



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:13 AM GMT

PDB ID : 2NQ5
Title : Crystal structure of methyltransferase from Streptococcus mutans
Authors : Fedorov, A.A.; Fedorov, E.V.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-10-30
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

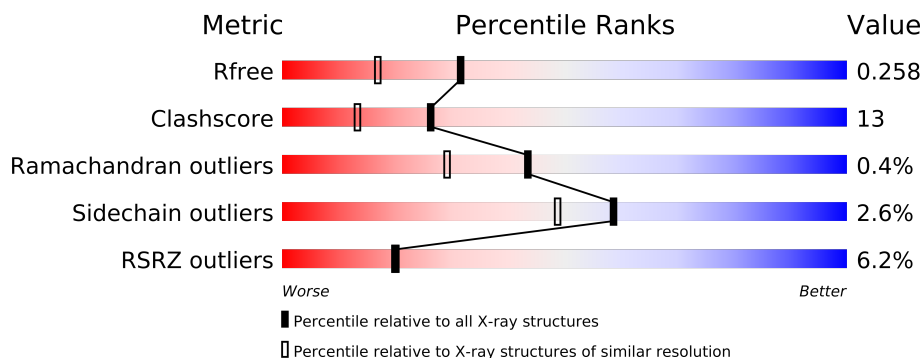
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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 ≥ 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	755	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5980 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 5-methyltetrahydropteroyltriglutamate--homocysteinemethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	0	0	0
			5632	3623	943	1059	7			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	CLONING ARTIFACT	UNP Q8CWX6
A	0	SER	-	CLONING ARTIFACT	UNP Q8CWX6
A	1	LEU	-	CLONING ARTIFACT	UNP Q8CWX6
A	746	GLU	-	CLONING ARTIFACT	UNP Q8CWX6
A	747	GLY	-	CLONING ARTIFACT	UNP Q8CWX6
A	748	HIS	-	EXPRESSION TAG	UNP Q8CWX6
A	749	HIS	-	EXPRESSION TAG	UNP Q8CWX6
A	750	HIS	-	EXPRESSION TAG	UNP Q8CWX6
A	751	HIS	-	EXPRESSION TAG	UNP Q8CWX6
A	752	HIS	-	EXPRESSION TAG	UNP Q8CWX6
A	753	HIS	-	EXPRESSION TAG	UNP Q8CWX6

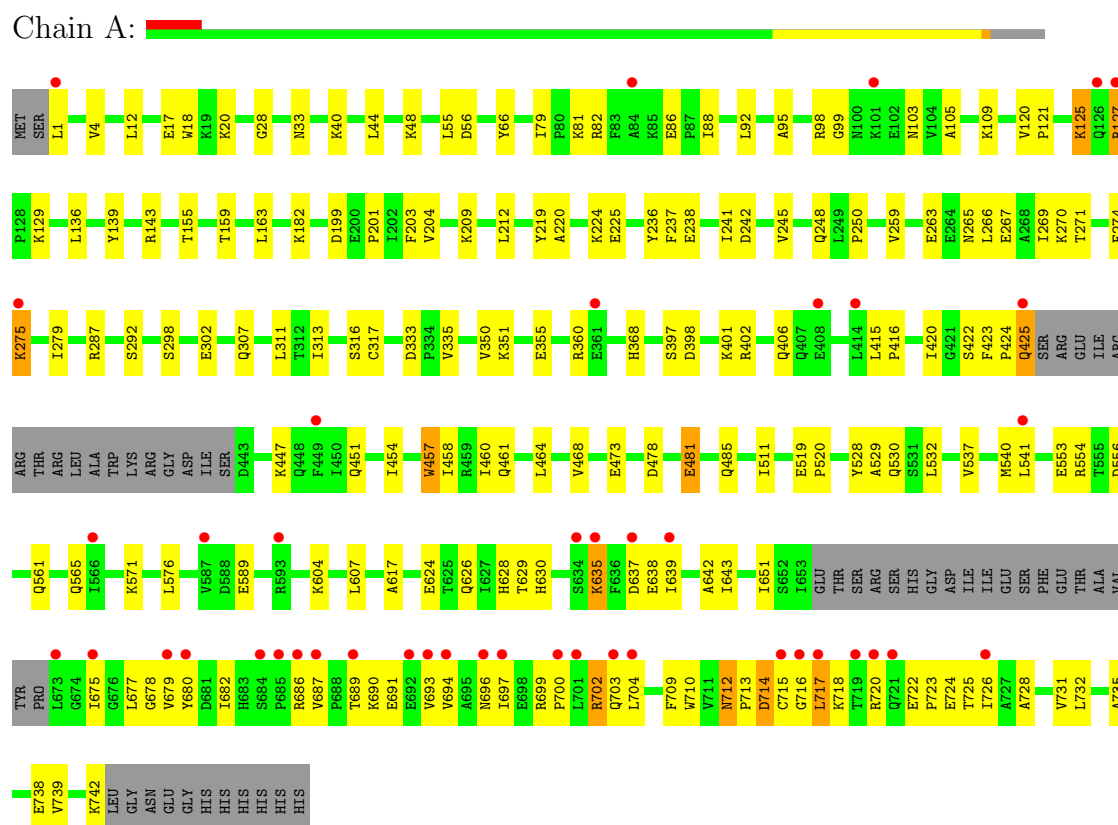
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	348	Total	O	0	0
			348	348		

