Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2026 – 05:19 pm BST

PDB ID	:	4C1N / pdb_00004c1n
Title	:	Corrinoid protein reactivation complex with activator
Authors	:	Hennig, S.E.; Goetzl, S.; Jeoung, J.H.; Bommer, M.; Lendzian, F.; Hildebrandt, P.; Dobbek, H.
Deposited on	:	2013-08-13
Resolution	:	2.53 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:

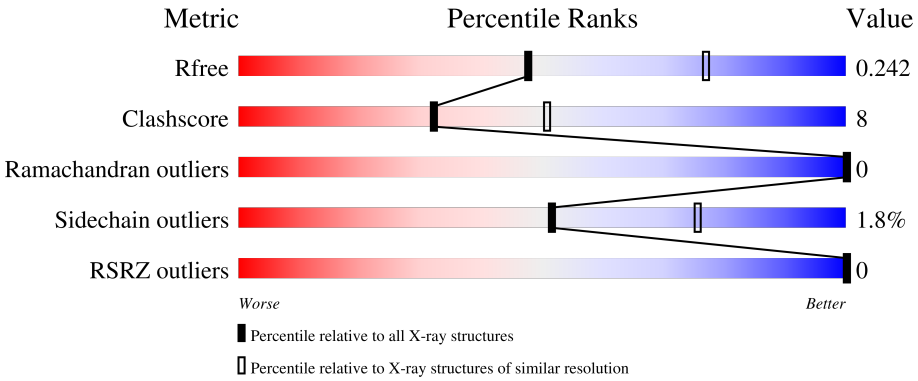
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.53 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	442	81% 19%
1	C	442	81% 17% •
1	E	442	82% 17% •
1	G	442	76% 23% •
2	B	309	79% 21%

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Mol	Chain	Length	Quality of chain
2	D	309	82% 17%
2	F	309	78% 20%
2	H	309	78% 21%
3	I	509	83% 17%
3	J	509	81% 18%
3	X	509	84% 15%
4	K	510	84% 16%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 40155 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 CARBON MONOXIDE DEHYDROGENASE CORRINOID/ IRON-SULFUR PROTEIN, GAMMA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3389	2186	559	634	10			
1	C	442	Total	C	N	O	S	0	0	0
			3389	2186	559	634	10			
1	E	442	Total	C	N	O	S	0	0	0
			3389	2186	559	634	10			
1	G	441	Total	C	N	O	S	0	0	0
			3385	2184	558	633	10			

- Molecule 2 is a protein called CO DEHYDROGENASE/ACETYL-COA SYNTHASE, IRON-SULFUR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	309	Total	C	N	O	S	0	0	0
			2368	1518	393	441	16			
2	D	309	Total	C	N	O	S	0	0	0
			2368	1518	393	441	16			
2	F	309	Total	C	N	O	S	0	0	0
			2368	1518	393	441	16			
2	H	309	Total	C	N	O	S	0	0	0
			2368	1518	393	441	16			

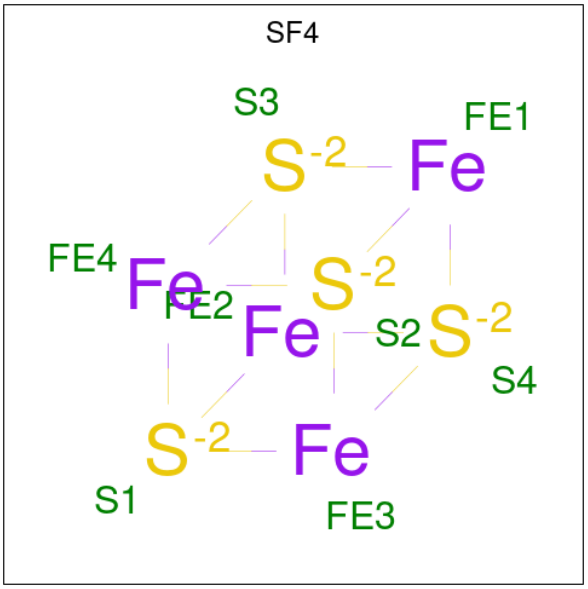
- Molecule 3 is a protein called IRON-SULFUR CLUSTER BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	509	Total	C	N	O	S	1	0	0
			3882	2474	652	740	16			
3	J	509	Total	C	N	O	S	1	0	0
			3882	2474	652	740	16			
3	X	509	Total	C	N	O	S	0	0	0
			3882	2474	652	740	16			

- Molecule 4 is a protein called IRON-SULFUR CLUSTER BINDING PROTEIN.

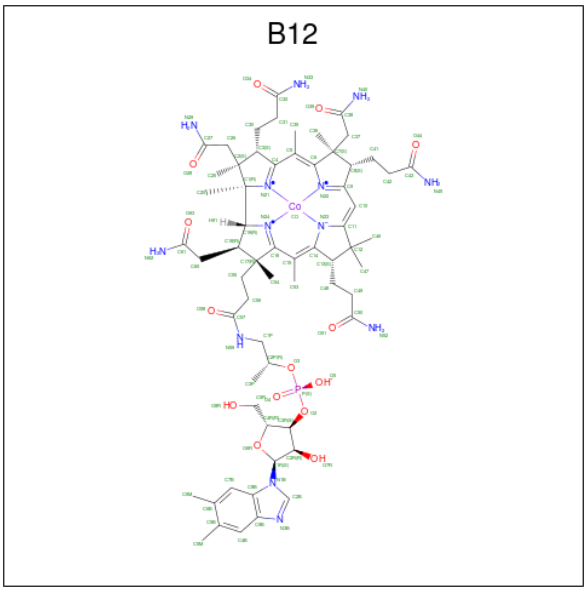
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	K	510	3891	2479	653	743	16	0	0	0

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	S			
5	A	1	8	4	4		0	0
5	C	1	Total	Fe	S		0	0
			8	4	4			
5	E	1	Total	Fe	S		0	0
			8	4	4			
5	G	1	Total	Fe	S		0	0
			8	4	4			

- Molecule 6 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
6	I	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
6	K	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
6	X	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	119	Total	O	0	0
			119	119		
7	B	51	Total	O	0	0
			51	51		
7	C	116	Total	O	0	0
			116	116		
7	D	49	Total	O	0	0
			49	49		
7	E	120	Total	O	0	0
			120	120		
7	F	69	Total	O	0	0
			69	69		
7	G	80	Total	O	0	0
			80	80		
7	H	43	Total	O	0	0
			43	43		

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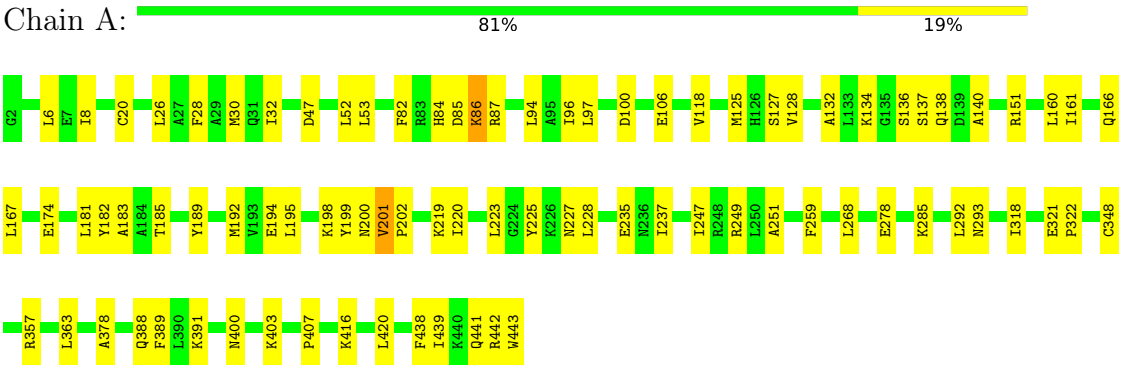
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	157	Total O 157 157	0	0
7	J	130	Total O 130 130	0	0
7	K	121	Total O 121 121	0	0
7	X	143	Total O 143 143	0	0

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.

