



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:41 AM GMT

PDB ID : 2BB6  
Title : Structure of Cobalamin-complexed Bovine Transcobalamin in Monoclinic Crystal Form  
Authors : Wuerges, J.; Garau, G.; Geremia, S.; Fedosov, S.N.; Petersen, T.E.; Randaccio, L.  
Deposited on : 2005-10-17  
Resolution : 2.00 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  
<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

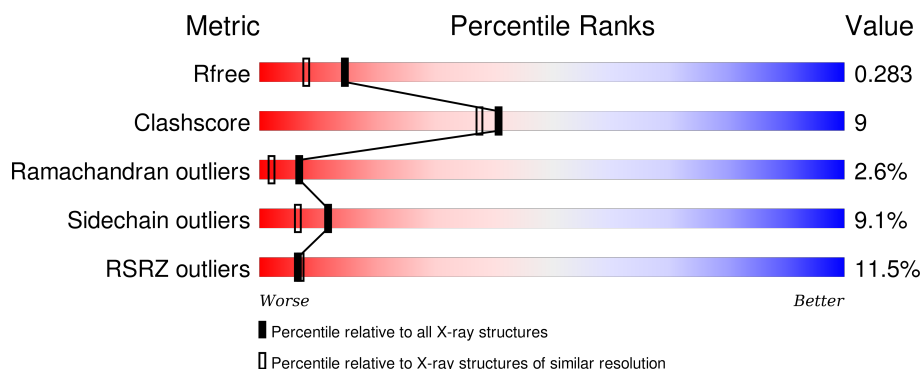
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 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	414	 11% 82% 14% . .
1	B	414	 11% 82% 13% .
1	C	414	 12% 82% 15% .
1	D	414	 12% 80% 16% . .

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	901	-	-	-	X
2	CL	B	902	-	-	-	X
2	CL	D	903	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14148 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.

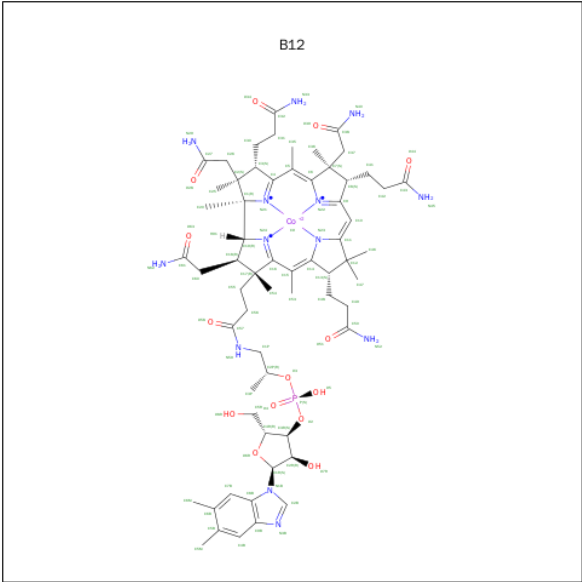
- Molecule 1 is a protein called Transcobalamin II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3254	2057	587	597	13			
1	B	414	Total	C	N	O	S	0	0	0
			3254	2057	587	597	13			
1	C	414	Total	C	N	O	S	0	0	0
			3254	2057	587	597	13			
1	D	414	Total	C	N	O	S	0	0	0
			3254	2057	587	597	13			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: C<sub>62</sub>H<sub>89</sub>CoN<sub>13</sub>O<sub>14</sub>P).



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

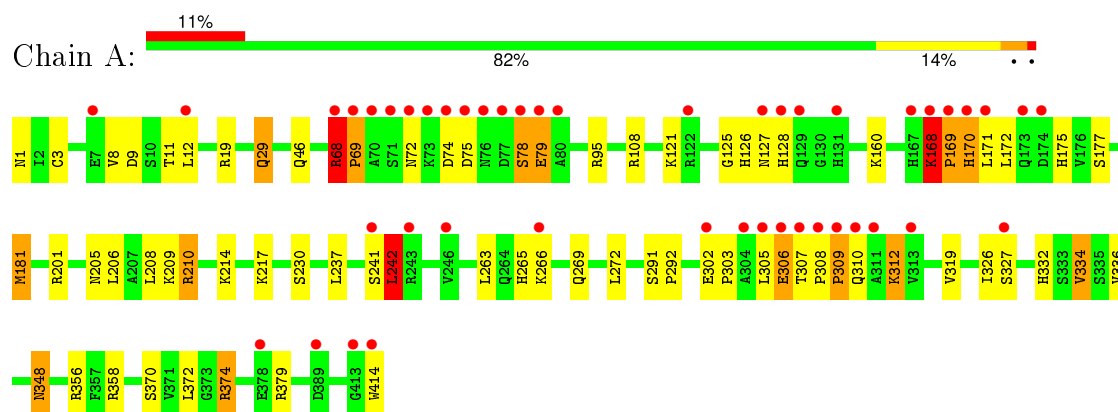
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	181	Total	O	0	0
			181	181		
4	B	204	Total	O	0	0
			204	204		
4	C	198	Total	O	0	0
			198	198		
4	D	181	Total	O	0	0
			181	181		

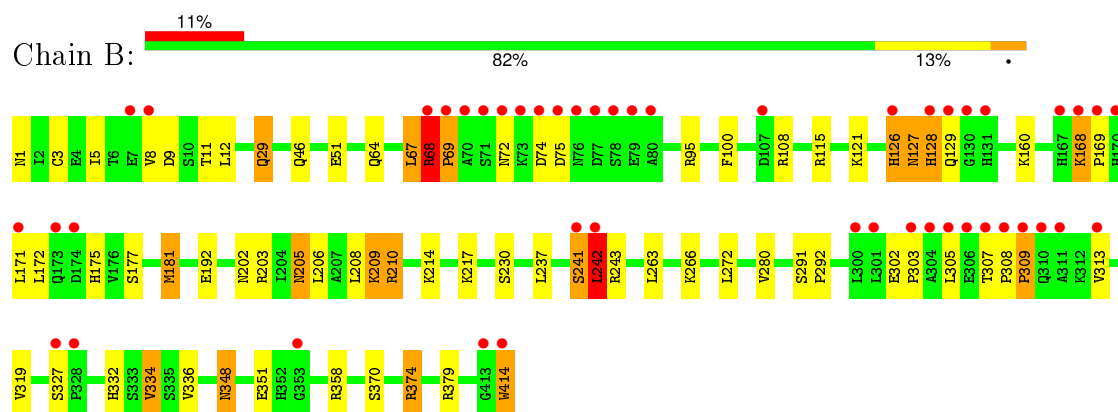
### 3 Residue-property plots [i](#)

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.

