Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 11:04 PM EST

PDB ID	:	3B0H
Title	:	Assimilatory nitrite reductase (Nii4) from tobbaco root
Authors	:	Nakano, S.; Takahashi, M.; Sakamoto, A.; Morikawa, H.; Katayanagi, K.
Deposited on	:	2011-06-09
Resolution	:	2.31 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

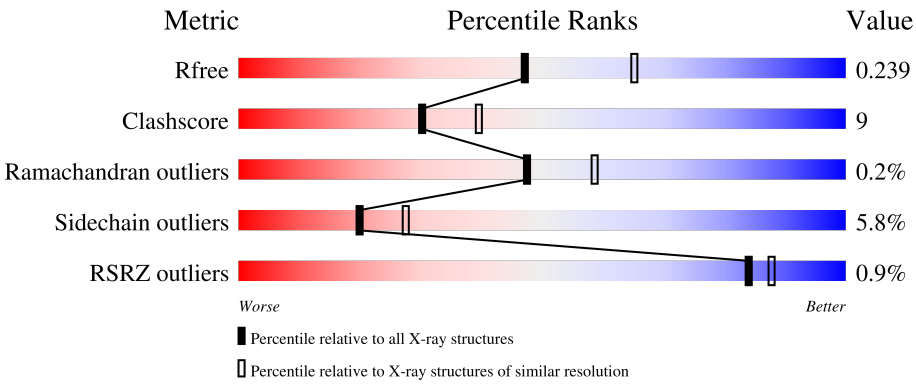
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	588	% 72% 16% • 9%
1	B	588	73% 16% • 9%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SRM	A	601	X	-	-	-
2	SRM	B	601	X	-	-	-
3	SF4	A	602	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9117 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 Nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4239	2675	753	787	24	0	0	0
1	B	535	4233	2672	752	785	24	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP Q76KA9
A	-24	GLY	-	expression tag	UNP Q76KA9
A	-23	HIS	-	expression tag	UNP Q76KA9
A	-22	HIS	-	expression tag	UNP Q76KA9
A	-21	HIS	-	expression tag	UNP Q76KA9
A	-20	HIS	-	expression tag	UNP Q76KA9
A	-19	HIS	-	expression tag	UNP Q76KA9
A	-18	HIS	-	expression tag	UNP Q76KA9
A	-17	HIS	-	expression tag	UNP Q76KA9
A	-16	HIS	-	expression tag	UNP Q76KA9
A	-15	HIS	-	expression tag	UNP Q76KA9
A	-14	HIS	-	expression tag	UNP Q76KA9
A	-13	SER	-	expression tag	UNP Q76KA9
A	-12	SER	-	expression tag	UNP Q76KA9
A	-11	GLY	-	expression tag	UNP Q76KA9
A	-10	HIS	-	expression tag	UNP Q76KA9
A	-9	ILE	-	expression tag	UNP Q76KA9
A	-8	GLU	-	expression tag	UNP Q76KA9
A	-7	GLY	-	expression tag	UNP Q76KA9
A	-6	ARG	-	expression tag	UNP Q76KA9
A	-5	HIS	-	expression tag	UNP Q76KA9
A	-4	MET	-	expression tag	UNP Q76KA9
B	-25	MET	-	expression tag	UNP Q76KA9
B	-24	GLY	-	expression tag	UNP Q76KA9
B	-23	HIS	-	expression tag	UNP Q76KA9

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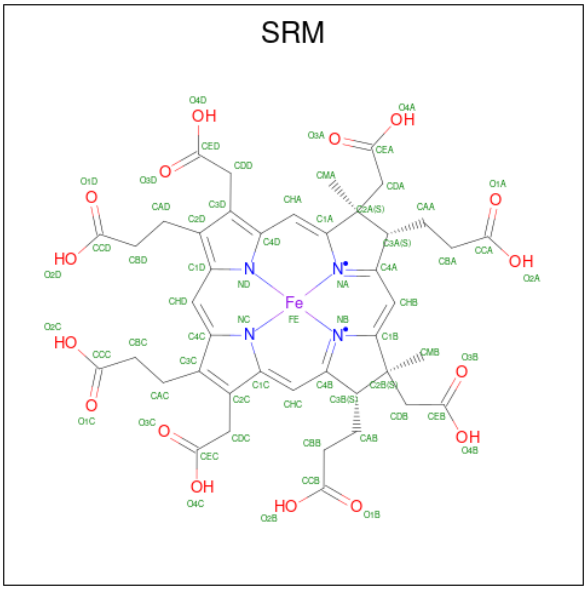
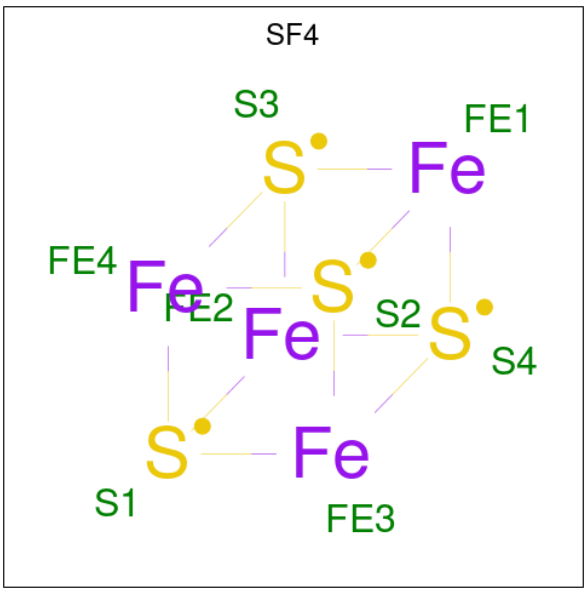
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	HIS	-	expression tag	UNP Q76KA9
B	-21	HIS	-	expression tag	UNP Q76KA9
B	-20	HIS	-	expression tag	UNP Q76KA9
B	-19	HIS	-	expression tag	UNP Q76KA9
B	-18	HIS	-	expression tag	UNP Q76KA9
B	-17	HIS	-	expression tag	UNP Q76KA9
B	-16	HIS	-	expression tag	UNP Q76KA9
B	-15	HIS	-	expression tag	UNP Q76KA9
B	-14	HIS	-	expression tag	UNP Q76KA9
B	-13	SER	-	expression tag	UNP Q76KA9
B	-12	SER	-	expression tag	UNP Q76KA9
B	-11	GLY	-	expression tag	UNP Q76KA9
B	-10	HIS	-	expression tag	UNP Q76KA9
B	-9	ILE	-	expression tag	UNP Q76KA9
B	-8	GLU	-	expression tag	UNP Q76KA9
B	-7	GLY	-	expression tag	UNP Q76KA9
B	-6	ARG	-	expression tag	UNP Q76KA9
B	-5	HIS	-	expression tag	UNP Q76KA9
B	-4	MET	-	expression tag	UNP Q76KA9

- Molecule 2 is SIROHEME (three-letter code: SRM) (formula: $C_{42}H_{44}FeN_4O_{16}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	63	42	1	4	16	0	0
			Total	C	Fe	N	O		
2	B	1	63	42	1	4	16	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0
5	B	2	Total Cl 2 2	0	0

- Molecule 6 is water.

