



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 05:56 AM EDT

PDB ID : 6CDK / pdb_00006cdk
Title : Characterization of the P1+ intermediate state of nitrogenase P-cluster
Authors : Keable, S.M.; Zadvornyy, O.A.; Rasmussen, A.J.; Danyal, K.; Eilers, B.J.;
Prussia, G.A.; LeVan, A.X.; Seefeldt, L.C.; Peters, J.W.
Deposited on : 2018-02-08
Resolution : 2.10 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 ⓘ 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 ⓘ](#)) 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

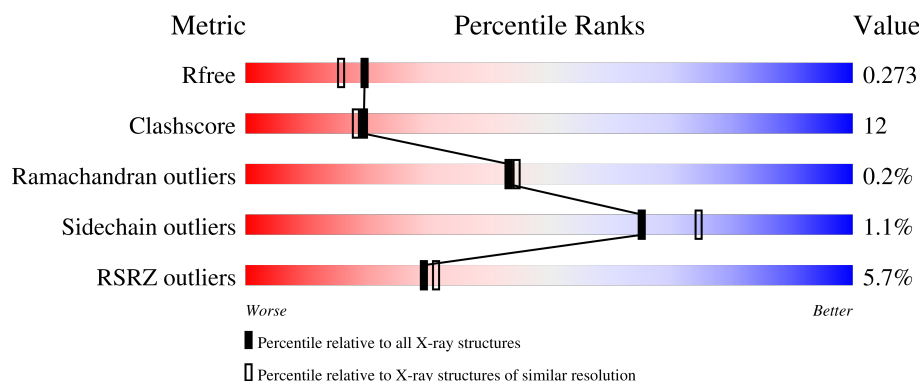
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	492	7% 74% 20% • 5%
1	C	492	8% 74% 19% • 5%
2	B	523	4% 83% 15% •
2	D	523	4% 83% 15% •

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	CLF	C	503	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16611 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.

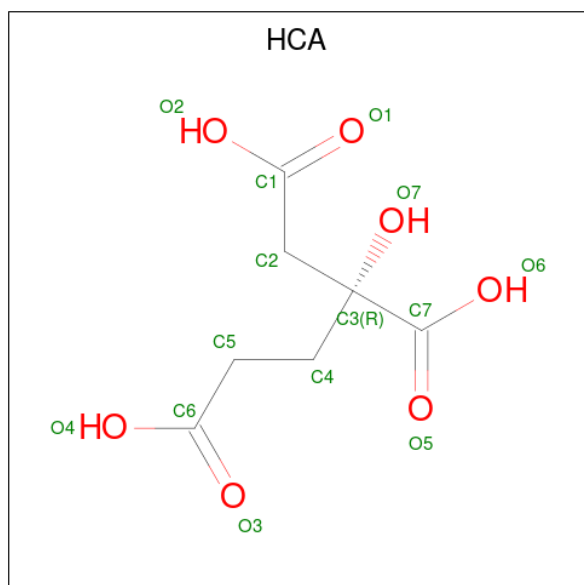
- Molecule 1 is a protein called Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3716	2363	633	696	24			
1	C	466	Total	C	N	O	S	0	0	0
			3711	2361	632	693	25			

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

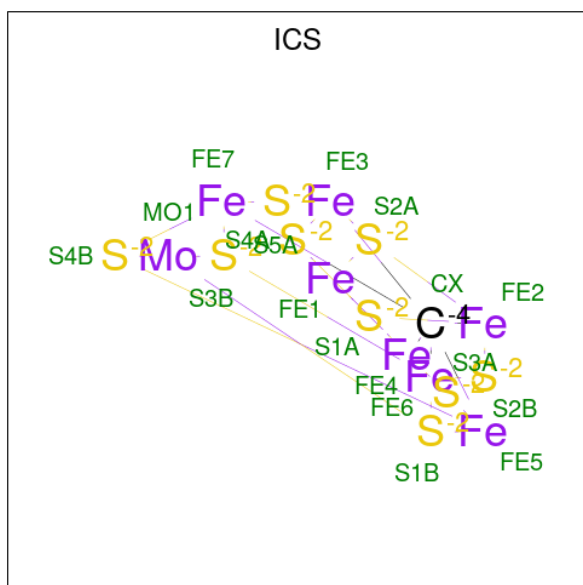
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4173	2666	705	774	28			

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



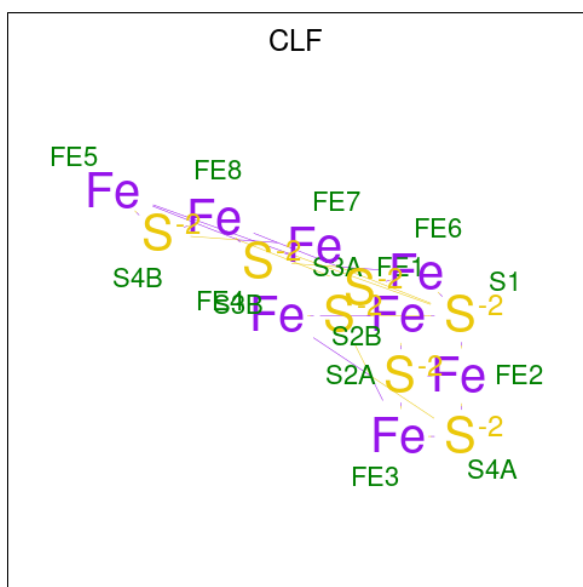
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	7	7		
3	C	1	Total	C	O	0	0
			14	7	7		

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



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

- Molecule 5 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe_8S_7).



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

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

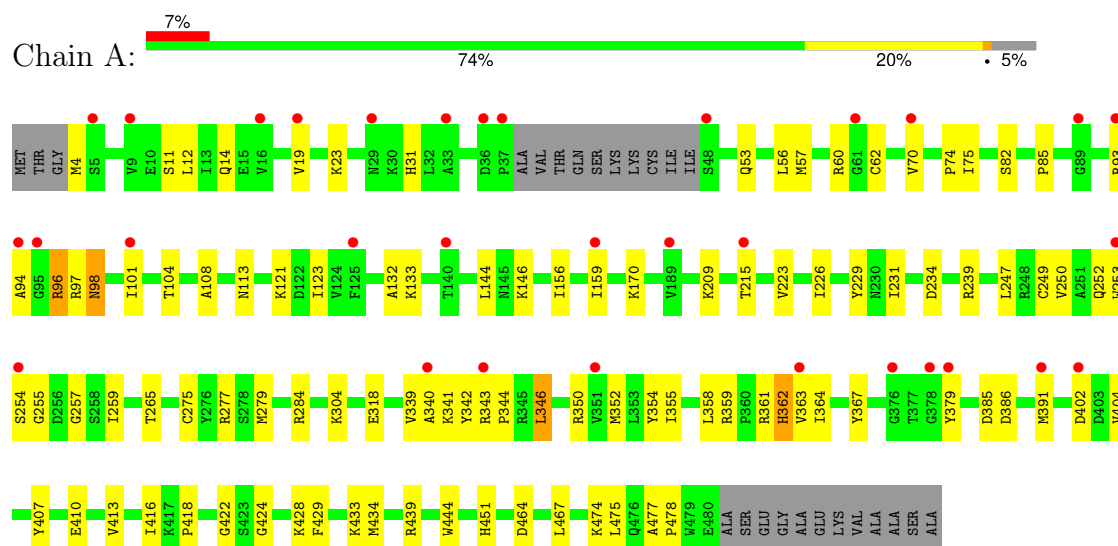
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	158	Total	O	0	0
			158	158		
7	B	215	Total	O	0	0
			215	215		
7	C	154	Total	O	0	0
			154	154		
7	D	214	Total	O	0	0
			214	214		

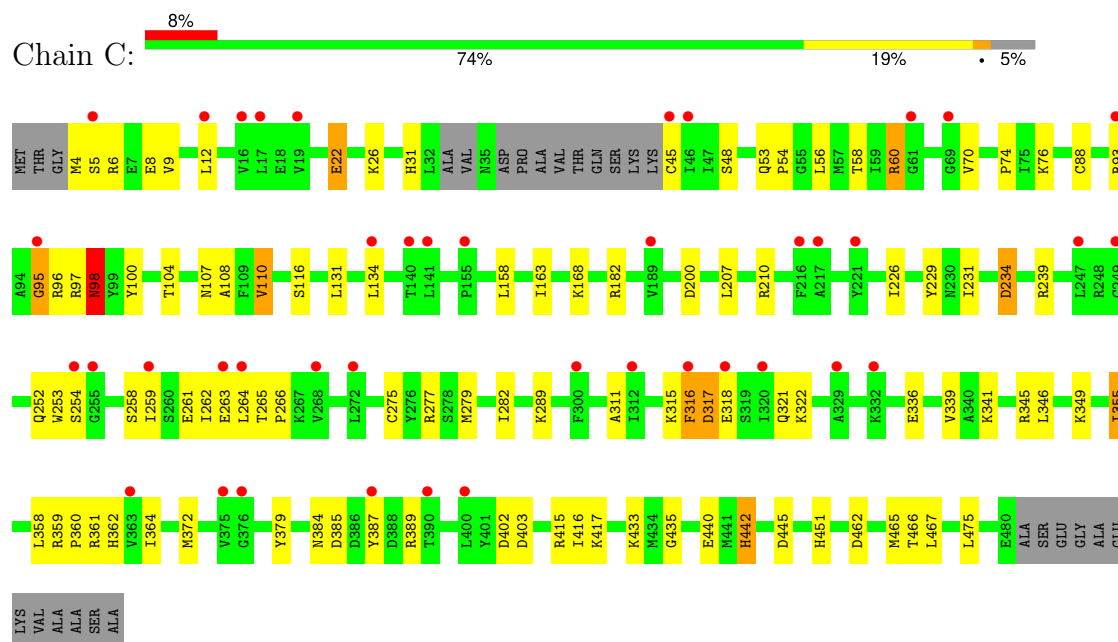
3 Residue-property plots [i](#)

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.

