



Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 07:44 PM GMT

PDB ID : 4AAY
Title : Crystal Structure of the arsenite oxidase protein complex from Rhizobium species strain NT-26
Authors : Oke, M.; Santini, J.M.; Naismith, J.H.
Deposited on : 2011-12-05
Resolution : 2.70 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>

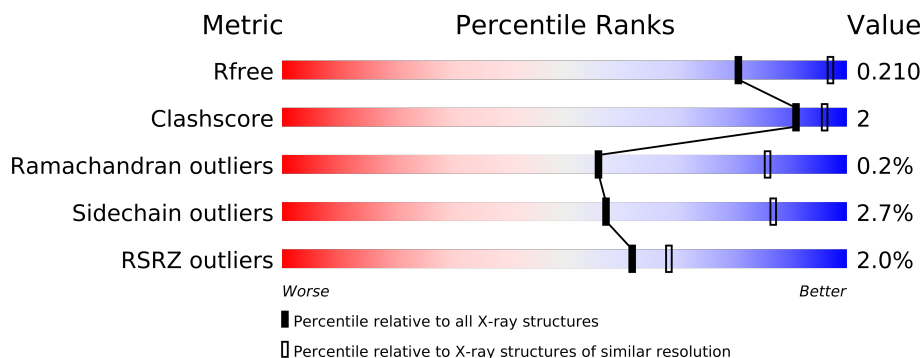
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22714
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) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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	845	
1	C	845	
1	E	845	
1	G	845	
2	B	175	
2	D	175	
2	F	175	
2	H	175	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	O	G	2003	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 30609 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.

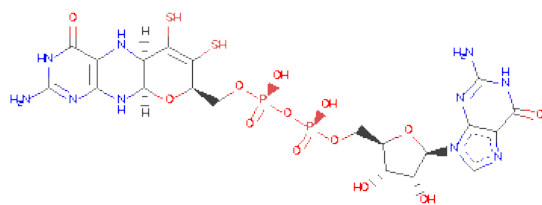
- Molecule 1 is a protein called AROA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	843	Total	C	N	O	S	0	0	0
			6545	4088	1167	1253	37			
1	C	843	Total	C	N	O	S	0	1	0
			6551	4092	1168	1254	37			
1	E	843	Total	C	N	O	S	0	0	0
			6545	4088	1167	1253	37			
1	G	843	Total	C	N	O	S	0	0	0
			6545	4088	1167	1253	37			

- Molecule 2 is a protein called AROB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			995	629	166	198	2			
2	D	132	Total	C	N	O	S	0	0	0
			995	629	166	198	2			
2	F	132	Total	C	N	O	S	0	0	0
			995	629	166	198	2			
2	H	132	Total	C	N	O	S	0	0	0
			995	629	166	198	2			

- Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONEGUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	G	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	G	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

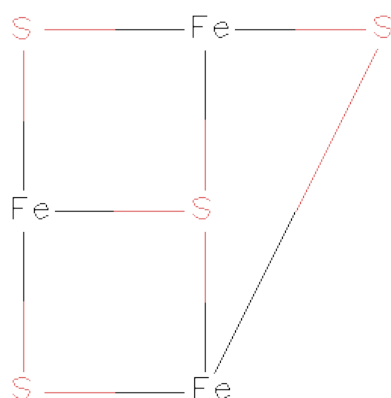
- Molecule 4 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	O	0	0
			1	1		
4	A	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		

- Molecule 5 is MOLYBDENUM(IV) ION (three-letter code: 4MO) (formula: Mo).

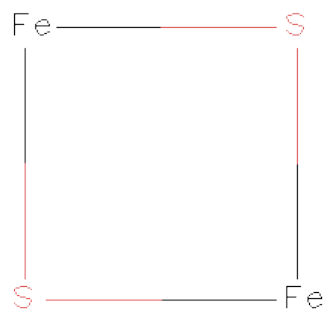
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mo	0	0
			1	1		
5	A	1	Total	Mo	0	0
			1	1		
5	C	1	Total	Mo	0	0
			1	1		
5	E	1	Total	Mo	0	0
			1	1		

- Molecule 6 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			7	3	4		
6	C	1	Total	Fe	S	0	0
			7	3	4		
6	E	1	Total	Fe	S	0	0
			7	3	4		
6	G	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	D	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		
7	H	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is water.

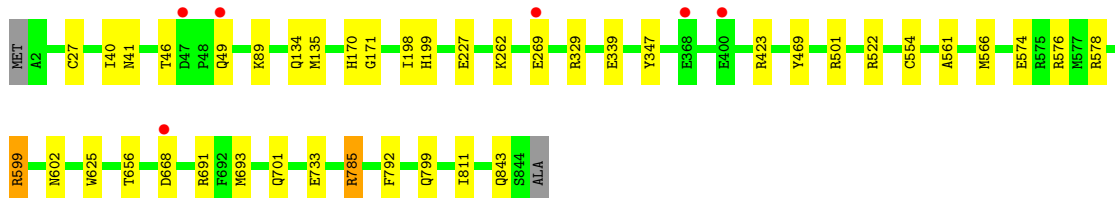
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total	O	0	0
			6	6		
8	C	2	Total	O	0	0
			2	2		
8	E	5	Total	O	0	0
			5	5		
8	G	2	Total	O	0	0
			2	2		

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.

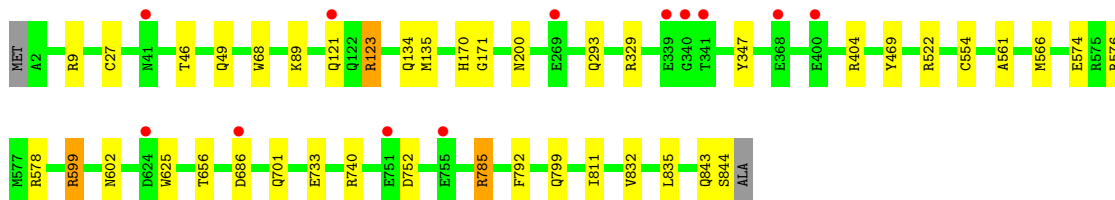
• Molecule 1: AROA

Chain A: 