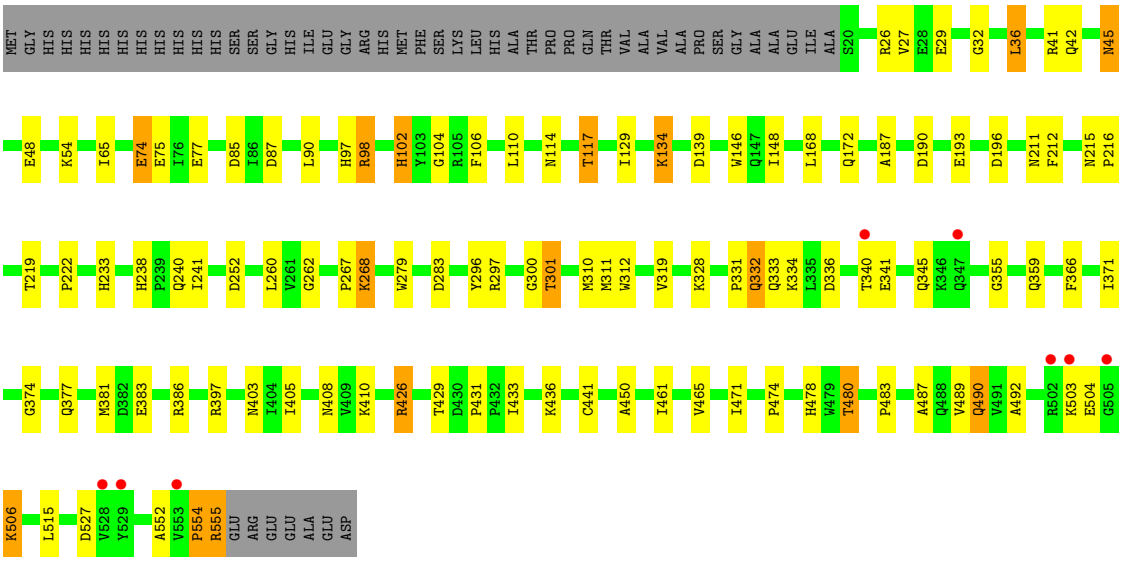
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	239	239	239	0	0
			Total	O		
6	B	258	258	258	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

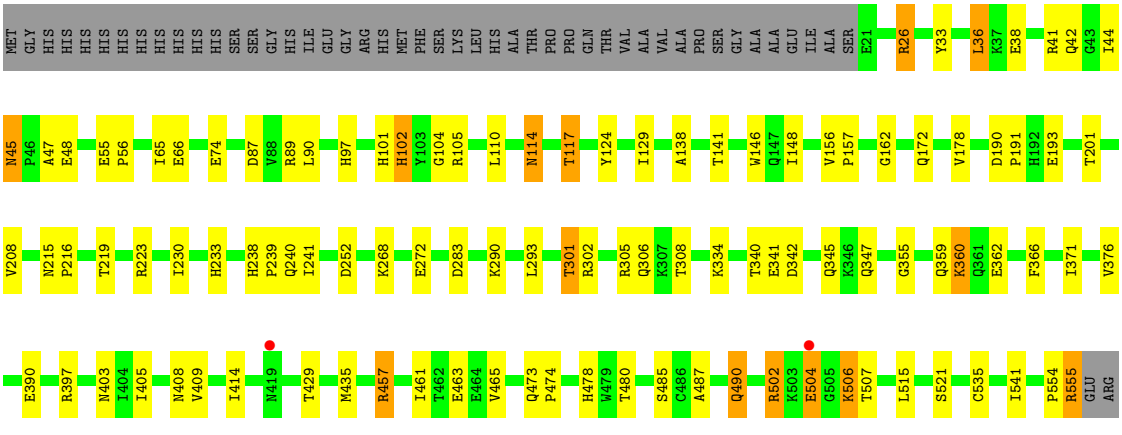
• Molecule 1: Nitrite reductase

Chain A:



• Molecule 1: Nitrite reductase

Chain B:



GLU
GLU
ALA
GLU
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.34Å 112.08Å 92.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.25 – 2.31 45.41 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.25-2.31) 99.2 (45.41-2.31)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	4.47 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.178 , 0.241 0.177 , 0.239	Depositor DCC
R_{free} test set	2311 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9117	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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 45.45 % 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 1.3199e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SF4, K, SRM

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	0.64	0/4323	0.73	1/5848 (0.0%)
1	B	0.67	0/4317	0.74	0/5840
All	All	0.65	0/8640	0.73	1/11688 (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
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	LEU	CA-CB-CG	5.38	127.68	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	110	LEU	Peptide