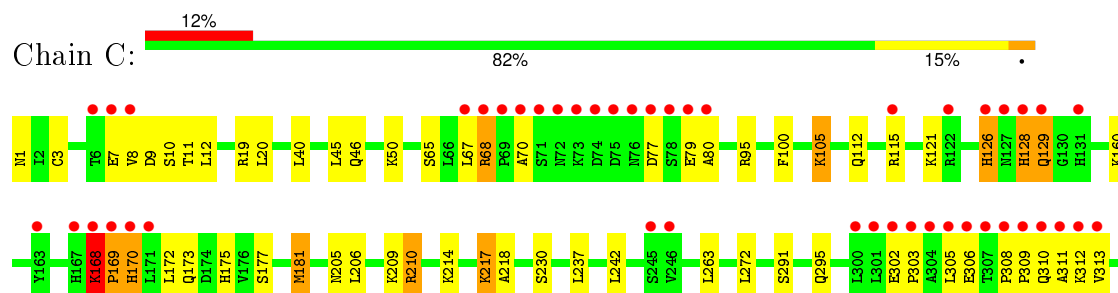
#### • Molecule 1: Transcobalamin II



#### • Molecule 1: Transcobalamin II

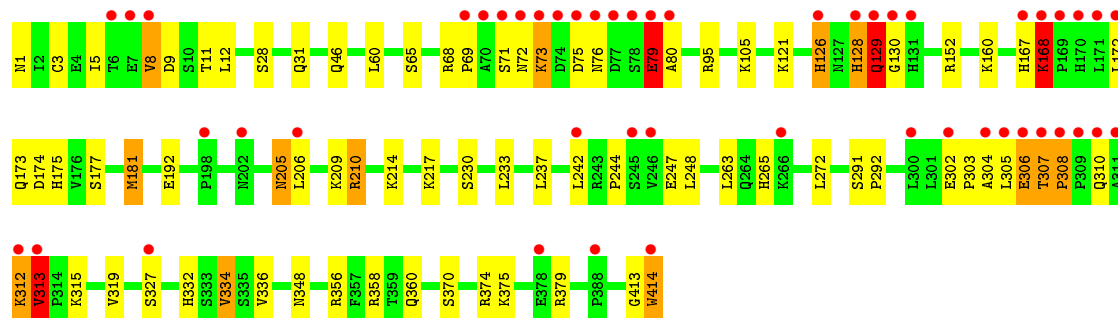
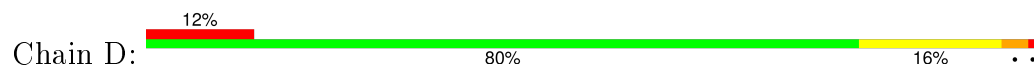


#### • Molecule 1: Transcobalamin II





• Molecule 1: Transcobalamin II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.83Å 100.66Å 99.14Å 90.00° 97.16° 90.00°	Depositor
Resolution (Å)	18.00 – 2.00 44.81 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.8 (18.00-2.00) 96.3 (44.81-1.95)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.241 , 0.280 0.252 , 0.283	Depositor DCC
$R_{free}$ test set	4895 reflections (4.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.1	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	5 of 130819 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14148	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.75 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.0232e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, CL

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	0.55	0/3319	0.65	0/4491
1	B	0.54	0/3319	0.65	0/4491
1	C	0.55	0/3319	0.62	0/4491
1	D	0.55	0/3319	0.65	0/4491
All	All	0.55	0/13276	0.64	0/17964

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	D	0	4
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	ARG	Peptide
1	B	67	LEU	Mainchain,Peptide
1	B	68	ARG	Peptide
1	D	129	GLN	Peptide
1	D	167	HIS	Peptide
1	D	168	LYS	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	D	313	VAL	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3254	0	3317	51	0
1	B	3254	0	3317	50	0
1	C	3254	0	3317	66	1
1	D	3254	0	3317	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	91	0	88	11	0
3	B	91	0	88	10	0
3	C	91	0	88	10	0
3	D	91	0	88	7	0
4	A	181	0	0	7	0
4	B	204	0	0	14	0
4	C	198	0	0	14	1
4	D	181	0	0	6	0
All	All	14148	0	13620	232	1

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 9.

All (232) 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:C:10:SER:CB	1:D:129:GLN:HA	1.63	1.29
1:C:10:SER:HB2	1:D:129:GLN:CA	1.66	1.24
1:B:100:PHE:HD2	4:B:1092:HOH:O	0.93	1.20
1:B:100:PHE:CD2	4:B:1092:HOH:O	1.67	1.13
4:C:993:HOH:O	1:D:129:GLN:HB2	1.52	1.06
1:B:68:ARG:HG3	1:B:108:ARG:HH12	1.24	1.02

