Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2026 – 10:14 PM EDT

PDB ID	:	5KOH / pdb_00005koh
Title	:	Nitrogenase MoFeP from Gluconacetobacter diazotrophicus in dithionite reduced state
Authors	:	Owens, C.P.; Tezcan, F.A.
Deposited on	:	2016-06-30
Resolution	:	1.83 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:

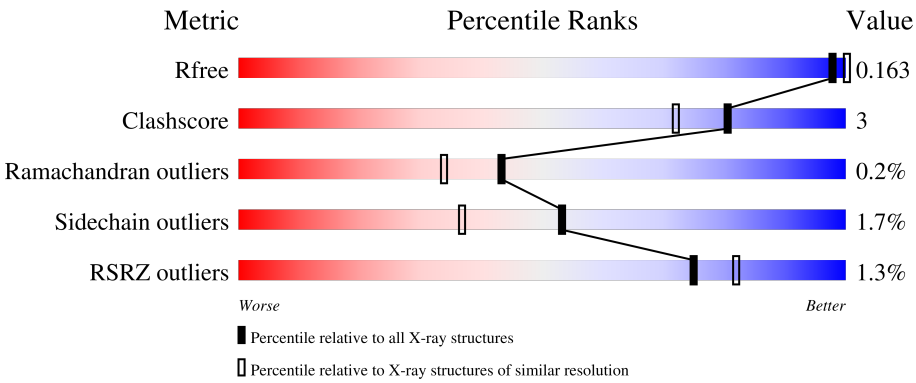
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.83 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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	499	2% 90% 7% •
1	C	499	2% 90% 6% •
2	B	511	% 95% 5% •
2	D	511	% 95% 5%

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
5	MRD	A	503	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 17785 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.

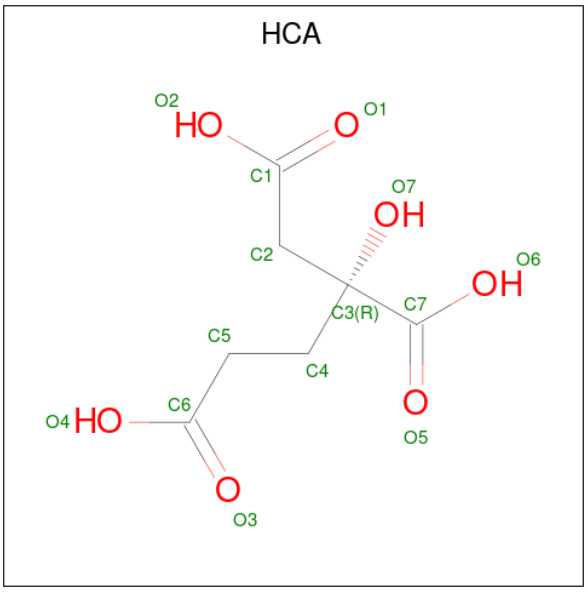
- Molecule 1 is a protein called Nitrogenase protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	483	3823	2433	669	701	20	0	1	0
1	C	482	3816	2427	664	704	21	0	1	0

- Molecule 2 is a protein called Nitrogenase FeMo beta subunit protein NifK.

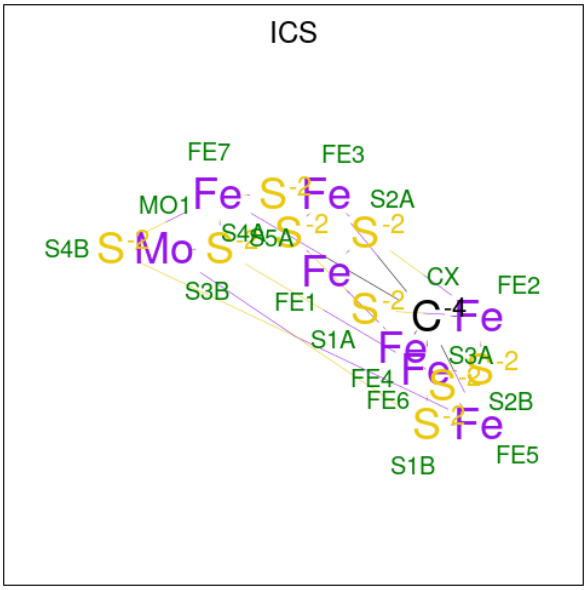
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	510	4032	2565	680	764	23	0	5	0
2	D	510	4015	2553	676	763	23	0	2	0

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



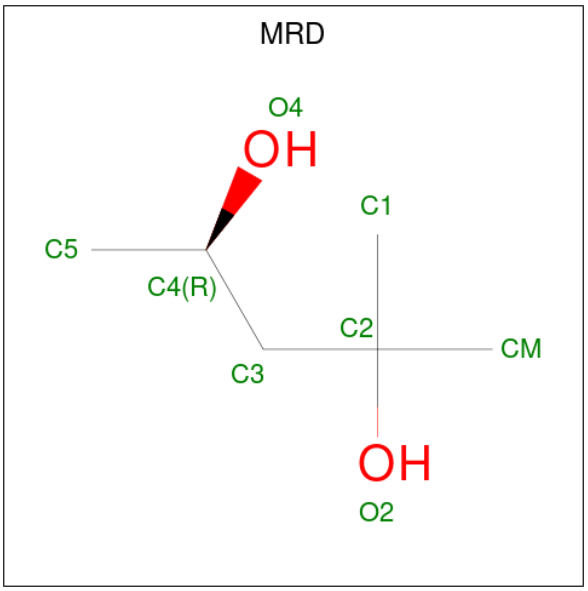
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	14	7	7	0	0
			Total	C	O		
3	C	1	14	7	7	0	0

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula: CFe_7MoS_9).