5.2 Too-close contacts (i)

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	4239	0	4269	77	0
1	B	4233	0	4264	80	0
2	A	63	0	34	2	0
2	B	63	0	34	2	0
3	A	8	0	0	2	0
3	B	8	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	239	0	0	7	0
6	B	258	0	0	13	0
All	All	9117	0	8601	160	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (160) 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:B:502:ARG:HH11	1:B:507:THR:HB	1.17	1.09
1:A:503:LYS:HG3	1:A:504:GLU:H	1.25	1.00
1:A:117:THR:HG21	1:A:146:TRP:HE1	1.28	0.97
1:B:359:GLN:HE22	1:B:408:ASN:H	1.08	0.95
1:A:359:GLN:HE22	1:A:408:ASN:H	1.09	0.95
1:B:342:ASP:HB2	6:B:753:HOH:O	1.70	0.92
1:B:490:GLN:H	1:B:490:GLN:HE21	1.17	0.92
1:A:97:HIS:HE1	1:A:104:GLY:H	1.12	0.91
1:B:301:THR:HG23	6:B:887:HOH:O	1.71	0.90
1:A:341:GLU:O	6:A:1151:HOH:O	1.91	0.88
1:A:359:GLN:NE2	1:A:408:ASN:H	1.73	0.86
1:B:341:GLU:HB2	6:B:741:HOH:O	1.75	0.86
1:B:190:ASP:HB3	1:B:193:GLU:HB3	1.57	0.85
1:A:333:GLN:O	6:A:1061:HOH:O	1.95	0.84
1:A:331:PRO:O	1:A:332:GLN:HB2	1.79	0.83
1:A:426:ARG:HG2	1:A:426:ARG:HH11	1.44	0.82
1:B:233:HIS:HD2	1:B:345:GLN:H	1.28	0.82
1:B:359:GLN:NE2	1:B:408:ASN:H	1.79	0.81
1:A:503:LYS:HG3	1:A:504:GLU:N	1.95	0.81
1:A:233:HIS:HD2	1:A:345:GLN:H	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LYS:CG	1:A:504:GLU:H	1.93	0.79
1:B:33:TYR:CD1	1:B:55:GLU:HG2	2.18	0.78
1:A:490:GLN:HE21	1:A:490:GLN:H	1.29	0.78
1:B:502:ARG:NH1	1:B:507:THR:HB	1.97	0.77
1:A:252:ASP:HB3	6:A:1031:HOH:O	1.84	0.75
1:A:233:HIS:CD2	1:A:345:GLN:H	2.04	0.74
1:B:233:HIS:CD2	1:B:345:GLN:H	2.07	0.72
1:B:117:THR:HG21	1:B:146:TRP:HE1	1.57	0.69
1:B:268:LYS:HD2	1:B:306:GLN:HB3	1.74	0.69
1:A:359:GLN:HE22	1:A:408:ASN:N	1.87	0.69
1:B:490:GLN:H	1:B:490:GLN:NE2	1.91	0.69
1:B:457:ARG:HE	1:B:535:CYS:HB3	1.57	0.68
1:B:435:MET:CE	1:B:463:GLU:HG3	2.24	0.68
1:B:301:THR:CG2	6:B:887:HOH:O	2.36	0.67
1:B:555:ARG:HH21	1:B:555:ARG:HG3	1.60	0.67
1:A:97:HIS:CE1	1:A:104:GLY:H	2.04	0.66
1:A:134:LYS:H	1:A:134:LYS:HD2	1.61	0.65
1:B:45:ASN:HD21	1:B:47:ALA:HB3	1.62	0.65
1:A:75:GLU:OE2	6:A:1126:HOH:O	2.14	0.64
1:B:238:HIS:HD2	6:B:719:HOH:O	1.80	0.64
1:B:555:ARG:HG3	1:B:555:ARG:NH2	2.12	0.64
1:A:340:THR:HG23	1:A:341:GLU:HG2	1.79	0.63
1:B:26:ARG:NH2	6:B:763:HOH:O	2.19	0.62
1:A:190:ASP:HB3	1:A:193:GLU:HB3	1.82	0.62
1:B:87:ASP:OD2	1:B:97:HIS:HD2	1.83	0.61
1:A:98:ARG:HB2	1:A:102:HIS:HB3	1.82	0.60
1:B:97:HIS:HE1	1:B:104:GLY:H	1.48	0.60
1:B:359:GLN:HE21	1:B:366:PHE:HB3	1.66	0.60
1:B:45:ASN:HD22	1:B:47:ALA:H	1.48	0.59
1:B:252:ASP:HB3	6:B:743:HOH:O	2.01	0.59
1:A:359:GLN:HE21	1:A:366:PHE:HB3	1.67	0.59
1:B:341:GLU:CB	6:B:741:HOH:O	2.41	0.59
1:B:240:GLN:HB2	1:B:272:GLU:HG2	1.85	0.58
1:B:359:GLN:HE22	1:B:408:ASN:N	1.90	0.58
1:A:503:LYS:HE3	1:A:504:GLU:HB2	1.85	0.57
1:A:87:ASP:OD2	1:A:97:HIS:HD2	1.87	0.57
1:B:555:ARG:HH21	1:B:555:ARG:CG	2.18	0.56
1:B:555:ARG:HH21	1:B:555:ARG:HA	1.70	0.56
1:A:301:THR:HB	6:A:1068:HOH:O	2.05	0.56
1:B:172:GLN:HE22	1:B:215:ASN:H	1.54	0.56
1:A:134:LYS:H	1:A:134:LYS:CD	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASN:ND2	1:B:47:ALA:HB3	2.20	0.56
1:B:138:ALA:HB3	1:B:376:VAL:HG23	1.88	0.56
1:A:211:ASN:O	1:A:212:PHE:HB2	2.05	0.55
1:A:433:ILE:HD11	1:A:474:PRO:HA	1.89	0.55
1:A:36:LEU:HD13	1:A:41:ARG:HD3	1.89	0.55
1:A:490:GLN:H	1:A:490:GLN:NE2	2.03	0.54
1:B:42:GLN:NE2	6:B:841:HOH:O	2.41	0.53
1:A:97:HIS:HE1	1:A:104:GLY:N	1.94	0.53
1:B:216:PRO:HA	1:B:219:THR:OG1	2.09	0.53
1:B:87:ASP:OD2	1:B:97:HIS:CD2	2.61	0.53
1:B:301:THR:HB	6:B:771:HOH:O	2.08	0.53
1:A:238:HIS:HD2	6:A:1027:HOH:O	1.92	0.52
1:A:503:LYS:HE2	1:A:506:LYS:HD3	1.91	0.52
1:B:26:ARG:NE	6:B:763:HOH:O	2.31	0.52
1:B:45:ASN:HD22	1:B:47:ALA:N	2.06	0.52
1:A:331:PRO:O	1:A:332:GLN:CB	2.53	0.52
1:A:461:ILE:O	1:A:465:VAL:HG23	2.10	0.52
1:A:45:ASN:ND2	1:A:48:GLU:H	2.07	0.52