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLU:HG3	1:B:115:ARG:HH22	1.17	1.02
1:C:168:LYS:HB3	1:C:169:PRO:CD	1.91	0.99
1:C:414:TRP:HZ2	3:C:0:B12:H521	1.04	0.95
1:A:168:LYS:HB3	1:A:169:PRO:HD2	1.49	0.92
1:C:168:LYS:HB3	1:C:169:PRO:HD2	1.51	0.92
3:C:0:B12:H351	3:C:0:B12:H362	1.55	0.88
1:B:5:ILE:HG13	4:B:1038:HOH:O	1.76	0.85
4:A:1069:HOH:O	1:C:217:LYS:HB2	1.77	0.85
1:A:306:GLU:HG3	1:B:115:ARG:NH2	1.90	0.84
3:D:0:B12:H362	3:D:0:B12:H351	1.59	0.84
1:A:266:LYS:HG2	1:A:269:GLN:NE2	1.92	0.84
1:A:125:GLY:O	1:A:127:ASN:N	2.11	0.83
3:A:0:B12:H351	3:A:0:B12:H362	1.59	0.82
1:B:280:VAL:HG12	4:B:1038:HOH:O	1.78	0.82
1:C:100:PHE:HB2	4:C:908:HOH:O	1.78	0.82
1:C:9:ASP:HB2	4:C:1034:HOH:O	1.78	0.81
1:C:168:LYS:CB	1:C:169:PRO:HD2	2.10	0.81
1:A:125:GLY:C	1:A:127:ASN:H	1.86	0.80
3:B:0:B12:H362	3:B:0:B12:H351	1.66	0.78
1:A:241:SER:O	1:A:242:LEU:HB2	1.83	0.77
1:A:332:HIS:HD2	1:A:334:VAL:HG12	1.49	0.76
1:D:332:HIS:HD2	1:D:334:VAL:HG12	1.50	0.76
1:A:170:HIS:HB3	1:A:214:LYS:NZ	2.02	0.74
1:B:68:ARG:HG3	1:B:108:ARG:NH1	2.00	0.74
1:C:332:HIS:HD2	1:C:334:VAL:HG12	1.53	0.74
1:B:332:HIS:HD2	1:B:334:VAL:HG12	1.53	0.73
3:C:0:B12:H552	3:C:0:B12:H531	1.70	0.73
1:C:302:GLU:HG2	1:C:303:PRO:HD2	1.70	0.72
1:C:100:PHE:CD2	4:C:908:HOH:O	2.42	0.72
1:B:208:LEU:HD13	1:B:242:LEU:HD11	1.71	0.71
1:C:100:PHE:HD2	4:C:908:HOH:O	1.72	0.71
1:C:312:LYS:HG3	1:C:313:VAL:H	1.55	0.70
1:A:302:GLU:HG2	1:A:303:PRO:HD2	1.72	0.70
1:B:414:TRP:HZ2	3:B:0:B12:H521	1.37	0.70
1:D:302:GLU:HG2	1:D:303:PRO:HD2	1.72	0.70
1:B:351:GLU:HG3	4:B:911:HOH:O	1.93	0.69
1:A:208:LEU:HD13	1:A:242:LEU:HD11	1.73	0.69
1:D:128:HIS:O	1:D:130:GLY:N	2.26	0.69
1:B:100:PHE:CB	4:B:1092:HOH:O	2.39	0.68
1:A:170:HIS:HB3	1:A:214:LYS:HZ2	1.57	0.68
1:B:302:GLU:HG2	1:B:303:PRO:HD2	1.74	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:GLN:HB3	4:D:1054:HOH:O	1.93	0.67
1:B:280:VAL:CG1	4:B:1038:HOH:O	2.39	0.67
1:D:414:TRP:HZ2	3:D:0:B12:H521	1.44	0.65
1:B:100:PHE:HB2	4:B:1092:HOH:O	1.94	0.65
1:D:265:HIS:HD2	4:D:1047:HOH:O	1.80	0.65
1:A:266:LYS:HG2	1:A:269:GLN:HE22	1.60	0.65
1:B:209:LYS:HD3	1:B:243:ARG:HD2	1.79	0.64
1:C:217:LYS:HE3	4:C:1068:HOH:O	1.98	0.64
1:B:241:SER:O	1:B:242:LEU:HB2	1.96	0.64
1:A:68:ARG:HB3	1:A:69:PRO:CD	2.26	0.64
1:D:332:HIS:CD2	1:D:334:VAL:HG12	2.32	0.64
1:C:126:HIS:H	1:C:128:HIS:CE1	2.16	0.63
1:C:10:SER:HB2	1:D:129:GLN:HA	0.76	0.63
1:B:67:LEU:O	1:B:69:PRO:HD2	1.99	0.63
1:A:332:HIS:CD2	1:A:334:VAL:HG12	2.33	0.62
1:B:210:ARG:HD3	1:B:214:LYS:HE2	1.82	0.61
1:C:100:PHE:N	4:C:908:HOH:O	2.32	0.61
3:B:0:B12:H552	3:B:0:B12:H531	1.83	0.61
1:C:332:HIS:CD2	1:C:334:VAL:HG12	2.33	0.61
1:C:210:ARG:HD3	1:C:214:LYS:HE2	1.83	0.61
1:B:168:LYS:HB3	1:B:169:PRO:HD2	1.83	0.61
3:A:0:B12:H552	3:A:0:B12:H531	1.83	0.60
1:B:319:VAL:HG12	1:B:334:VAL:HG22	1.84	0.60
3:C:0:B12:H302	3:C:0:B12:H353	1.83	0.60
1:D:121:LYS:HG3	1:D:160:LYS:HG3	1.85	0.59
1:A:326:ILE:HD13	4:A:1049:HOH:O	2.03	0.59
1:C:100:PHE:CB	4:C:908:HOH:O	2.40	0.58
1:B:332:HIS:CD2	1:B:334:VAL:HG12	2.36	0.58
1:A:210:ARG:HD3	1:A:214:LYS:HE2	1.86	0.58
1:D:9:ASP:OD2	1:D:11:THR:OG1	2.18	0.58
1:A:242:LEU:HD13	4:A:1045:HOH:O	2.03	0.58
1:B:121:LYS:HG3	1:B:160:LYS:HG3	1.86	0.58
1:A:319:VAL:HG12	1:A:334:VAL:HG22	1.86	0.58
1:D:306:GLU:O	1:D:307:THR:HB	2.03	0.58