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: 5-methyltetrahydropteroyltriglutamate--homocysteinemethyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.29Å 99.19Å 78.62Å 90.00° 109.25° 90.00°	Depositor
Resolution (Å)	24.96 – 1.90 29.07 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.5 (24.96-1.90) 96.3 (29.07-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 1.88Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.258 0.228 , 0.258	Depositor DCC
R_{free} test set	2919 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 40.4	EDS
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 60109 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5980	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.35	0/5752	0.58	0/7801

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	TYR	Sidechain

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	5632	0	5660	150	0
2	A	348	0	0	3	0
All	All	5980	0	5660	150	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 13.

All (150) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:143:ARG:HG3	1:A:143:ARG:HH11	1.36	0.91
1:A:4:VAL:HG23	1:A:55:LEU:HA	1.52	0.91
1:A:125:LYS:H	1:A:125:LYS:HD2	1.39	0.88
1:A:553:GLU:HG2	2:A:978:HOH:O	1.75	0.87
1:A:630:HIS:NE2	1:A:715:CYS:SG	2.53	0.81
1:A:717:LEU:O	1:A:717:LEU:HD23	1.83	0.78
1:A:425:GLN:N	1:A:425:GLN:HE21	1.82	0.77
1:A:275:LYS:HD3	1:A:275:LYS:O	1.83	0.77
1:A:720:ARG:HH12	1:A:724:GLU:HB3	1.48	0.77
1:A:313:ILE:HG22	1:A:350:VAL:HG13	1.67	0.76
1:A:717:LEU:HD21	1:A:725:THR:HG21	1.68	0.75
1:A:458:ILE:HD12	1:A:532:LEU:HD12	1.70	0.74
1:A:626:GLN:HE21	1:A:628:HIS:HE1	1.35	0.73
1:A:722:GLU:HB3	1:A:723:PRO:HD3	1.71	0.72
1:A:626:GLN:NE2	1:A:628:HIS:HE1	1.89	0.71
1:A:127:ARG:HD2	1:A:127:ARG:O	1.91	0.71
1:A:511:ILE:O	1:A:554:ARG:HG3	1.92	0.70
1:A:626:GLN:HE21	1:A:628:HIS:CE1	2.10	0.69
1:A:637:ASP:OD1	1:A:638:GLU:HG2	1.94	0.67
1:A:481:GLU:O	1:A:485:GLN:HG3	1.94	0.67
1:A:397:SER:OG	1:A:401:LYS:HE2	1.95	0.67
1:A:457:TRP:O	1:A:461:GLN:HG3	1.95	0.66
1:A:292:SER:O	1:A:368:HIS:HE1	1.78	0.66
1:A:127:ARG:HE	1:A:129:LYS:HD3	1.60	0.66
1:A:245:VAL:O	1:A:248:GLN:HG2	1.96	0.66
1:A:635:LYS:NZ	1:A:635:LYS:HB2	2.11	0.65
1:A:143:ARG:CG	1:A:143:ARG:HH11	2.10	0.65
1:A:447:LYS:O	1:A:451:GLN:HG3	1.96	0.65
1:A:88:ILE:N	1:A:88:ILE:HD12	2.11	0.65
1:A:263:GLU:O	1:A:267:GLU:HG3	1.98	0.64
1:A:159:THR:O	1:A:163:LEU:HD13	1.98	0.63
1:A:473:GLU:OE2	1:A:540:MET:HG2	1.99	0.63
1:A:4:VAL:CG2	1:A:55:LEU:HA	2.28	0.62
1:A:639:ILE:O	1:A:643:ILE:HG12	1.99	0.62
1:A:717:LEU:HD21	1:A:725:THR:CG2	2.29	0.62