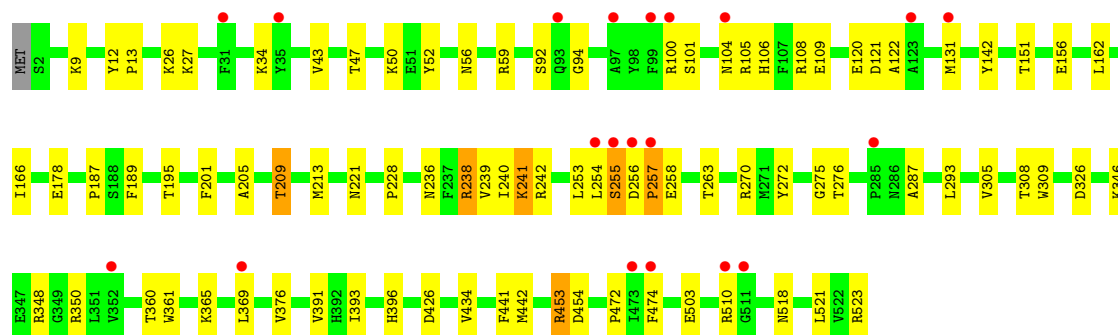
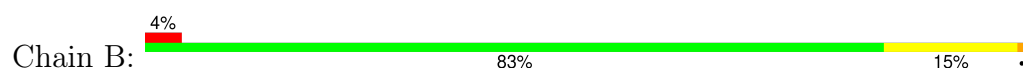
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



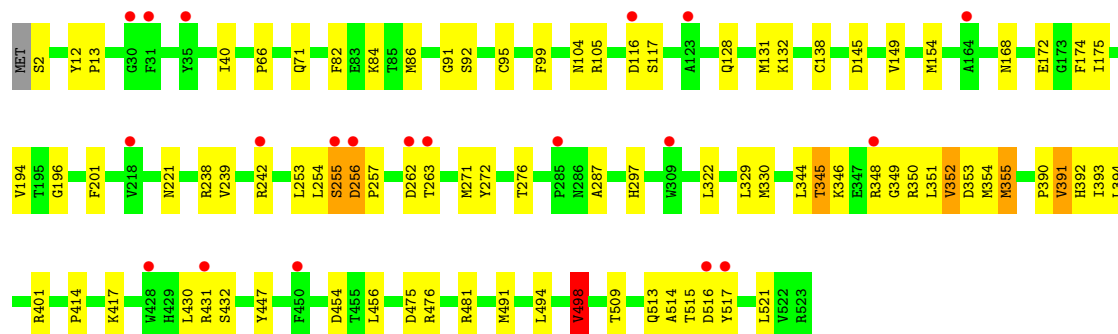
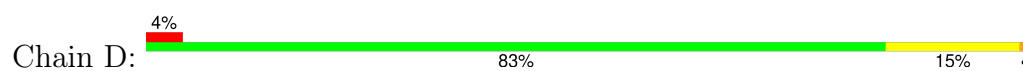
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain



• Molecule 2: Nitrogenase molybdenum-iron protein beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.88Å 130.78Å 80.79Å 90.00° 110.85° 90.00°	Depositor
Resolution (Å)	50.01 – 2.10 50.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	57.1 (50.01-2.10) 57.1 (50.01-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.232 , 0.263 0.246 , 0.273	Depositor DCC
R_{free} test set	3543 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	1.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16611	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: HCA, FE, CLF, ICS

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	0.98	5/3803 (0.1%)	1.11	10/5127 (0.2%)
1	C	0.94	3/3796 (0.1%)	1.08	12/5114 (0.2%)
2	B	0.93	6/4280 (0.1%)	1.05	3/5786 (0.1%)
2	D	0.92	6/4279 (0.1%)	1.08	8/5785 (0.1%)
All	All	0.94	20/16158 (0.1%)	1.08	33/21812 (0.2%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	VAL	C-O	-7.49	1.14	1.24
2	D	346	LYS	C-O	-7.16	1.15	1.24
2	D	345	THR	C-O	-7.02	1.16	1.24
2	B	236	ASN	C-O	-6.99	1.16	1.24
2	B	238	ARG	C-O	-6.87	1.15	1.24
1	C	95	GLY	C-O	-6.82	1.15	1.23
2	B	239	VAL	C-O	-6.31	1.16	1.24
1	A	257	GLY	C-O	-6.27	1.16	1.23
2	B	241	LYS	C-O	-6.18	1.16	1.24
2	D	353	ASP	C-O	-6.14	1.17	1.24
1	C	97	ARG	C-O	-6.00	1.16	1.24
1	C	98	ASN	CA-CB	5.68	1.59	1.52
2	D	355	MET	C-O	-5.56	1.17	1.24
1	A	259	ILE	C-O	-5.53	1.17	1.24
2	D	352	VAL	C-O	-5.45	1.17	1.24
1	A	96	ARG	C-O	-5.37	1.17	1.23
2	B	240	ILE	C-O	-5.26	1.18	1.24
2	D	354	MET	C-O	-5.18	1.17	1.24
1	A	346	LEU	C-O	-5.14	1.17	1.24
2	B	242	ARG	C-O	-5.01	1.18	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	92	SER	N-CA-C	11.01	126.57	110.28
2	D	255	SER	N-CA-C	8.56	123.03	112.58
1	C	316	PHE	N-CA-C	7.49	122.64	112.68
1	C	259	ILE	N-CA-C	7.43	118.20	110.62
2	D	498	VAL	CB-CA-C	-6.99	102.70	112.14
1	C	60	ARG	N-CA-C	6.95	119.80	110.35
1	C	110	VAL	N-CA-C	6.79	116.94	110.42
1	A	279	MET	N-CA-C	6.68	121.38	112.30
2	D	92	SER	N-CA-CB	-6.68	100.15	109.97
1	C	76	LYS	N-CA-C	6.50	119.18	111.71
2	D	432	SER	N-CA-C	-6.29	103.72	111.40
1	A	75	ILE	CA-C-N	6.27	128.59	120.44
1	A	75	ILE	C-N-CA	6.27	128.59	120.44
1	C	442	HIS	N-CA-C	-6.25	102.02	111.34
1	C	45	CYS	N-CA-C	6.22	128.41	111.00
2	B	391	VAL	N-CA-C	6.15	116.89	110.62
1	A	215	THR	N-CA-C	5.97	119.67	112.38
2	D	104	ASN	CB-CA-C	-5.97	100.53	110.68
2	D	256	ASP	N-CA-C	5.95	121.57	109.60
1	A	341	LYS	N-CA-C	5.89	120.62	112.90
1	C	22	GLU	N-CA-C	5.86	118.14	111.11
2	B	109	GLU	N-CA-CB	-5.74	103.18	109.72
1	A	255	GLY	N-CA-C	-5.70	99.67	113.18
2	B	109	GLU	N-CA-C	5.70	117.15	110.31
1	A	60	ARG	N-CA-C	5.62	117.99	110.35
2	D	391	VAL	N-CA-C	5.58	115.78	110.42
1	C	88	CYS	N-CA-C	5.53	117.74	111.11
1	C	417	LYS	CB-CA-C	-5.39	105.64	110.71
1	A	424	GLY	N-CA-C	5.37	120.82	112.60
1	C	234	ASP	N-CA-C	5.31	118.55	111.75
1	A	341	LYS	N-CA-CB	-5.15	102.61	110.33
1	C	6	ARG	N-CA-C	5.14	116.69	111.14
1	A	350	ARG	N-CA-C	5.09	117.27	109.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3716	0	3641	100	0
1	C	3711	0	3642	116	0
2	B	4174	0	4087	88	0
2	D	4173	0	4087	84	0
3	A	14	0	6	0	0
3	C	14	0	6	1	0
4	A	18	0	0	0	0
4	C	18	0	0	3	0
5	A	15	0	0	2	0
5	C	15	0	0	6	0
6	B	2	0	0	0	0
7	A	158	0	0	21	0
7	B	215	0	0	19	0
7	C	154	0	0	23	0
7	D	214	0	0	21	0
All	All	16611	0	15469	362	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 12.