1:D:319:VAL:HG12	1:D:334:VAL:HG22	1.85	0.57
1:C:312:LYS:NZ	1:C:312:LYS:HA	2.18	0.57
1:D:414:TRP:HZ2	3:D:0:B12:N52	2.02	0.57
1:C:319:VAL:HG12	1:C:334:VAL:HG22	1.86	0.57
1:C:121:LYS:HG3	1:C:160:LYS:HG3	1.87	0.57
1:A:121:LYS:HG3	1:A:160:LYS:HG3	1.87	0.57
1:C:45:LEU:HD22	4:D:1032:HOH:O	2.03	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ASP:OD2	1:C:11:THR:OG1	2.22	0.57
1:D:68:ARG:HB2	4:D:1082:HOH:O	2.05	0.56
1:A:201:ARG:HG2	4:A:1055:HOH:O	2.06	0.56
1:B:126:HIS:O	1:B:127:ASN:HB2	2.04	0.56
1:D:210:ARG:HD3	1:D:214:LYS:HE2	1.88	0.55
1:B:307:THR:C	1:B:309:PRO:HD3	2.27	0.55
1:A:125:GLY:C	1:A:127:ASN:N	2.59	0.54
1:D:302:GLU:CG	1:D:303:PRO:HD2	2.37	0.54
1:C:302:GLU:CG	1:C:303:PRO:HD2	2.37	0.54
1:B:160:LYS:NZ	4:B:1066:HOH:O	2.40	0.54
1:A:9:ASP:OD2	1:A:11:THR:OG1	2.24	0.54
1:B:9:ASP:OD2	1:B:11:THR:OG1	2.24	0.53
3:A:0:B12:H353	3:A:0:B12:H302	1.90	0.53
1:D:128:HIS:C	1:D:130:GLY:H	2.12	0.53
1:A:168:LYS:HB3	1:A:169:PRO:CD	2.31	0.53
1:A:302:GLU:CG	1:A:303:PRO:HD2	2.37	0.53
1:D:168:LYS:HE2	1:D:210:ARG:HH22	1.73	0.52
1:C:20:LEU:HD12	1:C:40:LEU:HD21	1.91	0.52
1:C:351:GLU:OE1	1:C:351:GLU:HA	2.09	0.52
1:B:307:THR:O	1:B:309:PRO:HD3	2.10	0.52
1:B:1:ASN:ND2	1:B:3:CYS:HB2	2.25	0.52
1:D:315:LYS:HG2	4:D:1006:HOH:O	2.11	0.51
1:B:175:HIS:HE1	3:B:0:B12:C5	2.23	0.51
3:B:0:B12:H482	3:B:0:B12:H533	1.91	0.51
1:C:126:HIS:N	1:C:128:HIS:CE1	2.78	0.51
1:A:310:GLN:HB2	1:A:312:LYS:HB2	1.93	0.51
1:D:79:GLU:O	1:D:79:GLU:CG	2.59	0.51
1:A:1:ASN:ND2	1:A:3:CYS:HB2	2.27	0.50
1:D:358:ARG:HB2	1:D:370:SER:HB3	1.94	0.50
1:A:68:ARG:HB3	1:A:69:PRO:HD3	1.94	0.50
1:C:9:ASP:HB3	1:C:12:LEU:HD12	1.92	0.50
1:A:358:ARG:HB2	1:A:370:SER:HB3	1.94	0.50
1:C:358:ARG:NH1	4:C:1055:HOH:O	2.44	0.50
1:B:334:VAL:HG11	1:B:348:ASN:HD21	1.77	0.50
1:A:175:HIS:HE1	3:A:0:B12:C5	2.25	0.49
1:A:9:ASP:HB3	1:A:12:LEU:HD12	1.94	0.49
1:C:352:HIS:CD2	4:C:992:HOH:O	2.65	0.49
1:D:28:SER:OG	1:D:31:GLN:HG3	2.13	0.49
1:B:302:GLU:CG	1:B:303:PRO:HD2	2.40	0.49
1:D:304:ALA:HB1	1:D:306:GLU:OE1	2.13	0.49
1:C:20:LEU:HD12	1:C:40:LEU:CD2	2.43	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:PRO:HB3	1:D:248:LEU:HD23	1.93	0.49
1:B:374:ARG:NH2	4:B:1046:HOH:O	2.01	0.49
1:B:51:GLU:HG2	4:B:1022:HOH:O	2.13	0.48
3:D:0:B12:H533	3:D:0:B12:H482	1.94	0.48
3:A:0:B12:H471	3:A:0:B12:H491	1.94	0.48
1:C:358:ARG:HG3	4:C:1055:HOH:O	2.12	0.48
3:B:0:B12:H471	3:B:0:B12:H491	1.96	0.48
1:B:9:ASP:HB3	1:B:12:LEU:HD12	1.96	0.48
1:C:168:LYS:O	1:C:170:HIS:N	2.47	0.47
1:B:358:ARG:HB2	1:B:370:SER:HB3	1.97	0.47
1:B:1:ASN:HD21	1:B:3:CYS:HB2	1.78	0.47
1:A:68:ARG:HG3	1:A:108:ARG:HH12	1.78	0.47
3:C:0:B12:H351	3:C:0:B12:C36	2.31	0.47
1:C:112:GLN:HA	1:C:115:ARG:HG2	1.95	0.47
3:A:0:B12:H531	3:A:0:B12:H543	1.97	0.47
1:A:265:HIS:CD2	4:B:1066:HOH:O	2.68	0.47
1:D:214:LYS:NZ	4:D:1068:HOH:O	2.48	0.47
1:C:358:ARG:HB2	1:C:370:SER:HB3	1.97	0.47
1:C:68:ARG:HD3	1:C:70:ALA:HB3	1.97	0.47
1:C:177:SER:O	1:C:181:MET:HG3	2.14	0.47
1:A:201:ARG:HA	4:A:1064:HOH:O	2.14	0.47
1:B:126:HIS:CD2	1:B:128:HIS:H	2.34	0.46
1:C:67:LEU:HD13	1:C:105:LYS:HD2	1.96	0.46
1:C:168:LYS:C	1:C:170:HIS:H	2.18	0.46
1:A:170:HIS:HB3	1:A:214:LYS:HZ1	1.78	0.46
1:C:168:LYS:C	1:C:170:HIS:N	2.69	0.46
1:A:334:VAL:HG23	1:A:336:VAL:HG13	1.96	0.46
1:D:1:ASN:ND2	1:D:3:CYS:HB2	2.31	0.46
1:A:1:ASN:HD21	1:A:3:CYS:HB2	1.79	0.46