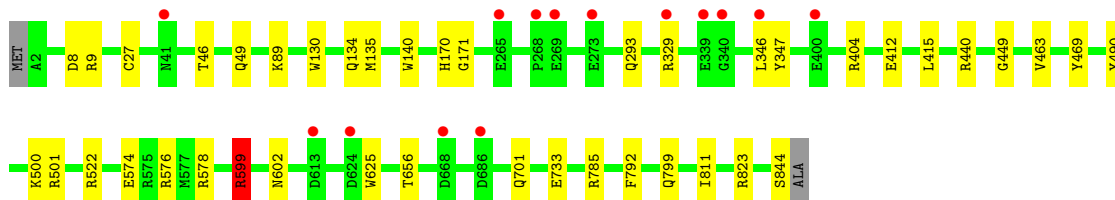
• Molecule 1: AROA

Chain C: 



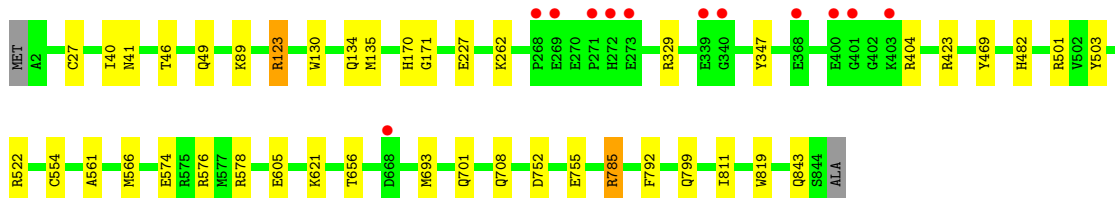
• Molecule 1: AROA

Chain E: 

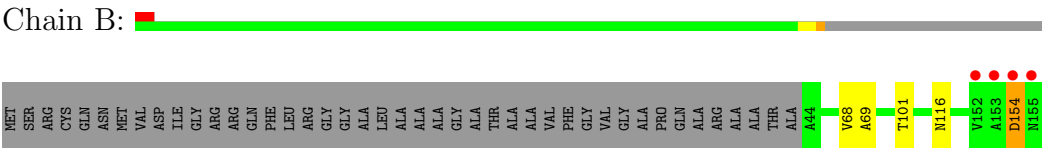


• Molecule 1: AROA

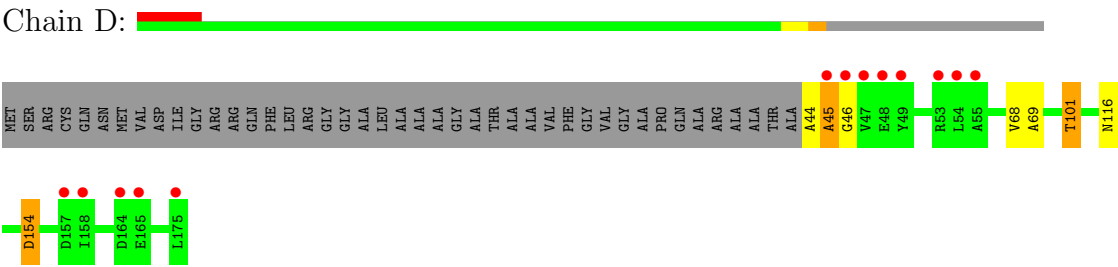
Chain G: 



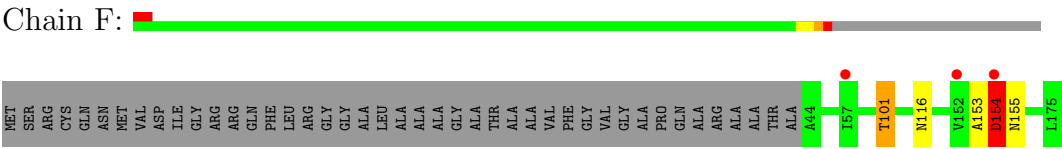
● Molecule 2: AROB



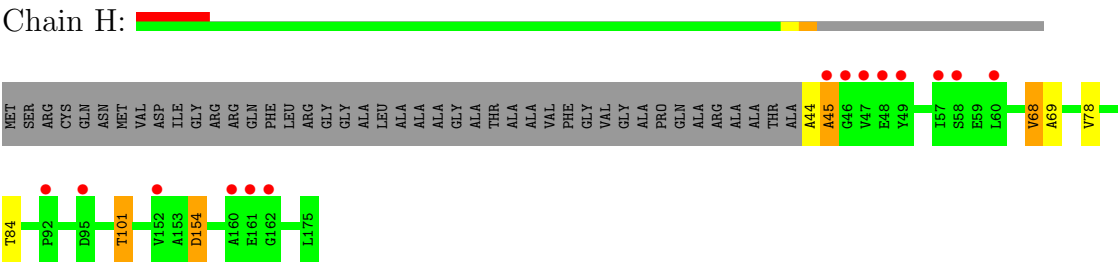
● Molecule 2: AROB



● Molecule 2: AROB



● Molecule 2: AROB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.13Å 232.96Å 141.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.87 – 2.70 43.52 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (141.87-2.70) 99.9 (43.52-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.193 , 0.211 0.193 , 0.210	Depositor DCC
R_{free} test set	6818 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.8	EDS
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 135725 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30609	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: 4MO, F3S, FES, O, MGD

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	0.60	0/6693	0.67	4/9068 (0.0%)
1	C	0.59	1/6702 (0.0%)	0.68	4/9080 (0.0%)
1	E	0.58	1/6693 (0.0%)	0.69	6/9068 (0.1%)
1	G	0.58	2/6693 (0.0%)	0.68	4/9068 (0.0%)
2	B	0.47	0/1018	0.61	0/1387
2	D	0.47	0/1018	0.67	1/1387 (0.1%)
2	F	0.50	0/1018	0.69	1/1387 (0.1%)
2	H	0.49	0/1018	0.63	0/1387
All	All	0.58	4/30853 (0.0%)	0.67	20/41832 (0.0%)