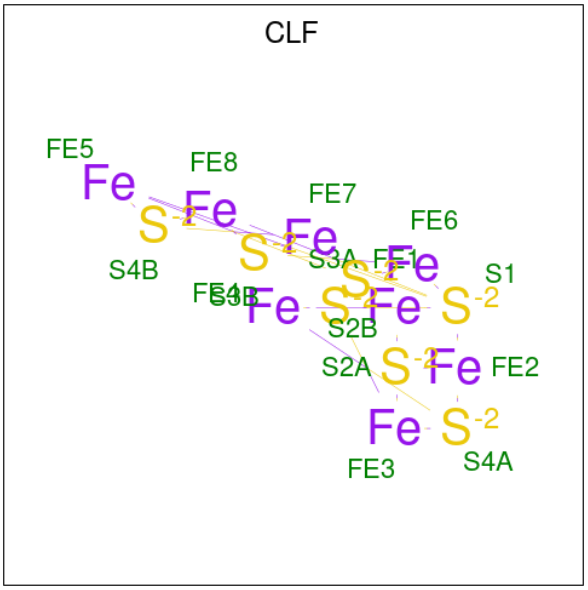
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	Mo	S		
4	A	1	18	1	7	1	9	0	0
			Total	C	Fe	Mo	S		
4	C	1	18	1	7	1	9	0	0

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0

- Molecule 6 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe_8S_7).

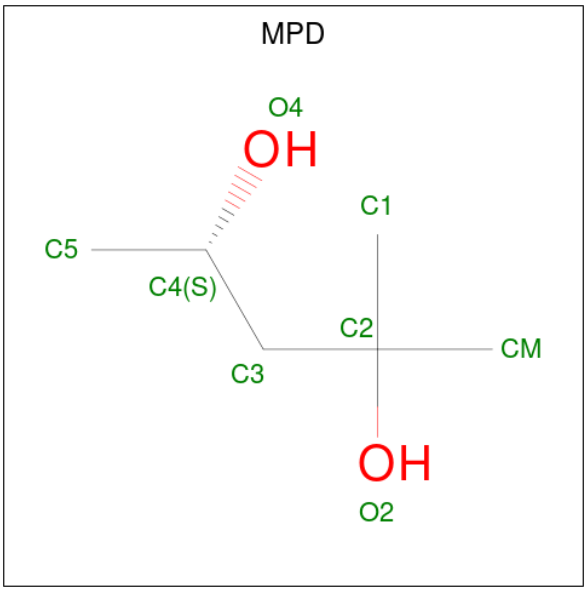


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Fe S 15 8 7	0	0
6	C	1	Total Fe S 15 8 7	0	0

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
7	B	2	2	2	0	0

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	C	1	8	6	2	0	0

- Molecule 9 is water.

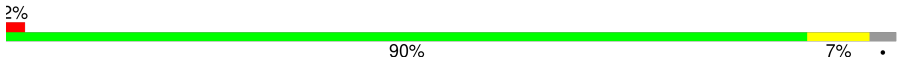
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	443	443	443	0	0
			Total	O		
9	B	545	545	545	0	0
			Total	O		
9	C	440	440	440	0	0
			Total	O		
9	D	551	551	551	0	0

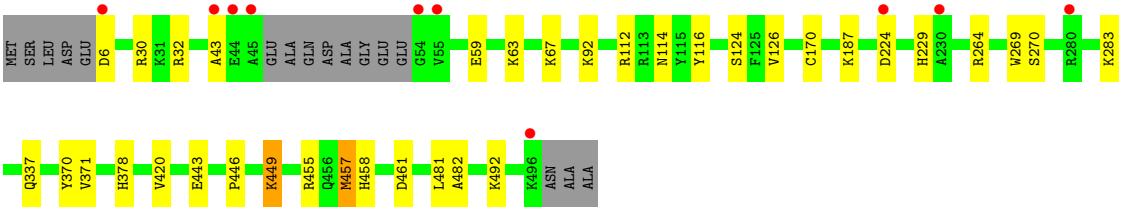
3 Residue-property plots (i)

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: Nitrogenase protein alpha chain

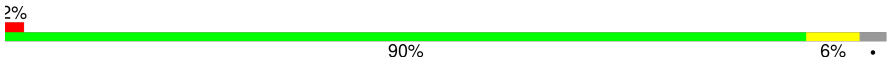
Chain A:

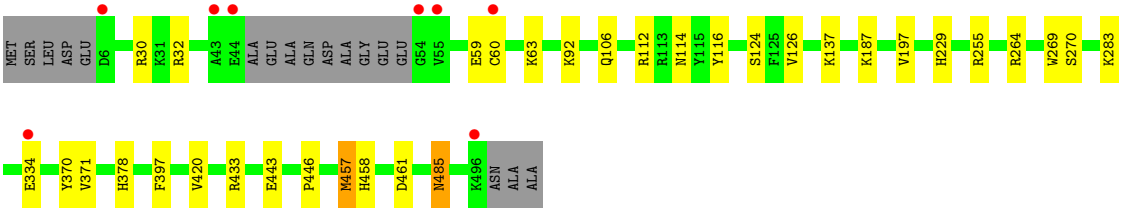




• Molecule 1: Nitrogenase protein alpha chain

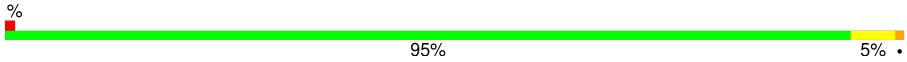
Chain C:

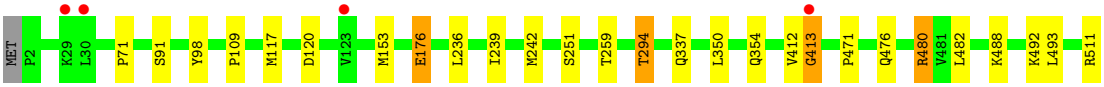




• Molecule 2: Nitrogenase FeMo beta subunit protein NifK

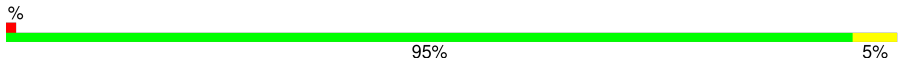
Chain B:

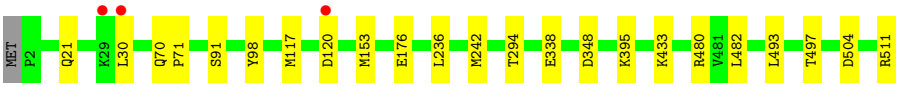




• Molecule 2: Nitrogenase FeMo beta subunit protein NifK

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	202.60Å 202.60Å 132.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	143.26 – 1.83 143.26 – 1.83	Depositor EDS
% Data completeness (in resolution range)	100.0 (143.26-1.83) 100.0 (143.26-1.83)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	0.43	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.129 , 0.150 0.142 , 0.163	Depositor DCC
R_{free} test set	11943 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	14.5	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.3	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	17785	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: CLF, FE, MPD, HCA, ICS, MRD

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	1.14	3/3918 (0.1%)	1.09	4/5291 (0.1%)
1	C	1.21	8/3911 (0.2%)	1.10	6/5283 (0.1%)
2	B	1.14	3/4150 (0.1%)	1.02	9/5621 (0.2%)
2	D	1.15	3/4124 (0.1%)	1.00	1/5586 (0.0%)
All	All	1.16	17/16103 (0.1%)	1.05	20/21781 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	B	0	1
All	All	0	3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	511	ARG	C-O	10.79	1.45	1.23
2	D	511	ARG	C-O	9.24	1.42	1.23
2	B	413	GLY	N-CA	9.06	1.60	1.45
1	A	449	LYS	CD-CE	8.96	1.79	1.52
1	C	255	ARG	CD-NE	-7.87	1.35	1.46
2	B	511	ARG	CA-C	6.92	1.67	1.52
1	A	457	MET	CG-SD	6.09	1.96	1.80
2	D	511	ARG	CA-C	6.08	1.65	1.52
1	C	485	ASN	CB-CG	-5.99	1.37	1.52
2	D	70	GLN	CA-CB	5.84	1.59	1.54
1	C	433	ARG	CA-C	-5.82	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	433	ARG	C-O	-5.67	1.21	1.23
1	C	255	ARG	CZ-NH2	-5.65	1.26	1.33
1	C	197	VAL	C-O	5.61	1.30	1.24
1	A	170	CYS	CA-C	5.50	1.58	1.52
1	C	397	PHE	N-CA	5.39	1.51	1.46
1	C	457	MET	CG-SD	5.27	1.94	1.80

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	457	MET	CG-SD-CE	-18.83	59.47	100.90
1	C	457	MET	CG-SD-CE	-18.66	59.85	100.90
1	A	449	LYS	CD-CE-NZ	-14.60	65.19	111.90
2	B	511	ARG	CA-C-O	-13.96	97.06	120.80
1	C	255	ARG	NE-CZ-NH2	-13.48	107.07	119.20
2	D	511	ARG	CA-C-O	-12.79	99.06	120.80
1	C	255	ARG	NE-CZ-NH1	9.72	131.22	121.50
2	B	480[A]	ARG	NE-CZ-NH1	-7.94	113.56	121.50
2	B	480[B]	ARG	NE-CZ-NH1	-7.94	113.56	121.50
1	C	255	ARG	CD-NE-CZ	7.68	135.15	124.40
2	B	413	GLY	N-CA-C	6.90	122.26	114.67
2	B	412	VAL	CA-C-N	-6.82	105.97	121.19
2	B	412	VAL	C-N-CA	-6.82	105.97	121.19
2	B	412	VAL	O-C-N	-6.81	115.24	121.91
1	C	264	ARG	CB-CG-CD	-5.76	98.04	111.30
1	A	264	ARG	CB-CG-CD	5.35	123.61	111.30
1	C	255	ARG	CG-CD-NE	-5.16	100.64	112.00
2	B	294	THR	CA-C-N	-5.13	113.26	118.85
2	B	294	THR	C-N-CA	-5.13	113.26	118.85
1	A	224	ASP	N-CA-C	5.01	117.57	110.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ARG	Sidechain
2	B	413	GLY	Peptide
1	C	112	ARG	Sidechain