1:C:311:ALA:O	1:C:312:LYS:HB2	2.15	0.46
1:D:175:HIS:HE1	3:D:0:B12:C5	2.29	0.46
1:C:1:ASN:ND2	1:C:3:CYS:HB2	2.31	0.45
1:C:414:TRP:HZ2	3:C:0:B12:N52	1.89	0.45
1:D:312:LYS:O	1:D:313:VAL:HG13	2.16	0.45
1:C:19:ARG:HG2	4:C:1059:HOH:O	2.16	0.45
1:C:175:HIS:HE1	3:C:0:B12:C5	2.29	0.45
1:C:68:ARG:HG2	1:C:70:ALA:HB3	1.99	0.45
1:C:50:LYS:HE2	4:C:987:HOH:O	2.15	0.45
1:C:126:HIS:H	1:C:128:HIS:HE1	1.65	0.45
1:B:74:ASP:N	1:B:74:ASP:OD1	2.49	0.44
1:A:334:VAL:HG11	1:A:348:ASN:HD21	1.83	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:SER:O	1:D:181:MET:HG3	2.17	0.44
1:C:168:LYS:CB	1:C:169:PRO:CD	2.67	0.44
1:A:68:ARG:H	1:A:108:ARG:HH22	1.66	0.44
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.87	0.44
1:A:29:GLN:HB3	1:A:29:GLN:HE21	1.58	0.44
1:A:175:HIS:CE1	3:A:0:B12:C6	3.01	0.44
1:B:192:GLU:OE1	1:B:205:ASN:ND2	2.51	0.44
1:A:374:ARG:NH2	4:A:966:HOH:O	2.26	0.43
3:A:0:B12:C35	3:A:0:B12:H362	2.40	0.43
3:C:0:B12:H533	3:C:0:B12:H482	1.99	0.43
1:D:307:THR:HA	1:D:308:PRO:HD2	1.76	0.43
1:B:95:ARG:O	1:B:292:PRO:HG3	2.18	0.43
1:B:29:GLN:HE21	1:B:29:GLN:HB3	1.63	0.43
1:B:334:VAL:HG23	1:B:336:VAL:HG13	1.99	0.43
1:D:126:HIS:HB2	1:D:128:HIS:CE1	2.54	0.43
1:A:356:ARG:HG2	1:A:372:LEU:HA	1.99	0.43
1:C:20:LEU:CD1	1:C:40:LEU:CD2	2.97	0.43
1:C:10:SER:CB	1:D:129:GLN:CA	2.53	0.42
1:B:203:ARG:HD2	4:B:1075:HOH:O	2.18	0.42
3:A:0:B12:H533	3:A:0:B12:H482	2.00	0.42
3:C:0:B12:H362	3:C:0:B12:C35	2.39	0.42
3:B:0:B12:H91	3:B:0:B12:H262	1.84	0.42
1:D:334:VAL:HG23	1:D:336:VAL:HG13	2.00	0.42
1:A:95:ARG:HD2	1:A:95:ARG:HA	1.88	0.42
1:A:78:SER:O	1:A:79:GLU:HB3	2.19	0.42
1:D:192:GLU:OE1	1:D:205:ASN:ND2	2.52	0.42
1:D:128:HIS:C	1:D:130:GLY:N	2.73	0.42
1:D:95:ARG:O	1:D:292:PRO:HG3	2.19	0.42
3:B:0:B12:C47	3:B:0:B12:H491	2.50	0.42
3:D:0:B12:H552	3:D:0:B12:H531	2.02	0.42
1:B:128:HIS:CG	1:B:129:GLN:N	2.88	0.42
1:D:1:ASN:HD21	1:D:3:CYS:HB2	1.84	0.42
1:B:305:LEU:HB2	4:B:1098:HOH:O	2.20	0.42
1:B:177:SER:O	1:B:181:MET:HG3	2.19	0.42
1:C:413:GLY:O	1:C:414:TRP:HB3	2.20	0.42
1:B:175:HIS:CE1	3:B:0:B12:C6	3.03	0.42
3:B:0:B12:H353	3:B:0:B12:H302	2.01	0.42
1:C:10:SER:HB2	1:D:129:GLN:C	2.33	0.41
1:C:327:SER:HB3	4:C:985:HOH:O	2.19	0.41
1:C:217:LYS:HE2	1:C:218:ALA:N	2.36	0.41
3:D:0:B12:H362	3:D:0:B12:C35	2.39	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ARG:HG2	4:A:1054:HOH:O	2.21	0.41
1:C:334:VAL:HG23	1:C:336:VAL:HG13	2.02	0.41
1:C:1:ASN:HD21	1:C:3:CYS:HB2	1.84	0.41
1:D:233:LEU:HA	1:D:233:LEU:HD23	1.95	0.41
1:A:168:LYS:CB	1:A:169:PRO:HD2	2.36	0.41
1:C:20:LEU:CD1	1:C:40:LEU:HD21	2.50	0.41
1:B:319:VAL:CG1	1:B:334:VAL:HG22	2.49	0.41
1:A:177:SER:O	1:A:181:MET:HG3	2.20	0.41
1:D:413:GLY:O	1:D:414:TRP:HB3	2.21	0.41
3:A:0:B12:H252	3:A:0:B12:C61	2.51	0.41
1:D:95:ARG:HA	1:D:95:ARG:HD2	1.89	0.41
1:A:319:VAL:CG1	1:A:334:VAL:HG22	2.50	0.41
1:D:5:ILE:HG22	1:D:8:VAL:HG22	2.02	0.41
1:C:168:LYS:HB3	1:C:169:PRO:HD3	1.93	0.40
1:C:319:VAL:CG1	1:C:334:VAL:HG22	2.51	0.40
1:D:68:ARG:NH2	1:D:80:ALA:O	2.54	0.40
1:A:95:ARG:O	1:A:292:PRO:HG3	2.21	0.40
1:C:95:ARG:HA	1:C:95:ARG:HD2	1.89	0.40
1:C:68:ARG:NH2	1:C:80:ALA:O	2.54	0.40
1:C:175:HIS:CE1	3:C:0:B12:C6	3.05	0.40
3:A:0:B12:H262	3:A:0:B12:H91	2.00	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:GLN:NE2	4:C:1094:HOH:O[2_655]	2.10	0.10