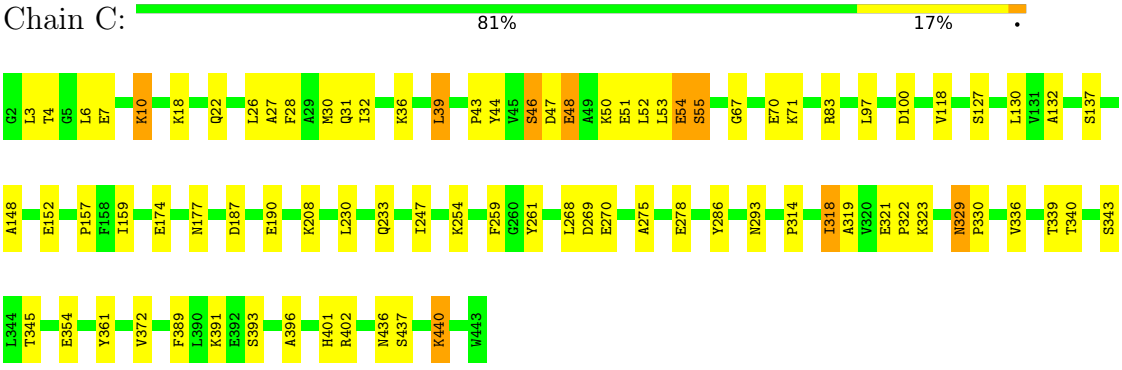
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE CORRINOID/IRON-SULFUR PROTEIN, GAMMA SUBUNIT

Chain A:



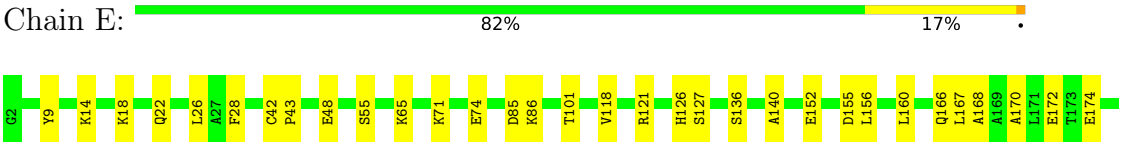
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE CORRINOID/IRON-SULFUR PROTEIN, GAMMA SUBUNIT

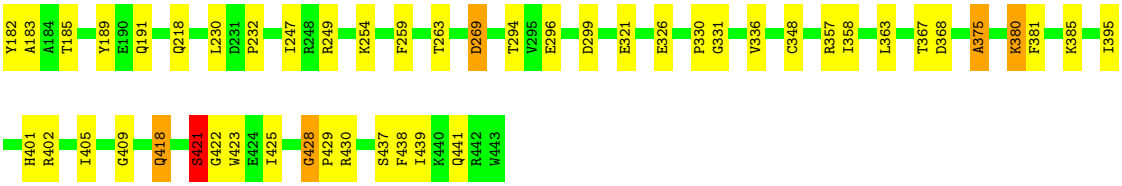
Chain C:



• Molecule 1: CARBON MONOXIDE DEHYDROGENASE CORRINOID/IRON-SULFUR PROTEIN, GAMMA SUBUNIT

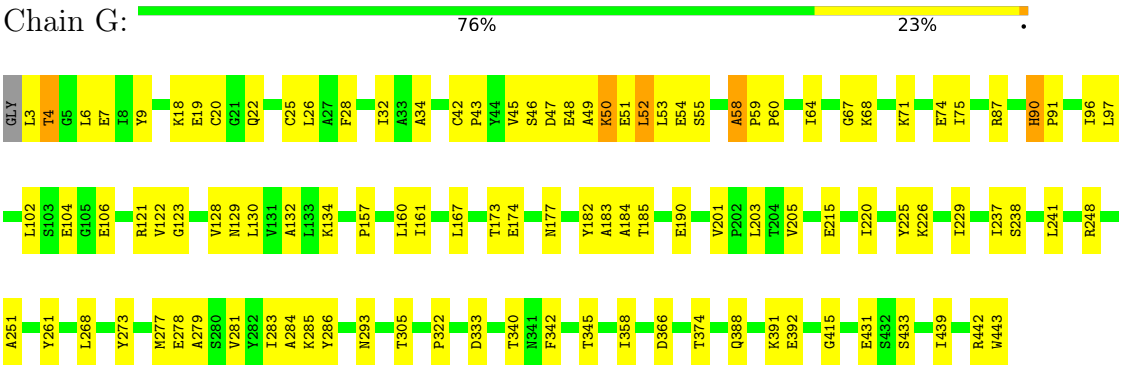
Chain E:





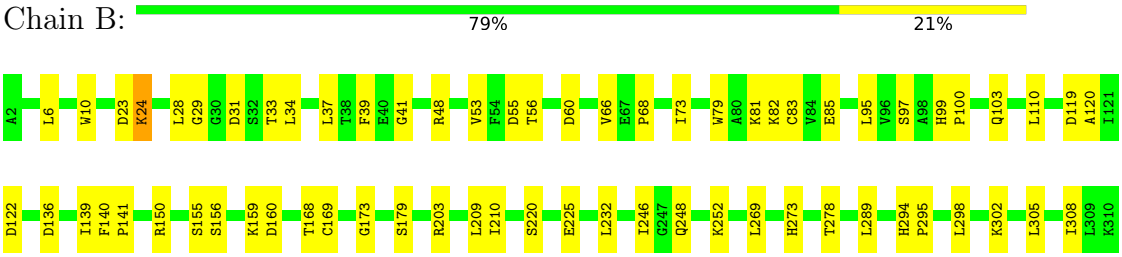
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE CORRINOID/IRON-SULFUR PROTEIN, GAMMA SUBUNIT

Chain G:



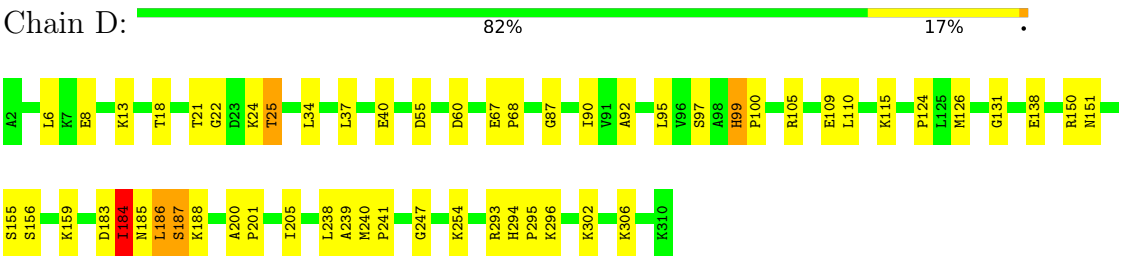
• Molecule 2: CO DEHYDROGENASE/ACETYL-COA SYNTHASE, IRON-SULFUR PROTEIN

Chain B:



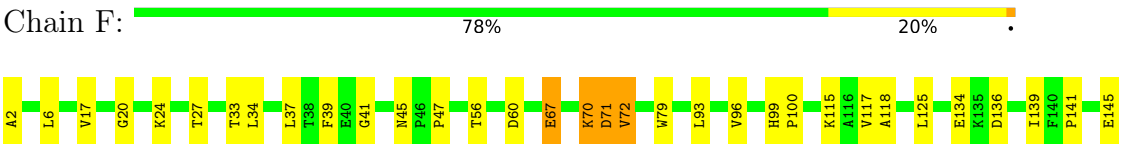
• Molecule 2: CO DEHYDROGENASE/ACETYL-COA SYNTHASE, IRON-SULFUR PROTEIN

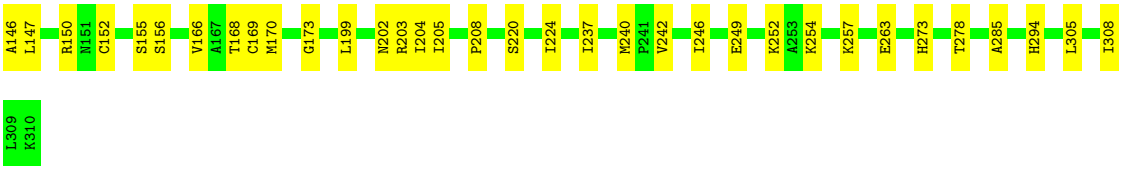
Chain D:



• Molecule 2: CO DEHYDROGENASE/ACETYL-COA SYNTHASE, IRON-SULFUR PROTEIN

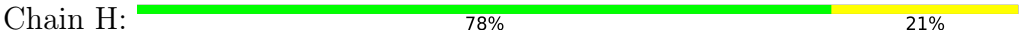
Chain F:

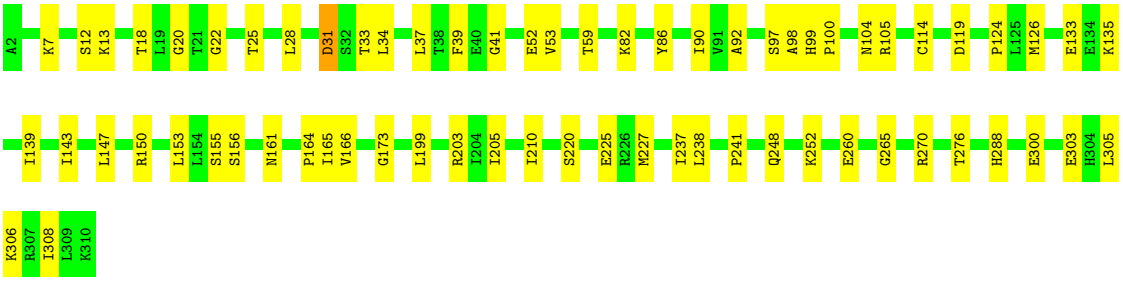




• Molecule 2: CO DEHYDROGENASE/ACETYL-COA SYNTHASE, IRON-SULFUR PROTEIN

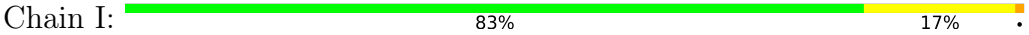
Chain H:

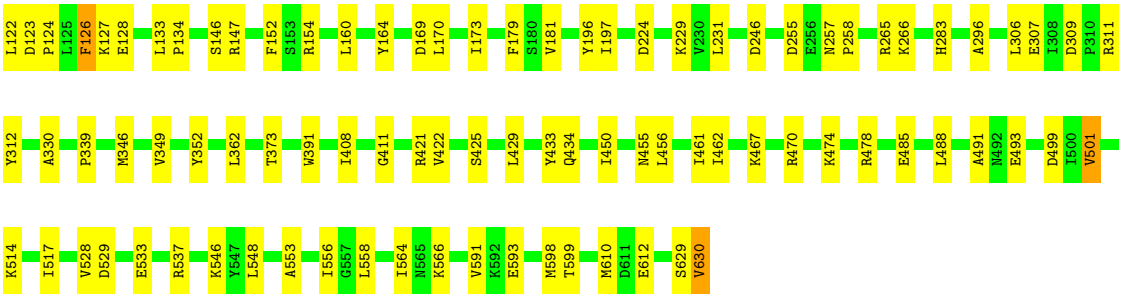




• Molecule 3: IRON-SULFUR CLUSTER BINDING PROTEIN

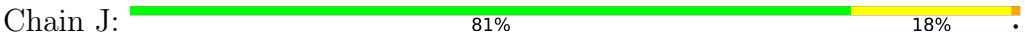
Chain I:

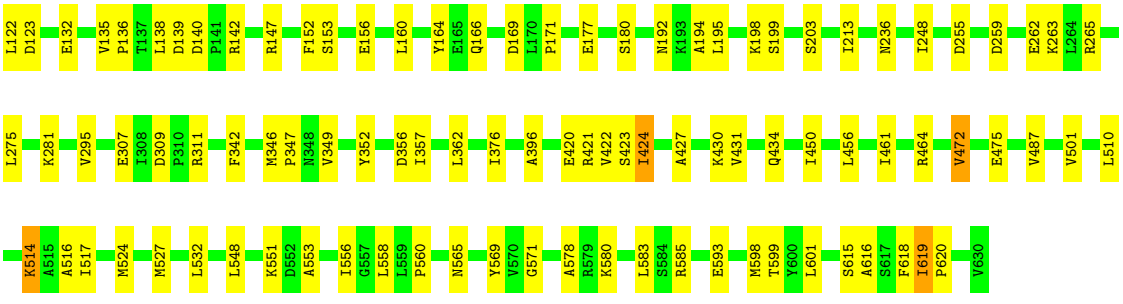




• Molecule 3: IRON-SULFUR CLUSTER BINDING PROTEIN

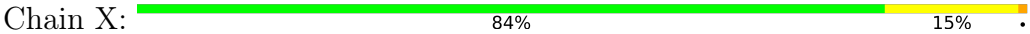
Chain J:

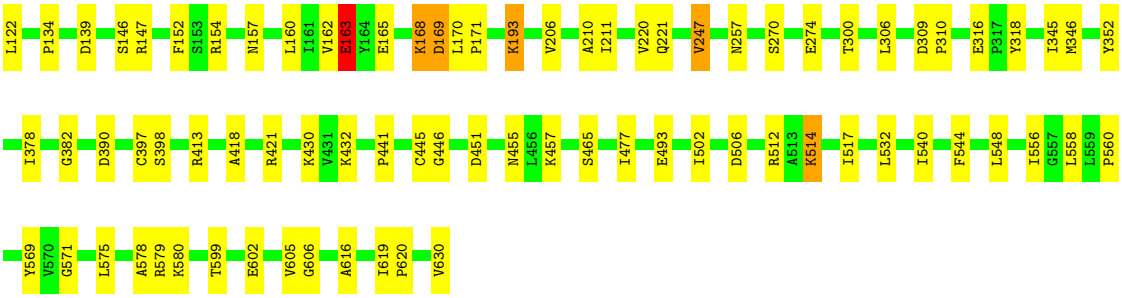




• Molecule 3: IRON-SULFUR CLUSTER BINDING PROTEIN

Chain X:





• Molecule 4: IRON-SULFUR CLUSTER BINDING PROTEIN

Chain K:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.13Å 128.18Å 163.37Å 77.61° 82.25° 88.76°	Depositor
Resolution (Å)	30.63 – 2.53 30.63 – 2.53	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.63-2.53) 96.0 (30.63-2.53)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.191 , 0.243 0.193 , 0.242	Depositor DCC
R_{free} test set	8449 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 23.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	40155	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.29% 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: SF4, B12

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	0.52	2/3459 (0.1%)	0.76	3/4703 (0.1%)
1	C	0.47	0/3459	0.77	4/4703 (0.1%)
1	E	0.68	5/3459 (0.1%)	0.81	4/4703 (0.1%)
1	G	0.40	1/3455 (0.0%)	0.77	5/4698 (0.1%)
2	B	0.53	2/2419 (0.1%)	0.78	5/3289 (0.2%)
2	D	0.56	5/2419 (0.2%)	0.77	3/3289 (0.1%)
2	F	0.39	0/2419	0.78	5/3289 (0.2%)
2	H	0.31	0/2419	0.76	0/3289
3	I	0.37	2/3944 (0.1%)	0.74	3/5342 (0.1%)
3	J	0.60	8/3944 (0.2%)	0.79	4/5342 (0.1%)
3	X	0.54	2/3944 (0.1%)	0.76	2/5342 (0.0%)
4	K	0.55	4/3953 (0.1%)	0.77	4/5354 (0.1%)
All	All	0.51	31/39293 (0.1%)	0.77	42/53343 (0.1%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	309	ASP	C-N	9.19	1.41	1.33
3	J	424	ILE	C-O	-7.47	1.15	1.24
3	J	156	GLU	CA-C	-6.09	1.45	1.52
3	J	423	SER	C-O	-5.83	1.17	1.24
2	D	185	ASN	C-O	-5.83	1.17	1.24
4	K	308	ILE	C-O	-5.81	1.17	1.24
3	J	618	PHE	C-O	-5.58	1.17	1.23
3	J	619	ILE	C-O	-5.52	1.18	1.24
1	A	201	VAL	C-N	5.41	1.40	1.33
3	X	162	VAL	C-O	-5.39	1.18	1.24
3	X	512	ARG	C-O	-5.37	1.17	1.24
3	I	123	ASP	C-N	5.36	1.40	1.33
4	K	310	PRO	N-CD	5.32	1.55	1.47
3	J	516	ALA	C-O	-5.32	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	PRO	N-CD	5.30	1.55	1.47
2	D	188	LYS	C-O	-5.29	1.18	1.24
2	D	186	LEU	C-O	-5.25	1.18	1.24
1	E	429	PRO	N-CD	5.23	1.55	1.47
3	J	615	SER	C-O	-5.23	1.17	1.24
1	E	375	ALA	C-O	-5.20	1.18	1.24
1	G	52	LEU	CA-C	-5.17	1.45	1.52
1	E	428	GLY	C-N	5.16	1.39	1.33
2	D	184	ILE	C-O	-5.15	1.18	1.24
2	B	82	LYS	C-O	-5.14	1.18	1.24
1	E	170	ALA	C-O	-5.12	1.18	1.24
3	J	510	LEU	C-O	-5.10	1.18	1.24
4	K	628	PRO	N-CD	5.08	1.54	1.47
2	B	83	CYS	C-O	-5.07	1.18	1.24
3	I	126	PHE	C-O	-5.07	1.17	1.24
1	E	430	ARG	C-O	-5.03	1.18	1.24
2	D	187	SER	C-O	-5.01	1.18	1.24

