



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:28 PM GMT

PDB ID : 1NQE  
Title : OUTER MEMBRANE COBALAMIN TRANSPORTER (BTUB) FROM E. COLI  
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Deposited on : 2003-01-21  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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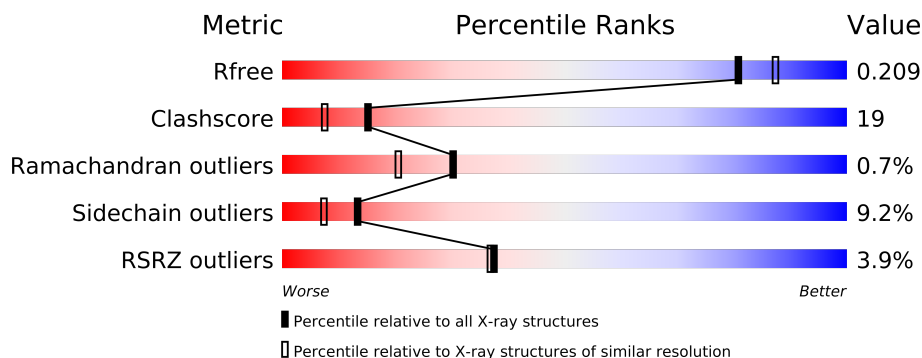
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	594	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	C8E	A	800	-	X
3	C8E	A	801	-	X
3	C8E	A	802	-	X
3	C8E	A	803	-	X
3	C8E	A	805	-	X
3	C8E	A	806	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4733 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

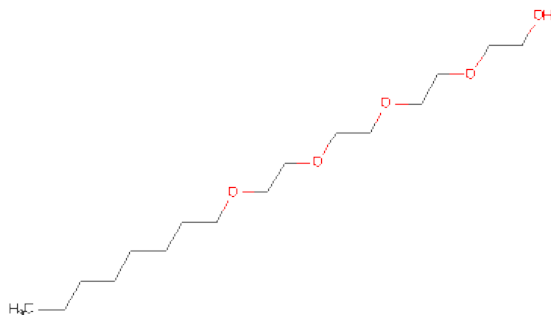
- Molecule 1 is a protein called Vitamin B12 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4350	2742	748	858	2			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	235	Total	O	0	0
			235	235		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.59Å 81.59Å 210.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.92 – 2.00 24.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (24.92-2.00) 99.6 (24.87-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.194 , 0.232 0.209 , 0.209	Depositor DCC
$R_{free}$ test set	2818 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 65.4	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55457 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, C8E