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	3823	0	3739	33	0
1	C	3816	0	3721	15	0
2	B	4032	0	3909	26	0
2	D	4015	0	3881	15	0
3	A	14	0	6	2	0
3	C	14	0	6	1	0
4	A	18	0	0	0	0
4	C	18	0	0	0	0
5	A	16	0	28	6	0
6	A	15	0	0	0	0
6	C	15	0	0	0	0
7	B	2	0	0	0	0
8	C	8	0	14	4	0
9	A	443	0	0	6	1
9	B	545	0	0	2	0
9	C	440	0	0	3	0
9	D	551	0	0	2	0
All	All	17785	0	15304	82	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (82) 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:A:449:LYS:CD	1:A:449:LYS:CE	1.79	1.58
1:A:449:LYS:CD	1:A:449:LYS:NZ	1.75	1.46
1:A:449:LYS:NZ	1:A:449:LYS:HD2	1.58	1.16
2:B:480[A]:ARG:NH2	2:D:480:ARG:HH22	1.51	1.07
2:B:480[A]:ARG:HH21	2:D:480:ARG:NH2	1.57	1.01
1:A:449:LYS:CD	1:A:449:LYS:HZ2	1.74	0.95
2:B:480[A]:ARG:NH2	2:D:480:ARG:NH2	2.18	0.88
2:B:117:MET:HE2	2:B:153:MET:SD	2.15	0.87
1:A:449:LYS:CD	1:A:449:LYS:HZ3	1.64	0.87
2:D:117:MET:HE2	2:D:153:MET:SD	2.15	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:480[A]:ARG:HH21	2:D:480:ARG:HH22	1.14	0.85
2:B:476[A]:GLN:HG3	2:B:480[A]:ARG:HH12	1.46	0.81
1:A:449:LYS:HD2	1:A:449:LYS:HZ3	1.23	0.79
2:B:480[A]:ARG:HE	2:D:480:ARG:HH12	1.33	0.76
2:D:21:GLN:HG2	9:D:915:HOH:O	1.88	0.73
2:B:471:PRO:HG2	2:B:480[A]:ARG:NH1	2.04	0.71
2:B:476[A]:GLN:HG3	2:B:480[A]:ARG:NH1	2.06	0.70
1:A:449:LYS:CE	1:A:449:LYS:CG	2.72	0.64
2:D:242:MET:HE3	2:D:338:GLU:CD	2.23	0.64
1:A:449:LYS:HE3	2:D:348:ASP:OD1	1.98	0.63
1:A:32:ARG:HD2	9:A:966:HOH:O	1.97	0.62
1:C:446:PRO:HG2	8:C:503:MPD:HM1	1.80	0.62
2:B:471:PRO:HG2	2:B:480[A]:ARG:HH11	1.64	0.61
1:C:443:GLU:HA	8:C:503:MPD:HM2	1.84	0.60
1:A:6:ASP:N	9:A:603:HOH:O	2.36	0.58
1:A:449:LYS:HD2	1:A:449:LYS:HZ2	1.46	0.58
2:B:480[B]:ARG:HG2	2:B:480[B]:ARG:HH11	1.69	0.56
1:A:43:ALA:HA	1:A:59:GLU:HG2	1.87	0.56
2:B:354:GLN:OE1	1:C:485:ASN:ND2	2.39	0.56
2:B:91:SER:OG	2:B:153:MET:HG2	2.06	0.56
2:D:71:PRO:HB2	2:D:98:TYR:CZ	2.40	0.56
1:A:449:LYS:HE2	2:B:259:THR:OG1	2.06	0.55
2:D:91:SER:OG	2:D:153:MET:HG2	2.07	0.55
2:B:480[B]:ARG:NH1	2:B:480[B]:ARG:CG	2.64	0.55
1:A:92:LYS:O	1:A:124:SER:HA	2.08	0.54
2:B:471:PRO:CG	2:B:480[A]:ARG:NH1	2.70	0.54
2:D:395:LYS:NZ	9:D:701:HOH:O	2.30	0.54
8:C:503:MPD:O4	8:C:503:MPD:CM	2.56	0.53
1:A:370:TYR:CZ	1:A:420:VAL:HG12	2.46	0.51
1:A:229:HIS:O	1:A:283:LYS:HE3	2.11	0.51
2:B:471:PRO:O	2:B:480[B]:ARG:HD2	2.12	0.50
1:C:334:GLU:H	1:C:334:GLU:CD	2.19	0.50
1:A:116:TYR:CE1	1:A:126:VAL:HB	2.46	0.50
1:C:32:ARG:HD2	9:C:979:HOH:O	2.11	0.50
1:C:229:HIS:O	1:C:283:LYS:HE3	2.12	0.49
1:C:116:TYR:CE1	1:C:126:VAL:HB	2.47	0.49
2:B:71:PRO:HB2	2:B:98:TYR:CZ	2.48	0.49
1:A:446:PRO:HB2	5:A:503:MRD:HMC1	1.94	0.49
1:C:370:TYR:CZ	1:C:420:VAL:HG12	2.47	0.48
1:A:443:GLU:HA	5:A:503:MRD:CM	2.43	0.48
5:A:503:MRD:O4	5:A:503:MRD:HMC2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:NH2	9:A:609:HOH:O	2.47	0.48
1:C:443:GLU:HA	8:C:503:MPD:CM	2.43	0.47
1:C:458:HIS:HB3	3:C:501:HCA:O5	2.14	0.47
1:A:30:ARG:HD2	9:A:666:HOH:O	2.14	0.47
1:A:446:PRO:HG2	5:A:503:MRD:HMC1	1.98	0.46
1:A:449:LYS:HZ1	2:B:109:PRO:HD3	1.81	0.46
1:C:92:LYS:O	1:C:124:SER:HA	2.16	0.45
2:D:497:THR:O	2:D:504:ASP:HA	2.17	0.45
1:A:337:GLN:CD	9:A:658:HOH:O	2.59	0.45
2:B:488:LYS:HD2	9:B:904:HOH:O	2.17	0.44
1:C:30:ARG:HD2	9:C:625:HOH:O	2.17	0.44
2:B:239:ILE:HA	2:B:242:MET:HE3	2.00	0.44
2:B:480[A]:ARG:HH11	2:B:480[A]:ARG:HD2	1.27	0.43
5:A:503:MRD:CM	5:A:503:MRD:O4	2.66	0.43
2:B:337:GLN:NE2	9:B:712:HOH:O	2.51	0.43
2:D:242:MET:HE3	2:D:338:GLU:CG	2.49	0.43
1:A:455:ARG:HD3	1:A:482:ALA:HB2	1.99	0.43
1:A:187:LYS:HD2	9:A:633:HOH:O	2.18	0.43
1:A:67:LYS:NZ	2:B:120:ASP:OD2	2.52	0.43
2:B:476[A]:GLN:CG	2:B:480[A]:ARG:HH12	2.22	0.42
1:C:187:LYS:HD2	9:C:647:HOH:O	2.19	0.42
1:A:458:HIS:HB3	3:A:501:HCA:O6	2.20	0.42
1:A:269:TRP:HA	1:A:270:SER:HA	1.76	0.42
1:A:443:GLU:HA	5:A:503:MRD:HMC2	2.02	0.41
1:A:481:LEU:C	1:A:481:LEU:HD12	2.45	0.41
1:C:457:MET:HB3	1:C:457:MET:HE3	1.76	0.41
1:C:269:TRP:HA	1:C:270:SER:HA	1.84	0.41
1:A:458:HIS:CG	3:A:501:HCA:H52	2.56	0.41
1:A:457:MET:HB3	1:A:457:MET:HE3	1.80	0.40
2:B:176:GLU:H	2:B:176:GLU:HG2	1.74	0.40
2:D:242:MET:HE1	2:D:338:GLU:HG2	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1033:HOH:O	9:A:1033:HOH:O[7_556]	2.09	0.11