1:A:29:GLU:OE1	1:A:32:GLY:N	2.33	0.51
1:A:117:THR:HG21	1:A:146:TRP:NE1	2.11	0.51
1:A:431:PRO:HG2	1:A:436:LYS:HG2	1.93	0.50
1:A:172:GLN:HE22	1:A:215:ASN:H	1.59	0.50
1:B:45:ASN:ND2	1:B:48:GLU:H	2.10	0.50
1:A:426:ARG:HG2	1:A:426:ARG:NH1	2.20	0.49
2:A:601:SRM:HBB1	2:A:601:SRM:HHC	1.93	0.49
1:B:554:PRO:O	1:B:555:ARG:HB2	2.13	0.49
1:B:178:VAL:HB	1:B:208:VAL:HG11	1.94	0.49
1:B:478:HIS:HD2	1:B:487:ALA:O	1.96	0.49
1:B:38:GLU:HG3	6:B:938:HOH:O	2.13	0.48
1:B:102:HIS:CE1	1:B:105:ARG:HD2	2.48	0.48
1:A:355:GLY:HA2	1:A:429:THR:HB	1.93	0.48
1:B:191:PRO:HA	1:B:360:LYS:HB3	1.94	0.48
1:A:554:PRO:O	1:A:555:ARG:C	2.52	0.48
1:A:331:PRO:O	6:A:1075:HOH:O	2.20	0.48
1:B:457:ARG:HE	1:B:535:CYS:CB	2.27	0.48
1:A:54:LYS:HE2	1:A:85:ASP:OD2	2.12	0.48
1:A:503:LYS:CG	1:A:504:GLU:N	2.64	0.47
1:A:371:ILE:HG12	1:A:403:ASN:HA	1.97	0.47
1:A:74:GLU:OE2	1:A:77:GLU:HB2	2.15	0.47
1:A:478:HIS:HD2	1:A:487:ALA:O	1.98	0.47
1:B:178:VAL:HG11	1:B:208:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ARG:O	1:B:44:ILE:HG12	2.15	0.47
1:B:223:ARG:HD3	1:B:308:THR:OG1	2.15	0.47
1:B:435:MET:HE3	1:B:463:GLU:HG3	1.96	0.47
1:B:490:GLN:HE21	1:B:490:GLN:N	1.99	0.47
1:A:65:ILE:HD13	1:A:90:LEU:HD21	1.96	0.46
1:A:279:TRP:O	1:A:336:ASP:HB2	2.15	0.46
1:B:56:PRO:HG3	1:B:89:ARG:HG2	1.96	0.46
1:A:490:GLN:HE21	1:A:490:GLN:N	2.05	0.46
1:A:240:GLN:HG2	1:A:241:ILE:HG23	1.97	0.46
1:B:461:ILE:O	1:B:465:VAL:HG23	2.16	0.46
1:B:371:ILE:HG12	1:B:403:ASN:HA	1.98	0.46
1:B:555:ARG:HH21	1:B:555:ARG:CA	2.27	0.46
1:B:48:GLU:HG3	1:B:302:ARG:HB3	1.99	0.45
1:A:433:ILE:HD11	1:A:474:PRO:CA	2.47	0.44
1:A:478:HIS:HB2	1:A:492:ALA:HB2	1.98	0.44
1:B:101:HIS:HE1	6:B:803:HOH:O	1.99	0.44
1:B:36:LEU:HD13	1:B:41:ARG:HD3	1.99	0.44
1:B:230:ILE:HD12	1:B:230:ILE:N	2.32	0.44
1:B:230:ILE:CG1	1:B:239:PRO:HG3	2.47	0.44
1:B:65:ILE:HD13	1:B:90:LEU:HD21	2.00	0.44
1:A:296:TYR:CD2	1:A:310:MET:HG3	2.53	0.44
1:B:124:TYR:CZ	1:B:162:GLY:HA3	2.52	0.44
1:A:262:GLY:O	1:A:311:MET:HB2	2.17	0.44
1:A:480:THR:HB	1:A:489:VAL:HG13	1.99	0.43
1:B:138:ALA:HB3	1:B:376:VAL:CG2	2.48	0.43
1:A:216:PRO:HA	1:A:219:THR:OG1	2.18	0.43
1:A:129:ILE:CG2	1:A:148:ILE:HB	2.48	0.43
1:B:506:LYS:H	1:B:506:LYS:HG3	1.66	0.43
1:A:383:GLU:CD	1:A:386:ARG:HH21	2.21	0.43
1:A:139:ASP:HA	1:A:374:GLY:O	2.19	0.42
1:A:431:PRO:HG2	1:A:436:LYS:CG	2.48	0.42
1:A:74:GLU:OE2	1:A:74:GLU:O	2.37	0.42
1:B:156:VAL:HB	1:B:157:PRO:HD3	2.02	0.42
1:A:268:LYS:HE3	1:A:312:TRP:CH2	2.55	0.42
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.83	0.42
1:A:27:VAL:HG21	1:A:297:ARG:HG2	2.02	0.41
1:A:267:PRO:HB3	1:A:483:PRO:HB2	2.02	0.41
1:B:473:GLN:HA	1:B:474:PRO:HD3	1.94	0.41
2:A:601:SRM:HHB	3:A:602:SF4:S1	2.59	0.41
1:B:114:ASN:HB2	1:B:201:THR:OG1	2.20	0.41
1:B:397:ARG:HB2	1:B:405:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:VAL:CG1	1:B:414:ILE:HD13	2.50	0.41
2:B:601:SRM:HHA	2:B:601:SRM:HDA2	1.81	0.41
1:A:450:ALA:HB2	3:A:602:SF4:S2	2.61	0.41
1:A:397:ARG:HB2	1:A:405:ILE:HB	2.03	0.41
1:B:129:ILE:CG2	1:B:148:ILE:HB	2.51	0.41
1:B:141:THR:HB	2:B:601:SRM:HAB1	2.02	0.41
1:B:435:MET:CE	1:B:463:GLU:CG	2.97	0.41
1:B:355:GLY:HA2	1:B:429:THR:HB	2.03	0.41
1:B:435:MET:HE1	1:B:463:GLU:HG3	2.03	0.41
1:A:377:GLN:O	1:A:381:MET:HG3	2.21	0.40
1:A:97:HIS:HB2	1:A:106:PHE:CE1	2.56	0.40
1:A:328:LYS:HA	1:A:333:GLN:OE1	2.22	0.40
1:A:110:LEU:HD13	1:A:168:LEU:HD13	2.03	0.40
1:A:187:ALA:HB1	1:A:196:ASP:OD2	2.21	0.40
1:A:222:PRO:HG2	1:A:300:GLY:HA3	2.04	0.40
1:A:471:ILE:HD12	1:A:552:ALA:HB2	2.03	0.40
1:B:238:HIS:HB3	1:B:241:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	534/588 (91%)	505 (95%)	28 (5%)	1 (0%)	47 58
1	B	533/588 (91%)	513 (96%)	19 (4%)	1 (0%)	47 58
All	All	1067/1176 (91%)	1018 (95%)	47 (4%)	2 (0%)	47 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	PRO