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	0.85	6/4455 (0.1%)	0.97	21/6059 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	GLN	CD-NE2	10.38	1.58	1.32
1	A	571	LYS	CE-NZ	9.21	1.72	1.49
1	A	571	LYS	CD-CE	7.90	1.71	1.51
1	A	537	GLN	CD-OE1	6.34	1.37	1.24
1	A	226	ARG	CG-CD	5.18	1.64	1.51
1	A	426	THR	CB-CG2	-5.01	1.35	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	537	GLN	OE1-CD-NE2	-8.74	101.80	121.90
1	A	498	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	A	134	ASP	CB-CG-OD2	7.02	124.62	118.30
1	A	515	ASP	CB-CG-OD2	6.63	124.26	118.30
1	A	497	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	A	162	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	513	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	548	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	81	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	447	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	84	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	439	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	492	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	485	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	274	ASP	CB-CG-OD2	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	153	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	571	LYS	CD-CE-NZ	-5.21	99.70	111.70
1	A	84	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	53	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	6	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4350	0	4109	141	0
2	A	1	0	0	0	0
3	A	147	0	238	35	0
4	A	235	0	0	10	0
All	All	4733	0	4347	167	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (167) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:571:LYS:NZ	1:A:571:LYS:CE	1.72	1.49
3:A:802:C8E:H52	3:A:802:C8E:C1	1.49	1.31
1:A:169:LEU:HD13	1:A:170:GLY:N	1.67	1.09
3:A:802:C8E:C5	3:A:802:C8E:H13	1.79	1.09
1:A:169:LEU:C	1:A:169:LEU:HD13	1.75	1.04
3:A:802:C8E:H52	3:A:802:C8E:H13	0.97	0.96
3:A:802:C8E:C5	3:A:802:C8E:C1	2.40	0.96
3:A:803:C8E:H13	3:A:805:C8E:C14	1.97	0.95
1:A:198:LEU:HD13	1:A:199:SER:N	1.82	0.94
1:A:169:LEU:C	1:A:169:LEU:CD1	2.37	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:48:ARG:HH12	1:A:519:THR:HG21	1.37	0.90
1:A:197:PHE:HD2	1:A:227:THR:HG22	1.35	0.90
1:A:197:PHE:CD2	1:A:227:THR:HG22	2.08	0.88
1:A:411:ASP:H	1:A:455:ASN:HD21	1.18	0.88
3:A:802:C8E:H52	3:A:802:C8E:H12	1.57	0.87
1:A:527:TYR:CE1	1:A:540:LYS:HG3	2.10	0.87
1:A:160:LEU:HD23	1:A:166:VAL:HG21	1.55	0.86
1:A:516:TRP:CE3	1:A:551:VAL:HG13	2.11	0.85
1:A:506:GLN:HE22	1:A:519:THR:CG2	1.91	0.83
1:A:198:LEU:HD13	1:A:198:LEU:C	2.00	0.81
3:A:803:C8E:H13	3:A:805:C8E:H141	1.62	0.80
1:A:169:LEU:HD13	1:A:170:GLY:CA	2.12	0.78
1:A:135:GLU:H	1:A:157:GLN:HE22	1.32	0.78
1:A:539:VAL:CG2	1:A:540:LYS:N	2.48	0.77
1:A:580:GLN:HG2	4:A:953:HOH:O	1.83	0.77
1:A:426:THR:CG2	1:A:431:TRP:HE1	1.96	0.77
1:A:198:LEU:C	1:A:198:LEU:CD1	2.53	0.76
1:A:144:TRP:C	1:A:144:TRP:CD1	2.61	0.73
1:A:404:PHE:O	1:A:404:PHE:HD2	1.71	0.73