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
2	D	0	2
2	F	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	140	TRP	CD2-CE2	5.51	1.48	1.41
1	C	68	TRP	CD2-CE2	5.21	1.47	1.41
1	G	819	TRP	CD2-CE2	5.09	1.47	1.41
1	G	130	TRP	CD2-CE2	5.02	1.47	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	599	ARG	NE-CZ-NH1	11.08	125.84	120.30
1	E	599	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	C	123	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	G	123	ARG	NE-CZ-NH2	-9.17	115.71	120.30
1	G	123	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	C	123	ARG	NE-CZ-NH2	-8.42	116.09	120.30
2	F	154	ASP	CB-CG-OD2	7.32	124.88	118.30
1	E	8	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	785	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	E	599	ARG	CD-NE-CZ	6.08	132.11	123.60
2	D	46	GLY	N-CA-C	-5.86	98.45	113.10
1	A	785	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	E	785	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	C	134	GLN	CB-CA-C	-5.45	99.49	110.40
1	A	668	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	501	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	E	501	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	123	ARG	CB-CG-CD	5.18	125.06	111.60
1	G	123	ARG	CB-CG-CD	5.05	124.73	111.60
1	G	501	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	44	ALA	Peptide
2	D	45	ALA	Peptide
2	F	153	ALA	Peptide

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	6545	0	38	14	0
1	C	6551	0	38	12	1
1	E	6545	0	38	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	6545	0	38	12	0
2	B	995	0	4	3	0
2	D	995	0	4	6	0
2	F	995	0	4	1	0
2	H	995	0	4	4	0
3	A	94	0	44	0	0
3	C	94	0	44	0	0
3	E	94	0	44	0	0
3	G	94	0	44	0	0
4	A	1	0	0	0	0
4	C	1	0	0	1	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	A	7	0	0	0	0
6	C	7	0	0	0	0
6	E	7	0	0	0	0
6	G	7	0	0	0	0
7	B	4	0	0	0	0
7	D	4	0	0	0	0
7	F	4	0	0	0	0
7	H	4	0	0	0	0
8	A	6	0	0	0	0
8	C	2	0	0	0	0
8	E	5	0	0	0	0
8	G	2	0	0	0	0
All	All	30609	0	344	61	1

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 2.

All (61) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:752:ASP:OD1	1:G:785:ARG:NH1	2.09	0.85
1:C:752:ASP:OD1	1:C:785:ARG:NH1	2.10	0.84
1:C:599:ARG:NH1	1:C:602:ASN:OD1	2.16	0.79
1:A:599:ARG:NH1	1:A:602:ASN:OD1	2.16	0.79
1:A:843:GLN:OE1	2:B:116:ASN:ND2	2.16	0.77
1:E:130:TRP:CB	1:E:135:MET:CE	2.63	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:599:ARG:NH1	1:E:602:ASN:OD1	2.22	0.73
2:D:45:ALA:CB	1:E:9:ARG:CZ	2.72	0.68
1:A:135:MET:CE	1:A:554:CYS:O	2.42	0.67
1:E:130:TRP:CE3	1:E:135:MET:CE	2.79	0.66
1:C:561:ALA:O	1:C:566:MET:CE	2.48	0.61
1:G:40:ILE:O	1:G:41:ASN:OD1	2.19	0.60
1:A:40:ILE:O	1:A:41:ASN:OD1	2.20	0.59
1:A:561:ALA:O	1:A:566:MET:CE	2.53	0.56
1:E:599:ARG:NH2	1:E:625:TRP:O	2.40	0.54
1:A:599:ARG:NH2	1:A:625:TRP:O	2.41	0.54
1:C:599:ARG:NH2	1:C:625:TRP:O	2.42	0.52
1:G:561:ALA:O	1:G:566:MET:CE	2.56	0.52
2:D:68:VAL:CG1	2:D:69:ALA:N	2.74	0.50
2:H:44:ALA:O	2:H:45:ALA:CB	2.59	0.50
1:G:574:GLU:OE1	1:G:576:ARG:NH1	2.45	0.50
1:C:574:GLU:OE1	1:C:576:ARG:NH1	2.45	0.50
1:A:574:GLU:OE1	1:A:576:ARG:NH1	2.45	0.50
2:B:68:VAL:CG1	2:B:69:ALA:N	2.76	0.49
1:E:574:GLU:OE1	1:E:576:ARG:NH1	2.45	0.49
1:G:578:ARG:CD	1:G:656:THR:O	2.61	0.49
1:E:578:ARG:CD	1:E:656:THR:O	2.60	0.49
1:E:170:HIS:ND1	1:E:171:GLY:O	2.47	0.48
1:C:135:MET:CE	1:C:554:CYS:O	2.60	0.48
1:C:9:ARG:NH2	2:D:45:ALA:CB	2.76	0.48
1:G:170:HIS:ND1	1:G:171:GLY:O	2.45	0.48
1:A:170:HIS:ND1	1:A:171:GLY:O	2.47	0.48
1:C:170:HIS:ND1	1:C:171:GLY:O	2.47	0.48
1:C:578:ARG:CD	1:C:656:THR:O	2.62	0.47
1:E:293:GLN:NE2	1:E:844:SER:HB3	2.29	0.47
1:A:578:ARG:CD	1:A:656:THR:O	2.62	0.47
2:D:101:THR:O	2:D:101:THR:CG2	2.63	0.47
2:H:68:VAL:CG1	2:H:69:ALA:N	2.77	0.47
1:A:423:ARG:CA	1:A:693:MET:CE	2.92	0.47
1:G:605:GLU:OE2	1:G:621:LYS:NZ	2.49	0.46
2:D:154:ASP:N	2:D:154:ASP:OD1	2.49	0.46
2:H:154:ASP:N	2:H:154:ASP:OD1	2.49	0.45
1:G:135:MET:CE	1:G:554:CYS:O	2.64	0.45
1:G:423:ARG:CA	1:G:693:MET:CE	2.94	0.45
1:E:415:LEU:C	1:E:415:LEU:CD2	2.85	0.45
1:C:293:GLN:NE2	1:C:844:SER:HB2	2.32	0.44
1:C:200:ASN:ND2	4:C:2003:O:O	2.50	0.44
2:H:101:THR:O	2:H:101:THR:CG2	2.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:227:GLU:OE1	1:G:262:LYS:NZ	2.51	0.44
1:E:412:GLU:OE1	1:E:449:GLY:N	2.51	0.44
2:D:45:ALA:CB	1:E:9:ARG:NH2	2.81	0.43
1:C:740:ARG:O	1:C:835:LEU:CD2	2.66	0.43
1:A:227:GLU:OE1	1:A:262:LYS:NZ	2.52	0.42
1:E:130:TRP:CA	1:E:135:MET:CE	2.98	0.42
2:B:154:ASP:OD1	2:B:154:ASP:N	2.52	0.42
1:A:339:GLU:CG	1:G:755:GLU:O	2.69	0.41
2:F:101:THR:O	2:F:101:THR:CG2	2.69	0.41
1:A:269:GLU:OE1	1:E:823:ARG:NH1	2.54	0.41
1:A:198:ILE:CG2	1:A:199:HIS:N	2.84	0.41
1:G:482:HIS:ND1	1:G:503:TYR:OH	2.54	0.40
1:E:490:TYR:O	1:E:500:LYS:CE	2.70	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	Distance(Å)	Clash(Å)
1:C:686:ASP:O	1:C:686:ASP:O[2_545]	1.73	0.47