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Mol	Chain	Res	Type
1	B	504	GLU

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	465/506 (92%)	440 (95%)	25 (5%)	22 30
1	B	464/506 (92%)	435 (94%)	29 (6%)	18 24
All	All	929/1012 (92%)	875 (94%)	54 (6%)	20 27

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	36	LEU
1	A	42	GLN
1	A	45	ASN
1	A	74	GLU
1	A	98	ARG
1	A	102	HIS
1	A	114	ASN
1	A	117	THR
1	A	134	LYS
1	A	268	LYS
1	A	283	ASP
1	A	301	THR
1	A	319	VAL
1	A	332	GLN
1	A	334	LYS
1	A	410	LYS
1	A	426	ARG
1	A	441	CYS
1	A	480	THR
1	A	490	GLN
1	A	506	LYS

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Mol	Chain	Res	Type
1	A	515	LEU
1	A	527	ASP
1	A	555	ARG
1	B	26	ARG
1	B	36	LEU
1	B	45	ASN
1	B	66	GLU
1	B	74	GLU
1	B	102	HIS
1	B	114	ASN
1	B	117	THR
1	B	283	ASP
1	B	290	LYS
1	B	301	THR
1	B	305	ARG
1	B	334	LYS
1	B	340	THR
1	B	347	GLN
1	B	360	LYS
1	B	362	GLU
1	B	390	GLU
1	B	457	ARG
1	B	480	THR
1	B	485	SER
1	B	490	GLN
1	B	502	ARG
1	B	504	GLU
1	B	506	LYS
1	B	515	LEU
1	B	521	SER
1	B	541	ILE
1	B	555	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	97	HIS
1	A	172	GLN
1	A	177	ASN
1	A	202	ASN
1	A	233	HIS

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Mol	Chain	Res	Type
1	A	238	HIS
1	A	306	GLN
1	A	359	GLN
1	A	370	HIS
1	A	377	GLN
1	A	411	ASN
1	A	473	GLN
1	A	478	HIS
1	A	490	GLN
1	B	42	GLN
1	B	45	ASN
1	B	97	HIS
1	B	101	HIS
1	B	172	GLN
1	B	177	ASN
1	B	202	ASN
1	B	206	GLN
1	B	211	ASN
1	B	233	HIS
1	B	238	HIS
1	B	306	GLN
1	B	345	GLN
1	B	359	GLN
1	B	370	HIS
1	B	377	GLN
1	B	425	ASN
1	B	437	ASN
1	B	478	HIS
1	B	490	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 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	SF4	A	602	1	0,12,12	-	-	-		
2	SRM	A	601	6,1	68,70,70	1.61	9 (13%)	81,112,112	2.27	20 (24%)
2	SRM	B	601	6,1	68,70,70	1.48	10 (14%)	81,112,112	2.12	22 (27%)
3	SF4	B	602	1	0,12,12	-	-	-		

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	SF4	A	602	1	-	-	0/6/5/5
2	SRM	A	601	6,1	1/1/19/23	15/38/126/126	-
2	SRM	B	601	6,1	1/1/19/23	14/38/126/126	-
3	SF4	B	602	1	-	-	0/6/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	SRM	C3C-C2C	5.89	1.49	1.36
2	B	601	SRM	C3C-C2C	5.87	1.49	1.36
2	A	601	SRM	FE-NC	5.24	2.16	1.95
2	B	601	SRM	C3D-C2D	3.72	1.47	1.39
2	A	601	SRM	C3D-C2D	3.69	1.47	1.39
2	B	601	SRM	FE-NC	2.87	2.06	1.95
2	A	601	SRM	CHD-C4C	2.82	1.39	1.35
2	A	601	SRM	C1C-NC	-2.80	1.34	1.39
2	A	601	SRM	CHA-C1A	2.55	1.40	1.35
2	A	601	SRM	C4C-NC	-2.51	1.34	1.39
2	B	601	SRM	CHA-C1A	2.43	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	SRM	CHD-C4C	2.28	1.38	1.35
2	A	601	SRM	FE-ND	2.25	2.14	1.96
2	B	601	SRM	C1C-NC	-2.20	1.35	1.39
2	A	601	SRM	FE-NA	2.14	2.08	1.97
2	B	601	SRM	FE-NB	2.11	2.08	1.97
2	B	601	SRM	C4C-C3C	2.08	1.48	1.45
2	B	601	SRM	O4A-CEA	-2.06	1.23	1.30
2	B	601	SRM	O2C-CCC	-2.05	1.23	1.30