1:A:539:VAL:HG22	1:A:540:LYS:N	2.01	0.73
1:A:397:ASN:H	1:A:400:GLN:HE21	1.37	0.72
1:A:506:GLN:NE2	1:A:519:THR:HB	2.04	0.72
1:A:160:LEU:HD23	1:A:166:VAL:CG2	2.19	0.72
1:A:146:SER:O	1:A:147:ASN:HB2	1.88	0.72
1:A:100:PRO:HG2	1:A:103:LEU:HD22	1.71	0.71
1:A:358:ARG:O	3:A:800:C8E:H82	1.90	0.71
1:A:506:GLN:HE22	1:A:519:THR:HG22	1.55	0.71
1:A:362:ASN:ND2	1:A:364:GLN:H	1.89	0.70
1:A:47:ARG:NH2	4:A:832:HOH:O	2.25	0.70
3:A:803:C8E:C1	3:A:805:C8E:C14	2.71	0.69
1:A:397:ASN:H	1:A:400:GLN:NE2	1.92	0.68
1:A:48:ARG:NH1	1:A:519:THR:HG21	2.10	0.66
1:A:516:TRP:CE3	1:A:551:VAL:CG1	2.78	0.66
3:A:803:C8E:H112	3:A:805:C8E:H82	1.78	0.66
1:A:534:TYR:CG	1:A:535:PRO:HA	2.30	0.66
1:A:369:GLY:C	3:A:800:C8E:H111	2.16	0.66
1:A:13:ASN:ND2	1:A:15:PHE:H	1.95	0.65
3:A:803:C8E:H13	3:A:805:C8E:O15	1.96	0.65
1:A:174:HIS:CE1	1:A:176:HIS:CE1	2.85	0.64
1:A:383:TYR:OH	1:A:426:THR:HB	1.98	0.64
1:A:407:ASN:C	1:A:407:ASN:HD22	2.00	0.64
1:A:144:TRP:HD1	1:A:144:TRP:C	2.02	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:571:LYS:CD	1:A:571:LYS:NZ	2.62	0.63
1:A:491:THR:HG23	1:A:493:THR:H	1.63	0.63
1:A:411:ASP:H	1:A:455:ASN:ND2	1.93	0.63
1:A:516:TRP:CZ3	1:A:551:VAL:HG13	2.33	0.62
1:A:114:ARG:HA	1:A:372:GLN:HE22	1.64	0.62
1:A:144:TRP:HD1	1:A:144:TRP:O	1.83	0.61
1:A:47:ARG:NH2	1:A:548:ASP:OD2	2.26	0.61
3:A:802:C8E:H101	3:A:802:C8E:H141	1.82	0.60
1:A:491:THR:CG2	1:A:493:THR:OG1	2.50	0.60
3:A:803:C8E:C1	3:A:805:C8E:H141	2.31	0.59
1:A:19:ARG:HE	1:A:26:THR:HG23	1.68	0.59
1:A:539:VAL:CG2	1:A:540:LYS:H	2.16	0.58
1:A:323:THR:HG23	1:A:324:PRO:HD2	1.85	0.58
1:A:135:GLU:H	1:A:157:GLN:NE2	1.98	0.58
1:A:527:TYR:CZ	1:A:540:LYS:HG3	2.37	0.58
1:A:510:GLN:NE2	4:A:902:HOH:O	2.37	0.58
1:A:488:ASN:CG	1:A:491:THR:HG22	2.25	0.57
1:A:426:THR:HG23	1:A:431:TRP:HE1	1.70	0.57
1:A:19:ARG:HE	1:A:26:THR:CG2	2.18	0.56
1:A:516:TRP:CZ3	1:A:551:VAL:CG1	2.88	0.56
1:A:174:HIS:C	1:A:174:HIS:CD2	2.77	0.56
1:A:539:VAL:HG23	1:A:540:LYS:H	1.70	0.56
1:A:245:LEU:HD23	1:A:246:TYR:N	2.22	0.55
1:A:358:ARG:O	3:A:800:C8E:C8	2.54	0.55
1:A:245:LEU:CD2	1:A:246:TYR:N	2.69	0.55
1:A:174:HIS:HE1	1:A:176:HIS:CE1	2.25	0.55
3:A:803:C8E:C11	3:A:805:C8E:H61	2.37	0.54
1:A:426:THR:HG22	1:A:431:TRP:HE1	1.73	0.54
1:A:13:ASN:HD22	1:A:15:PHE:H	1.54	0.54
1:A:362:ASN:HD22	1:A:365:PHE:H	1.56	0.54
1:A:13:ASN:HD22	1:A:13:ASN:C	2.10	0.54
1:A:534:TYR:CD2	1:A:535:PRO:HA	2.42	0.54
1:A:447:ASP:OD2	1:A:449:HIS:HB2	2.07	0.54
1:A:510:GLN:N	1:A:510:GLN:NE2	2.56	0.54
1:A:336:ARG:HD3	4:A:1010:HOH:O	2.08	0.54
1:A:407:ASN:ND2	1:A:409:ASN:H	2.07	0.53
1:A:491:THR:HG23	1:A:493:THR:OG1	2.09	0.53
1:A:506:GLN:NE2	1:A:519:THR:CB	2.72	0.53
1:A:368:HIS:HD2	4:A:957:HOH:O	1.92	0.52
1:A:358:ARG:C	3:A:800:C8E:H71	2.30	0.52
1:A:160:LEU:CD2	1:A:166:VAL:HG21	2.34	0.52
1:A:263:SER:OG	1:A:302:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:LEU:HD11	1:A:200:LYS:HG3	1.92	0.52
1:A:521:GLN:HE21	1:A:523:LEU:HD21	1.75	0.51
1:A:491:THR:HG21	1:A:493:THR:OG1	2.11	0.51
1:A:462:LYS:HB3	3:A:804:C8E:H172	1.92	0.51