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	841/845 (100%)	810 (96%)	30 (4%)	1 (0%)	59	89
1	C	842/845 (100%)	812 (96%)	29 (3%)	1 (0%)	59	89
1	E	841/845 (100%)	815 (97%)	25 (3%)	1 (0%)	59	89
1	G	841/845 (100%)	809 (96%)	31 (4%)	1 (0%)	59	89
2	B	130/175 (74%)	125 (96%)	5 (4%)	0	100	100
2	D	130/175 (74%)	126 (97%)	4 (3%)	0	100	100
2	F	130/175 (74%)	121 (93%)	7 (5%)	2 (2%)	15	38
2	H	130/175 (74%)	125 (96%)	4 (3%)	1 (1%)	27	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3885/4080 (95%)	3743 (96%)	135 (4%)	7 (0%)	56 86

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	154	ASP
2	H	45	ALA
2	F	155	ASN
1	E	811	ILE
1	A	811	ILE
1	G	811	ILE
1	C	811	ILE

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	677/678 (100%)	661 (98%)	16 (2%)	61 89
1	C	678/678 (100%)	658 (97%)	20 (3%)	55 85
1	E	677/678 (100%)	659 (97%)	18 (3%)	57 87
1	G	677/678 (100%)	660 (98%)	17 (2%)	60 89
2	B	105/130 (81%)	103 (98%)	2 (2%)	69 92
2	D	105/130 (81%)	102 (97%)	3 (3%)	55 85
2	F	105/130 (81%)	102 (97%)	3 (3%)	55 85
2	H	105/130 (81%)	100 (95%)	5 (5%)	35 68
All	All	3129/3232 (97%)	3045 (97%)	84 (3%)	57 87

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	CYS
1	A	46	THR
1	A	49	GLN
1	A	89	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	134	GLN
1	A	329	ARG
1	A	347	TYR
1	A	469	TYR
1	A	522	ARG
1	A	599	ARG
1	A	691	ARG
1	A	701	GLN
1	A	733	GLU
1	A	785	ARG
1	A	792	PHE
1	A	799	GLN
2	B	101	THR
2	B	154	ASP
1	C	27	CYS
1	C	46	THR
1	C	49	GLN
1	C	89	LYS
1	C	121[A]	GLN
1	C	121[B]	GLN
1	C	123	ARG
1	C	329	ARG
1	C	347	TYR
1	C	404	ARG
1	C	469	TYR
1	C	522	ARG
1	C	599	ARG
1	C	701	GLN
1	C	733	GLU
1	C	785	ARG
1	C	792	PHE
1	C	799	GLN
1	C	832	VAL
1	C	843	GLN
2	D	101	THR
2	D	116	ASN
2	D	154	ASP
1	E	27	CYS
1	E	46	THR
1	E	49	GLN
1	E	89	LYS
1	E	134	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	329	ARG
1	E	346	LEU
1	E	347	TYR
1	E	404	ARG
1	E	440	ARG
1	E	463	VAL
1	E	469	TYR
1	E	522	ARG
1	E	599	ARG
1	E	701	GLN
1	E	733	GLU
1	E	792	PHE
1	E	799	GLN
2	F	101	THR
2	F	116	ASN
2	F	154	ASP
1	G	27	CYS
1	G	46	THR
1	G	49	GLN
1	G	89	LYS
1	G	123	ARG
1	G	134	GLN
1	G	329	ARG
1	G	347	TYR
1	G	404	ARG
1	G	469	TYR
1	G	522	ARG
1	G	701	GLN
1	G	708	GLN
1	G	785	ARG
1	G	792	PHE
1	G	799	GLN
1	G	843	GLN
2	H	68	VAL
2	H	78	VAL
2	H	84	THR
2	H	101	THR
2	H	154	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	MGD	A	2001	5	52,52,52	1.44	7 (13%)	73,81,81	2.64	18 (24%)
3	MGD	A	2002	5	52,52,52	1.42	6 (11%)	73,81,81	2.59	20 (27%)
6	F3S	A	2005	1	3,9,9	19.63	3 (100%)	0,15,15	0.00	-
7	FES	B	2006	2	0,4,4	0.00	-	0,4,4	0.00	-
3	MGD	C	2001	5	52,52,52	1.55	9 (17%)	73,81,81	2.72	25 (34%)
3	MGD	C	2002	5	52,52,52	1.50	7 (13%)	73,81,81	2.22	17 (23%)
6	F3S	C	2005	1	3,9,9	18.87	3 (100%)	0,15,15	0.00	-
7	FES	D	2006	2	0,4,4	0.00	-	0,4,4	0.00	-
3	MGD	E	2001	5	52,52,52	1.54	8 (15%)	73,81,81	2.05	20 (27%)
3	MGD	E	2002	5	52,52,52	1.46	8 (15%)	73,81,81	2.61	20 (27%)
6	F3S	E	2005	1	3,9,9	19.10	3 (100%)	0,15,15	0.00	-
7	FES	F	2006	2	0,4,4	0.00	-	0,4,4	0.00	-
3	MGD	G	2001	5	52,52,52	1.42	8 (15%)	73,81,81	2.72	18 (24%)
3	MGD	G	2002	5	52,52,52	1.55	10 (19%)	73,81,81	2.55	20 (27%)
6	F3S	G	2005	1	3,9,9	19.21	3 (100%)	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FES	H	2006	2	0,4,4	0.00	-	0,4,4	0.00	-