All (362) 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)
2:B:106:HIS:HB2	2:B:474:PHE:HE1	1.11	1.16
1:A:93:ARG:HD2	1:A:113:ASN:HB2	1.23	1.14
1:C:435:GLY:HA2	1:C:475:LEU:HD11	1.43	1.00
1:C:440:GLU:HB2	1:C:445:ASP:OD1	1.62	0.99
1:C:289:LYS:HA	7:C:658:HOH:O	1.60	0.99
1:C:475:LEU:HG	7:C:606:HOH:O	1.63	0.98
2:B:101:SER:HB3	2:B:105:ARG:HH12	1.24	0.98
1:C:226:ILE:HD12	7:C:740:HOH:O	1.64	0.97
1:C:239:ARG:HE	1:C:252:GLN:HE21	1.07	0.96
1:A:284:ARG:HB3	7:A:676:HOH:O	1.65	0.96
2:B:255:SER:O	2:B:257:PRO:HD3	1.65	0.95
1:A:121:LYS:HE3	7:A:688:HOH:O	1.63	0.95
5:C:503:CLF:S3A	5:C:503:CLF:S2A	2.65	0.95
1:A:475:LEU:HD22	7:A:717:HOH:O	1.67	0.94
2:B:106:HIS:HB2	2:B:474:PHE:CE1	2.01	0.94
1:C:70:VAL:HA	1:C:96:ARG:NH1	1.82	0.93
2:D:271:MET:HG2	7:D:757:HOH:O	1.67	0.93
2:B:350:ARG:HD2	2:D:262:ASP:OD1	1.70	0.92
1:A:101:ILE:HG23	7:D:707:HOH:O	1.68	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:271:MET:HB3	7:D:757:HOH:O	1.69	0.91
1:C:253:TRP:CD2	7:C:740:HOH:O	2.23	0.91
1:A:226:ILE:HD13	1:A:253:TRP:CD1	2.04	0.91
1:A:93:ARG:HD2	1:A:113:ASN:CB	1.99	0.91
7:B:882:HOH:O	2:D:491:MET:SD	2.28	0.91
2:B:9:LYS:CD	7:B:750:HOH:O	2.19	0.90
2:D:271:MET:CB	7:D:757:HOH:O	2.19	0.90
7:B:882:HOH:O	2:D:491:MET:CE	2.20	0.90
1:C:435:GLY:CA	1:C:475:LEU:HD11	2.02	0.89
2:D:272:TYR:CD2	7:D:757:HOH:O	2.25	0.89
1:C:239:ARG:HE	1:C:252:GLN:NE2	1.71	0.86
2:B:106:HIS:CB	2:B:474:PHE:HE1	1.89	0.86
1:C:440:GLU:CB	1:C:445:ASP:OD1	2.24	0.85
2:D:271:MET:CG	7:D:757:HOH:O	2.20	0.85
2:B:101:SER:HB3	2:B:105:ARG:NH1	1.91	0.85
2:D:154:MET:HA	7:D:764:HOH:O	1.77	0.84
1:C:70:VAL:HA	1:C:96:ARG:HH11	1.39	0.84
2:D:345:THR:O	2:D:348:ARG:HG2	1.78	0.84
1:C:96:ARG:HE	1:C:231:ILE:HD11	1.43	0.83
1:C:317:ASP:O	1:C:321:GLN:CD	2.20	0.83
1:A:391:MET:HB2	7:A:620:HOH:O	1.79	0.82
1:C:317:ASP:O	1:C:321:GLN:NE2	2.12	0.81
1:A:359:ARG:O	1:A:363:VAL:HG22	1.80	0.81
1:C:31:HIS:HE1	7:C:623:HOH:O	1.65	0.80
1:A:226:ILE:CD1	1:A:253:TRP:CD1	2.63	0.79
2:B:92:SER:HB3	7:B:786:HOH:O	1.83	0.78
1:C:433:LYS:NZ	2:D:263:THR:O	2.17	0.78
2:B:360:THR:HA	1:C:465:MET:CE	2.13	0.78
7:B:882:HOH:O	2:D:491:MET:HE1	1.81	0.78
1:A:96:ARG:HD3	1:A:98:ASN:HD22	1.48	0.77
1:C:387:TYR:CD2	7:C:636:HOH:O	2.36	0.77
2:B:101:SER:CB	2:B:105:ARG:HH12	1.96	0.77
1:A:239:ARG:HD2	1:A:252:GLN:NE2	2.00	0.76
1:C:440:GLU:CG	1:C:445:ASP:OD1	2.34	0.76
1:C:70:VAL:HG13	1:C:96:ARG:HH12	1.48	0.76
2:D:431:ARG:NE	2:D:454:ASP:OD2	2.18	0.75
1:C:96:ARG:NH2	4:C:502:ICS:S5A	2.60	0.75
2:D:513:GLN:CG	7:D:707:HOH:O	2.35	0.74
2:D:401:ARG:HG3	7:D:777:HOH:O	1.88	0.73
2:B:350:ARG:HD2	2:D:262:ASP:CG	2.13	0.73
1:A:57:MET:HG2	2:B:100:ARG:NH1	2.04	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:MET:HG2	2:B:100:ARG:HH12	1.54	0.72
1:C:442:HIS:ND1	4:C:502:ICS:S4B	2.63	0.72
1:A:121:LYS:HE2	7:A:749:HOH:O	1.90	0.72
1:C:74:PRO:CB	1:C:254:SER:O	2.38	0.71
5:C:503:CLF:FE3	5:C:503:CLF:S4A	1.82	0.71
1:A:363:VAL:O	1:A:367:TYR:HD2	1.72	0.71
1:C:4:MET:HE2	1:C:12:LEU:HD22	1.73	0.70
2:D:272:TYR:CG	7:D:757:HOH:O	2.43	0.70
1:C:239:ARG:NE	1:C:252:GLN:HE21	1.85	0.70
5:C:503:CLF:S3A	5:C:503:CLF:FE1	1.83	0.70
1:A:11:SER:O	1:A:14:GLN:HG2	1.92	0.70
2:B:209:THR:HG21	2:B:309:TRP:HE1	1.57	0.69
2:D:351:LEU:HG	2:D:355:MET:HE2	1.75	0.69
1:A:339:VAL:CG2	1:A:343:ARG:HB2	2.23	0.69
2:B:166:ILE:HG13	7:B:733:HOH:O	1.93	0.69
2:D:513:GLN:HG3	7:D:707:HOH:O	1.93	0.69
5:C:503:CLF:S2A	5:C:503:CLF:FE3	1.84	0.68
1:C:96:ARG:NH2	1:C:229:TYR:CB	2.57	0.68
1:C:289:LYS:CA	7:C:658:HOH:O	2.30	0.68
1:C:96:ARG:NH2	1:C:229:TYR:CG	2.62	0.68
2:D:352:VAL:HA	2:D:355:MET:HE3	1.76	0.67
1:A:361:ARG:HG3	7:A:754:HOH:O	1.93	0.67
1:A:253:TRP:HE1	1:A:265:THR:HG21	1.60	0.67
5:C:503:CLF:S3A	5:C:503:CLF:FE3	1.85	0.67
1:A:361:ARG:NH2	1:A:386:ASP:OD1	2.27	0.67
1:C:210:ARG:NH1	1:C:264:LEU:CD1	2.59	0.66
1:C:440:GLU:HG3	1:C:445:ASP:OD1	1.94	0.66
1:A:339:VAL:HG23	1:A:343:ARG:HB2	1.76	0.66
2:B:209:THR:HG21	2:B:309:TRP:NE1	2.10	0.66
1:C:349:LYS:HE3	7:C:710:HOH:O	1.96	0.66
2:D:329:LEU:HD13	2:D:344:LEU:HD13	1.78	0.66
2:B:503:GLU:OE1	2:D:476:ARG:NH1	2.29	0.65
2:D:272:TYR:CE2	7:D:757:HOH:O	2.46	0.65
1:C:95:GLY:HA2	2:D:105:ARG:HH12	1.60	0.65
1:C:74:PRO:HB2	1:C:254:SER:O	1.94	0.65
1:C:5:SER:O	1:C:9:VAL:HG23	1.97	0.65
1:C:359:ARG:NH1	1:C:442:HIS:HA	2.12	0.65
1:A:252:GLN:OE1	2:B:27:LYS:HE3	1.97	0.64
1:C:385:ASP:O	1:C:389:ARG:NH1	2.29	0.64
1:C:58:THR:HG22	1:C:60:ARG:H	1.63	0.64
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:N	1:A:344:PRO:HD2	2.14	0.63
2:B:9:LYS:HD2	7:B:750:HOH:O	1.86	0.63
2:B:166:ILE:CD1	7:B:733:HOH:O	2.45	0.63
1:A:94:ALA:HB3	2:D:521:LEU:CD2	2.29	0.63
5:A:503:CLF:FE3	5:A:503:CLF:S4A	1.90	0.62
1:C:70:VAL:CA	1:C:96:ARG:NH1	2.62	0.62
2:B:100:ARG:O	2:B:104:ASN:CG	2.43	0.62
2:B:360:THR:HA	1:C:465:MET:HE1	1.79	0.62
2:D:431:ARG:HE	2:D:454:ASP:CG	2.07	0.62
1:A:352:MET:HE1	1:A:413:VAL:HA	1.82	0.61
5:C:503:CLF:S2A	5:C:503:CLF:FE1	1.91	0.61
2:D:329:LEU:CD1	2:D:344:LEU:HD13	2.30	0.61
1:C:22:GLU:CG	1:C:26:LYS:HE2	2.30	0.61
2:B:201:PHE:HZ	2:B:254:LEU:CD1	2.14	0.61
1:C:96:ARG:HH21	1:C:229:TYR:HB2	1.66	0.61
1:C:93:ARG:HA	7:C:673:HOH:O	1.99	0.60
2:D:128:GLN:HG3	2:D:132:LYS:HE2	1.83	0.60
2:B:472:PRO:HB2	2:B:474:PHE:CZ	2.35	0.60
1:C:158:LEU:HD12	7:D:764:HOH:O	2.02	0.60
1:C:182:ARG:CZ	7:C:651:HOH:O	2.50	0.60
2:B:510:ARG:O	2:B:510:ARG:HG2	2.02	0.60
1:A:410:GLU:HG3	1:A:434:MET:HE1	1.83	0.60
1:C:253:TRP:CE3	7:C:740:HOH:O	2.51	0.60
2:D:131:MET:HE1	2:D:149:VAL:HG21	1.84	0.59
1:C:93:ARG:HD3	2:D:447:TYR:CE1	2.37	0.59
2:B:254:LEU:O	2:B:255:SER:HB3	2.01	0.59
1:C:210:ARG:HH11	1:C:264:LEU:CD1	2.15	0.59
1:A:339:VAL:CG2	1:A:343:ARG:HD2	2.34	0.58
2:B:472:PRO:HB2	2:B:474:PHE:CE1	2.39	0.58
1:C:239:ARG:NE	1:C:252:GLN:NE2	2.47	0.58
2:D:513:GLN:C	7:D:706:HOH:O	2.46	0.58
1:A:226:ILE:CD1	1:A:253:TRP:NE1	2.67	0.57
1:C:96:ARG:HH21	1:C:229:TYR:CB	2.17	0.57
1:C:435:GLY:CA	1:C:475:LEU:CD1	2.81	0.57
1:C:96:ARG:HD3	1:C:98:ASN:HD22	1.69	0.57
2:D:82:PHE:CZ	2:D:255:SER:HB2	2.40	0.57
1:C:58:THR:HG23	1:C:403:ASP:OD1	2.05	0.57
2:D:255:SER:N	2:D:276:THR:OG1	2.38	0.57
1:A:93:ARG:NH1	7:A:602:HOH:O	2.35	0.57
2:B:263:THR:HG21	7:B:703:HOH:O	2.04	0.57
1:C:316:PHE:O	1:C:317:ASP:HB3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.87	0.57
2:D:431:ARG:NH2	7:D:703:HOH:O	2.37	0.56
2:B:255:SER:O	2:B:257:PRO:CD	2.46	0.56
2:B:100:ARG:O	2:B:104:ASN:ND2	2.39	0.56
1:A:429:PHE:CD1	2:B:108:ARG:O	2.59	0.56
2:B:441:PHE:HD2	7:B:796:HOH:O	1.88	0.56
2:D:390:PRO:HB2	2:D:393:ILE:HD11	1.88	0.56
2:B:510:ARG:HG2	2:D:456:LEU:HD23	1.86	0.56
1:C:200:ASP:HB2	7:C:638:HOH:O	2.04	0.56
1:A:93:ARG:O	1:A:94:ALA:HB3	2.06	0.55
1:A:339:VAL:HG13	1:A:340:ALA:N	2.21	0.55
1:A:277:ARG:HG2	7:A:608:HOH:O	2.07	0.55
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.42	0.55
2:B:360:THR:HA	1:C:465:MET:HE2	1.87	0.55
2:B:238:ARG:HE	2:B:258:GLU:HG3	1.71	0.55
1:C:226:ILE:HG22	1:C:279:MET:HB3	1.89	0.55
2:D:253:LEU:CD2	2:D:256:ASP:HB2	2.36	0.54
2:B:326:ASP:OD1	2:B:348:ARG:NE	2.39	0.54
1:C:54:PRO:HB3	2:D:116:ASP:O	2.06	0.54
1:A:361:ARG:HB3	1:A:379:TYR:OH	2.08	0.54
2:B:201:PHE:HZ	2:B:254:LEU:HD12	1.72	0.54
1:A:96:ARG:HD3	1:A:98:ASN:ND2	2.21	0.54
1:A:96:ARG:NH2	1:A:229:TYR:CG	2.76	0.54
1:A:346:LEU:HD21	1:A:464:ASP:HA	1.89	0.54
1:A:346:LEU:HD22	1:A:467:LEU:HD23	1.90	0.54
2:B:205:ALA:O	2:B:209:THR:HB	2.08	0.54
1:C:96:ARG:HD3	1:C:98:ASN:ND2	2.23	0.54
2:D:494:LEU:O	2:D:498:VAL:HG23	2.07	0.54
1:A:304:LYS:HE2	7:A:727:HOH:O	2.07	0.54
1:A:361:ARG:O	1:A:364:ILE:HG12	2.07	0.53
1:C:311:ALA:O	1:C:315:LYS:HG2	2.08	0.53
2:D:194:VAL:HB	2:D:297:HIS:CG	2.44	0.53
1:A:277:ARG:HB2	7:A:608:HOH:O	2.08	0.53
1:A:277:ARG:O	1:A:277:ARG:HD3	2.08	0.53
2:B:270:ARG:NH2	7:B:701:HOH:O	2.41	0.53
1:A:277:ARG:NH2	1:A:385:ASP:OD1	2.42	0.52
1:A:94:ALA:HB3	2:D:521:LEU:HD23	1.90	0.52
2:B:453:ARG:NH1	2:B:454:ASP:OD1	2.42	0.52
1:A:94:ALA:HB3	2:D:521:LEU:HD22	1.90	0.52
2:B:131:MET:HE3	7:B:733:HOH:O	2.10	0.52
2:B:434:VAL:HG11	2:B:442:MET:HE3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:TYR:HA	2:D:517:TYR:OH	2.10	0.51
2:B:369:LEU:C	2:B:369:LEU:HD12	2.35	0.51
2:D:116:ASP:OD1	2:D:116:ASP:C	2.53	0.51
1:A:146:LYS:NZ	7:A:605:HOH:O	2.43	0.51
7:A:665:HOH:O	2:B:120:GLU:HG3	2.11	0.51
2:B:518:ASN:O	2:B:523:ARG:NH2	2.40	0.51
1:C:346:LEU:HD22	1:C:467:LEU:HD23	1.93	0.51
1:A:363:VAL:O	1:A:367:TYR:CD2	2.60	0.50
1:A:475:LEU:O	7:A:601:HOH:O	2.19	0.50
1:A:475:LEU:CD2	7:A:717:HOH:O	2.43	0.50
2:D:82:PHE:CE1	2:D:255:SER:HB2	2.46	0.50
1:A:352:MET:HE3	1:A:418:PRO:HG3	1.92	0.50
1:A:444:TRP:HA	1:A:444:TRP:CE3	2.46	0.50
1:A:234:ASP:HB3	1:A:451:HIS:ND1	2.27	0.49
2:B:326:ASP:CG	2:B:348:ARG:HE	2.20	0.49
1:A:23:LYS:HB3	7:A:747:HOH:O	2.12	0.49
2:B:92:SER:CB	7:B:786:HOH:O	2.51	0.49
1:C:387:TYR:CG	7:C:636:HOH:O	2.62	0.49
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.95	0.49
1:C:53:GLN:HB2	1:C:56:LEU:HD12	1.94	0.49
1:C:355:ILE:HG22	1:C:442:HIS:CE1	2.47	0.49
1:A:144:LEU:CD1	2:B:43:VAL:HG21	2.41	0.49
1:A:97:ARG:O	1:A:231:ILE:HA	2.12	0.49
1:A:123:ILE:HG13	2:B:189:PHE:CG	2.47	0.49
1:A:156:ILE:O	1:A:159:ILE:HG22	2.13	0.49
1:C:435:GLY:HA3	1:C:475:LEU:CD1	2.43	0.49
2:B:106:HIS:CA	2:B:474:PHE:HE1	2.25	0.49
1:A:428:LYS:NZ	7:A:607:HOH:O	2.45	0.49
2:B:162:LEU:HB3	7:B:733:HOH:O	2.13	0.49
1:C:277:ARG:HD3	7:C:612:HOH:O	2.12	0.48
1:C:440:GLU:H	1:C:445:ASP:CG	2.20	0.48
1:C:104:THR:HA	1:C:108:ALA:O	2.13	0.48
7:C:611:HOH:O	2:D:66:PRO:HD2	2.13	0.48
1:A:223:VAL:HG11	1:A:247:LEU:HD13	1.95	0.48
1:A:339:VAL:HG13	1:A:340:ALA:H	1.77	0.48
1:C:234:ASP:HB3	1:C:451:HIS:ND1	2.28	0.48
1:A:444:TRP:HA	1:A:444:TRP:HE3	1.77	0.48
1:A:123:ILE:HA	1:A:159:ILE:HD11	1.96	0.48
1:C:258:SER:OG	1:C:261:GLU:HG3	2.13	0.48
1:C:116:SER:HB3	1:C:134:LEU:HD21	1.96	0.48
1:C:359:ARG:N	1:C:360:PRO:CD	2.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLY:HA2	1:A:439:ARG:O	2.13	0.48
1:C:360:PRO:HG2	1:C:379:TYR:CD2	2.49	0.48
2:D:2:SER:N	7:D:709:HOH:O	2.46	0.48
2:D:255:SER:O	2:D:257:PRO:HD3	2.13	0.48
2:B:9:LYS:HD3	7:B:750:HOH:O	2.03	0.48
2:B:56:ASN:OD1	2:B:59:ARG:NH1	2.46	0.48
1:C:210:ARG:NH1	1:C:264:LEU:HD13	2.29	0.48
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.49	0.47
2:B:166:ILE:HD11	7:B:733:HOH:O	2.13	0.47
1:C:442:HIS:HB3	3:C:501:HCA:O5	2.14	0.47
2:B:106:HIS:CA	2:B:474:PHE:CE1	2.97	0.47
1:C:263:GLU:O	1:C:266:PRO:HD2	2.14	0.47
1:A:226:ILE:HD12	1:A:253:TRP:NE1	2.29	0.47
1:C:70:VAL:CG1	1:C:96:ARG:HH12	2.22	0.47
1:C:253:TRP:CZ2	1:C:262:ILE:HG23	2.49	0.47
1:A:352:MET:HE2	1:A:416:ILE:HB	1.96	0.47
2:B:255:SER:N	2:B:276:THR:OG1	2.42	0.47
2:D:168:ASN:O	2:D:172:GLU:HG2	2.15	0.47
2:B:151:THR:CG2	2:B:162:LEU:HD11	2.44	0.47
1:A:339:VAL:HG22	1:A:343:ARG:HB2	1.94	0.47
1:C:462:ASP:HA	1:C:465:MET:HG2	1.97	0.47
1:A:343:ARG:N	1:A:344:PRO:CD	2.78	0.47
1:C:4:MET:SD	1:C:416:ILE:HD13	2.55	0.47
2:B:238:ARG:HE	2:B:258:GLU:CG	2.28	0.46
1:A:362:HIS:HD2	7:A:754:HOH:O	1.98	0.46
2:D:116:ASP:OD1	2:D:117:SER:N	2.48	0.46
2:D:348:ARG:HG3	2:D:349:GLY:N	2.29	0.46
2:B:472:PRO:CB	2:B:474:PHE:CZ	2.99	0.46
1:C:5:SER:O	1:C:8:GLU:HB2	2.14	0.46
1:C:107:ASN:HD22	2:D:40:ILE:HG12	1.79	0.46
1:C:346:LEU:CD2	1:C:467:LEU:HD23	2.46	0.46
1:A:239:ARG:NH1	1:A:249:CYS:HB2	2.30	0.46
2:B:9:LYS:CE	7:B:750:HOH:O	2.54	0.46
1:C:465:MET:HG3	1:C:466:THR:N	2.30	0.46
2:D:351:LEU:HG	2:D:355:MET:CE	2.45	0.46
2:D:513:GLN:HG2	7:D:707:HOH:O	2.07	0.46
1:A:94:ALA:CB	2:D:521:LEU:HD22	2.46	0.46
1:C:359:ARG:NH1	1:C:442:HIS:CA	2.78	0.46
1:C:266:PRO:CB	7:C:602:HOH:O	2.64	0.46
1:A:478:PRO:HB2	2:D:330:MET:SD	2.56	0.46
1:C:58:THR:HG22	1:C:60:ARG:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ASN:ND2	2:D:40:ILE:HD13	2.32	0.46
1:A:144:LEU:HD13	2:B:43:VAL:HG21	1.96	0.45
1:A:391:MET:CB	7:A:620:HOH:O	2.49	0.45
1:C:207:LEU:HD22	1:C:282:ILE:HD11	1.98	0.45
2:D:239:VAL:HG23	2:D:242:ARG:HH21	1.81	0.45
2:D:253:LEU:HD23	2:D:256:ASP:HB2	1.97	0.45
1:C:131:LEU:HA	1:C:134:LEU:HG	1.98	0.45
2:B:34:LYS:NZ	7:B:706:HOH:O	2.50	0.45
1:C:265:THR:N	1:C:266:PRO:CD	2.79	0.45
2:D:91:GLY:O	2:D:116:ASP:OD1	2.33	0.45
1:A:82:SER:N	7:A:611:HOH:O	2.49	0.45
2:B:9:LYS:HE2	7:B:750:HOH:O	2.14	0.45
1:A:277:ARG:HD3	1:A:277:ARG:C	2.42	0.45
2:D:514:ALA:N	7:D:706:HOH:O	2.50	0.45
1:C:345:ARG:HD3	7:C:738:HOH:O	2.16	0.45
2:D:351:LEU:CG	2:D:355:MET:HE2	2.45	0.45
1:A:31:HIS:HD2	1:A:402:ASP:OD2	2.01	0.44
2:B:396:HIS:CE1	2:B:426:ASP:HB3	2.53	0.44
1:C:318:GLU:HG3	1:C:322:LYS:HE3	2.00	0.44
1:A:475:LEU:HD13	7:A:717:HOH:O	2.17	0.44
7:C:611:HOH:O	2:D:66:PRO:CD	2.66	0.44
2:B:510:ARG:O	2:B:510:ARG:CG	2.65	0.44
2:D:84:LYS:HE2	2:D:145:ASP:OD2	2.18	0.44
2:D:86:MET:HG2	2:D:138:CYS:SG	2.57	0.44
2:B:121:ASP:OD1	2:B:122:ALA:N	2.51	0.44
2:B:346:LYS:O	2:B:350:ARG:HG3	2.18	0.44
2:B:369:LEU:HD11	2:B:393:ILE:HG23	1.98	0.44
1:A:433:LYS:NZ	2:B:263:THR:O	2.50	0.44
1:A:74:PRO:CB	1:A:254:SER:O	2.66	0.43
1:A:53:GLN:HB2	1:A:56:LEU:HD12	2.00	0.43
2:B:213:MET:HE2	2:B:308:THR:O	2.18	0.43
2:B:241:LYS:HD2	2:B:253:LEU:HD22	2.00	0.43
2:B:361:TRP:O	2:B:365:LYS:HE3	2.18	0.43
1:A:342:TYR:C	1:A:344:PRO:HD2	2.43	0.43
2:B:142:TYR:O	2:B:272:TYR:OH	2.33	0.43
2:B:369:LEU:CD1	2:B:376:VAL:HG13	2.48	0.43
1:C:12:LEU:HD13	1:C:415:ARG:HG2	2.01	0.43
2:D:516:ASP:O	2:D:517:TYR:C	2.61	0.43
1:A:226:ILE:HD12	1:A:253:TRP:CD1	2.50	0.43
1:C:158:LEU:CD1	7:D:764:HOH:O	2.63	0.43
1:A:85:PRO:HB2	5:A:503:CLF:S2B	2.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:LEU:CG	7:C:606:HOH:O	2.42	0.43
1:A:4:MET:HE1	1:A:12:LEU:HD22	2.01	0.42
2:D:394:LEU:HD13	2:D:430:LEU:HB2	2.01	0.42
1:C:475:LEU:CD2	7:C:606:HOH:O	2.64	0.42
1:A:70:VAL:HG13	1:A:96:ARG:NH2	2.33	0.42
1:A:19:VAL:HG11	1:A:407:TYR:CE2	2.55	0.42
2:B:47:THR:HA	2:B:52:TYR:CG	2.54	0.42
1:C:442:HIS:CE1	4:C:502:ICS:S1B	3.13	0.42
2:B:12:TYR:HA	2:B:13:PRO:HA	1.76	0.42
1:C:341:LYS:NZ	7:C:603:HOH:O	2.52	0.42
2:D:95:CYS:HB3	2:D:99:PHE:CZ	2.54	0.42
1:A:359:ARG:CZ	1:A:444:TRP:CZ2	3.03	0.42
1:C:163:ILE:HD11	1:C:182:ARG:HD2	2.02	0.42
2:D:221:ASN:OD1	2:D:287:ALA:HA	2.19	0.42
2:D:515:THR:HA	2:D:517:TYR:CE2	2.54	0.42
1:A:410:GLU:CG	1:A:434:MET:HE1	2.49	0.42
1:C:31:HIS:CE1	7:C:623:HOH:O	2.53	0.42
1:C:361:ARG:O	1:C:364:ILE:HG12	2.19	0.42
1:C:336:GLU:HA	1:C:339:VAL:HG22	2.01	0.42
1:C:349:LYS:HA	1:C:349:LYS:HD3	1.93	0.42
1:C:22:GLU:HG2	1:C:26:LYS:HE2	2.02	0.42
2:B:521:LEU:O	2:D:475:ASP:HB3	2.20	0.41
2:B:256:ASP:O	2:B:275:GLY:HA2	2.20	0.41
1:C:355:ILE:CG2	1:C:442:HIS:CE1	3.03	0.41
1:A:474:LYS:HB3	2:D:322:LEU:HD21	2.02	0.41
1:C:346:LEU:HD13	1:C:372:MET:HE2	2.02	0.41
1:C:359:ARG:HH12	1:C:442:HIS:C	2.27	0.41
2:B:101:SER:CB	2:B:105:ARG:NH1	2.68	0.41
2:D:12:TYR:HA	2:D:13:PRO:HA	1.80	0.41
1:A:429:PHE:CG	2:B:108:ARG:O	2.74	0.41
2:B:221:ASN:OD1	2:B:287:ALA:HA	2.21	0.41
2:D:71:GLN:O	2:D:196:GLY:HA3	2.21	0.41
2:D:201:PHE:HZ	2:D:254:LEU:HD12	1.86	0.41
1:A:62:CYS:HB3	2:B:94:GLY:HA3	2.03	0.41
1:A:277:ARG:HD3	7:A:619:HOH:O	2.21	0.41
1:C:74:PRO:HB3	1:C:254:SER:O	2.16	0.41
1:C:210:ARG:HH11	1:C:264:LEU:HD12	1.85	0.41
2:D:391:VAL:HG12	2:D:392:HIS:CE1	2.56	0.41
2:D:481:ARG:NH2	7:D:714:HOH:O	2.51	0.41
2:D:509:THR:O	2:D:516:ASP:HA	2.20	0.41
1:A:477:ALA:HB2	2:D:348:ARG:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:HIS:HD2	1:C:402:ASP:OD2	2.04	0.41
2:D:201:PHE:HZ	2:D:254:LEU:CD1	2.33	0.41
1:A:104:THR:HA	1:A:108:ALA:O	2.19	0.40
2:B:228:PRO:HA	2:B:293:LEU:HD12	2.03	0.40
1:C:48:SER:OG	1:C:384:ASN:ND2	2.52	0.40
2:B:305:VAL:O	2:B:309:TRP:HB2	2.22	0.40
1:C:96:ARG:CD	1:C:98:ASN:HD22	2.33	0.40
1:C:442:HIS:HB2	7:C:678:HOH:O	2.21	0.40
1:A:74:PRO:HB2	1:A:254:SER:O	2.21	0.40
1:A:132:ALA:HB1	1:A:170:LYS:HE3	2.03	0.40
2:D:262:ASP:OD1	7:D:701:HOH:O	2.22	0.40
2:B:156:GLU:HG3	2:B:187:PRO:HB3	2.03	0.40
2:D:414:PRO:HA	2:D:417:LYS:HD3	2.04	0.40
1:A:94:ALA:CB	2:D:521:LEU:CD2	2.99	0.40
2:D:132:LYS:HD3	2:D:174:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/492 (94%)	438 (95%)	24 (5%)	1 (0%)	43	44
1	C	461/492 (94%)	434 (94%)	26 (6%)	1 (0%)	43	44
2	B	520/523 (99%)	494 (95%)	24 (5%)	2 (0%)	30	28
2	D	520/523 (99%)	505 (97%)	15 (3%)	0	100	100
All	All	1964/2030 (97%)	1871 (95%)	89 (4%)	4 (0%)	43	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	317	ASP
1	A	318	GLU
2	B	255	SER
2	B	257	PRO