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	SRM	C4C-NC-C1C	8.08	113.26	105.35
2	B	601	SRM	C4C-NC-C1C	7.09	112.30	105.35
2	B	601	SRM	CAA-C3A-C4A	6.73	123.06	111.19
2	A	601	SRM	C1A-NA-C4A	6.41	112.49	105.23
2	A	601	SRM	CAA-C3A-C4A	6.10	121.95	111.19
2	B	601	SRM	CAB-C3B-C4B	6.10	121.94	111.19
2	B	601	SRM	C1A-NA-C4A	5.42	111.37	105.23
2	A	601	SRM	C2A-C1A-CHA	5.21	128.30	123.54
2	A	601	SRM	CAB-C3B-C4B	4.85	119.74	111.19
2	A	601	SRM	C2B-C1B-CHB	4.83	127.95	123.54
2	B	601	SRM	C4B-NB-C1B	4.78	110.65	105.23
2	A	601	SRM	C4B-NB-C1B	4.26	110.06	105.23
2	A	601	SRM	CBD-CAD-C2D	-3.92	105.93	112.62
2	A	601	SRM	CHD-C4C-NC	-3.62	120.51	124.43
2	B	601	SRM	O4A-CEA-O3A	-3.57	114.41	123.30
2	B	601	SRM	C3B-C4B-NB	-3.43	104.11	110.85
2	B	601	SRM	C4D-CHA-C1A	-3.40	123.39	130.12
2	B	601	SRM	C2A-C3A-C4A	3.00	104.75	100.90
2	A	601	SRM	C4C-C3C-C2C	-2.95	103.44	106.86
2	A	601	SRM	C3B-C4B-NB	-2.89	105.16	110.85
2	B	601	SRM	CBB-CAB-C3B	-2.73	106.85	114.73
2	A	601	SRM	C1C-CHC-C4B	-2.72	120.06	126.62
2	B	601	SRM	C4C-C3C-C2C	-2.61	103.84	106.86
2	A	601	SRM	O2A-CCA-O1A	-2.59	116.85	123.30
2	A	601	SRM	CHD-C4C-C3C	2.57	129.09	124.93
2	A	601	SRM	CEC-CDC-C2C	-2.51	107.28	113.79
2	A	601	SRM	C2C-C1C-NC	-2.48	107.91	110.32
2	A	601	SRM	O4B-CEB-O3B	-2.47	117.15	123.30
2	B	601	SRM	C2A-C1A-CHA	2.42	125.75	123.54
2	B	601	SRM	O2C-CCC-O1C	-2.34	117.48	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	SRM	CBD-CAD-C2D	-2.29	108.71	112.62
2	B	601	SRM	O2A-CCA-CBA	2.27	121.32	114.03
2	B	601	SRM	O4B-CEB-O3B	-2.26	117.67	123.30
2	A	601	SRM	O4D-CED-O3D	-2.25	117.70	123.30
2	A	601	SRM	CAD-CBD-CCD	-2.23	107.50	113.76
2	B	601	SRM	CEC-CDC-C2C	-2.21	108.06	113.79
2	B	601	SRM	C3D-CDD-CED	-2.19	111.59	114.21
2	B	601	SRM	CMA-C2A-C3A	2.17	116.09	112.08
2	A	601	SRM	CHC-C1C-C2C	2.16	128.44	124.94
2	B	601	SRM	O2D-CCD-CBD	2.08	120.72	114.03
2	B	601	SRM	C3B-C4B-CHC	2.06	127.78	123.32
2	B	601	SRM	C2B-C1B-NB	-2.04	107.94	111.21

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	SRM	NC
2	B	601	SRM	NC

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	SRM	C2A-C3A-CAA-CBA
2	A	601	SRM	C4A-C3A-CAA-CBA
2	B	601	SRM	C2A-C3A-CAA-CBA
2	B	601	SRM	C4C-C3C-CAC-CBC
2	A	601	SRM	C1A-C2A-CDA-CEA
2	A	601	SRM	C3A-C2A-CDA-CEA
2	B	601	SRM	C2B-CDB-CEB-O4B
2	A	601	SRM	C3B-C2B-CDB-CEB
2	B	601	SRM	C3A-C2A-CDA-CEA
2	B	601	SRM	C3B-C2B-CDB-CEB
2	B	601	SRM	C2C-C3C-CAC-CBC
2	B	601	SRM	C4A-C3A-CAA-CBA
2	B	601	SRM	CAB-CBB-CCB-O1B
2	B	601	SRM	CAB-CBB-CCB-O2B
2	A	601	SRM	CAA-CBA-CCA-O1A
2	A	601	SRM	CAB-CBB-CCB-O1B
2	A	601	SRM	CAA-CBA-CCA-O2A
2	A	601	SRM	CAB-CBB-CCB-O2B
2	B	601	SRM	CAA-CBA-CCA-O2A
2	A	601	SRM	CAC-CBC-CCC-O2C

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Mol	Chain	Res	Type	Atoms
2	A	601	SRM	CAD-CBD-CCD-O1D
2	B	601	SRM	CAA-CBA-CCA-O1A
2	B	601	SRM	CAC-CBC-CCC-O2C
2	A	601	SRM	CMA-C2A-CDA-CEA
2	A	601	SRM	CAC-CBC-CCC-O1C
2	B	601	SRM	CAC-CBC-CCC-O1C
2	A	601	SRM	CAD-CBD-CCD-O2D
2	B	601	SRM	CAD-CBD-CCD-O1D
2	A	601	SRM	C3A-CAA-CBA-CCA

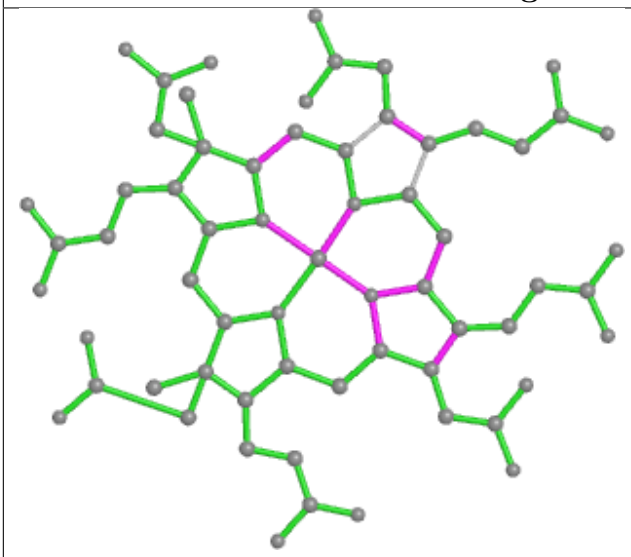
There are no ring outliers.

3 monomers are involved in 5 short contacts:

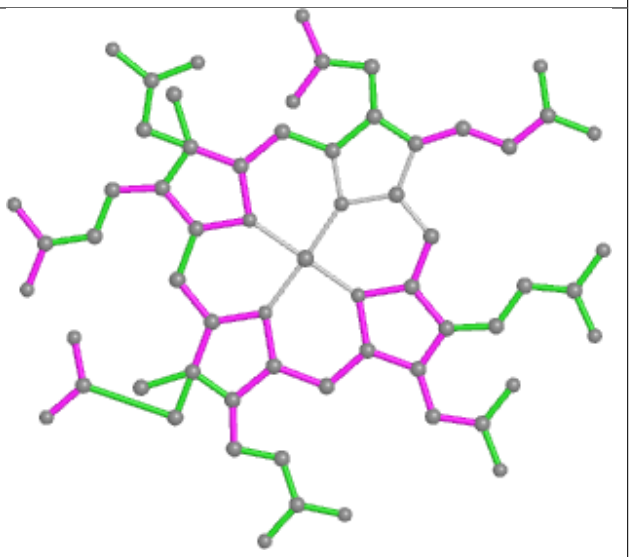
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	SF4	2	0
2	A	601	SRM	2	0
2	B	601	SRM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