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	412/414 (100%)	388 (94%)	10 (2%)	14 (3%)	5	1
1	B	412/414 (100%)	382 (93%)	21 (5%)	9 (2%)	8	3
1	C	412/414 (100%)	384 (93%)	19 (5%)	9 (2%)	8	3
1	D	412/414 (100%)	388 (94%)	13 (3%)	11 (3%)	6	2
All	All	1648/1656 (100%)	1542 (94%)	63 (4%)	43 (3%)	7	2

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	69	PRO
1	A	72	ASN
1	A	126	HIS
1	A	242	LEU
1	B	69	PRO
1	B	126	HIS
1	B	127	ASN
1	B	242	LEU
1	C	168	LYS
1	C	169	PRO
1	C	170	HIS
1	D	73	LYS
1	D	76	ASN
1	D	129	GLN
1	A	74	ASP
1	A	79	GLU
1	A	307	THR
1	C	128	HIS
1	C	129	GLN
1	D	69	PRO
1	D	71	SER
1	D	72	ASN
1	D	308	PRO
1	A	168	LYS
1	A	78	SER
1	A	128	HIS
1	B	128	HIS
1	C	310	GLN
1	D	79	GLU
1	D	128	HIS
1	D	168	LYS
1	D	307	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	75	ASP
1	A	169	PRO
1	B	75	ASP
1	C	79	GLU
1	C	309	PRO
1	B	168	LYS
1	B	309	PRO
1	B	308	PRO
1	C	308	PRO
1	A	309	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	358/358 (100%)	329 (92%)	29 (8%)	15	9
1	B	358/358 (100%)	328 (92%)	30 (8%)	14	8
1	C	358/358 (100%)	327 (91%)	31 (9%)	13	7
1	D	358/358 (100%)	317 (88%)	41 (12%)	7	4
All	All	1432/1432 (100%)	1301 (91%)	131 (9%)	12	6

