HG22	1:A:1032:GLN:C	2.41	0.41
1:A:975:ARG:O	1:A:978:LYS:HB3	2.21	0.41
1:A:693:ILE:HD13	1:A:697:LEU:CD2	2.51	0.41
1:A:741:GLU:O	1:A:742:GLN:HB2	2.20	0.41
1:A:1072:LEU:O	1:A:1075:ALA:HB3	2.21	0.41
1:A:760:ASP:O	1:A:763:LYS:HB3	2.21	0.41
1:A:1163:MET:CE	1:A:1176:SER:HB3	2.51	0.41
1:A:693:ILE:HD13	1:A:697:LEU:HD22	2.03	0.40
1:A:842:THR:HG21	1:A:856:TYR:HB2	2.03	0.40
1:A:759:HIS:H	1:A:759:HIS:HD1	1.69	0.40
1:A:905:THR:HB	1:A:907:GLU:OE1	2.21	0.40
1:A:754:VAL:HG13	1:A:813:GLU:HB3	2.03	0.40
1:A:663:LEU:HD23	1:A:696:PRO:CG	2.52	0.40
1:A:814:MET:CE	1:A:832:ILE:HG23	2.52	0.40
1:A:723:ARG:O	1:A:727:GLN:HG3	2.22	0.40
1:A:657:TRP:O	1:A:662:ARG:CD	2.69	0.40
1:A:990:GLU:CB	1:A:992:THR:HG23	2.51	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	575/579 (99%)	486 (84%)	69 (12%)	20 (4%)	4 30

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	690	CYS
1	A	914	PHE
1	A	966	ASP
1	A	687	THR
1	A	811	LEU
1	A	876	ARG
1	A	967	GLU
1	A	1024	ASN
1	A	1166	THR
1	A	743	CYS
1	A	1054	LYS
1	A	851	SER
1	A	1017	GLU
1	A	1110	VAL
1	A	1154	LEU
1	A	1111	TYR
1	A	754	VAL
1	A	1185	PRO
1	A	1211	VAL
1	A	689	PRO

### 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	483/484 (100%)	477 (99%)	6 (1%)	78	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	688	ARG
1	A	690	CYS
1	A	743	CYS
1	A	899	PRO
1	A	1099	PHE
1	A	1130	TYR

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	684	GLN
1	A	702	ASN
1	A	727	GLN
1	A	764	ASN
1	A	849	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](#)

1 ligand is 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	3	74,101,101	2.62	27 (36%)	111,166,166	2.15	35 (31%)