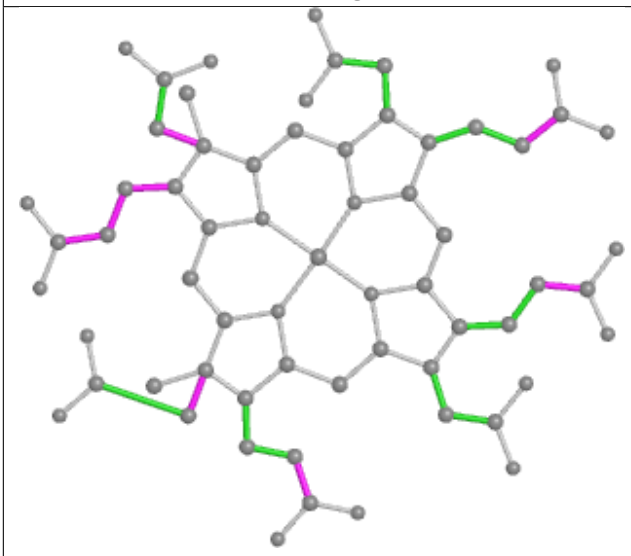
Ligand SRM A 601



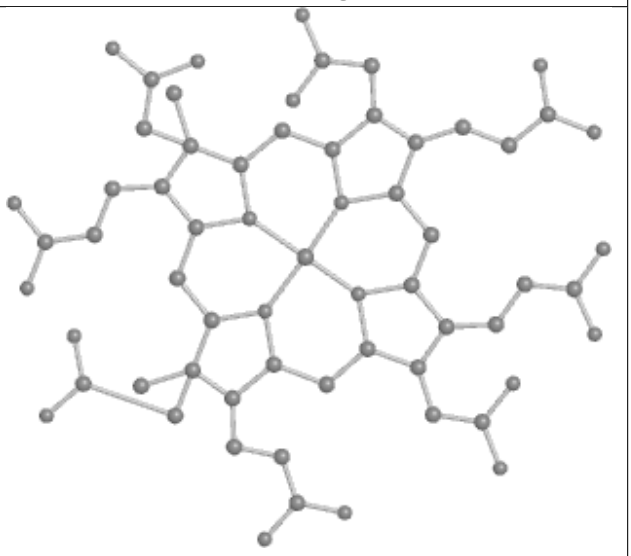
Bond lengths



Bond angles

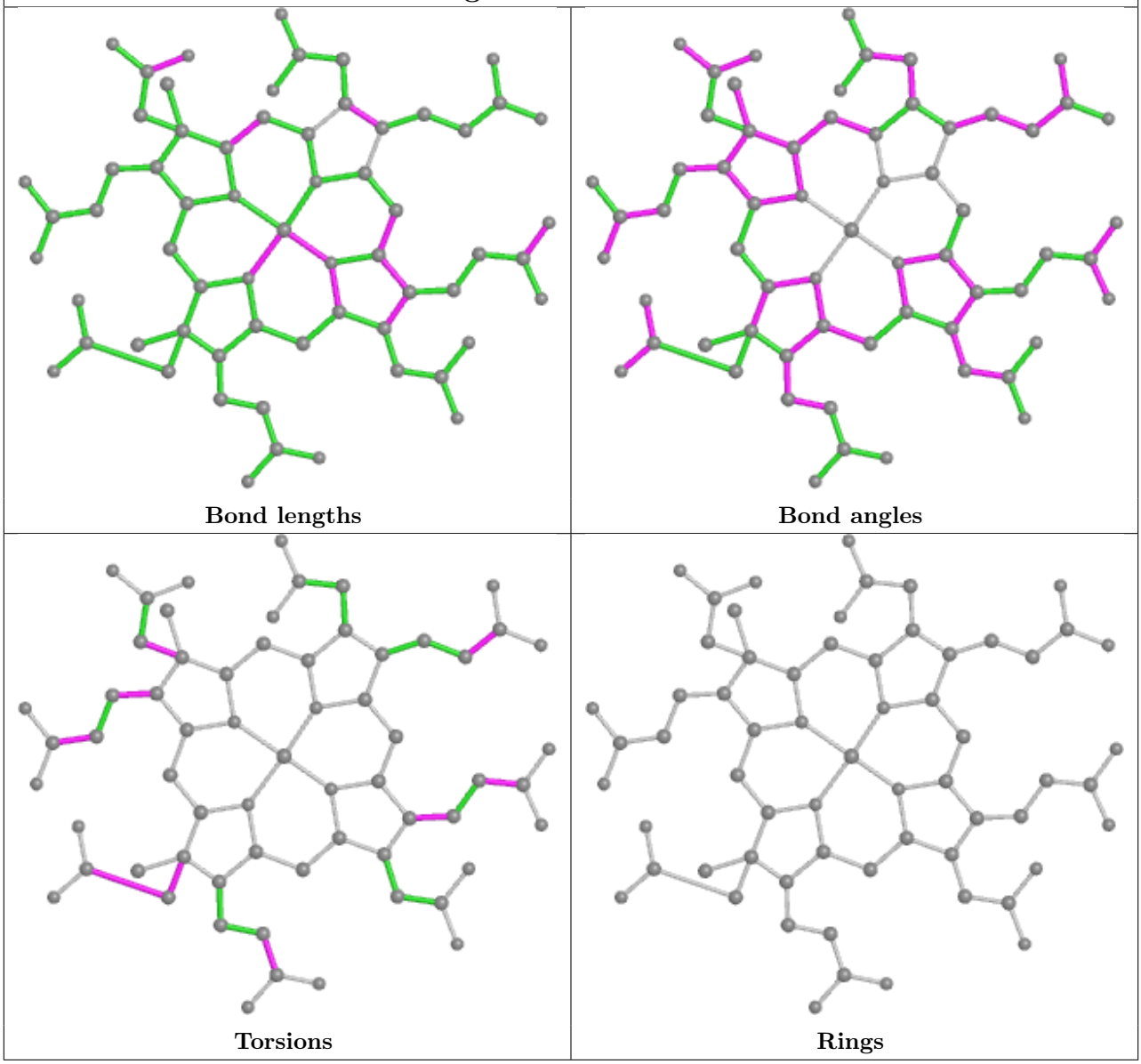


Torsions



Rings

Ligand SRM B 601



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	536/588 (91%)	-0.36	8 (1%)	73	79	14, 24, 39, 59	0
1	B	535/588 (90%)	-0.38	2 (0%)	92	95	14, 24, 39, 60	0
All	All	1071/1176 (91%)	-0.37	10 (0%)	84	88	14, 24, 39, 60	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	LYS	3.9
1	A	340	THR	2.7
1	A	529	TYR	2.5
1	A	347	GLN	2.4
1	A	553	VAL	2.4
1	A	505	GLY	2.2
1	A	502	ARG	2.1
1	B	504	GLU	2.1
1	A	528	VAL	2.0
1	B	419	ASN	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 monosaccharides in this entry.