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	156	GLU	N-CA-C	-14.10	87.57	109.85
1	G	48	GLU	N-CA-C	8.04	119.82	111.14
3	J	357	ILE	N-CA-C	7.67	117.74	110.53
3	X	168	LYS	N-CA-C	7.14	119.06	111.28
2	F	72	VAL	N-CA-C	7.07	118.89	112.17
1	C	329	ASN	CA-C-N	7.01	127.46	120.52
1	C	329	ASN	C-N-CA	7.01	127.46	120.52
1	C	46	SER	N-CA-C	6.38	118.95	110.53
3	I	123	ASP	CA-C-N	-6.20	113.90	120.03
3	I	123	ASP	C-N-CA	-6.20	113.90	120.03
1	E	428	GLY	CA-C-N	-6.18	113.91	120.03
1	E	428	GLY	C-N-CA	-6.18	113.91	120.03
1	E	421	SER	N-CA-C	6.15	117.79	111.14
1	E	423	TRP	N-CA-C	-6.11	100.20	109.85
1	A	201	VAL	CA-C-N	-5.90	113.89	120.14
1	A	201	VAL	C-N-CA	-5.90	113.89	120.14
3	X	163	GLU	N-CA-C	5.77	118.95	110.59
4	K	309	ASP	CA-C-N	-5.71	114.43	120.94
4	K	309	ASP	C-N-CA	-5.71	114.43	120.94
3	J	615	SER	N-CA-C	5.71	118.44	111.82
1	A	285	LYS	N-CA-C	5.62	117.73	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	90	HIS	CA-C-N	5.55	125.56	119.90
1	G	90	HIS	C-N-CA	5.55	125.56	119.90
2	B	99	HIS	CA-C-N	5.50	125.32	119.28
2	B	99	HIS	C-N-CA	5.50	125.32	119.28
1	C	48	GLU	N-CA-C	-5.49	105.30	111.28
1	G	58	ALA	CA-C-N	5.43	125.97	120.38
1	G	58	ALA	C-N-CA	5.43	125.97	120.38
2	B	24	LYS	N-CA-C	-5.37	106.50	112.57
2	D	25	THR	N-CA-C	5.25	118.37	109.76
4	K	627	PHE	CA-C-N	-5.24	113.23	119.05
4	K	627	PHE	C-N-CA	-5.24	113.23	119.05
3	J	376	ILE	N-CA-C	5.23	115.65	108.12
2	D	99	HIS	CA-C-N	5.16	124.82	119.56
2	D	99	HIS	C-N-CA	5.16	124.82	119.56
2	F	294	HIS	CA-C-N	5.08	124.87	119.28
2	F	294	HIS	C-N-CA	5.08	124.87	119.28
2	B	294	HIS	CA-C-N	5.08	124.68	119.05
2	B	294	HIS	C-N-CA	5.08	124.68	119.05
2	F	67	GLU	CA-C-N	-5.07	114.60	119.87
2	F	67	GLU	C-N-CA	-5.07	114.60	119.87
3	I	124	PRO	N-CA-C	5.01	118.93	111.41

There are no chirality outliers.

There are no planarity outliers.

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	3389	0	3467	60	0
1	C	3389	0	3467	60	0
1	E	3389	0	3467	55	0
1	G	3385	0	3464	83	0
2	B	2368	0	2402	40	0
2	D	2368	0	2402	34	0
2	F	2368	0	2402	44	0
2	H	2368	0	2402	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	3882	0	3973	59	0
3	J	3882	0	3973	61	0
3	X	3882	0	3973	60	0
4	K	3891	0	3979	52	0
5	A	8	0	0	1	0
5	C	8	0	0	0	0
5	E	8	0	0	0	0
5	G	8	0	0	1	0
6	C	91	0	88	9	0
6	I	91	0	88	10	0
6	K	91	0	88	5	0
6	X	91	0	88	5	0
7	A	119	0	0	11	0
7	B	51	0	0	6	0
7	C	116	0	0	11	0
7	D	49	0	0	5	0
7	E	120	0	0	17	0
7	F	69	0	0	5	0
7	G	80	0	0	18	1
7	H	43	0	0	4	0
7	I	157	0	0	13	0
7	J	130	0	0	20	0
7	K	121	0	0	14	0
7	X	143	0	0	15	1
All	All	40155	0	39723	629	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 8.