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	MGD	A	2001	5	-	0/22/66/66	0/6/6/6
3	MGD	A	2002	5	-	0/22/66/66	0/6/6/6
6	F3S	A	2005	1	-	0/0/24/24	0/0/3/3
7	FES	B	2006	2	-	0/0/4/4	0/1/1/1
3	MGD	C	2001	5	-	0/22/66/66	0/6/6/6
3	MGD	C	2002	5	-	0/22/66/66	0/6/6/6
6	F3S	C	2005	1	-	0/0/24/24	0/0/3/3
7	FES	D	2006	2	-	0/0/4/4	0/1/1/1
3	MGD	E	2001	5	-	0/22/66/66	0/6/6/6
3	MGD	E	2002	5	-	0/22/66/66	0/6/6/6
6	F3S	E	2005	1	-	0/0/24/24	0/0/3/3
7	FES	F	2006	2	-	0/0/4/4	0/1/1/1
3	MGD	G	2001	5	-	0/22/66/66	0/6/6/6
3	MGD	G	2002	5	-	0/22/66/66	0/6/6/6
6	F3S	G	2005	1	-	0/0/24/24	0/0/3/3
7	FES	H	2006	2	-	0/0/4/4	0/1/1/1

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2005	F3S	S3-FE4	-22.18	2.18	2.33
6	E	2005	F3S	S3-FE4	-21.72	2.18	2.33
6	G	2005	F3S	S3-FE3	-21.08	2.19	2.33
6	G	2005	F3S	S3-FE4	-19.26	2.20	2.33
6	C	2005	F3S	S3-FE1	-19.10	2.20	2.33
6	C	2005	F3S	S3-FE3	-18.90	2.20	2.33
6	C	2005	F3S	S3-FE4	-18.59	2.20	2.33
6	A	2005	F3S	S3-FE1	-18.36	2.20	2.33
6	E	2005	F3S	S3-FE1	-18.18	2.21	2.33
6	A	2005	F3S	S3-FE3	-18.07	2.21	2.33
6	G	2005	F3S	S3-FE1	-17.09	2.21	2.33
6	E	2005	F3S	S3-FE3	-17.09	2.21	2.33
3	E	2001	MGD	C17-C16	5.50	1.48	1.41
3	C	2002	MGD	C17-C16	5.36	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2002	MGD	C17-C16	5.31	1.48	1.41
3	G	2001	MGD	C17-C16	4.60	1.47	1.41
3	C	2001	MGD	C17-C16	4.59	1.47	1.41
3	A	2002	MGD	C17-C16	4.56	1.47	1.41
3	A	2001	MGD	C4-N9	-4.55	1.31	1.37
3	C	2001	MGD	C4-N9	-4.53	1.31	1.37
3	A	2001	MGD	C17-C16	4.15	1.46	1.41
3	G	2001	MGD	C5-N7	-4.10	1.33	1.38
3	E	2001	MGD	C4-N9	-3.89	1.32	1.37
3	E	2001	MGD	C5-N7	-3.80	1.33	1.38
3	E	2002	MGD	C4-N9	-3.70	1.32	1.37
3	C	2001	MGD	C5-N7	-3.61	1.33	1.38
3	A	2002	MGD	C5-N7	-3.59	1.33	1.38
3	G	2001	MGD	C4-N9	-3.53	1.32	1.37
3	G	2002	MGD	C5-N7	-3.41	1.34	1.38
3	G	2002	MGD	C16-C21	3.38	1.48	1.41
3	E	2002	MGD	C17-C16	3.38	1.45	1.41
3	C	2002	MGD	C5-C4	3.34	1.48	1.40
3	E	2002	MGD	C5-N7	-3.30	1.34	1.38
3	C	2002	MGD	C4-N9	-3.24	1.33	1.37
3	A	2002	MGD	C4-N9	-3.24	1.33	1.37
3	C	2001	MGD	C2-N2	2.92	1.36	1.32
3	A	2001	MGD	C17-N18	-2.90	1.32	1.36
3	G	2002	MGD	C4-N9	-2.89	1.33	1.37
3	E	2002	MGD	C5-C4	2.81	1.46	1.40
3	G	2002	MGD	C5-C4	2.80	1.46	1.40
3	C	2002	MGD	C16-C21	2.80	1.47	1.41
3	C	2002	MGD	C2-N3	2.72	1.36	1.33
3	E	2001	MGD	C16-C21	2.71	1.47	1.41
3	G	2001	MGD	C16-C21	2.67	1.47	1.41
3	E	2001	MGD	C2-N2	2.66	1.36	1.32
3	G	2002	MGD	C19-N19	2.60	1.36	1.32
3	G	2001	MGD	C19-N19	2.59	1.36	1.32
3	A	2001	MGD	C5-N7	-2.59	1.35	1.38
3	C	2001	MGD	C16-N15	-2.58	1.32	1.38
3	C	2001	MGD	C16-C21	2.58	1.47	1.41
3	C	2001	MGD	C19-N19	2.57	1.36	1.32
3	A	2002	MGD	C16-C21	2.52	1.46	1.41
3	C	2002	MGD	C5-N7	-2.47	1.35	1.38
3	G	2002	MGD	C19-N20	2.46	1.36	1.33
3	A	2001	MGD	C5-C4	2.44	1.46	1.40
3	G	2001	MGD	C16-N15	-2.44	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2002	MGD	C19-N19	2.37	1.35	1.32
3	G	2001	MGD	C12-S12	-2.36	1.68	1.75
3	G	2002	MGD	C2-N3	2.33	1.36	1.33
3	E	2002	MGD	C12-S12	-2.30	1.68	1.75
3	G	2001	MGD	C5-C4	2.29	1.45	1.40
3	C	2002	MGD	C19-N19	2.26	1.35	1.32
3	G	2002	MGD	C2-N2	2.24	1.35	1.32
3	G	2002	MGD	C12-S12	-2.24	1.68	1.75
3	A	2002	MGD	C5-C4	2.23	1.45	1.40
3	E	2002	MGD	O4'-C1'	2.17	1.44	1.41
3	E	2001	MGD	C6-N1	-2.17	1.33	1.36
3	E	2002	MGD	O11-C11	-2.13	1.40	1.43
3	A	2001	MGD	C13-S13	-2.09	1.68	1.75
3	E	2001	MGD	C16-N15	-2.09	1.33	1.38
3	C	2001	MGD	C5-C4	2.08	1.45	1.40
3	A	2002	MGD	C17-N18	-2.05	1.33	1.36
3	A	2001	MGD	C16-N15	-2.04	1.33	1.38
3	C	2001	MGD	C13-S13	-2.01	1.69	1.75
3	E	2001	MGD	C8-N9	-2.00	1.33	1.36