1:A:135:GLU:OE1	1:A:135:GLU:HA	2.10	0.50
1:A:527:TYR:CE1	1:A:540:LYS:CG	2.90	0.50
1:A:245:LEU:C	1:A:245:LEU:CD2	2.79	0.50
1:A:407:ASN:C	1:A:407:ASN:ND2	2.65	0.49
1:A:13:ASN:O	1:A:14:ARG:HB2	2.12	0.49
1:A:368:HIS:HE1	4:A:847:HOH:O	1.95	0.49
1:A:169:LEU:O	1:A:169:LEU:CD1	2.61	0.49
1:A:174:HIS:HB2	1:A:198:LEU:HD22	1.95	0.48
3:A:803:C8E:H82	3:A:806:C8E:H22	1.96	0.48
1:A:583:GLY:O	1:A:585:GLU:HG3	2.14	0.48
1:A:407:ASN:HD22	1:A:409:ASN:H	1.60	0.48
1:A:488:ASN:HB3	1:A:491:THR:HG22	1.96	0.48
1:A:404:PHE:CD2	1:A:404:PHE:O	2.58	0.47
1:A:196:GLY:N	1:A:228:ASN:HD22	2.12	0.47
1:A:519:THR:HG23	4:A:872:HOH:O	2.15	0.47
1:A:516:TRP:CD2	1:A:551:VAL:CG1	2.98	0.47
1:A:346:GLN:NE2	3:A:805:C8E:H202	2.30	0.47
1:A:519:THR:CG2	4:A:872:HOH:O	2.63	0.46
1:A:506:GLN:HE22	1:A:519:THR:CB	2.27	0.46
1:A:506:GLN:NE2	1:A:519:THR:CG2	2.70	0.46
3:A:803:C8E:H111	3:A:805:C8E:H61	1.97	0.46
1:A:17:GLN:OE1	1:A:21:THR:HG22	2.15	0.46
1:A:13:ASN:ND2	1:A:13:ASN:C	2.69	0.45
1:A:144:TRP:CD1	1:A:144:TRP:O	2.65	0.45
1:A:404:PHE:C	1:A:404:PHE:CD2	2.89	0.45
1:A:8:LEU:HD13	1:A:16:GLU:OE2	2.16	0.45
1:A:516:TRP:CH2	1:A:551:VAL:HG11	2.52	0.45
3:A:802:C8E:C14	3:A:802:C8E:C10	2.94	0.45
3:A:803:C8E:H22	3:A:805:C8E:H142	1.98	0.45
1:A:362:ASN:HD22	1:A:364:GLN:H	1.59	0.45
1:A:436:TYR:O	3:A:804:C8E:H202	2.17	0.45
1:A:372:GLN:NE2	4:A:809:HOH:O	2.49	0.45
1:A:426:THR:HG23	1:A:431:TRP:NE1	2.32	0.44
1:A:160:LEU:HD13	1:A:160:LEU:HA	1.60	0.44
1:A:146:SER:O	1:A:147:ASN:CB	2.62	0.44
3:A:803:C8E:H71	3:A:803:C8E:H101	1.25	0.44
1:A:369:GLY:HA3	3:A:800:C8E:C11	2.48	0.44
3:A:804:C8E:H82	3:A:804:C8E:H112	1.21	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:488:ASN:HB3	1:A:491:THR:CG2	2.47	0.44
1:A:169:LEU:O	1:A:169:LEU:HD12	2.18	0.43
1:A:162:ASP:C	1:A:163:LYS:CG	2.86	0.43
3:A:803:C8E:H172	3:A:803:C8E:H142	1.44	0.43
3:A:801:C8E:H142	4:A:861:HOH:O	2.18	0.43
1:A:164:THR:OG1	1:A:208:HIS:CD2	2.72	0.43
1:A:245:LEU:C	1:A:245:LEU:HD22	2.40	0.43
1:A:308:HIS:HB3	1:A:347:GLN:HE21	1.83	0.43
3:A:805:C8E:H161	3:A:805:C8E:H191	1.76	0.43
1:A:555:VAL:HG12	1:A:556:THR:HG23	2.02	0.42
3:A:805:C8E:H52	3:A:806:C8E:H41	2.01	0.42
1:A:526:ARG:C	1:A:527:TYR:HD1	2.23	0.42
1:A:245:LEU:HD22	1:A:246:TYR:N	2.34	0.42
1:A:160:LEU:CD2	1:A:166:VAL:CG2	2.95	0.42
1:A:157:GLN:C	1:A:158:GLN:HG2	2.40	0.42
1:A:462:LYS:HB3	3:A:804:C8E:H201	2.02	0.42
1:A:174:HIS:HB2	1:A:198:LEU:CD2	2.49	0.42
3:A:801:C8E:H131	3:A:801:C8E:H102	1.44	0.41
1:A:84:ARG:HH11	1:A:318:GLN:HE22	1.67	0.41
1:A:488:ASN:CB	1:A:491:THR:HG22	2.50	0.41
1:A:491:THR:OG1	1:A:493:THR:HG23	2.20	0.41
1:A:163:LYS:HB3	1:A:209:ASN:O	2.21	0.41
1:A:330:GLU:HG3	1:A:330:GLU:H	1.55	0.41
3:A:800:C8E:H112	3:A:800:C8E:H141	1.07	0.40
1:A:31:ARG:O	1:A:31:ARG:HD3	2.21	0.40
1:A:291:ASP:HA	1:A:326:THR:HG23	2.03	0.40
1:A:142:ALA:HB1	1:A:151:ASN:O	2.21	0.40
1:A:407:ASN:HD22	1:A:408:PRO:N	2.18	0.40
3:A:801:C8E:H141	3:A:801:C8E:H171	1.73	0.40
1:A:411:ASP:N	1:A:455:ASN:HD21	2.00	0.40
1:A:594:PHE:N	1:A:594:PHE:CD1	2.90	0.40