All (629) 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:G:46:SER:O	7:G:2006:HOH:O	1.59	1.17
1:G:284:ALA:O	7:G:2051:HOH:O	1.70	1.06
1:E:367:THR:O	1:E:380:LYS:NZ	1.90	1.04
1:A:86:LYS:HD2	1:A:87:ARG:HG2	1.42	1.01
7:J:2066:HOH:O	3:X:169:ASP:HB3	1.60	0.99
7:J:2066:HOH:O	3:X:169:ASP:CB	2.11	0.98
1:E:428:GLY:O	7:E:2109:HOH:O	1.89	0.89
1:E:269:ASP:O	7:E:2077:HOH:O	1.88	0.89
3:X:122:LEU:O	7:X:2006:HOH:O	1.92	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:457:LYS:NZ	7:K:2080:HOH:O	2.05	0.86
3:X:163:GLU:HG3	7:X:2027:HOH:O	1.76	0.85
3:X:580:LYS:O	7:X:2126:HOH:O	1.94	0.85
1:C:319:ALA:O	7:C:2087:HOH:O	1.92	0.84
3:J:514:LYS:NZ	3:J:616:ALA:O	2.11	0.83
1:G:9:TYR:OH	7:G:2002:HOH:O	1.93	0.81
1:C:46:SER:O	1:C:50:LYS:HG3	1.81	0.80
6:C:1444:B12:O5	7:C:2098:HOH:O	1.98	0.80
3:X:257:ASN:OD1	7:X:2055:HOH:O	1.99	0.80
1:G:366:ASP:OD1	7:G:2058:HOH:O	2.00	0.79
1:G:129:ASN:ND2	7:G:2025:HOH:O	2.15	0.78
2:H:90:ILE:HG22	2:H:124:PRO:HG2	1.66	0.78
2:D:159:LYS:NZ	7:D:2025:HOH:O	2.16	0.77
1:G:174:GLU:OE2	1:G:177:ASN:ND2	2.17	0.77
3:J:475:GLU:O	7:J:2104:HOH:O	2.01	0.77
7:E:2067:HOH:O	2:F:308:ILE:O	2.04	0.76
1:C:43:PRO:HG3	3:X:154:ARG:HH21	1.49	0.76
1:C:286:TYR:O	7:C:2070:HOH:O	2.04	0.75
4:K:529:ASP:OD1	7:K:2098:HOH:O	2.05	0.75
3:X:390:ASP:OD1	7:X:2079:HOH:O	2.02	0.75
2:B:203:ARG:NH2	7:B:2032:HOH:O	2.17	0.75
1:E:152:GLU:OE2	7:E:2051:HOH:O	2.05	0.75
1:A:194:GLU:OE1	7:A:2058:HOH:O	2.04	0.74
1:G:46:SER:O	1:G:50:LYS:HD3	1.86	0.74
3:J:356:ASP:OD2	7:J:2077:HOH:O	2.05	0.73
2:B:29:GLY:O	7:B:2009:HOH:O	2.06	0.73
1:G:74:GLU:O	7:G:2009:HOH:O	2.05	0.73
3:X:477:ILE:O	7:X:2103:HOH:O	2.06	0.73
2:B:141:PRO:HA	2:B:168:THR:HG21	1.71	0.72
1:A:251:ALA:O	7:A:2020:HOH:O	2.06	0.72
1:G:51:GLU:CD	1:G:51:GLU:H	1.98	0.72
1:G:392:GLU:O	7:G:2067:HOH:O	2.08	0.71
7:J:2032:HOH:O	3:X:163:GLU:OE2	2.07	0.71
1:A:357:ARG:HH12	2:B:100:PRO:HB3	1.53	0.71
1:A:388:GLN:HA	1:A:391:LYS:HE2	1.71	0.71
2:H:22:GLY:N	7:H:2008:HOH:O	2.22	0.71
3:J:138:LEU:O	7:J:2013:HOH:O	2.09	0.71
1:A:348:CYS:O	7:A:2095:HOH:O	2.08	0.71
1:G:431:GLU:OE2	7:G:2075:HOH:O	2.08	0.71
1:G:433:SER:OG	7:G:2073:HOH:O	2.08	0.71
3:I:546:LYS:NZ	7:I:2137:HOH:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LYS:NZ	7:A:2106:HOH:O	2.09	0.70
3:I:629:SER:O	7:I:2154:HOH:O	2.10	0.70
2:H:205:ILE:HG12	2:H:241:PRO:HG2	1.72	0.70
3:J:420:GLU:OE2	7:J:2088:HOH:O	2.08	0.70
1:A:195:LEU:HA	1:A:198:LYS:HE3	1.74	0.69
7:A:2001:HOH:O	3:I:529:ASP:OD2	2.10	0.69
3:J:262:GLU:OE1	7:J:2051:HOH:O	2.10	0.69
3:X:606:GLY:O	7:X:2131:HOH:O	2.10	0.69
4:K:140:ASP:OD2	7:K:2015:HOH:O	2.11	0.68
4:K:291:MET:O	7:K:2050:HOH:O	2.10	0.68
1:A:220:ILE:HA	1:A:223:LEU:HD12	1.75	0.68
3:I:422:VAL:HG21	3:I:488:LEU:HD11	1.75	0.68
1:A:268:LEU:HD22	1:A:293:ASN:HB2	1.76	0.68
3:J:180:SER:O	7:J:2027:HOH:O	2.12	0.67
1:C:7:GLU:HA	1:C:10:LYS:HE3	1.77	0.67
3:I:612:GLU:OE1	7:I:2153:HOH:O	2.12	0.67
2:D:187:SER:OG	7:D:2028:HOH:O	2.12	0.67
1:A:160:LEU:HB3	1:A:167:LEU:HD22	1.77	0.67
1:E:218:GLN:OE1	7:E:2062:HOH:O	2.12	0.66
1:E:172:GLU:OE2	7:E:2053:HOH:O	2.13	0.66
2:F:141:PRO:HA	2:F:168:THR:HG21	1.75	0.66
1:A:201:VAL:O	1:A:225:TYR:OH	2.08	0.66
1:A:441:GLN:NE2	7:A:2116:HOH:O	2.28	0.66
1:C:318:ILE:HD13	1:C:318:ILE:N	2.11	0.66
1:E:294:THR:HG22	1:E:296:GLU:H	1.59	0.66
3:I:311:ARG:NH2	7:I:2074:HOH:O	2.27	0.66
3:J:265:ARG:HD2	3:J:307:GLU:HB2	1.77	0.66
3:X:514:LYS:NZ	3:X:616:ALA:O	2.29	0.66
1:A:47:ASP:OD1	7:A:2015:HOH:O	2.14	0.65
6:C:1444:B12:O28	7:C:2111:HOH:O	2.13	0.65
6:I:1631:B12:O44	7:I:2075:HOH:O	2.13	0.65
1:E:168:ALA:O	7:E:2053:HOH:O	2.14	0.65
3:X:579:ARG:NH2	7:X:2124:HOH:O	2.27	0.65
2:B:85:GLU:OE2	7:B:2022:HOH:O	2.15	0.65
1:E:86:LYS:NZ	7:E:2031:HOH:O	2.29	0.65
4:K:630:VAL:HG22	7:K:2080:HOH:O	1.96	0.65
2:F:71:ASP:HB2	2:F:72:VAL:HG13	1.78	0.64
3:I:265:ARG:HD2	3:I:307:GLU:HB2	1.80	0.64
1:E:326:GLU:OE1	7:E:2086:HOH:O	2.15	0.64
3:J:349:VAL:HG21	3:J:598:MET:HE2	1.79	0.64
2:F:252:LYS:NZ	7:F:2061:HOH:O	2.21	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:GLY:O	2:D:302:LYS:NZ	2.31	0.64
2:D:138:GLU:OE1	7:D:2022:HOH:O	2.15	0.63
3:I:537:ARG:HA	3:I:566:LYS:HB3	1.81	0.63
2:H:119:ASP:OD1	2:H:150:ARG:NH2	2.31	0.63
1:C:174:GLU:OE2	1:C:177:ASN:ND2	2.31	0.62
1:E:172:GLU:HA	1:E:172:GLU:OE1	1.98	0.62
3:J:424:ILE:HG23	3:J:431:VAL:HG22	1.82	0.62
1:A:20:CYS:HB3	5:A:1444:SF4:S1	2.40	0.62
1:A:86:LYS:CD	1:A:87:ARG:HG2	2.26	0.61
4:K:362:LEU:HG	4:K:580:LYS:HD3	1.82	0.61
3:X:134:PRO:O	3:X:147:ARG:NH1	2.33	0.61
3:I:470:ARG:HH12	3:I:474:LYS:HA	1.64	0.61
1:G:388:GLN:HA	1:G:391:LYS:HE2	1.83	0.61
6:C:1444:B12:H362	6:C:1444:B12:H351	1.83	0.61
2:F:224:ILE:HD12	2:F:242:VAL:HG11	1.83	0.60
1:G:190:GLU:OE2	7:G:2036:HOH:O	2.16	0.60
1:G:102:LEU:HB3	1:G:106:GLU:HB2	1.83	0.60
1:G:50:LYS:O	1:G:50:LYS:HG2	2.01	0.60
2:B:31:ASP:OD1	7:B:2009:HOH:O	2.17	0.60
1:E:85:ASP:OD2	7:E:2027:HOH:O	2.17	0.60
1:C:336:VAL:HG12	1:C:361:TYR:HB2	1.84	0.59
6:I:1631:B12:H362	6:I:1631:B12:H351	1.84	0.59
6:K:1631:B12:H362	6:K:1631:B12:H351	1.84	0.59
2:B:33:THR:HB	2:B:41:GLY:HA3	1.85	0.59
6:K:1631:B12:O28	7:K:2121:HOH:O	2.17	0.59