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2001	MGD	C6-C5-N7	16.35	136.34	134.14
3	A	2001	MGD	C6-C5-N7	16.29	136.33	134.14
3	C	2001	MGD	C6-C5-N7	15.53	136.23	134.14
3	A	2002	MGD	C6-C5-N7	13.06	135.90	134.14
3	E	2002	MGD	C6-C5-N7	12.53	135.83	134.14
3	G	2002	MGD	C6-C5-N7	11.38	135.67	134.14
3	G	2002	MGD	C4'-O4'-C1'	-7.95	100.98	109.72
3	C	2002	MGD	C4'-O4'-C1'	-7.43	101.55	109.72
3	E	2002	MGD	O11-C23-N22	-7.09	100.91	109.03
3	E	2002	MGD	C4'-O4'-C1'	-6.39	102.69	109.72
3	E	2001	MGD	C6-C5-N7	6.37	135.00	134.14
3	C	2002	MGD	C6-N1-C2	6.30	123.76	120.20
3	A	2002	MGD	C4'-O4'-C1'	-6.22	102.88	109.72
3	A	2002	MGD	C5-C4-N3	-6.17	118.97	126.07
3	E	2002	MGD	C5-C4-N3	-6.08	119.07	126.07
3	G	2002	MGD	O11-C23-N22	-5.86	102.32	109.03
3	G	2002	MGD	C5-C4-N3	-5.74	119.45	126.07
3	C	2002	MGD	C6-C5-N7	5.53	134.88	134.14
3	G	2002	MGD	N3-C4-N9	5.48	134.95	126.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2001	MGD	N3-C4-N9	5.46	134.91	126.91
3	C	2002	MGD	O11-C23-N22	-5.29	102.97	109.03
3	C	2002	MGD	C17-N18-C19	5.24	123.16	120.20
3	C	2002	MGD	N3-C4-N9	5.20	134.54	126.91
3	E	2001	MGD	C5-C4-N3	-5.14	120.15	126.07
3	C	2001	MGD	C17-N18-C19	5.11	123.09	120.20
3	G	2001	MGD	C5-C4-N3	-4.93	120.39	126.07
3	A	2002	MGD	O11-C23-C14	4.93	112.87	108.99
3	G	2001	MGD	C10-C11-C12	4.89	116.75	110.98
3	A	2002	MGD	C17-N18-C19	4.86	122.95	120.20
3	C	2001	MGD	C6-N1-C2	4.85	122.94	120.20
3	A	2002	MGD	N3-C4-N9	4.82	133.98	126.91
3	C	2002	MGD	C5-C4-N3	-4.72	120.63	126.07
3	A	2001	MGD	C10-C11-C12	4.70	116.52	110.98
3	E	2001	MGD	C23-C14-N15	4.67	114.91	108.34
3	C	2001	MGD	C5-C4-N3	-4.62	120.75	126.07
3	A	2001	MGD	C23-C14-N15	4.60	114.80	108.34
3	G	2001	MGD	N2-C2-N3	-4.59	114.31	120.28
3	G	2001	MGD	N2-C2-N1	4.53	122.68	117.82
3	G	2001	MGD	C2-N3-C4	4.48	120.68	115.30
3	E	2002	MGD	N3-C4-N9	4.46	133.44	126.91
3	C	2002	MGD	C14-C23-N22	4.28	116.06	110.06
3	C	2001	MGD	C23-C14-N15	4.26	114.33	108.34
3	G	2002	MGD	C2-N3-C4	4.25	120.40	115.30
3	A	2001	MGD	C5-C4-N3	-4.22	121.21	126.07
3	G	2001	MGD	N3-C4-N9	4.17	133.03	126.91
3	A	2001	MGD	C1'-N9-C4	-4.14	119.48	126.64
3	G	2001	MGD	PA-O3B-PB	-4.14	120.47	131.93
3	G	2002	MGD	C23-C14-N15	4.11	114.12	108.34
3	A	2002	MGD	C2-N3-C4	4.04	120.15	115.30
3	E	2001	MGD	C10-C11-C12	4.01	115.70	110.98
3	C	2001	MGD	N3-C4-N9	3.99	132.76	126.91
3	A	2002	MGD	C4-C5-N7	-3.99	105.56	109.41
3	G	2002	MGD	C6-N1-C2	3.90	122.40	120.20
3	E	2002	MGD	C2-N3-C4	3.90	119.98	115.30
3	A	2001	MGD	N3-C4-N9	3.87	132.59	126.91
3	C	2001	MGD	C1'-N9-C4	-3.82	120.03	126.64
3	E	2002	MGD	O11-C23-C14	3.79	111.98	108.99
3	C	2001	MGD	C2-N3-C4	3.78	119.83	115.30
3	G	2001	MGD	C14-C23-N22	3.77	115.34	110.06
3	A	2001	MGD	C6-N1-C2	3.75	122.32	120.20
3	C	2002	MGD	C8-N9-C4	3.75	110.00	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2001	MGD	C10-C11-C12	3.71	115.36	110.98
3	A	2002	MGD	C23-C14-N15	3.70	113.54	108.34
3	E	2002	MGD	C14-C23-N22	3.65	115.18	110.06
3	A	2001	MGD	C2-N3-C4	3.61	119.64	115.30
3	A	2001	MGD	C17-C16-C21	3.57	117.80	114.56
3	C	2001	MGD	O3B-PA-O3A	-3.55	93.50	102.91
3	E	2001	MGD	C8-N9-C4	3.54	109.84	106.96
3	A	2001	MGD	PA-O3B-PB	-3.54	122.13	131.93
3	E	2001	MGD	C2-N3-C4	3.54	119.55	115.30
3	E	2001	MGD	C17-C16-C21	3.48	117.71	114.56
3	E	2002	MGD	C17-N18-C19	3.44	122.14	120.20
3	E	2002	MGD	C6-N1-C2	3.43	122.14	120.20
3	A	2001	MGD	N22-C21-N20	3.42	122.06	116.62
3	E	2002	MGD	C4-C5-N7	-3.37	106.15	109.41
3	G	2001	MGD	C17-C16-C21	3.31	117.56	114.56
3	A	2002	MGD	O11-C23-N22	-3.31	105.24	109.03
3	G	2002	MGD	C17-N18-C19	3.25	122.04	120.20
3	E	2001	MGD	C1'-N9-C4	-3.24	121.04	126.64
3	G	2001	MGD	C23-C14-N15	3.23	112.88	108.34
3	C	2001	MGD	C8-N9-C4	3.22	109.58	106.96
3	C	2002	MGD	N22-C21-N20	3.21	121.74	116.62
3	G	2002	MGD	O4'-C1'-N9	3.19	115.04	108.10
3	A	2002	MGD	N2-C2-N3	-3.18	116.15	120.28
3	C	2001	MGD	PA-O3B-PB	-3.13	123.27	131.93
3	G	2001	MGD	C1'-N9-C4	-3.12	121.24	126.64
3	E	2002	MGD	C23-C14-N15	3.04	112.61	108.34
3	C	2001	MGD	C17-C16-C21	3.01	117.28	114.56
3	C	2001	MGD	N22-C21-N20	2.96	121.34	116.62
3	G	2002	MGD	C14-C23-N22	2.96	114.21	110.06
3	C	2001	MGD	N19-C19-N18	2.96	120.99	117.82
3	A	2001	MGD	C8-N9-C4	2.95	109.36	106.96
3	G	2001	MGD	N22-C21-N20	2.93	121.28	116.62
3	C	2001	MGD	C4-C5-N7	-2.92	106.59	109.41
3	E	2002	MGD	N22-C21-N20	2.92	121.26	116.62
3	E	2001	MGD	N2-C2-N3	-2.88	116.53	120.28
3	E	2001	MGD	PA-O3B-PB	-2.87	123.99	131.93
3	C	2001	MGD	C4'-O4'-C1'	-2.84	106.59	109.72
3	G	2002	MGD	N22-C21-N20	2.84	121.14	116.62
3	E	2001	MGD	C17-N18-C19	2.83	121.80	120.20
3	C	2002	MGD	C23-C14-N15	2.77	112.23	108.34
3	E	2001	MGD	N22-C21-N20	2.74	120.98	116.62
3	A	2001	MGD	N2-C2-N3	-2.73	116.73	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	MGD	N22-C21-N20	2.71	120.93	116.62
3	E	2001	MGD	C4'-O4'-C1'	-2.68	106.77	109.72
3	C	2001	MGD	N2-C2-N1	2.67	120.68	117.82
3	G	2001	MGD	C17-N18-C19	2.66	121.70	120.20
3	A	2001	MGD	C8-N9-C1'	2.66	131.16	126.15
3	A	2002	MGD	C14-C23-N22	2.63	113.74	110.06
3	G	2002	MGD	O11-C23-C14	2.61	111.04	108.99
3	E	2001	MGD	C14-C23-N22	2.59	113.69	110.06
3	G	2002	MGD	C17-C16-N15	2.54	122.71	119.07
3	G	2002	MGD	O4'-C1'-C2'	-2.53	103.01	106.69
3	A	2002	MGD	C17-C16-C21	2.50	116.83	114.56
3	A	2001	MGD	C17-C16-N15	2.49	122.63	119.07
3	C	2001	MGD	C14-C23-N22	2.49	113.55	110.06
3	A	2002	MGD	O3B-PB-O5'	2.47	109.46	102.91
3	C	2001	MGD	C17-C16-N15	2.45	122.58	119.07
3	G	2001	MGD	O3B-PA-O3A	-2.44	96.44	102.91
3	G	2002	MGD	C21-N22-C23	-2.43	119.86	124.06
3	C	2001	MGD	N2-C2-N3	-2.42	117.13	120.28
3	E	2001	MGD	N2-C2-N1	2.41	120.40	117.82
3	G	2001	MGD	C4-C5-N7	-2.40	107.09	109.41
3	E	2001	MGD	C6-N1-C2	2.38	121.55	120.20
3	E	2001	MGD	O4'-C4'-C3'	2.35	109.94	105.16
3	C	2002	MGD	C2-N3-C4	2.31	118.07	115.30
3	E	2002	MGD	O4'-C1'-C2'	-2.29	103.36	106.69
3	C	2001	MGD	C16-C21-N22	2.28	120.73	118.34
3	C	2002	MGD	O4'-C1'-C2'	-2.27	103.38	106.69
3	C	2002	MGD	C17-C16-N15	2.26	122.31	119.07
3	G	2001	MGD	C8-N9-C1'	2.25	130.39	126.15
3	E	2001	MGD	N19-C19-N20	-2.24	117.38	120.29
3	G	2001	MGD	N19-C19-N20	-2.23	117.40	120.29
3	C	2002	MGD	O3B-PB-O5'	2.22	108.81	102.91
3	C	2001	MGD	C8-N9-C1'	2.22	130.32	126.15
3	G	2002	MGD	C8-N9-C4	2.19	108.73	106.96
3	E	2002	MGD	N19-C19-N18	2.18	120.16	117.82
3	C	2001	MGD	C19-N20-C21	2.18	122.45	116.20
3	E	2002	MGD	N2-C2-N3	-2.16	117.47	120.28
3	A	2001	MGD	C16-C21-N22	2.15	120.59	118.34
3	A	2001	MGD	N2-C2-N1	2.14	120.11	117.82
3	E	2002	MGD	C23-O11-C11	2.11	115.74	111.89
3	E	2002	MGD	C17-C16-C21	2.11	116.48	114.56
3	E	2002	MGD	O4'-C1'-N9	2.11	112.69	108.10
3	A	2001	MGD	N19-C19-N20	-2.10	117.57	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	MGD	C17-C16-N15	2.10	122.07	119.07
3	A	2002	MGD	C8-N9-C4	2.08	108.65	106.96
3	E	2001	MGD	C17-C16-N15	2.08	122.06	119.07
3	C	2002	MGD	C4-C5-N7	-2.08	107.40	109.41
3	C	2001	MGD	N19-C19-N20	-2.07	117.61	120.29
3	G	2002	MGD	C4-C5-N7	-2.06	107.42	109.41
3	G	2002	MGD	PA-O3B-PB	-2.05	126.24	131.93
3	A	2002	MGD	C6-N1-C2	2.05	121.36	120.20
3	C	2002	MGD	C1'-N9-C4	-2.05	123.10	126.64
3	A	2002	MGD	O11-C11-C10	-2.03	103.58	108.81
3	G	2002	MGD	O11-C11-C10	-2.02	103.59	108.81
3	A	2002	MGD	C21-N22-C23	-2.01	120.59	124.06
3	E	2002	MGD	C10-C11-C12	2.00	113.34	110.98