1:A:738:GLU:O	1:A:742:LYS:HD3	2.00	0.61
1:A:333:ASP:OD1	1:A:335:VAL:HG12	1.99	0.61
1:A:607:LEU:HD13	1:A:639:ILE:HG23	1.82	0.60
1:A:28:GLY:HA2	2:A:1090:HOH:O	2.01	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:125:LYS:HD2	1:A:125:LYS:N	2.16	0.59
1:A:604:LYS:HG2	2:A:1009:HOH:O	2.04	0.58
1:A:425:GLN:OE1	1:A:718:LYS:HE3	2.04	0.58
1:A:82:ARG:HB2	1:A:103:ASN:ND2	2.18	0.58
1:A:699:ARG:O	1:A:702:ARG:HB3	2.02	0.58
1:A:298:SER:O	1:A:302:GLU:HG3	2.04	0.57
1:A:690:LYS:HG2	1:A:731:VAL:HG23	1.85	0.57
1:A:626:GLN:HG2	1:A:628:HIS:CE1	2.40	0.56
1:A:351:LYS:O	1:A:355:GLU:HG3	2.05	0.56
1:A:424:PRO:HD3	1:A:717:LEU:CD2	2.36	0.56
1:A:81:LYS:HE3	1:A:81:LYS:HA	1.87	0.55
1:A:143:ARG:HG3	1:A:143:ARG:NH1	2.14	0.55
1:A:398:ASP:O	1:A:402:ARG:HG3	2.06	0.55
1:A:704:LEU:HD12	1:A:704:LEU:N	2.21	0.55
1:A:201:PRO:O	1:A:204:VAL:HG22	2.06	0.55
1:A:17:GLU:HA	1:A:20:LYS:HE3	1.87	0.55
1:A:267:GLU:O	1:A:271:THR:HG23	2.07	0.54
1:A:720:ARG:HH12	1:A:724:GLU:CB	2.20	0.54
1:A:109:LYS:HG3	1:A:120:VAL:HG21	1.90	0.53
1:A:693:VAL:O	1:A:697:ILE:HG22	2.08	0.53
1:A:720:ARG:HG3	1:A:720:ARG:HH11	1.73	0.53
1:A:678:GLY:HA2	1:A:712:ASN:O	2.09	0.52
1:A:136:LEU:C	1:A:136:LEU:HD13	2.29	0.52
1:A:4:VAL:HG11	1:A:351:LYS:HA	1.92	0.52
1:A:127:ARG:HH11	1:A:127:ARG:HG2	1.73	0.52
1:A:460:ILE:O	1:A:464:LEU:HG	2.10	0.51
1:A:630:HIS:HE2	1:A:715:CYS:HA	1.76	0.51
1:A:415:LEU:HD13	1:A:697:ILE:HD11	1.92	0.51
1:A:287:ARG:HG3	1:A:317:CYS:SG	2.51	0.51
1:A:98:ARG:C	1:A:105:ALA:HB2	2.31	0.51
1:A:677:LEU:HD11	1:A:709:PHE:HD2	1.76	0.51
1:A:682:ILE:HD12	1:A:682:ILE:C	2.31	0.51
1:A:423:PHE:HA	1:A:717:LEU:HD22	1.93	0.51
1:A:425:GLN:HE22	1:A:718:LYS:HG2	1.76	0.51
1:A:275:LYS:HD3	1:A:275:LYS:C	2.31	0.50
1:A:397:SER:CB	1:A:401:LYS:HE2	2.42	0.50
1:A:704:LEU:HD12	1:A:704:LEU:H	1.77	0.49
1:A:313:ILE:CG2	1:A:350:VAL:HG13	2.40	0.49
1:A:422:SER:O	1:A:717:LEU:HB3	2.12	0.49
1:A:702:ARG:HG3	1:A:703:GLN:HG3	1.94	0.49
1:A:629:THR:O	1:A:651:ILE:HA	2.13	0.48
1:A:677:LEU:HD11	1:A:709:PHE:CD2	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:561:GLN:O	1:A:565:GLN:HG3	2.13	0.48
1:A:139:TYR:CZ	1:A:143:ARG:HD3	2.49	0.48
1:A:451:GLN:HB3	1:A:528:TYR:CE2	2.48	0.47
1:A:680:TYR:HD1	1:A:713:PRO:HB3	1.79	0.47
1:A:40:LYS:O	1:A:44:LEU:HG	2.15	0.47
1:A:4:VAL:HG22	1:A:56:ASP:OD2	2.15	0.47
1:A:709:PHE:N	1:A:709:PHE:CD1	2.83	0.47
1:A:224:LYS:NZ	1:A:225:GLU:OE2	2.47	0.47
1:A:651:ILE:HG23	1:A:651:ILE:O	2.15	0.47
1:A:266:LEU:HG	1:A:270:LYS:HE2	1.97	0.47
1:A:478:ASP:HB3	1:A:481:GLU:HB3	1.96	0.47
1:A:704:LEU:CD1	1:A:704:LEU:H	2.28	0.46
1:A:689:THR:O	1:A:693:VAL:HG22	2.15	0.46