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	480/499 (96%)	460 (96%)	20 (4%)	0	100	100
1	C	479/499 (96%)	461 (96%)	18 (4%)	0	100	100
2	B	513/511 (100%)	505 (98%)	6 (1%)	2 (0%)	30	18
2	D	510/511 (100%)	502 (98%)	7 (1%)	1 (0%)	43	34
All	All	1982/2020 (98%)	1928 (97%)	51 (3%)	3 (0%)	43	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	294	THR
2	D	294	THR
2	B	251	SER

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	399/413 (97%)	393 (98%)	6 (2%)	57	42
1	C	400/413 (97%)	390 (98%)	10 (2%)	42	24
2	B	432/428 (101%)	426 (99%)	6 (1%)	59	45
2	D	429/428 (100%)	422 (98%)	7 (2%)	55	39
All	All	1660/1682 (99%)	1631 (98%)	29 (2%)	53	37

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	114	ASN
1	A	371	VAL
1	A	378	HIS
1	A	461	ASP
1	A	492	LYS
2	B	176	GLU
2	B	236	LEU
2	B	350	LEU
2	B	482	LEU
2	B	492	LYS
2	B	493	LEU
1	C	59	GLU
1	C	60[A]	CYS
1	C	60[B]	CYS
1	C	63	LYS
1	C	106	GLN
1	C	114	ASN
1	C	137	LYS
1	C	371	VAL
1	C	378	HIS
1	C	461	ASP
2	D	30	LEU
2	D	120	ASP
2	D	176	GLU
2	D	236	LEU
2	D	433	LYS
2	D	482	LEU
2	D	493	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	378	HIS
1	A	384	ASN
1	C	106	GLN
1	C	129	GLN
1	C	378	HIS
2	D	302	GLN
2	D	337	GLN
2	D	476	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
4	ICS	C	502	1,3	6,30,30	2.15	4 (66%)	-		
3	HCA	A	501	4	13,13,13	1.15	1 (7%)	15,18,18	1.54	3 (20%)
6	CLF	A	505	1,2	0,24,24	-	-	-		
5	MRD	A	504	-	7,7,7	0.41	0	9,10,10	0.67	0
3	HCA	C	501	4	13,13,13	1.86	4 (30%)	15,18,18	1.63	3 (20%)
4	ICS	A	502	1,3	6,30,30	1.48	1 (16%)	-		
5	MRD	A	503	-	7,7,7	0.82	0	9,10,10	1.11	0
8	MPD	C	503	-	7,7,7	1.00	0	9,10,10	1.25	1 (11%)
6	CLF	C	504	1,2	0,24,24	-	-	-		

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	HCA	A	501	4	-	2/17/17/17	-
6	CLF	A	505	1,2	-	-	0/12/10/10
5	MRD	A	504	-	-	3/5/5/5	-
3	HCA	C	501	4	-	1/17/17/17	-
5	MRD	A	503	-	-	1/5/5/5	-
8	MPD	C	503	-	-	2/5/5/5	-
6	CLF	C	504	1,2	-	-	0/12/10/10