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	398/415 (96%)	393 (99%)	5 (1%)	61	69
1	C	398/415 (96%)	394 (99%)	4 (1%)	68	76
2	B	454/455 (100%)	448 (99%)	6 (1%)	61	69
2	D	454/455 (100%)	450 (99%)	4 (1%)	70	78
All	All	1704/1740 (98%)	1685 (99%)	19 (1%)	65	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	133	LYS
1	A	209	LYS
1	A	355	ILE
1	A	362	HIS
2	B	26	LYS
2	B	50	LYS
2	B	178	GLU
2	B	195	THR
2	B	209	THR
2	B	453	ARG
1	C	98	ASN
1	C	168	LYS
1	C	355	ILE
1	C	362	HIS
2	D	175	ILE
2	D	238	ARG
2	D	350	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	498	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	98	ASN
1	A	285	HIS
1	A	362	HIS
2	B	286	ASN
2	B	457	HIS
1	C	14	GLN
1	C	31	HIS
1	C	98	ASN
1	C	252	GLN
1	C	321	GLN
1	C	362	HIS
1	C	384	ASN
2	D	163	ASN
2	D	338	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	A	502	1,3	6,30,30	1.37	1 (16%)	-		
3	HCA	A	501	4	13,13,13	1.52	2 (15%)	15,18,18	2.47	5 (33%)
5	CLF	A	503	1,2	0,24,24	-	-	-		
5	CLF	C	503	1,2	0,24,24	-	-	-		
4	ICS	C	502	1,3	6,30,30	1.45	1 (16%)	-		
3	HCA	C	501	4	13,13,13	1.46	3 (23%)	15,18,18	1.70	4 (26%)