1:A:220:ALA:HA	1:A:250:PRO:HG3	1.97	0.46
1:A:79:ILE:HD13	1:A:92:LEU:HD21	1.97	0.46
1:A:236:TYR:O	1:A:237:PHE:HB2	2.15	0.46
1:A:88:ILE:CD1	1:A:88:ILE:N	2.79	0.46
1:A:44:LEU:O	1:A:48:LYS:HG3	2.16	0.46
1:A:735:ALA:O	1:A:739:VAL:HG23	2.16	0.45
1:A:680:TYR:CD1	1:A:713:PRO:HB3	2.51	0.45
1:A:639:ILE:HG22	1:A:639:ILE:O	2.16	0.45
1:A:259:VAL:HB	1:A:316:SER:OG	2.16	0.45
1:A:720:ARG:NH1	1:A:724:GLU:HB3	2.26	0.45
1:A:12:LEU:HA	1:A:18:TRP:HB3	1.98	0.45
1:A:458:ILE:HD11	1:A:529:ALA:HA	1.99	0.44
1:A:265:ASN:O	1:A:269:ILE:HG12	2.17	0.44
1:A:686:ARG:O	1:A:720:ARG:NH2	2.50	0.44
1:A:571:LYS:HB2	1:A:617:ALA:HA	1.99	0.44
1:A:691:GLU:O	1:A:694:VAL:HG12	2.18	0.44
1:A:675:ILE:HD11	1:A:709:PHE:CE2	2.53	0.44
1:A:687:VAL:HG13	1:A:687:VAL:O	2.18	0.44
1:A:554:ARG:HB3	1:A:556:ASP:OD1	2.18	0.44
1:A:530:GLN:NE2	1:A:537:VAL:H	2.16	0.44
1:A:127:ARG:HG2	1:A:127:ARG:NH1	2.33	0.44
1:A:86:GLU:HB2	1:A:92:LEU:HD13	2.00	0.44
1:A:270:LYS:HA	1:A:307:GLN:HE21	1.83	0.43
1:A:589:GLU:OE1	1:A:589:GLU:HA	2.18	0.43
1:A:540:MET:O	1:A:541:LEU:HD23	2.18	0.43
1:A:415:LEU:N	1:A:416:PRO:HD3	2.31	0.43
1:A:519:GLU:HB2	1:A:520:PRO:HD2	2.00	0.43
1:A:722:GLU:O	1:A:726:ILE:HG22	2.18	0.43
1:A:728:ALA:O	1:A:731:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:95:ALA:O	1:A:99:GLY:N	2.49	0.43
1:A:212:LEU:HD11	1:A:242:ASP:OD2	2.19	0.43
1:A:690:LYS:O	1:A:694:VAL:HG12	2.19	0.43
1:A:274:PHE:HB3	1:A:279:ILE:HD11	2.01	0.43
1:A:639:ILE:HG22	1:A:642:ALA:HB3	2.00	0.42
1:A:406:GLN:HG2	1:A:624:GLU:O	2.18	0.42
1:A:699:ARG:N	1:A:700:PRO:HD2	2.33	0.42
1:A:635:LYS:HZ2	1:A:635:LYS:HB2	1.80	0.42
1:A:702:ARG:HD2	1:A:702:ARG:O	2.18	0.42
1:A:454:ILE:O	1:A:458:ILE:HG13	2.19	0.42
1:A:99:GLY:N	1:A:105:ALA:HB2	2.35	0.42
1:A:203:PHE:O	1:A:241:ILE:HG12	2.19	0.42
1:A:182:LYS:C	1:A:182:LYS:HD3	2.40	0.42
1:A:451:GLN:HB3	1:A:528:TYR:CZ	2.55	0.42
1:A:732:LEU:HD23	1:A:732:LEU:C	2.40	0.42
1:A:425:GLN:HE21	1:A:425:GLN:H	1.62	0.41
1:A:682:ILE:HG21	1:A:716:GLY:O	2.19	0.41
1:A:704:LEU:N	1:A:704:LEU:CD1	2.84	0.41
1:A:155:THR:HA	1:A:199:ASP:HB2	2.01	0.41
1:A:420:ILE:HG13	1:A:714:ASP:O	2.21	0.41
1:A:691:GLU:C	1:A:694:VAL:HG12	2.41	0.41
1:A:679:VAL:HG12	1:A:696:ASN:HB3	2.03	0.41
1:A:630:HIS:CD2	1:A:715:CYS:SG	3.14	0.41
1:A:693:VAL:HG23	1:A:735:ALA:CB	2.51	0.41
1:A:143:ARG:CG	1:A:143:ARG:NH1	2.72	0.40
1:A:120:VAL:HA	1:A:121:PRO:HD3	1.94	0.40
1:A:468:VAL:HG21	1:A:710:TRP:CZ3	2.56	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	700/755 (93%)	676 (97%)	21 (3%)	3 (0%)	43 29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	714	ASP
1	A	717	LEU
1	A	66	TYR