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	HCA	C3-C7	-3.33	1.50	1.53
4	C	502	ICS	S2B-FE2	-3.00	2.17	2.24
3	C	501	HCA	C2-C3	2.96	1.57	1.54
4	C	502	ICS	S5A-FE7	-2.70	2.18	2.24
4	A	502	ICS	S2B-FE6	-2.57	2.18	2.24
3	A	501	HCA	C2-C3	2.48	1.57	1.54
3	C	501	HCA	C4-C5	2.41	1.58	1.53
4	C	502	ICS	S5A-FE3	-2.37	2.19	2.24
4	C	502	ICS	S2B-FE6	-2.35	2.19	2.24
3	C	501	HCA	O4-C6	-2.01	1.24	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	HCA	O6-C7-C3	4.30	121.39	113.14
3	A	501	HCA	C4-C5-C6	3.62	121.17	112.77
8	C	503	MPD	CM-C2-C1	-2.91	104.11	110.63
3	C	501	HCA	C4-C5-C6	2.66	118.93	112.77
3	C	501	HCA	O5-C7-C3	-2.57	117.12	122.09
3	A	501	HCA	O3-C6-C5	-2.54	115.05	123.09
3	A	501	HCA	O7-C3-C7	-2.06	106.04	108.96

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	HCA	C2-C3-C4-C5
3	C	501	HCA	C2-C3-C4-C5
5	A	504	MRD	C1-C2-C3-C4
8	C	503	MPD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	A	503	MRD	O2-C2-C3-C4
5	A	504	MRD	O2-C2-C3-C4
5	A	504	MRD	CM-C2-C3-C4
8	C	503	MPD	CM-C2-C3-C4
3	A	501	HCA	O1-C1-C2-C3

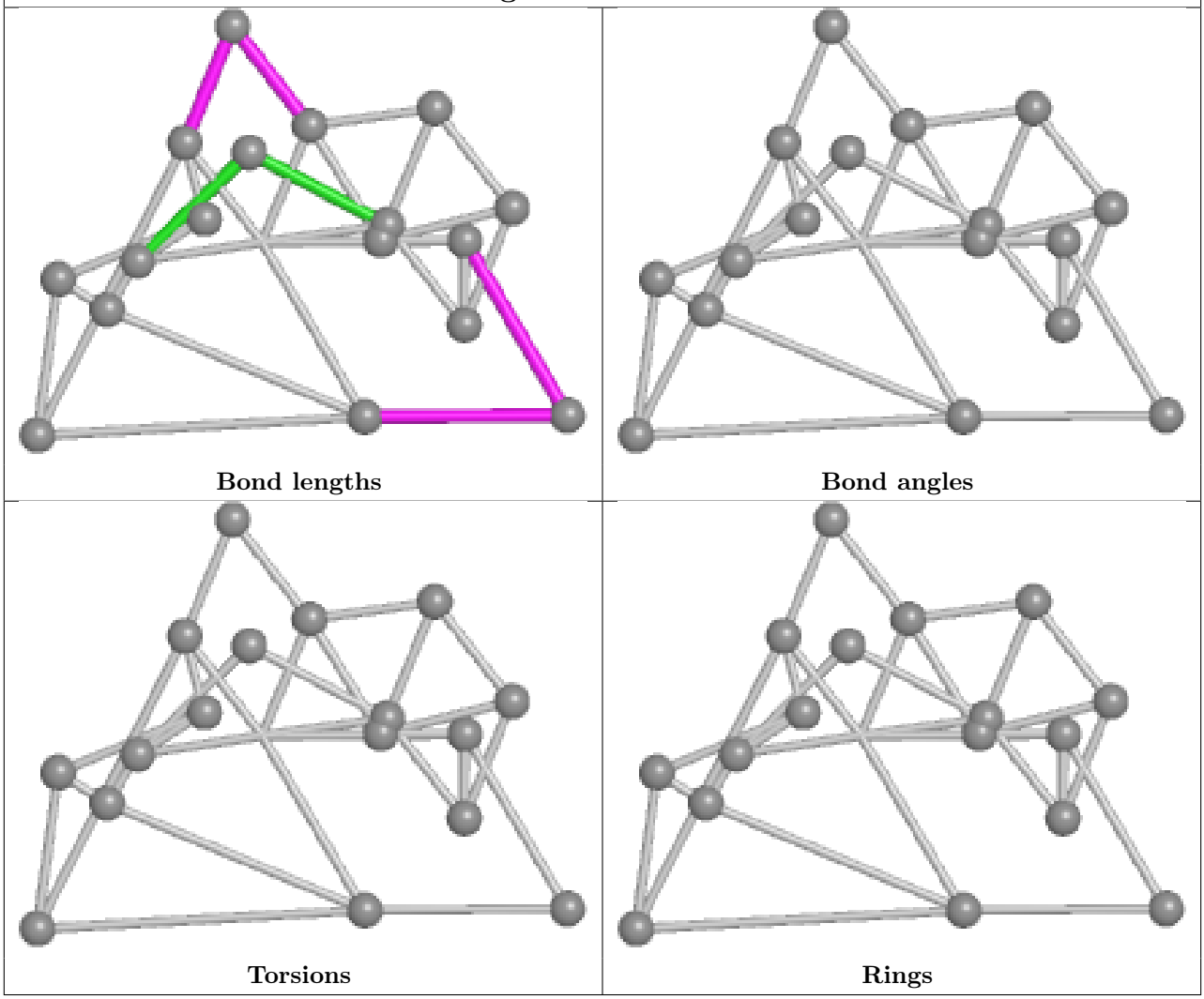
There are no ring outliers.