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, 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	843/845 (99%)	-0.35	6 (0%) 84 89	44, 49, 70, 93	0
1	C	843/845 (99%)	-0.30	12 (1%) 72 77	45, 49, 72, 104	0
1	E	843/845 (99%)	-0.33	14 (1%) 67 73	45, 51, 77, 105	0
1	G	843/845 (99%)	-0.31	12 (1%) 72 77	44, 53, 83, 112	0
2	B	132/175 (75%)	0.12	4 (3%) 48 54	49, 69, 105, 133	0
2	D	132/175 (75%)	0.57	13 (9%) 8 8	47, 68, 240, 343	0
2	F	132/175 (75%)	0.09	3 (2%) 57 64	49, 69, 96, 105	0
2	H	132/175 (75%)	0.46	14 (10%) 7 7	49, 78, 168, 322	0
All	All	3900/4080 (95%)	-0.24	78 (2%) 62 68	44, 52, 85, 343	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	46	GLY	8.5
2	H	46	GLY	8.1
2	D	45	ALA	7.9
2	H	45	ALA	7.3
2	D	47	VAL	6.1
2	D	164	ASP	5.3
2	H	47	VAL	5.1
1	E	269	GLU	5.0
1	C	340	GLY	4.9
1	E	400	GLU	4.7
1	G	400	GLU	4.7
2	D	165	GLU	4.6
1	A	269	GLU	4.4
2	D	53	ARG	4.3
2	H	162	GLY	3.9
2	D	49	TYR	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	273	GLU	3.8
1	C	339	GLU	3.7
2	H	57	ILE	3.7
1	A	400	GLU	3.7
1	C	400	GLU	3.5
1	G	269	GLU	3.5
2	D	54	LEU	3.5
2	D	48	GLU	3.4
2	H	48	GLU	3.3
1	E	268	PRO	3.2
1	G	401	GLY	3.1
1	G	340	GLY	3.0
1	E	340	GLY	2.9
1	G	339	GLU	2.9
2	B	154	ASP	2.9
1	C	269	GLU	2.9
1	E	339	GLU	2.8
2	B	153	ALA	2.8
1	G	668	ASP	2.8
2	D	55	ALA	2.8
1	E	265	GLU	2.7
2	D	158	ILE	2.6
1	E	346	LEU	2.6
1	C	341	THR	2.6
1	E	41	ASN	2.6
1	G	271	PRO	2.5
1	E	686	ASP	2.5
2	H	95	ASP	2.5
1	C	686	ASP	2.4
2	F	152	VAL	2.4
2	H	58	SER	2.4
1	A	49	GLN	2.4
1	C	624	ASP	2.4
1	E	668	ASP	2.4
1	E	329	ARG	2.4
2	H	160	ALA	2.3
2	H	49	TYR	2.3
2	F	154	ASP	2.3
1	G	268	PRO	2.3
1	E	624	ASP	2.3
1	G	272	HIS	2.3
2	H	161	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	41	ASN	2.2
1	G	403	LYS	2.2
1	A	47	ASP	2.2
2	H	92	PRO	2.2
1	A	668	ASP	2.2
1	G	368	GLU	2.2
2	H	152	VAL	2.2
1	E	273	GLU	2.2
2	B	155	ASN	2.2
2	B	152	VAL	2.2
1	C	121[A]	GLN	2.1
2	D	175	LEU	2.1
2	H	60	LEU	2.1
1	C	368	GLU	2.1
2	F	57	ILE	2.1
1	A	368	GLU	2.1
1	C	751	GLU	2.1
2	D	157	ASP	2.1
1	C	755	GLU	2.0
1	E	613	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 ⓘ