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	-	7/17/17/17	-
5	CLF	A	503	1,2	-	-	0/12/10/10
5	CLF	C	503	1,2	-	-	0/12/10/10
3	HCA	C	501	4	-	2/17/17/17	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	HCA	O5-C7	3.57	1.33	1.22
3	C	501	HCA	O4-C6	-2.55	1.22	1.30
3	C	501	HCA	O5-C7	2.46	1.29	1.22
4	C	502	ICS	S3A-FE4	-2.43	2.19	2.24
3	A	501	HCA	O4-C6	-2.38	1.22	1.30
4	A	502	ICS	S3A-FE5	2.29	2.30	2.24
3	C	501	HCA	O1-C1	2.17	1.29	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HCA	O7-C3-C7	-6.40	99.88	108.96
3	A	501	HCA	O5-C7-C3	-3.41	115.48	122.09
3	C	501	HCA	O7-C3-C4	3.30	114.16	108.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HCA	O7-C3-C4	3.03	113.72	108.88
3	C	501	HCA	O4-C6-C5	3.02	123.53	114.00
3	A	501	HCA	O4-C6-C5	2.92	123.22	114.00
3	C	501	HCA	C4-C5-C6	2.77	119.19	112.77
3	C	501	HCA	O4-C6-O3	-2.35	117.28	123.33
3	A	501	HCA	O3-C6-C5	-2.18	116.18	123.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