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	608/651 (93%)	592 (97%)	16 (3%)	59 49

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	33	ASN
1	A	125	LYS
1	A	127	ARG
1	A	209	LYS
1	A	238	GLU
1	A	275	LYS
1	A	311	LEU
1	A	360	ARG
1	A	425	GLN
1	A	457	TRP
1	A	481	GLU
1	A	576	LEU
1	A	635	LYS
1	A	702	ARG
1	A	712	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	50	GLN
1	A	103	ASN

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Mol	Chain	Res	Type
1	A	115	ASN
1	A	368	HIS
1	A	425	GLN
1	A	530	GLN
1	A	586	GLN
1	A	626	GLN
1	A	628	HIS
1	A	696	ASN
1	A	703	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 ⓘ

There are no ligands in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	706/755 (93%)	0.31	44 (6%) 20 20	12, 21, 43, 52	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	704	LEU	5.4
1	A	449	PHE	5.3
1	A	639	ILE	4.7
1	A	703	GLN	4.7
1	A	715	CYS	4.7
1	A	414	LEU	4.6
1	A	716	GLY	4.5
1	A	361	GLU	4.3
1	A	680	TYR	4.3
1	A	692	GLU	4.3
1	A	685	PRO	4.1
1	A	697	ILE	4.0
1	A	1	LEU	3.9
1	A	635	LYS	3.9
1	A	687	VAL	3.7
1	A	679	VAL	3.5
1	A	673	LEU	3.4
1	A	126	GLN	3.3
1	A	726	ILE	3.3
1	A	689	THR	3.3
1	A	720	ARG	3.3
1	A	701	LEU	3.1
1	A	408	GLU	3.0
1	A	593	ARG	3.0
1	A	700	PRO	2.9
1	A	675	ILE	2.9
1	A	541	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	721	GLN	2.9
1	A	587	VAL	2.8
1	A	127	ARG	2.7
1	A	634	SER	2.6
1	A	719	THR	2.6
1	A	696	ASN	2.6
1	A	275	LYS	2.5
1	A	686	ARG	2.5
1	A	566	ILE	2.3
1	A	101	LYS	2.3
1	A	84	ALA	2.2
1	A	717	LEU	2.2
1	A	693	VAL	2.1
1	A	425	GLN	2.1
1	A	694	VAL	2.0
1	A	684	SER	2.0
1	A	637	ASP	2.0

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.