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, 95th 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 ²)	Q<0.9
4	O	G	2003	1/1	0.20	2.68	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	O	C	2003	1/1	0.21	1.58	56,56,56,56	0
3	MGD	E	2002	47/47	0.19	1.29	52,53,56,57	0
3	MGD	E	2001	47/47	0.15	1.02	53,54,57,57	0
3	MGD	G	2001	47/47	0.15	1.00	52,55,57,58	0
4	O	A	2003	1/1	0.17	0.82	55,55,55,55	0
3	MGD	A	2002	47/47	0.17	0.70	48,51,51,52	0
3	MGD	C	2001	47/47	0.16	0.68	52,53,54,55	0
3	MGD	C	2002	47/47	0.17	0.55	50,52,55,55	0
3	MGD	A	2001	47/47	0.15	0.51	51,53,54,55	0
3	MGD	G	2002	47/47	0.16	0.41	53,55,58,59	0
4	O	E	2003	1/1	0.12	-0.54	57,57,57,57	0
6	F3S	E	2005	7/7	0.11	-0.62	56,56,57,57	0
6	F3S	G	2005	7/7	0.11	-0.89	56,57,57,57	0
5	4MO	C	2004	1/1	0.12	-0.98	54,54,54,54	0
5	4MO	E	2004	1/1	0.10	-1.01	57,57,57,57	0
6	F3S	C	2005	7/7	0.10	-1.13	54,55,56,57	0
5	4MO	A	2004	1/1	0.10	-1.17	53,53,53,53	0
6	F3S	A	2005	7/7	0.09	-1.32	53,54,55,55	0
5	4MO	G	2004	1/1	0.10	-1.52	56,56,56,56	0
7	FES	H	2006	4/4	0.07	-1.88	81,81,82,88	0
7	FES	D	2006	4/4	0.05	-2.16	79,80,83,86	0
7	FES	B	2006	4/4	0.07	-2.48	74,79,82,85	0
7	FES	F	2006	4/4	0.06	-2.86	74,76,77,84	0

6.5 Other polymers ⓘ

There are no such residues in this entry.