4 monomers are involved in 13 short contacts:

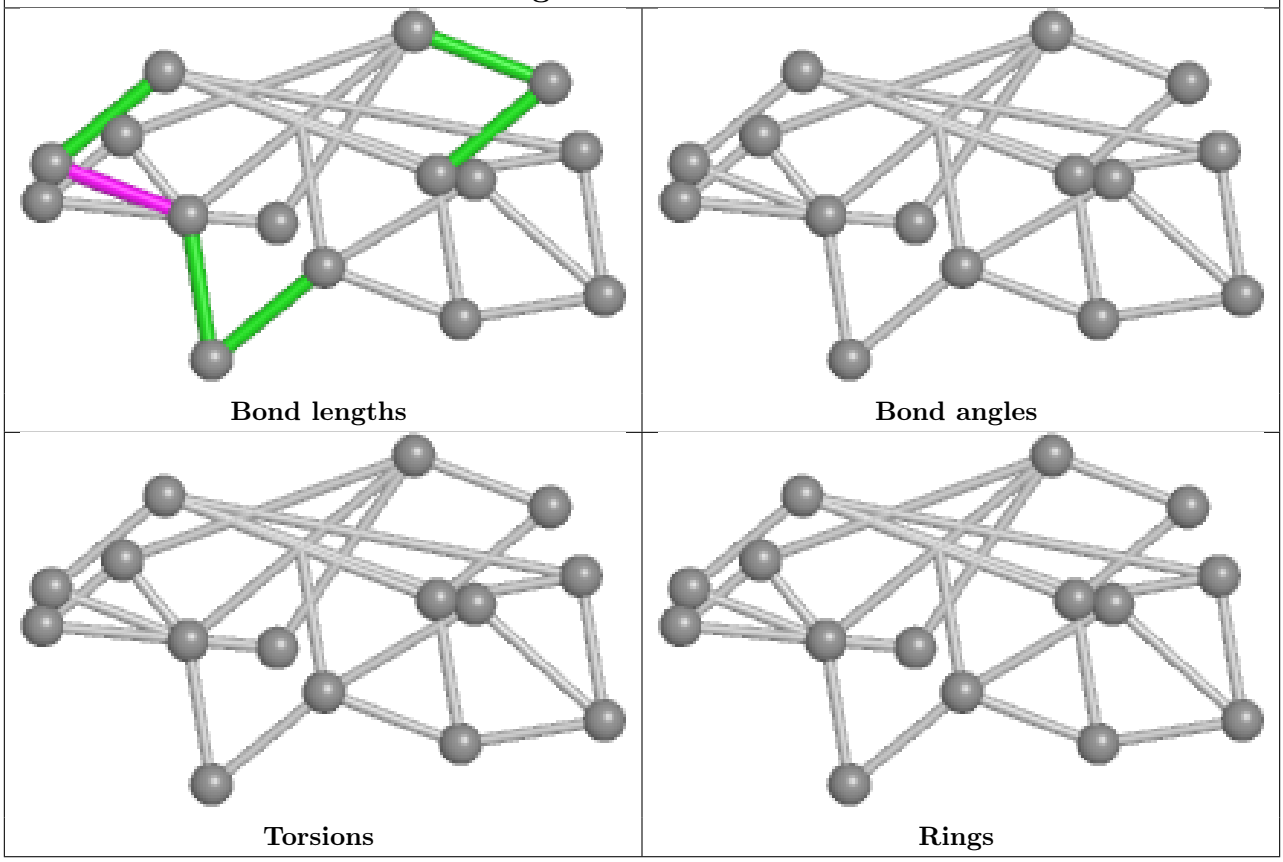
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	HCA	2	0
3	C	501	HCA	1	0
5	A	503	MRD	6	0
8	C	503	MPD	4	0

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 ICS C 502



Ligand ICS A 502



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	483/499 (96%)	-0.48	10 (2%)	63	71	10, 15, 36, 81	1 (0%)
1	C	482/499 (96%)	-0.50	8 (1%)	69	77	9, 15, 31, 59	1 (0%)
2	B	510/511 (99%)	-0.56	4 (0%)	82	88	8, 14, 29, 50	5 (0%)
2	D	510/511 (99%)	-0.59	3 (0%)	85	90	9, 14, 28, 44	2 (0%)
All	All	1985/2020 (98%)	-0.53	25 (1%)	75	82	8, 14, 31, 81	9 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	4.1
1	C	55	VAL	3.2
1	C	54	GLY	3.1
1	A	224	ASP	3.0
1	A	6	ASP	2.9
1	A	496	LYS	2.9
1	A	44	GLU	2.8
2	B	413	GLY	2.7
1	A	55	VAL	2.7
1	A	54	GLY	2.6
1	C	60[A]	CYS	2.5
1	C	496	LYS	2.5
2	D	120	ASP	2.5
1	A	230	ALA	2.4
1	C	44	GLU	2.3
1	C	334	GLU	2.3
1	C	43	ALA	2.3
1	C	6	ASP	2.3
1	A	43	ALA	2.2
2	B	29	LYS	2.2
2	D	29	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	30	LEU	2.1
2	B	30	LEU	2.1
2	B	123	VAL	2.1
1	A	280	ARG	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 oligosaccharides in this entry.