1:G:226:LYS:HG2	1:G:261:TYR:HE1	1.67	0.58
1:C:54:GLU:HG3	1:C:55:SER:N	2.18	0.58
6:X:1631:B12:H362	6:X:1631:B12:H351	1.85	0.58
2:H:13:LYS:NZ	7:H:2006:HOH:O	2.36	0.58
4:K:265:ARG:HD2	4:K:307:GLU:HB2	1.84	0.58
2:B:159:LYS:O	7:B:2030:HOH:O	2.17	0.58
1:G:34:ALA:O	1:G:87:ARG:NH2	2.36	0.58
1:C:354:GLU:OE2	7:C:2095:HOH:O	2.17	0.58
2:F:33:THR:HB	2:F:41:GLY:HA3	1.85	0.58
3:I:373:THR:OG1	7:I:2087:HOH:O	2.13	0.58
3:I:362:LEU:HD22	3:I:591:VAL:HB	1.86	0.57
2:B:269:LEU:O	2:B:273:HIS:ND1	2.38	0.57
1:C:36:LYS:NZ	7:C:2004:HOH:O	2.37	0.57
1:G:279:ALA:O	1:G:283:ILE:HG13	2.04	0.57
4:K:206:VAL:HG12	4:K:225:LEU:HD12	1.86	0.57
1:E:160:LEU:HB3	1:E:167:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:266:LYS:NZ	7:I:2064:HOH:O	2.19	0.57
3:J:192:ASN:ND2	7:J:2019:HOH:O	2.32	0.57
3:X:221:GLN:HG3	3:X:575:LEU:HD21	1.87	0.57
2:D:239:ALA:O	7:D:2042:HOH:O	2.17	0.56
4:K:381:ASN:OD1	6:K:1631:B12:N40	2.37	0.56
1:A:400:ASN:OD1	7:A:2105:HOH:O	2.17	0.56
6:C:1444:B12:H491	6:C:1444:B12:H533	1.86	0.56
3:I:169:ASP:OD1	3:I:169:ASP:N	2.38	0.56
3:J:132:GLU:O	7:J:2009:HOH:O	2.18	0.56
1:E:348:CYS:SG	6:X:1631:B12:O8R	2.60	0.56
3:X:163:GLU:OE1	3:X:193:LYS:NZ	2.32	0.56
2:D:34:LEU:HB2	2:D:37:LEU:HD12	1.88	0.56
1:G:45:VAL:CG1	1:G:46:SER:HA	2.35	0.56
1:G:19:GLU:O	3:I:154:ARG:NH2	2.39	0.56
3:I:312:TYR:CZ	4:K:175:ARG:HD3	2.40	0.56
4:K:362:LEU:HD22	4:K:591:VAL:HB	1.89	0.55
2:B:136:ASP:HA	2:B:139:ILE:HG12	1.89	0.55
1:G:49:ALA:HA	1:G:51:GLU:OE1	2.06	0.55
1:G:342:PHE:HB3	1:G:345:THR:HG22	1.86	0.55
3:X:540:ILE:HD13	3:X:548:LEU:HD23	1.87	0.55
1:A:237:ILE:HD13	1:A:278:GLU:HG3	1.86	0.55
2:B:95:LEU:HD23	2:B:110:LEU:HD13	1.87	0.55
2:D:92:ALA:HB2	2:D:126:MET:HE3	1.88	0.55
2:D:21:THR:O	2:D:24:LYS:HB2	2.06	0.55
1:G:45:VAL:N	1:G:46:SER:HA	2.21	0.55
3:J:580:LYS:O	7:J:2125:HOH:O	2.18	0.55
3:X:514:LYS:HE3	3:X:556:ILE:O	2.07	0.55
1:G:4:THR:HG23	1:G:6:LEU:H	1.71	0.55
2:D:55:ASP:OD2	2:D:97:SER:OG	2.22	0.55
2:H:7:LYS:NZ	2:H:39:PHE:O	2.32	0.55
1:G:160:LEU:HB3	1:G:167:LEU:HD22	1.89	0.54
3:J:160:LEU:HD11	3:J:194:ALA:HB2	1.87	0.54
1:G:238:SER:O	7:G:2044:HOH:O	2.18	0.54
3:I:408:ILE:HB	3:I:411:GLY:HA3	1.89	0.54
2:B:60:ASP:OD1	2:B:60:ASP:N	2.38	0.54
3:X:345:ILE:O	7:X:2065:HOH:O	2.18	0.54
3:J:548:LEU:HD11	3:J:553:ALA:HB2	1.90	0.54
2:F:220:SER:O	2:F:224:ILE:HG12	2.07	0.54
1:G:268:LEU:HD22	1:G:293:ASN:HB2	1.89	0.54
3:X:451:ASP:OD1	3:X:455:ASN:ND2	2.40	0.54
3:I:173:ILE:HG21	3:I:197:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:277:MET:HE1	2:H:300:GLU:HB3	1.89	0.54
2:H:59:THR:N	7:H:2020:HOH:O	2.39	0.54
3:J:169:ASP:OD1	3:J:169:ASP:N	2.41	0.54
2:B:81:LYS:HE2	2:B:120:ALA:HB1	1.90	0.53
1:G:47:ASP:OD1	1:G:50:LYS:HE2	2.08	0.53
7:G:2012:HOH:O	2:H:225:GLU:OE1	2.19	0.53
2:B:66:VAL:HG13	2:B:73:ILE:HD12	1.89	0.53
2:D:8:GLU:N	2:D:40:GLU:OE1	2.41	0.53
3:I:255:ASP:OD1	3:I:311:ARG:NE	2.42	0.53
1:C:389:PHE:O	1:C:393:SER:OG	2.16	0.53
1:G:374:THR:HG21	6:K:1631:B12:H491	1.90	0.53
7:E:2060:HOH:O	2:F:2:ALA:N	2.42	0.53
2:F:202:ASN:O	7:F:2007:HOH:O	2.18	0.53
1:E:232:PRO:HD2	7:E:2065:HOH:O	2.07	0.53
3:I:433:TYR:OH	3:I:493:GLU:OE1	2.26	0.53
2:F:34:LEU:HB2	2:F:37:LEU:HD12	1.91	0.52
1:E:249:ARG:HD3	2:F:6:LEU:HD22	1.91	0.52
4:K:336:GLU:OE2	7:K:2046:HOH:O	2.19	0.52
4:K:421:ARG:HG3	4:K:434:GLN:HB3	1.91	0.52
3:X:418:ALA:HB1	3:X:445:CYS:HB3	1.90	0.52
1:E:247:ILE:HG23	1:E:259:PHE:HB3	1.90	0.52
3:I:478:ARG:O	3:I:485:GLU:N	2.39	0.52
4:K:408:ILE:HG22	7:K:2071:HOH:O	2.09	0.52
2:F:145:GLU:OE2	7:F:2036:HOH:O	2.19	0.52
6:I:1631:B12:H533	6:I:1631:B12:H491	1.91	0.52
4:K:222:LEU:HD21	4:K:285:VAL:HG21	1.90	0.52
1:E:367:THR:C	1:E:380:LYS:HZ1	2.18	0.51
3:I:306:LEU:HB3	4:K:164:TYR:HE1	1.75	0.51
1:E:22:GLN:NE2	3:J:139:ASP:O	2.43	0.51
2:F:249:GLU:OE1	7:F:2061:HOH:O	2.19	0.51
3:I:122:LEU:N	7:I:2007:HOH:O	2.43	0.51
3:I:517:ILE:HD12	3:I:558:LEU:HD11	1.91	0.51
1:C:437:SER:HA	1:C:440:LYS:HD3	1.91	0.51
2:F:173:GLY:HA2	2:F:203:ARG:HH22	1.76	0.51
3:J:524:MET:HG2	3:J:601:LEU:HD12	1.93	0.51
1:G:4:THR:N	1:G:7:GLU:OE1	2.35	0.51
1:A:6:LEU:HD11	3:I:528:VAL:HG22	1.93	0.51
2:D:60:ASP:OD1	2:D:60:ASP:N	2.40	0.51
3:I:164:TYR:HE1	4:K:306:LEU:HB3	1.76	0.51
3:J:487:VAL:HA	3:J:501:VAL:HG12	1.93	0.51
1:E:254:LYS:HG3	2:F:6:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:436:VAL:HA	7:K:2079:HOH:O	2.10	0.51
1:A:8:ILE:HG23	1:A:53:LEU:HD13	1.92	0.51
1:C:22:GLN:NE2	3:X:139:ASP:O	2.42	0.51
2:F:60:ASP:OD1	2:F:60:ASP:N	2.43	0.51
1:C:130:LEU:HD23	1:C:159:ILE:HD11	1.92	0.51
2:H:126:MET:HE2	2:H:153:LEU:HD23	1.93	0.51
3:J:553:ALA:HB1	3:J:558:LEU:HB3	1.93	0.51
1:C:396:ALA:O	1:C:402:ARG:NH2	2.43	0.50
1:G:121:ARG:NH1	1:G:305:THR:OG1	2.41	0.50
3:I:309:ASP:HB3	4:K:171:PRO:HG2	1.93	0.50
4:K:377:ASP:OD1	7:K:2065:HOH:O	2.20	0.50
1:A:249:ARG:HB3	2:B:6:LEU:HD23	1.94	0.50
1:C:254:LYS:HE3	2:D:6:LEU:HD13	1.93	0.50
2:D:21:THR:HG22	2:D:22:GLY:N	2.26	0.50
2:D:184:ILE:HD11	2:D:238:LEU:HD11	1.93	0.50
7:J:2053:HOH:O	3:X:168:LYS:NZ	2.43	0.50
3:X:630:VAL:HA	7:X:2135:HOH:O	2.11	0.50
1:E:385:LYS:NZ	7:E:2096:HOH:O	2.14	0.50
2:B:173:GLY:HA2	2:B:203:ARG:HH22	1.75	0.50
2:B:179:SER:HB3	2:B:209:LEU:HD21	1.94	0.50