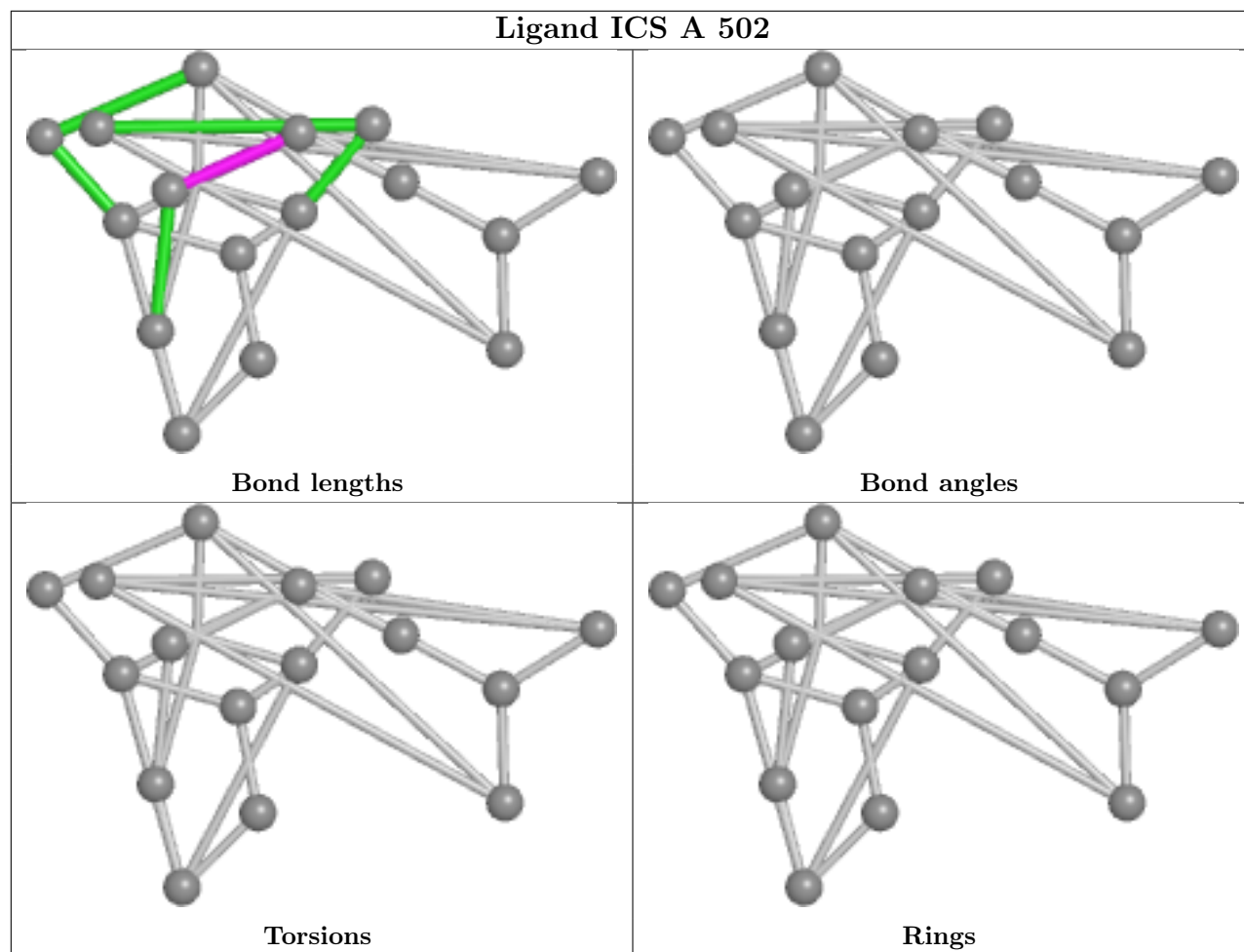
Mol	Chain	Res	Type	Atoms
3	A	501	HCA	C2-C3-C4-C5
3	A	501	HCA	C7-C3-C4-C5
3	A	501	HCA	O7-C3-C4-C5
3	A	501	HCA	C3-C4-C5-C6
3	C	501	HCA	C2-C3-C4-C5
3	A	501	HCA	O2-C1-C2-C3
3	A	501	HCA	O1-C1-C2-C3
3	A	501	HCA	C4-C5-C6-O4
3	C	501	HCA	C4-C5-C6-O3