6.4 Ligands (i)

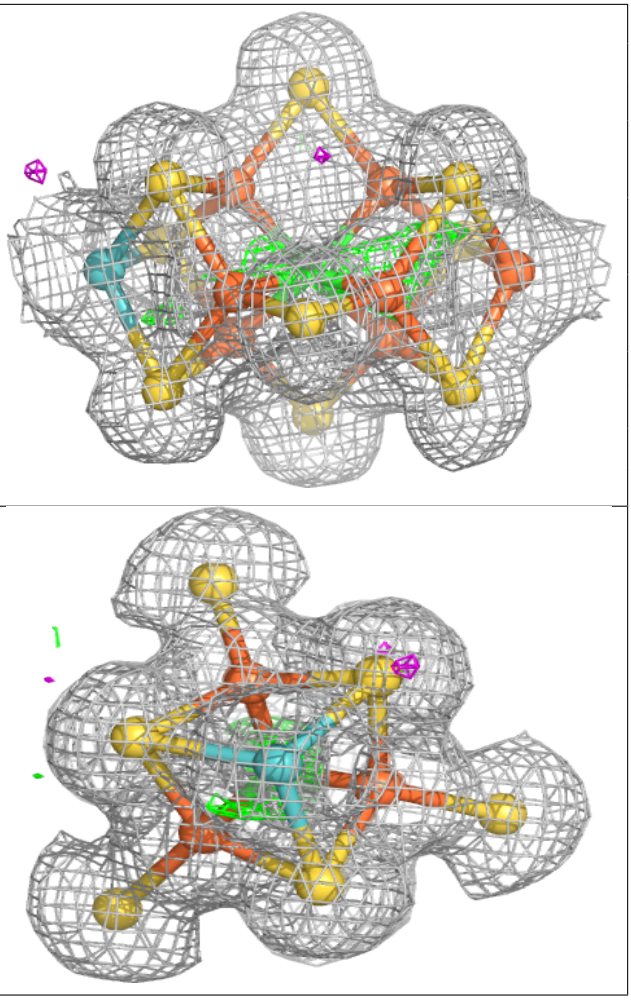
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MPD	C	503	8/8	0.88	0.13	18,25,30,32	0
5	MRD	A	503	8/8	0.90	0.13	19,25,30,31	0
5	MRD	A	504	8/8	0.91	0.12	27,33,35,43	0
7	FE	B	601	1/1	0.98	0.13	31,31,31,31	0
3	HCA	A	501	14/14	0.98	0.05	9,11,14,16	0
7	FE	B	602	1/1	0.99	0.16	31,31,31,31	0
3	HCA	C	501	14/14	0.99	0.04	8,11,14,14	0
6	CLF	C	504	15/15	1.00	0.01	10,10,12,14	0
4	ICS	A	502	18/18	1.00	0.02	9,11,12,12	0
4	ICS	C	502	18/18	1.00	0.02	9,10,11,12	0
6	CLF	A	505	15/15	1.00	0.02	9,11,13,15	2

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.

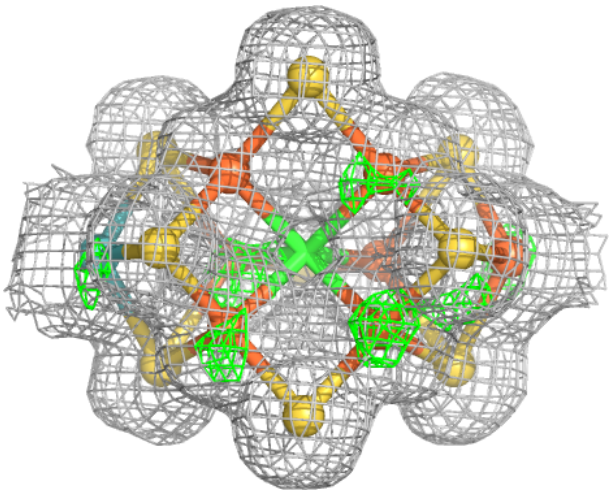
Electron density around ICS A 502:

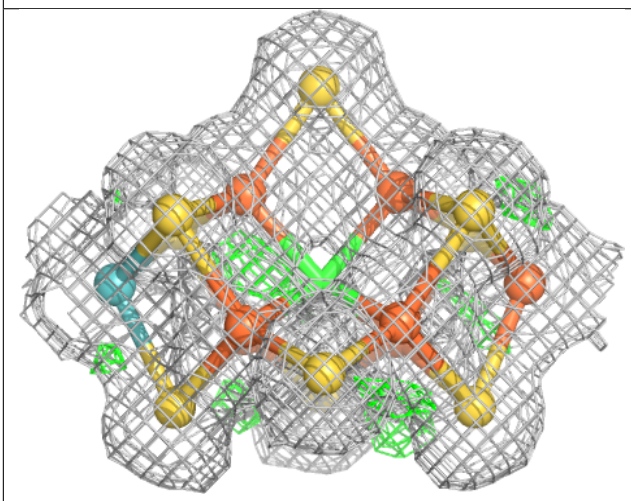
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

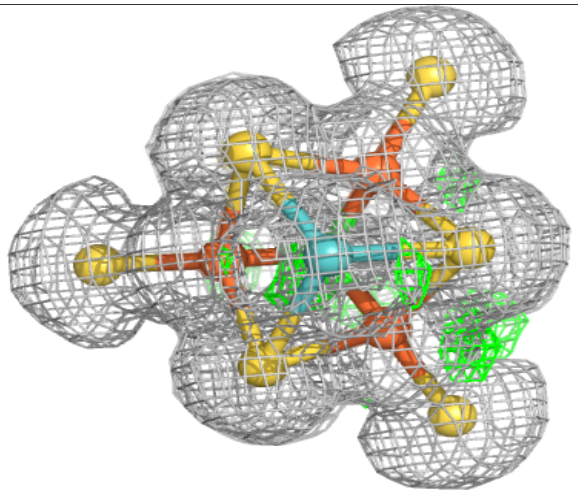


Electron density around ICS C 502:

$2mF_o$-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.