1:E:358:ILE:HD13	1:E:439:ILE:HG13	1.94	0.50
3:I:533:GLU:O	7:I:2135:HOH:O	2.19	0.50
1:E:357:ARG:NH2	2:F:134:GLU:OE2	2.45	0.50
1:G:96:ILE:HG12	1:G:128:VAL:HG11	1.94	0.50
1:G:97:LEU:HA	1:G:132:ALA:HB3	1.94	0.50
3:J:396:ALA:O	7:J:2083:HOH:O	2.19	0.50
1:C:118:VAL:HG12	1:C:127:SER:OG	2.12	0.49
1:C:4:THR:OG1	1:C:7:GLU:HG3	2.12	0.49
1:E:368:ASP:OD2	7:E:2092:HOH:O	2.19	0.49
1:G:45:VAL:N	1:G:46:SER:CA	2.75	0.49
3:I:128:GLU:OE2	3:I:196:TYR:OH	2.30	0.49
1:G:3:LEU:N	1:G:7:GLU:OE1	2.45	0.49
1:G:201:VAL:O	1:G:225:TYR:OH	2.24	0.49
3:X:382:GLY:HA3	3:X:397:CYS:SG	2.52	0.49
1:C:48:GLU:O	1:C:51:GLU:HG2	2.12	0.49
1:E:182:TYR:CG	1:E:183:ALA:HB2	2.48	0.49
2:F:56:THR:HG22	2:F:96:VAL:HG23	1.95	0.49
1:G:51:GLU:O	1:G:54:GLU:HG3	2.12	0.49
1:G:415:GLY:O	7:G:2069:HOH:O	2.20	0.49
1:G:439:ILE:HG23	1:G:443:TRP:HB3	1.93	0.49
2:H:97:SER:HB2	2:H:105:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:461:ILE:HG22	3:I:462:ILE:HG23	1.94	0.49
2:B:169:CYS:O	2:B:203:ARG:NH2	2.46	0.49
1:G:130:LEU:HD23	1:G:157:PRO:HG2	1.94	0.49
1:C:70:GLU:HG2	1:C:71:LYS:HG2	1.94	0.49
3:J:421:ARG:HB2	3:J:434:GLN:HB3	1.93	0.49
3:J:517:ILE:HD12	3:J:558:LEU:HD21	1.95	0.49
1:A:219:LYS:O	1:A:223:LEU:HG	2.13	0.49
2:B:23:ASP:OD1	7:B:2005:HOH:O	2.19	0.49
2:F:147:LEU:HA	2:F:150:ARG:NH2	2.27	0.49
3:I:485:GLU:HB3	3:I:501:VAL:HG21	1.95	0.49
2:F:118:ALA:HB2	2:F:125:LEU:HD22	1.94	0.49
3:X:378:ILE:HG12	3:X:544:PHE:HD2	1.78	0.49
1:A:106:GLU:O	7:A:2035:HOH:O	2.20	0.49
1:A:151:ARG:NH2	1:A:174:GLU:OE2	2.44	0.49
2:D:22:GLY:O	2:D:25:THR:HG23	2.12	0.49
3:I:246:ASP:HB2	7:I:2156:HOH:O	2.11	0.49
7:C:2095:HOH:O	2:D:131:GLY:O	2.20	0.48
3:I:134:PRO:O	3:I:147:ARG:NH1	2.46	0.48
1:C:268:LEU:HD22	1:C:293:ASN:HB2	1.94	0.48
1:E:437:SER:O	1:E:441:GLN:HG2	2.13	0.48
1:G:18:LYS:HD2	3:I:146:SER:HB3	1.94	0.48
3:I:349:VAL:HG21	3:I:598:MET:HE2	1.95	0.48
3:I:421:ARG:HB2	3:I:434:GLN:HB3	1.95	0.48
2:F:27:THR:OG1	2:F:45:ASN:OD1	2.31	0.48
3:J:342:PHE:N	7:J:2060:HOH:O	2.03	0.48
2:F:169:CYS:O	2:F:203:ARG:NH2	2.47	0.48
4:K:487:VAL:HA	4:K:501:VAL:HG12	1.96	0.48
2:B:119:ASP:OD1	2:B:150:ARG:NH1	2.45	0.48
2:H:31:ASP:OD1	7:H:2011:HOH:O	2.19	0.48
2:F:20:GLY:HA3	2:F:24:LYS:O	2.14	0.48
3:X:446:GLY:HA3	3:X:544:PHE:HE1	1.77	0.48
1:C:18:LYS:NZ	3:X:146:SER:OG	2.43	0.48
1:E:375:ALA:HB1	1:E:381:PHE:HB2	1.96	0.48
4:K:393:VAL:HG13	4:K:601:LEU:HD13	1.94	0.48
1:A:97:LEU:HA	1:A:132:ALA:HB3	1.96	0.47
1:A:198:LYS:HD2	1:A:199:TYR:CE1	2.49	0.47
2:B:139:ILE:HG13	2:B:140:PHE:N	2.29	0.47
2:H:133:GLU:O	2:H:161:ASN:ND2	2.48	0.47
4:K:514:LYS:HE3	4:K:556:ILE:O	2.14	0.47
1:E:140:ALA:HA	1:E:166:GLN:HG2	1.96	0.47
2:H:265:GLY:O	2:H:270:ARG:NH2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:425:SER:HB2	7:I:2108:HOH:O	2.13	0.47
3:X:170:LEU:N	3:X:171:PRO:CD	2.77	0.47
1:C:30:MET:HE2	3:J:527:MET:HE3	1.96	0.47
1:E:155:ASP:OD1	1:E:155:ASP:N	2.46	0.47
1:G:20:CYS:HB3	5:G:1444:SF4:S1	2.55	0.47
1:G:45:VAL:HG13	1:G:46:SER:HA	1.97	0.47
2:H:104:ASN:ND2	2:H:104:ASN:O	2.47	0.47
3:J:281:LYS:HA	3:J:281:LYS:HD3	1.60	0.47
4:K:174:LEU:HD23	4:K:181:VAL:HG11	1.96	0.47
1:A:96:ILE:HG12	1:A:128:VAL:HG11	1.96	0.47
1:A:407:PRO:HB3	6:I:1631:B12:C8B	2.45	0.47
2:B:155:SER:HA	2:B:156:SER:HA	1.59	0.47
1:C:28:PHE:O	1:C:32:ILE:HG12	2.15	0.47
6:C:1444:B12:H601	6:C:1444:B12:H262	1.96	0.47
2:D:18:THR:O	2:D:151:ASN:ND2	2.47	0.47
1:G:67:GLY:HA3	1:G:157:PRO:HB3	1.96	0.47
1:G:358:ILE:HD13	1:G:439:ILE:HG13	1.97	0.47
3:I:296:ALA:HB2	3:I:346:MET:HG3	1.97	0.47
3:J:309:ASP:HB3	3:X:171:PRO:HG2	1.96	0.47
3:J:619:ILE:HA	3:J:620:PRO:HA	1.74	0.47
2:F:17:VAL:HG11	2:F:205:ILE:HD11	1.97	0.47
3:I:133:LEU:HB2	3:I:179:PHE:HB3	1.96	0.47
1:E:363:LEU:HD21	1:E:395:ILE:HG21	1.96	0.47
3:J:236:ASN:HB2	3:J:275:LEU:HD21	1.97	0.47
1:C:401:HIS:O	1:C:402:ARG:NH1	2.41	0.47
1:E:421:SER:N	1:E:422:GLY:HA2	2.30	0.47
2:F:204:ILE:HB	2:F:240:MET:SD	2.55	0.47
3:J:427:ALA:HA	3:J:472:VAL:HG13	1.96	0.47
1:E:418:GLN:HG3	1:E:425:ILE:H	1.80	0.46
1:G:4:THR:HG23	1:G:6:LEU:N	2.29	0.46
2:H:155:SER:HA	2:H:156:SER:HA	1.56	0.46
3:X:247:VAL:HG13	3:X:300:THR:HG21	1.96	0.46
1:G:285:LYS:C	1:G:286:TYR:CG	2.93	0.46
1:A:378:ALA:HB2	6:I:1631:B12:H421	1.97	0.46
1:E:71:LYS:HD3	1:E:156:LEU:HD23	1.96	0.46
1:G:64:ILE:HG21	1:G:229:ILE:HD11	1.96	0.46
1:E:294:THR:HG21	1:E:299:ASP:OD2	2.15	0.46
2:H:227:MET:HG2	2:H:238:LEU:HD11	1.96	0.46
3:J:514:LYS:HE3	3:J:556:ILE:O	2.15	0.46
1:A:52:LEU:HA	1:E:55:SER:HB3	1.97	0.46
2:F:47:PRO:HG2	2:F:305:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:114:CYS:HB3	2:H:147:LEU:HD11	1.96	0.46
2:H:18:THR:HG23	2:H:25:THR:HG23	1.96	0.46
3:I:456:LEU:HD22	3:I:461:ILE:HG21	1.98	0.46
3:J:450:ILE:HG23	3:J:556:ILE:HD13	1.98	0.46
3:X:270:SER:O	3:X:274:GLU:HG3	2.15	0.46
1:E:121:ARG:HB2	1:E:126:HIS:CD2	2.50	0.46
1:G:122:VAL:HG21	7:G:2020:HOH:O	2.15	0.46
3:I:593:GLU:HG2	7:I:2146:HOH:O	2.15	0.46
7:J:2066:HOH:O	3:X:169:ASP:HB2	1.95	0.46
3:X:457:LYS:NZ	7:X:2099:HOH:O	2.11	0.46
3:J:456:LEU:HD22	3:J:461:ILE:HG21	1.98	0.46
4:K:126:PHE:CE1	4:K:291:MET:HG3	2.50	0.46
4:K:346:MET:HE3	4:K:591:VAL:HG21	1.97	0.46
2:B:298:LEU:O	2:B:302:LYS:HB2	2.16	0.46