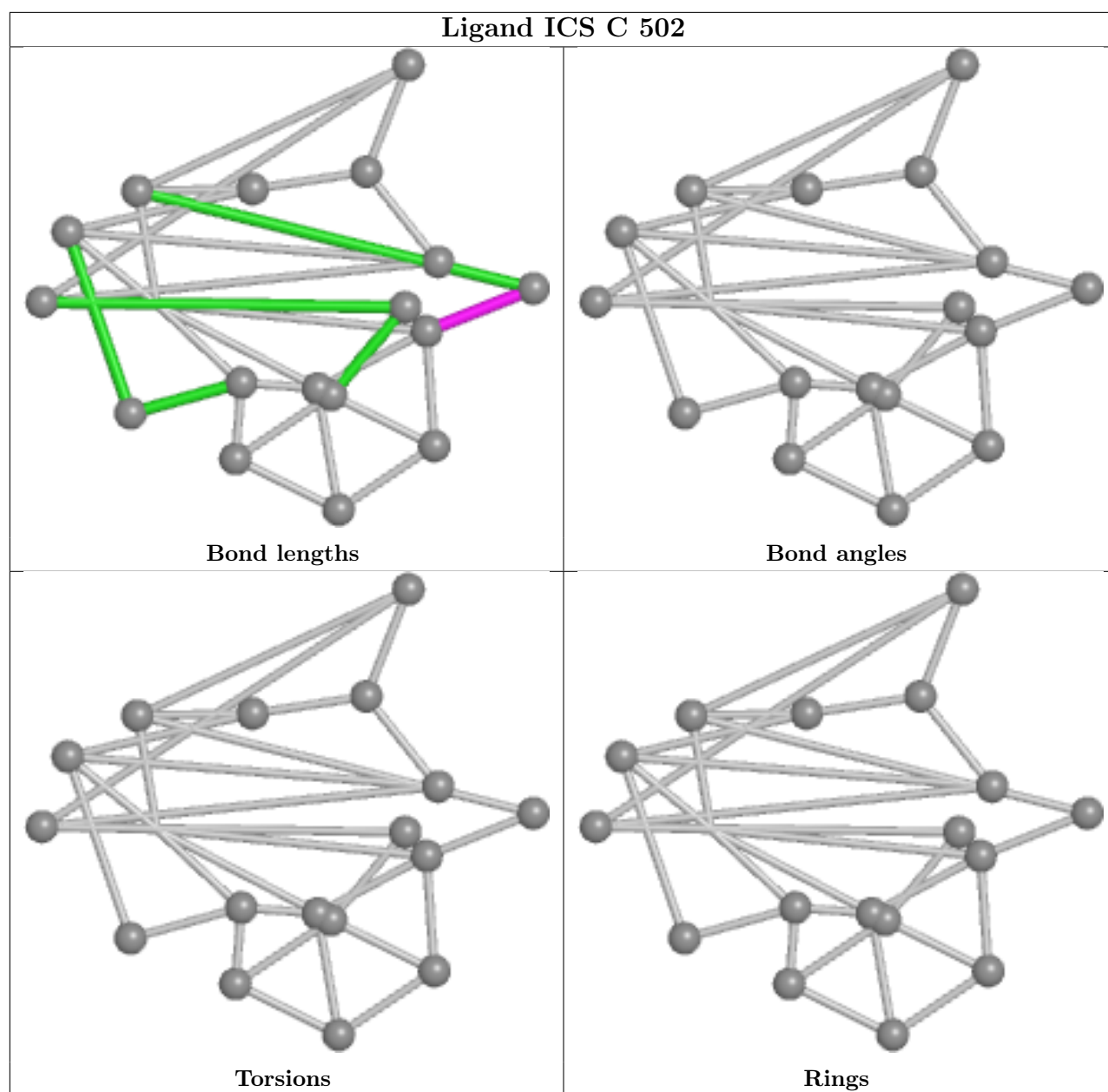
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	CLF	2	0
5	C	503	CLF	6	0
4	C	502	ICS	3	0
3	C	501	HCA	1	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 than 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.





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

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	467/492 (94%)	0.77	32 (6%)	23	24	25, 40, 61, 84	0
1	C	466/492 (94%)	0.84	41 (8%)	15	16	27, 44, 63, 81	0
2	B	522/523 (99%)	0.55	20 (3%)	44	46	25, 39, 58, 88	0
2	D	522/523 (99%)	0.50	20 (3%)	44	46	25, 37, 57, 74	0
All	All	1977/2030 (97%)	0.66	113 (5%)	29	31	25, 40, 61, 88	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	GLY	6.7
2	D	516	ASP	5.3
2	D	116	ASP	5.2
2	B	256	ASP	5.2
1	C	329	ALA	5.0
2	D	255	SER	4.8
2	D	517	TYR	4.6
2	D	263	THR	4.2
1	A	363	VAL	4.1
2	D	431	ARG	4.0
1	C	376	GLY	3.9
1	A	253	TRP	3.7
2	B	474	PHE	3.7
1	A	254	SER	3.4
1	C	254	SER	3.4
1	C	17	LEU	3.3
1	C	249	CYS	3.3
1	A	94	ALA	3.2
1	C	45	CYS	3.2
1	C	400	LEU	3.1
1	A	93	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	140	THR	3.0
2	B	123	ALA	3.0
1	A	5	SER	3.0
1	C	316	PHE	3.0
1	C	69	GLY	3.0
1	C	255	GLY	2.9
1	C	390	THR	2.9
1	C	300	PHE	2.9
1	C	259	ILE	2.9
1	C	189	VAL	2.8
2	B	35	TYR	2.8
1	A	343	ARG	2.8
1	A	33	ALA	2.8
1	A	125	PHE	2.8
1	C	332	LYS	2.8
1	A	48	SER	2.7
2	D	30	GLY	2.7
2	B	254	LEU	2.7
1	A	9	VAL	2.7
2	B	352	VAL	2.7
1	C	268	VAL	2.7
2	D	262	ASP	2.7
2	D	450	PHE	2.7
1	C	387	TYR	2.7
1	C	363	VAL	2.7
1	C	140	THR	2.6
1	A	29	ASN	2.6
1	C	247	LEU	2.6
1	C	312	ILE	2.6
2	B	511	GLY	2.6
2	D	164	ALA	2.6
2	D	256	ASP	2.6
1	A	378	GLY	2.5
1	C	216	PHE	2.5
1	C	46	ILE	2.5
1	A	340	ALA	2.5
1	C	5	SER	2.5
1	C	217	ALA	2.5
1	C	263	GLU	2.5
1	A	70	VAL	2.5
2	B	510	ARG	2.5
2	D	31	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	215	THR	2.4
1	A	19	VAL	2.4
1	C	320	ILE	2.4
2	B	97	ALA	2.4
1	A	36	ASP	2.4
1	A	159	ILE	2.4
2	B	255	SER	2.4
1	C	221	TYR	2.3
1	A	376	GLY	2.3
2	D	285	PRO	2.3
1	C	61	GLY	2.3
2	B	257	PRO	2.3
2	D	348	ARG	2.3
2	B	99	PHE	2.3
1	C	134	LEU	2.3
2	D	309	TRP	2.3
1	A	89	GLY	2.2
2	B	131	MET	2.2
2	B	369	LEU	2.2
2	B	31	PHE	2.2
2	B	104	ASN	2.2
2	B	473	ILE	2.2
2	D	218	VAL	2.2
2	D	123	ALA	2.2
1	C	12	LEU	2.2
1	C	93	ARG	2.2
2	B	285	PRO	2.2
1	C	19	VAL	2.2
1	C	375	VAL	2.2
1	C	272	LEU	2.2
1	A	351	VAL	2.1
2	D	242	ARG	2.1
1	C	318	GLU	2.1
1	C	16	VAL	2.1
1	C	95	GLY	2.1
1	A	379	TYR	2.1
1	A	101	ILE	2.1
2	B	100	ARG	2.1
1	C	264	LEU	2.1
1	A	402	ASP	2.1
1	A	37	PRO	2.1
1	C	155	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	61	GLY	2.1
1	A	189	VAL	2.1
1	A	391	MET	2.0
1	C	141	LEU	2.0
2	B	93	GLN	2.0
2	D	35	TYR	2.0
1	A	16	VAL	2.0
2	D	428	TRP	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](#)