There are no symmetry-related clashes.

## 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	541/594 (91%)	522 (96%)	15 (3%)	4 (1%)	30	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	456	GLU
1	A	513	ASP
1	A	121	ASP

### 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	457/495 (92%)	415 (91%)	42 (9%)	13	7

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	13	ASN
1	A	21	THR
1	A	31	ARG
1	A	47	ARG
1	A	60	SER
1	A	103	LEU
1	A	138	THR
1	A	144	TRP
1	A	155	SER
1	A	158	GLN
1	A	160	LEU
1	A	162	ASP
1	A	163	LYS
1	A	169	LEU
1	A	174	HIS
1	A	198	LEU
1	A	206	LEU
1	A	215	SER

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Mol	Chain	Res	Type
1	A	245	LEU
1	A	260	LEU
1	A	262	LYS
1	A	265	LEU
1	A	266	ILE
1	A	330	GLU
1	A	345	LEU
1	A	346	GLN
1	A	348	VAL
1	A	404	PHE
1	A	407	ASN
1	A	423	GLU
1	A	425	LEU
1	A	426	THR
1	A	510	GLN
1	A	511	LEU
1	A	519	THR
1	A	539	VAL
1	A	551	VAL
1	A	559	LEU
1	A	564	LYS
1	A	589	SER
1	A	594	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	98	GLN
1	A	147	ASN
1	A	150	GLN
1	A	157	GLN
1	A	159	GLN
1	A	174	HIS
1	A	176	HIS
1	A	208	HIS
1	A	225	ASN
1	A	248	GLN
1	A	295	GLN
1	A	302	ASN
1	A	318	GLN
1	A	320	GLN

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Mol	Chain	Res	Type
1	A	337	ASN
1	A	347	GLN
1	A	362	ASN
1	A	372	GLN
1	A	400	GLN
1	A	407	ASN
1	A	455	ASN
1	A	506	GLN
1	A	510	GLN
1	A	521	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	C8E	A	800	-	20,20,20	0.53	0	19,19,19	1.02	2 (10%)
3	C8E	A	801	-	20,20,20	0.59	0	19,19,19	0.86	0
3	C8E	A	802	-	20,20,20	0.40	0	19,19,19	0.75	0
3	C8E	A	803	-	20,20,20	0.38	0	19,19,19	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	C8E	A	804	-	20,20,20	0.40	0	19,19,19	0.74	0
3	C8E	A	805	-	20,20,20	0.56	0	19,19,19	0.44	0
3	C8E	A	806	-	20,20,20	0.56	0	19,19,19	0.47	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	C8E	A	800	-	-	0/18/18/18	0/0/0/0
3	C8E	A	801	-	-	0/18/18/18	0/0/0/0
3	C8E	A	802	-	-	0/18/18/18	0/0/0/0
3	C8E	A	803	-	-	0/18/18/18	0/0/0/0
3	C8E	A	804	-	-	0/18/18/18	0/0/0/0
3	C8E	A	805	-	-	0/18/18/18	0/0/0/0
3	C8E	A	806	-	-	0/18/18/18	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	C8E	O9-C8-C7	-2.26	100.92	109.88
3	A	800	C8E	O12-C11-C10	-2.22	100.38	110.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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	549/594 (92%)	-0.02	22 (4%) 36 36	28, 40, 67, 97	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ASP	5.7
1	A	162	ASP	5.7
1	A	277	TYR	5.6
1	A	328	TYR	5.3
1	A	177	GLY	5.0
1	A	144	TRP	4.4
1	A	594	PHE	4.3
1	A	512	TYR	4.0
1	A	592	TYR	3.7
1	A	241	ASP	3.6
1	A	288	ALA	3.4
1	A	404	PHE	3.2
1	A	242	THR	2.9
1	A	135	GLU	2.7
1	A	580	GLN	2.7
1	A	448	ASP	2.6
1	A	330	GLU	2.5
1	A	531	TYR	2.4
1	A	160	LEU	2.4
1	A	134	ASP	2.4
1	A	331	ASP	2.1
1	A	308	HIS	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	C8E	A	806	21/21	0.35	8.58	49,100,128,136	0
3	C8E	A	801	21/21	0.20	5.53	47,68,107,111	0
3	C8E	A	805	21/21	0.17	2.93	61,79,107,109	0
3	C8E	A	800	21/21	0.19	2.70	42,58,84,96	0
3	C8E	A	803	21/21	0.18	2.50	49,89,110,117	0
3	C8E	A	802	21/21	0.19	2.31	38,57,77,86	0
3	C8E	A	804	21/21	0.16	2.00	39,58,86,102	0
2	MG	A	595	1/1	0.06	-3.58	48,48,48,48	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.