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	29	GLN
1	A	46	GLN
1	A	68	ARG
1	A	168	LYS
1	A	170	HIS
1	A	171	LEU
1	A	172	LEU
1	A	181	MET
1	A	205	ASN
1	A	206	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	209	LYS
1	A	210	ARG
1	A	217	LYS
1	A	230	SER
1	A	237	LEU
1	A	242	LEU
1	A	263	LEU
1	A	272	LEU
1	A	291	SER
1	A	305	LEU
1	A	306	GLU
1	A	312	LYS
1	A	327	SER
1	A	334	VAL
1	A	348	ASN
1	A	374	ARG
1	A	379	ARG
1	A	414	TRP
1	B	8	VAL
1	B	29	GLN
1	B	46	GLN
1	B	64	GLN
1	B	68	ARG
1	B	72	ASN
1	B	171	LEU
1	B	172	LEU
1	B	181	MET
1	B	202	ASN
1	B	205	ASN
1	B	206	LEU
1	B	209	LYS
1	B	210	ARG
1	B	217	LYS
1	B	230	SER
1	B	237	LEU
1	B	241	SER
1	B	242	LEU
1	B	263	LEU
1	B	266	LYS
1	B	272	LEU
1	B	291	SER
1	B	313	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	327	SER
1	B	334	VAL
1	B	348	ASN
1	B	374	ARG
1	B	379	ARG
1	B	414	TRP
1	C	7	GLU
1	C	8	VAL
1	C	46	GLN
1	C	65	SER
1	C	68	ARG
1	C	77	ASP
1	C	105	LYS
1	C	126	HIS
1	C	129	GLN
1	C	168	LYS
1	C	172	LEU
1	C	173	GLN
1	C	181	MET
1	C	205	ASN
1	C	206	LEU
1	C	209	LYS
1	C	210	ARG
1	C	217	LYS
1	C	230	SER
1	C	237	LEU
1	C	242	LEU
1	C	263	LEU
1	C	272	LEU
1	C	291	SER
1	C	305	LEU
1	C	306	GLU
1	C	327	SER
1	C	334	VAL
1	C	374	ARG
1	C	379	ARG
1	C	414	TRP
1	D	8	VAL
1	D	12	LEU
1	D	46	GLN
1	D	60	LEU
1	D	65	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	73	LYS
1	D	75	ASP
1	D	79	GLU
1	D	105	LYS
1	D	126	HIS
1	D	152	ARG
1	D	168	LYS
1	D	172	LEU
1	D	173	GLN
1	D	174	ASP
1	D	181	MET
1	D	205	ASN
1	D	206	LEU
1	D	209	LYS
1	D	210	ARG
1	D	217	LYS
1	D	230	SER
1	D	237	LEU
1	D	242	LEU
1	D	247	GLU
1	D	263	LEU
1	D	272	LEU
1	D	291	SER
1	D	305	LEU
1	D	306	GLU
1	D	310	GLN
1	D	312	LYS
1	D	313	VAL
1	D	327	SER
1	D	334	VAL
1	D	348	ASN
1	D	356	ARG
1	D	374	ARG
1	D	375	LYS
1	D	379	ARG
1	D	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	63	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	205	ASN
1	A	269	GLN
1	A	348	ASN
1	A	360	GLN
1	B	1	ASN
1	B	63	GLN
1	B	348	ASN
1	B	360	GLN
1	C	1	ASN
1	C	63	GLN
1	C	128	HIS
1	C	129	GLN
1	C	173	GLN
1	C	205	ASN
1	C	348	ASN
1	C	360	GLN
1	D	1	ASN
1	D	63	GLN
1	D	128	HIS
1	D	205	ASN
1	D	348	ASN
1	D	360	GLN

### 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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
3	B12	A	0	1	74,101,101	0.86	2 (2%)	111,166,166	1.29	15 (13%)
3	B12	B	0	1	74,101,101	0.87	2 (2%)	111,166,166	1.36	11 (9%)
3	B12	C	0	1	74,101,101	0.83	2 (2%)	111,166,166	1.34	13 (11%)
3	B12	D	0	1	74,101,101	0.92	3 (4%)	111,166,166	1.46	18 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B12	A	0	1	-	0/51/223/223	0/3/11/11
3	B12	B	0	1	-	0/51/223/223	0/3/11/11
3	B12	C	0	1	-	0/51/223/223	0/3/11/11
3	B12	D	0	1	-	0/51/223/223	0/3/11/11

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	0	B12	C4B-C9B	-3.39	1.36	1.41
3	B	0	B12	C4B-C9B	-3.00	1.37	1.41
3	A	0	B12	C4B-C9B	-2.98	1.37	1.41
3	A	0	B12	C48-C13	-2.54	1.50	1.54
3	C	0	B12	C4B-C9B	-2.47	1.38	1.41
3	C	0	B12	C2B-N3B	-2.28	1.30	1.34
3	B	0	B12	C2B-N3B	-2.22	1.30	1.34
3	D	0	B12	C2B-N3B	-2.21	1.30	1.34
3	D	0	B12	C30-C3	2.02	1.57	1.54