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	3	-	0/51/223/223	0/3/11/11

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	B12	C1-C19	-3.90	1.46	1.55
2	A	1301	B12	C2-C3	-3.76	1.52	1.58
2	A	1301	B12	C43-N45	-3.22	1.22	1.32
2	A	1301	B12	C61-N62	-3.15	1.22	1.32
2	A	1301	B12	C50-N52	-2.99	1.23	1.32
2	A	1301	B12	C38-N40	-2.99	1.23	1.32
2	A	1301	B12	C32-N33	-2.97	1.23	1.32
2	A	1301	B12	C27-N29	-2.93	1.23	1.32
2	A	1301	B12	O8R-C5R	-2.71	1.30	1.42
2	A	1301	B12	C20-C1	2.04	1.57	1.53
2	A	1301	B12	C55-C56	2.06	1.58	1.53
2	A	1301	B12	C26-C2	2.23	1.61	1.55
2	A	1301	B12	C1-C2	2.82	1.65	1.58
2	A	1301	B12	C54-C17	2.84	1.59	1.54
2	A	1301	B12	C36-C7	3.29	1.60	1.54
2	A	1301	B12	C25-C2	3.53	1.61	1.54
2	A	1301	B12	C60-C18	3.76	1.62	1.54
2	A	1301	B12	C4B-C5B	4.12	1.49	1.37
2	A	1301	B12	C4B-C9B	4.67	1.48	1.41
2	A	1301	B12	C7B-C6B	4.70	1.50	1.37
2	A	1301	B12	C6B-C5B	4.71	1.53	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	B12	C8B-C9B	5.06	1.50	1.40
2	A	1301	B12	C7B-C8B	5.14	1.51	1.40
2	A	1301	B12	C30-C3	5.25	1.62	1.54
2	A	1301	B12	C41-C8	6.10	1.64	1.54
2	A	1301	B12	O6R-C1R	6.84	1.49	1.41
2	A	1301	B12	C48-C13	7.10	1.65	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	B12	C56-C57-N59	-4.46	108.71	116.46
2	A	1301	B12	C20-C1-C19	-4.33	105.14	109.38
2	A	1301	B12	C47-C12-C46	-3.66	100.53	109.56
2	A	1301	B12	C7-C6-N22	-3.25	104.10	110.81
2	A	1301	B12	C25-C2-C26	-2.63	104.05	109.73
2	A	1301	B12	C53-C15-C14	-2.46	113.85	118.25
2	A	1301	B12	C5M-C5B-C4B	-2.22	114.24	120.28
2	A	1301	B12	O5-P-O4	-2.18	112.21	118.70
2	A	1301	B12	C35-C5-C4	-2.17	114.35	118.25
2	A	1301	B12	O8R-C5R-C4R	-2.01	104.70	111.33
2	A	1301	B12	C5M-C5B-C6B	2.04	125.20	120.73
2	A	1301	B12	C48-C49-C50	2.11	119.23	112.53
2	A	1301	B12	C3R-C2R-C1R	2.16	105.17	99.98
2	A	1301	B12	C1P-N59-C57	2.24	128.32	122.68
2	A	1301	B12	O7R-C2R-C3R	2.37	117.99	111.16
2	A	1301	B12	C60-C18-C17	2.37	120.27	115.68
2	A	1301	B12	C60-C18-C19	2.39	121.31	114.64
2	A	1301	B12	C2-C26-C27	2.82	123.70	115.34
2	A	1301	B12	C26-C2-C1	2.94	114.67	110.00
2	A	1301	B12	C30-C3-C2	2.94	124.91	119.11
2	A	1301	B12	C7-C37-C38	3.08	123.88	114.11
2	A	1301	B12	O6R-C4R-C5R	3.11	115.91	109.17
2	A	1301	B12	C18-C17-C16	3.63	105.45	100.54
2	A	1301	B12	O58-C57-N59	3.67	130.22	122.94
2	A	1301	B12	O6R-C1R-N1B	3.79	116.04	108.10
2	A	1301	B12	P-O3-C2P	3.88	126.01	120.92
2	A	1301	B12	C56-C55-C17	3.95	123.85	115.57
2	A	1301	B12	C48-C13-C12	3.99	127.45	116.53
2	A	1301	B12	C53-C15-C16	4.43	126.19	118.25
2	A	1301	B12	C41-C8-C7	4.56	127.15	114.16
2	A	1301	B12	C2-C1-C19	4.62	126.53	118.56
2	A	1301	B12	C17-C18-C19	5.11	110.90	102.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	B12	C1-C19-C18	5.26	131.09	121.85
2	A	1301	B12	C2R-C1R-N1B	5.32	122.42	114.29
2	A	1301	B12	C1-C19-N24	5.79	113.22	106.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	B12	6	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	577/579 (99%)	0.23	26 (4%) 37 28	67, 113, 146, 157	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	679	THR	4.7
1	A	732	LEU	4.5
1	A	692	VAL	3.8
1	A	682	ALA	3.4
1	A	734	PRO	3.3
1	A	843	ALA	3.2
1	A	651	GLN	3.2
1	A	665	TYR	3.1
1	A	738	ALA	3.1
1	A	728	ALA	3.0
1	A	842	THR	3.0
1	A	681	GLU	2.9
1	A	689	PRO	2.8
1	A	696	PRO	2.8
1	A	896	ARG	2.6
1	A	678	ASP	2.5
1	A	1227	ASP	2.4
1	A	691	GLU	2.4
1	A	736	ILE	2.3
1	A	700	GLY	2.3
1	A	874	THR	2.2
1	A	731	TYR	2.2
1	A	741	GLU	2.2
1	A	878	ASP	2.2
1	A	739	SER	2.1
1	A	656	SER	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	B12	A	1301	91/91	0.92	0.28	0.57	99,108,136,140	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.