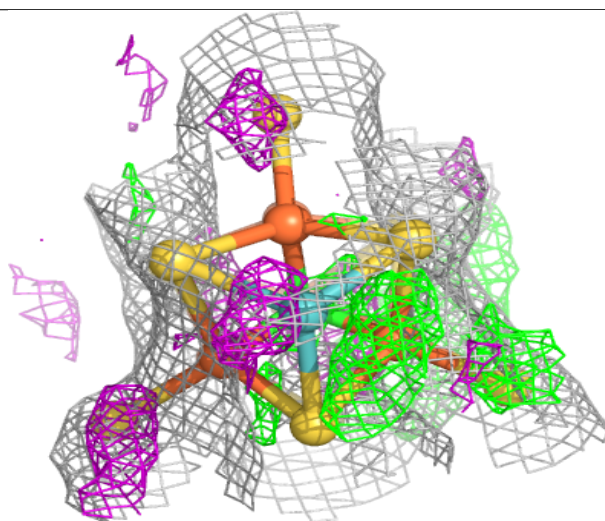
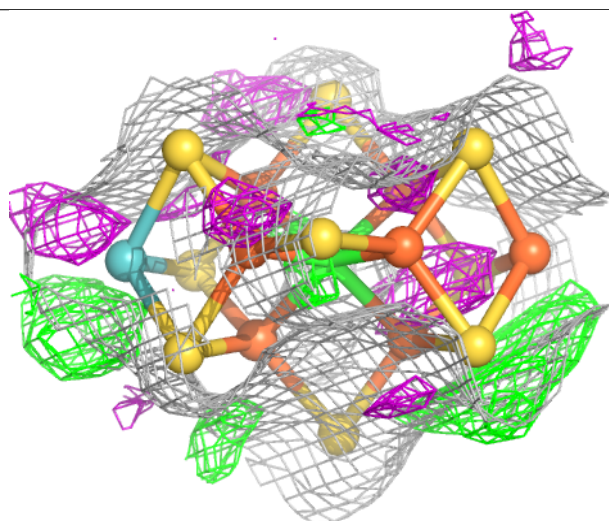
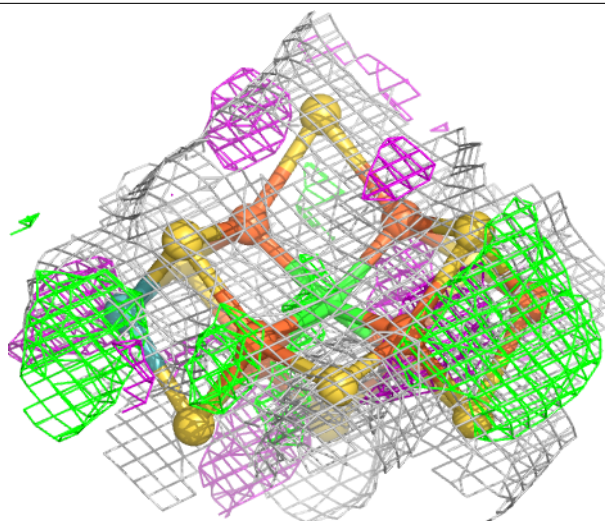
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HCA	C	501	14/14	0.92	0.14	26,30,35,35	0
5	CLF	C	503	15/15	0.92	0.09	28,30,36,40	0
5	CLF	A	503	15/15	0.94	0.08	23,25,27,29	0
3	HCA	A	501	14/14	0.94	0.10	28,32,36,40	0
4	ICS	C	502	18/18	0.96	0.07	27,31,34,34	0
6	FE	B	602	1/1	0.97	0.04	40,40,40,40	0
4	ICS	A	502	18/18	0.98	0.05	28,30,32,33	0
6	FE	B	601	1/1	0.99	0.03	40,40,40,40	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.

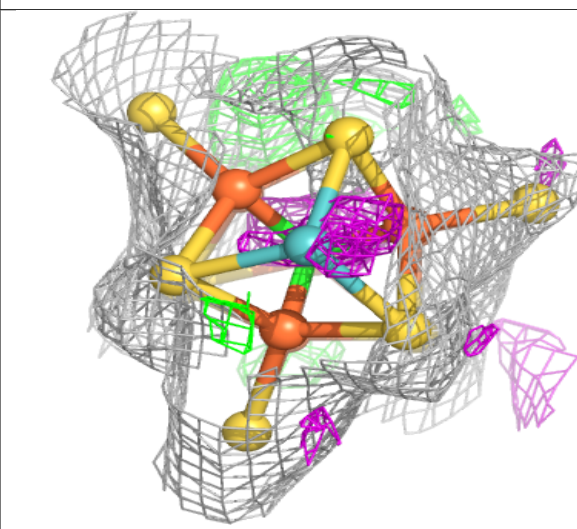
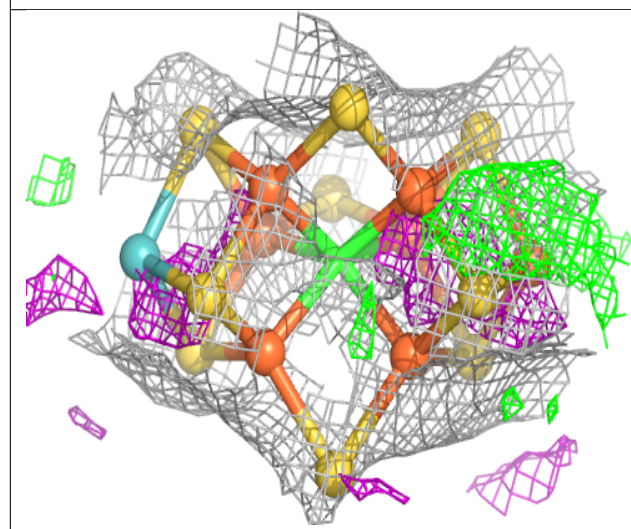
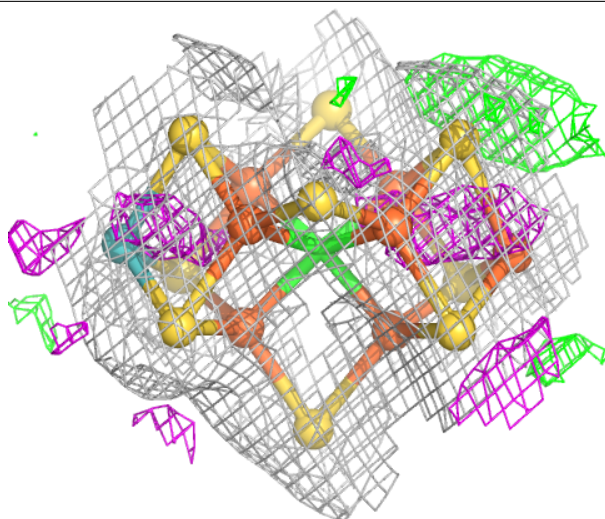
Electron density around ICS C 502:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.