6.4 Ligands (i)

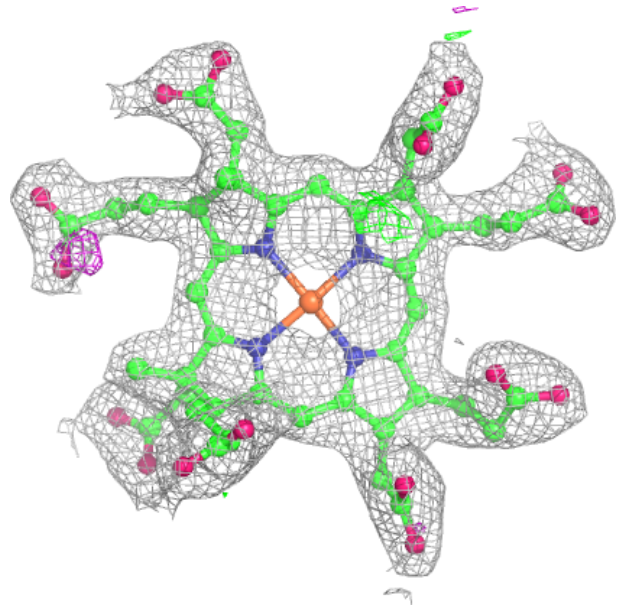
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

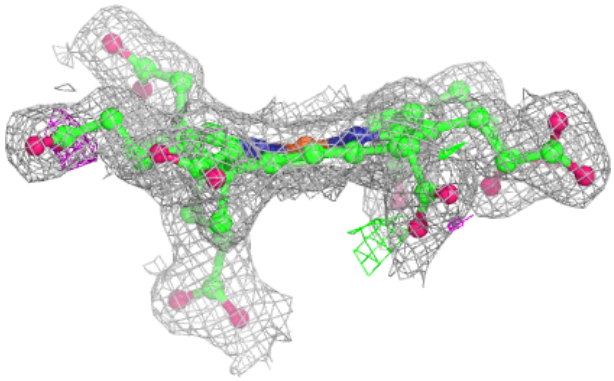
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	K	B	603	1/1	0.92	0.06	42,42,42,42	0
4	K	A	603	1/1	0.93	0.08	36,36,36,36	0
2	SRM	B	601	63/63	0.97	0.10	13,19,23,30	0
2	SRM	A	601	63/63	0.98	0.10	10,19,25,33	0
5	CL	A	604	1/1	0.98	0.06	28,28,28,28	0
3	SF4	B	602	8/8	0.99	0.07	19,21,21,23	0
3	SF4	A	602	8/8	0.99	0.07	19,20,22,23	0
5	CL	A	605	1/1	0.99	0.05	23,23,23,23	0
5	CL	B	604	1/1	0.99	0.06	26,26,26,26	0
5	CL	B	605	1/1	0.99	0.06	26,26,26,26	0

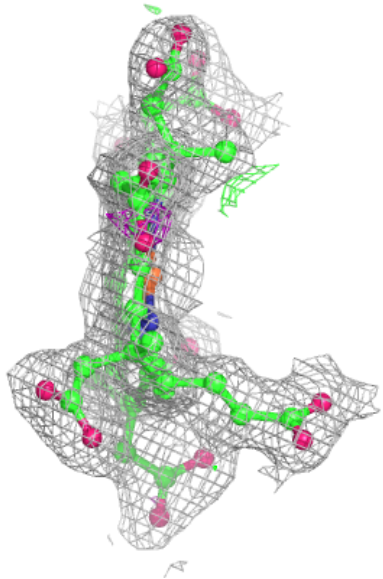
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SRM B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

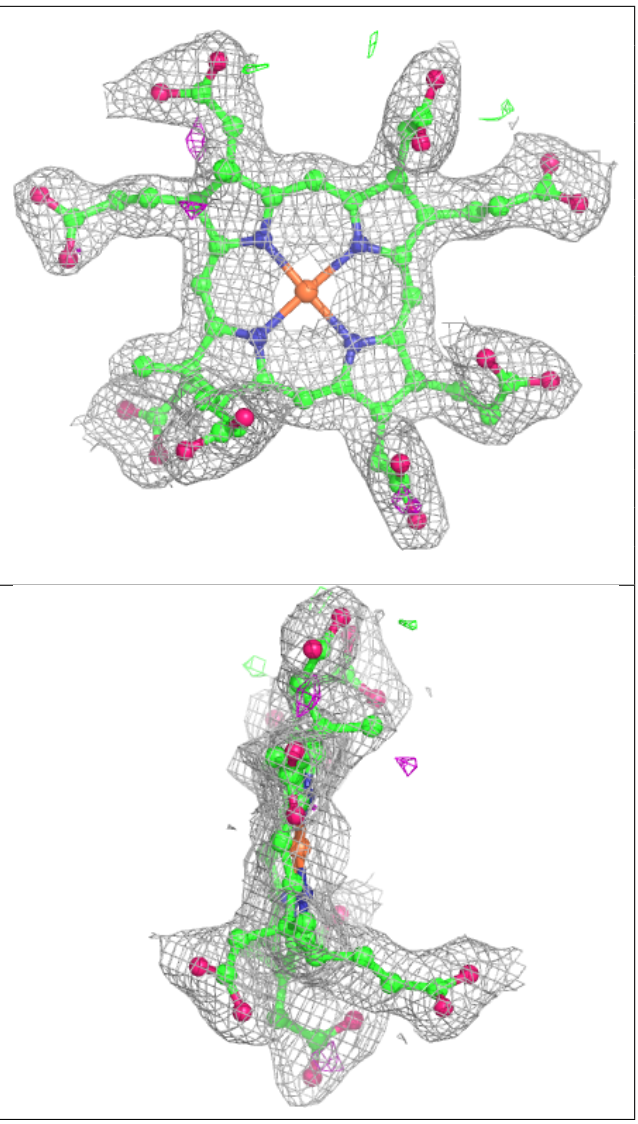






Electron density around SRM A 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.