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	0	B12	C2R-C1R-N1B	-6.85	103.82	114.29
3	D	0	B12	C2R-C1R-N1B	-6.75	103.98	114.29
3	C	0	B12	C2R-C1R-N1B	-6.70	104.05	114.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	0	B12	C2R-C1R-N1B	-6.18	104.85	114.29
3	D	0	B12	O2-P-O3	-4.03	96.24	100.07
3	B	0	B12	C25-C2-C26	-3.31	102.59	109.73
3	B	0	B12	C4B-C9B-C8B	-2.90	118.13	121.10
3	C	0	B12	C25-C2-C26	-2.87	103.54	109.73
3	A	0	B12	C25-C2-C26	-2.62	104.07	109.73
3	C	0	B12	C4B-C9B-C8B	-2.55	118.49	121.10
3	B	0	B12	C3-C4-C5	-2.52	123.38	131.88
3	D	0	B12	C9-C10-C11	-2.49	126.05	132.28
3	A	0	B12	C3-C4-C5	-2.42	123.72	131.88
3	C	0	B12	C3-C4-C5	-2.41	123.73	131.88
3	D	0	B12	C3-C4-C5	-2.32	124.04	131.88
3	A	0	B12	C13-C14-C15	-2.31	124.08	131.88
3	D	0	B12	C4B-C9B-C8B	-2.28	118.77	121.10
3	D	0	B12	C25-C2-C26	-2.28	104.82	109.73
3	A	0	B12	C9-C10-C11	-2.26	126.63	132.28
3	B	0	B12	C13-C14-C15	-2.23	124.34	131.88
3	A	0	B12	O2-P-O3	-2.18	97.99	100.07
3	D	0	B12	C55-C17-C18	-2.12	106.72	110.97
3	A	0	B12	C4B-C9B-C8B	-2.09	118.97	121.10
3	A	0	B12	C5R-C4R-C3R	-2.09	107.78	114.82
3	D	0	B12	C47-C12-C46	-2.05	104.50	109.56
3	C	0	B12	C9-C10-C11	-2.05	127.14	132.28
3	B	0	B12	C36-C7-C37	-2.00	107.44	110.81
3	C	0	B12	C18-C60-C61	2.00	118.86	113.92
3	B	0	B12	C36-C7-C8	2.00	115.86	112.24
3	D	0	B12	C4R-O6R-C1R	2.01	111.93	109.72
3	B	0	B12	C60-C18-C19	2.06	120.40	114.64
3	D	0	B12	C2P-C1P-N59	2.08	116.01	112.92
3	D	0	B12	C18-C17-C16	2.19	103.50	100.54
3	C	0	B12	C7B-C8B-C9B	2.22	122.74	120.54
3	C	0	B12	C60-C18-C19	2.22	120.84	114.64
3	A	0	B12	C2P-C1P-N59	2.27	116.28	112.92
3	A	0	B12	C1-C19-N24	2.32	109.01	106.20
3	A	0	B12	C7B-C8B-C9B	2.35	122.86	120.54
3	A	0	B12	C35-C5-C6	2.38	122.52	118.25
3	D	0	B12	C26-C2-C1	2.46	113.92	110.00
3	A	0	B12	C26-C2-C1	2.47	113.94	110.00
3	D	0	B12	C1-C19-N24	2.48	109.22	106.20
3	D	0	B12	C35-C5-C6	2.50	122.73	118.25
3	C	0	B12	C2P-C1P-N59	2.55	116.70	112.92
3	C	0	B12	C19-C1-N21	2.58	104.78	102.16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	0	B12	C19-C1-N21	2.66	104.87	102.16
3	A	0	B12	P-O3-C2P	2.72	124.49	120.92
3	D	0	B12	C18-C60-C61	2.80	120.84	113.92
3	C	0	B12	P-O3-C2P	2.98	124.83	120.92
3	C	0	B12	C20-C1-C2	3.06	118.86	113.26
3	B	0	B12	P-O3-C2P	3.06	124.94	120.92
3	C	0	B12	O6R-C1R-N1B	3.38	115.17	108.10
3	D	0	B12	C20-C1-C2	3.41	119.48	113.26
3	D	0	B12	O6R-C1R-N1B	3.42	115.26	108.10
3	B	0	B12	O6R-C1R-N1B	3.43	115.28	108.10
3	A	0	B12	O6R-C1R-N1B	4.02	116.52	108.10
3	B	0	B12	C7B-C8B-C9B	4.10	124.60	120.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	0	B12	11	0
3	B	0	B12	10	0
3	C	0	B12	10	0
3	D	0	B12	7	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	414/414 (100%)	0.67	46 (11%) 7 8	8, 30, 77, 151	0
1	B	414/414 (100%)	0.72	47 (11%) 7 7	8, 31, 77, 157	0
1	C	414/414 (100%)	0.79	49 (11%) 6 6	9, 33, 86, 221	0
1	D	414/414 (100%)	0.72	49 (11%) 6 6	11, 31, 79, 151	0
All	All	1656/1656 (100%)	0.72	191 (11%) 6 7	8, 31, 79, 221	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	LEU	14.1
1	D	72	ASN	13.8
1	D	73	LYS	12.7
1	C	71	SER	12.5
1	C	305	LEU	11.9
1	C	309	PRO	11.2
1	D	70	ALA	10.4
1	C	75	ASP	10.0
1	A	169	PRO	9.9
1	D	305	LEU	9.5
1	D	309	PRO	9.5
1	D	313	VAL	9.1
1	C	307	THR	9.1
1	C	78	SER	8.8
1	A	305	LEU	8.7
1	D	75	ASP	8.6
1	A	78	SER	8.5
1	D	76	ASN	8.3
1	B	75	ASP	8.2
1	B	309	PRO	8.2
1	C	169	PRO	8.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	304	ALA	8.2
1	C	76	ASN	8.0
1	D	307	THR	8.0
1	A	414	TRP	7.9
1	A	72	ASN	7.8
1	B	71	SER	7.8
1	C	72	ASN	7.8
1	A	73	LYS	7.7
1	B	311	ALA	7.6
1	B	169	PRO	7.5
1	C	308	PRO	7.5
1	C	303	PRO	7.4
1	A	168	LYS	7.3
1	A	74	ASP	7.3
1	A	71	SER	7.2
1	C	70	ALA	7.1
1	B	304	ALA	7.0
1	B	76	ASN	7.0
1	D	311	ALA	6.9
1	B	72	ASN	6.9
1	B	414	TRP	6.9
1	D	74	ASP	6.8
1	C	73	LYS	6.8
1	C	310	GLN	6.6
1	A	309	PRO	6.6
1	B	78	SER	6.5
1	D	310	GLN	6.4
1	D	169	PRO	6.3
1	D	69	PRO	6.3
1	B	310	GLN	6.3
1	A	311	ALA	6.2
1	B	73	LYS	6.2
1	C	77	ASP	6.1
1	D	129	GLN	6.1
1	C	74	ASP	6.1
1	C	167	HIS	6.1
1	A	413	GLY	5.9
1	D	308	PRO	5.9
1	D	71	SER	5.8
1	C	80	ALA	5.7
1	C	168	LYS	5.7
1	D	168	LYS	5.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	311	ALA	5.5
1	B	77	ASP	5.4
1	B	307	THR	5.4
1	D	414	TRP	5.3
1	A	128	HIS	5.3
1	A	171	LEU	5.2
1	C	126	HIS	5.2
1	C	171	LEU	5.0
1	B	308	PRO	4.9
1	D	7	GLU	4.9
1	A	310	GLN	4.9
1	A	327	SER	4.7
1	B	79	GLU	4.7
1	A	307	THR	4.6
1	A	80	ALA	4.6
1	B	168	LYS	4.6
1	B	327	SER	4.5
1	B	68	ARG	4.5
1	C	128	HIS	4.5
1	D	77	ASP	4.5
1	A	170	HIS	4.5
1	A	76	ASN	4.4
1	D	126	HIS	4.4
1	C	129	GLN	4.4
1	A	79	GLU	4.4
1	B	313	VAL	4.4
1	A	313	VAL	4.4
1	A	173	GLN	4.4
1	D	131	HIS	4.4
1	B	70	ALA	4.3
1	B	128	HIS	4.3
1	C	300	LEU	4.2
1	D	128	HIS	4.2
1	B	129	GLN	4.1
1	D	80	ALA	4.1
1	D	312	LYS	4.1
1	B	173	GLN	4.1
1	C	306	GLU	4.0
1	B	174	ASP	3.9
1	C	7	GLU	3.9
1	A	69	PRO	3.9
1	A	241	SER	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	327	SER	3.8
1	A	167	HIS	3.8
1	C	6	THR	3.7
1	D	171	LEU	3.7
1	C	414	TRP	3.7
1	D	167	HIS	3.7
1	D	78	SER	3.6
1	B	7	GLU	3.6
1	C	313	VAL	3.5
1	B	170	HIS	3.5
1	A	77	ASP	3.5
1	A	127	ASN	3.5
1	D	79	GLU	3.4
1	D	266	LYS	3.2
1	B	131	HIS	3.2
1	A	68	ARG	3.2
1	D	246	VAL	3.2
1	C	327	SER	3.2
1	C	79	GLU	3.2
1	B	303	PRO	3.1
1	C	170	HIS	3.1
1	C	69	PRO	3.1
1	A	70	ALA	3.0
1	D	242	LEU	3.0
1	A	174	ASP	3.0
1	D	378	GLU	2.9
1	A	131	HIS	2.9
1	D	130	GLY	2.9
1	D	304	ALA	2.9
1	B	126	HIS	2.9
1	B	171	LEU	2.9
1	B	306	GLU	2.9
1	C	115	ARG	2.9
1	D	306	GLU	2.7
1	B	74	ASP	2.7
1	D	6	THR	2.7
1	B	300	LEU	2.7
1	B	241	SER	2.7
1	B	107	ASP	2.7
1	A	266	LYS	2.7
1	B	242	LEU	2.6
1	C	246	VAL	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	127	ASN	2.6
1	B	80	ALA	2.5
1	A	7	GLU	2.5
1	C	312	LYS	2.5
1	C	163	TYR	2.4
1	D	170	HIS	2.4
1	D	245	SER	2.4
1	C	67	LEU	2.4
1	C	301	LEU	2.4
1	A	129	GLN	2.4
1	A	243	ARG	2.4
1	C	131	HIS	2.4
1	D	300	LEU	2.4
1	D	8	VAL	2.3
1	D	198	PRO	2.3
1	A	306	GLU	2.3
1	D	202	ASN	2.3
1	A	75	ASP	2.3
1	C	122	ARG	2.3
1	D	172	LEU	2.3
1	B	353	GLY	2.3
1	B	8	VAL	2.3
1	A	378	GLU	2.3
1	B	413	GLY	2.2
1	A	246	VAL	2.2
1	C	302	GLU	2.2
1	B	301	LEU	2.2
1	C	328	PRO	2.2
1	A	12	LEU	2.2
1	D	302	GLU	2.2
1	C	68	ARG	2.1
1	C	245	SER	2.1
1	B	328	PRO	2.1
1	C	8	VAL	2.1
1	B	167	HIS	2.1
1	B	69	PRO	2.1
1	A	122	ARG	2.1
1	A	308	PRO	2.0
1	A	304	ALA	2.0
1	D	206	LEU	2.0
1	D	388	PRO	2.0
1	A	302	GLU	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	130	GLY	2.0
1	A	389	ASP	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(Å <sup>2</sup> )	Q<0.9
2	CL	A	901	1/1	0.99	0.22	6.70	23,23,23,23	0
2	CL	B	902	1/1	1.00	0.15	2.96	24,24,24,24	0
2	CL	D	903	1/1	0.99	0.16	2.25	24,24,24,24	0
2	CL	C	904	1/1	0.99	0.10	0.19	23,23,23,23	0
3	B12	D	0	91/91	0.96	0.12	-0.04	9,15,28,42	0
3	B12	B	0	91/91	0.96	0.11	-0.06	7,14,27,44	0
3	B12	C	0	91/91	0.96	0.11	-0.07	7,15,31,44	0
3	B12	A	0	91/91	0.96	0.12	-0.12	7,13,21,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.