2:H:210:ILE:HG22	2:H:220:SER:HB3	1.98	0.46
3:X:579:ARG:NH2	7:X:2125:HOH:O	2.49	0.46
1:A:182:TYR:CG	1:A:183:ALA:HB2	2.51	0.46
2:D:105:ARG:HD2	2:D:109:GLU:OE2	2.17	0.46
1:E:191:GLN:OE1	7:E:2058:HOH:O	2.20	0.46
2:F:170:MET:HE2	2:F:199:LEU:HB2	1.96	0.46
3:J:198:LYS:NZ	7:J:2033:HOH:O	2.02	0.45
4:K:306:LEU:HD11	4:K:345:ILE:HG13	1.96	0.45
1:A:357:ARG:HH12	2:B:100:PRO:CB	2.27	0.45
7:A:2031:HOH:O	2:B:225:GLU:OE1	2.20	0.45
2:B:246:ILE:HD12	2:B:278:THR:HG22	1.98	0.45
1:C:43:PRO:HG2	1:C:44:TYR:CE2	2.51	0.45
3:X:517:ILE:HD12	3:X:558:LEU:HD11	1.99	0.45
1:C:47:ASP:HA	1:C:50:LYS:HD2	1.99	0.45
1:C:47:ASP:OD1	1:C:50:LYS:HD2	2.16	0.45
2:F:146:ALA:O	2:F:150:ARG:NH2	2.48	0.45
1:G:322:PRO:HB3	1:G:366:ASP:HB2	1.98	0.45
3:J:255:ASP:OD2	3:J:311:ARG:HG3	2.16	0.45
2:D:247:GLY:HA3	2:D:293:ARG:HG3	1.98	0.45
1:G:52:LEU:O	1:G:55:SER:HB3	2.17	0.45
3:I:224:ASP:HB2	3:I:231:LEU:HD11	1.98	0.45
3:I:491:ALA:N	3:I:499:ASP:OD1	2.49	0.45
3:J:164:TYR:HE1	3:X:306:LEU:HB3	1.80	0.45
3:X:169:ASP:OD1	3:X:169:ASP:N	2.47	0.45
1:E:118:VAL:HG22	1:E:127:SER:HB3	1.98	0.45
2:H:305:LEU:HA	2:H:308:ILE:HG22	1.99	0.45
2:B:160:ASP:HA	3:I:467:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:277:MET:SD	2:H:276:THR:HB	2.57	0.45
4:K:236:ASN:OD1	4:K:237:TYR:N	2.46	0.45
3:X:532:LEU:HD11	3:X:560:PRO:HB3	1.98	0.45
3:I:514:LYS:HD2	3:I:556:ILE:O	2.16	0.45
1:C:67:GLY:HA3	1:C:157:PRO:HB3	1.99	0.45
1:E:336:VAL:N	7:E:2088:HOH:O	2.02	0.45
3:X:352:TYR:CZ	6:X:1631:B12:H361	2.51	0.45
1:A:247:ILE:HG23	1:A:259:PHE:HB3	1.98	0.45
1:G:22:GLN:HG3	1:G:28:PHE:HA	1.97	0.45
6:I:1631:B12:H353	6:I:1631:B12:O34	2.17	0.45
4:K:556:ILE:O	4:K:620:PRO:HA	2.17	0.45
1:C:372:VAL:HB	7:C:2098:HOH:O	2.17	0.44
2:H:12:SER:OG	2:H:13:LYS:N	2.51	0.44
2:H:31:ASP:OD2	2:H:288:HIS:NE2	2.48	0.44
3:X:316:GLU:HA	3:X:318:TYR:N	2.33	0.44
3:X:421:ARG:HG2	3:X:451:ASP:OD2	2.17	0.44
1:A:185:THR:O	1:A:189:TYR:HB3	2.18	0.44
1:A:199:TYR:O	1:A:201:VAL:HG13	2.17	0.44
2:B:305:LEU:HA	2:B:308:ILE:HG22	1.99	0.44
2:F:155:SER:HA	2:F:156:SER:HA	1.64	0.44
3:J:152:PHE:CD1	3:J:160:LEU:HB2	2.53	0.44
3:J:527:MET:HG3	3:J:601:LEU:HD13	1.99	0.44
3:X:210:ALA:HB3	3:X:221:GLN:HB2	1.98	0.44
3:X:465:SER:O	7:X:2101:HOH:O	2.21	0.44
3:X:506:ASP:OD2	7:X:2085:HOH:O	2.21	0.44
1:C:345:THR:HA	6:C:1444:B12:H3P1	1.98	0.44
7:C:2112:HOH:O	3:J:248:ILE:HG12	2.18	0.44
2:D:67:GLU:HB3	2:D:68:PRO:HD3	2.00	0.44
1:E:65:LYS:HG2	1:E:74:GLU:HG2	1.99	0.44
2:F:93:LEU:HD22	2:F:117:VAL:HG21	1.98	0.44
2:F:224:ILE:HB	2:F:285:ALA:HB1	1.99	0.44
1:G:184:ALA:HB2	1:G:203:LEU:HD11	1.99	0.44
1:G:273:TYR:C	1:G:277:MET:HE2	2.43	0.44
4:K:478:ARG:NH1	7:K:2087:HOH:O	2.51	0.44
1:C:47:ASP:HA	1:C:50:LYS:HG3	1.99	0.44
6:C:1444:B12:H353	6:C:1444:B12:O34	2.17	0.44
2:D:115:LYS:HE3	2:D:150:ARG:NH2	2.33	0.44
2:F:208:PRO:HG2	2:F:224:ILE:HD11	1.99	0.44
1:G:134:LYS:HA	1:G:161:ILE:HB	1.99	0.44
2:H:248:GLN:O	2:H:252:LYS:HD2	2.17	0.44
3:I:231:LEU:O	3:I:283:HIS:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:398:SER:O	6:X:1631:B12:H542	2.18	0.44
1:A:438:PHE:CE1	1:A:442:ARG:HG3	2.52	0.44
2:D:155:SER:HA	2:D:156:SER:HA	1.60	0.44
3:J:213:ILE:HD12	3:J:295:VAL:HG13	2.00	0.44
4:K:234:LYS:NZ	4:K:278:GLN:HB3	2.33	0.44
6:K:1631:B12:H473	6:K:1631:B12:H482	1.86	0.44
3:X:569:TYR:CZ	3:X:571:GLY:HA2	2.52	0.44
1:A:118:VAL:HG13	1:A:127:SER:HB3	2.00	0.44
2:D:302:LYS:HB2	2:D:302:LYS:HE3	1.80	0.44
3:I:391:TRP:CH2	3:I:528:VAL:HG21	2.53	0.44
2:B:10:TRP:HB3	2:B:232:LEU:HB3	1.99	0.43
3:J:464:ARG:NH2	7:J:2101:HOH:O	2.50	0.43
1:C:97:LEU:HA	1:C:132:ALA:HB3	2.00	0.43
2:D:183:ASP:HB3	2:D:186:LEU:HB2	1.99	0.43
1:E:9:TYR:CE2	1:E:14:LYS:HE3	2.53	0.43
2:H:53:VAL:N	2:H:92:ALA:O	2.44	0.43
3:J:122:LEU:HD11	3:J:583:LEU:HD22	1.99	0.43
3:J:532:LEU:HD22	3:J:560:PRO:HB3	2.00	0.43
4:K:461:ILE:HA	4:K:472:VAL:HG11	2.00	0.43
1:A:118:VAL:HG12	1:A:125:MET:HE3	1.99	0.43
1:C:130:LEU:HD12	1:C:157:PRO:HG2	2.00	0.43
2:F:37:LEU:HD22	2:F:39:PHE:HE1	1.83	0.43
1:C:26:LEU:HB3	3:J:599:THR:OG1	2.19	0.43
2:D:90:ILE:HG12	2:D:124:PRO:HB2	2.01	0.43
1:E:185:THR:O	1:E:189:TYR:HB3	2.19	0.43
1:E:405:ILE:HD13	1:E:438:PHE:HE2	1.83	0.43
2:F:254:LYS:HA	2:F:257:LYS:HE2	2.00	0.43
3:I:450:ILE:HG23	3:I:556:ILE:HD13	2.01	0.43
4:K:135:VAL:HA	4:K:136:PRO:HD3	1.90	0.43
3:X:152:PHE:CD1	3:X:160:LEU:HB2	2.53	0.43
1:G:50:LYS:O	1:G:54:GLU:HG2	2.18	0.43
1:G:442:ARG:NH1	7:G:2078:HOH:O	2.42	0.43
2:B:37:LEU:HD22	2:B:39:PHE:HE2	1.84	0.43
1:C:321:GLU:HA	1:C:322:PRO:HD3	1.78	0.43
2:H:82:LYS:NZ	2:H:86:TYR:OH	2.52	0.43
3:J:203:SER:O	7:J:2007:HOH:O	2.21	0.43
4:K:485:GLU:CB	4:K:503:THR:HG22	2.49	0.43
2:B:48:ARG:HD3	2:B:48:ARG:HA	1.82	0.43
1:C:39:LEU:HD22	1:C:53:LEU:HD12	2.00	0.43
2:D:95:LEU:HD22	2:D:110:LEU:HD22	1.99	0.43
1:G:123:GLY:O	7:G:2023:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:TYR:HA	1:G:183:ALA:HA	1.75	0.43
4:K:376:ILE:HG22	4:K:384:MET:HB2	1.99	0.43
1:C:100:ASP:OD2	1:C:137:SER:OG	2.30	0.43
4:K:369:SER:O	4:K:389:LYS:N	2.49	0.43
1:A:82:PHE:O	1:A:85:ASP:HB2	2.19	0.43
2:B:53:VAL:HG22	2:B:79:TRP:CD1	2.54	0.43
1:E:330:PRO:HA	1:E:331:GLY:HA3	1.83	0.43
3:I:181:VAL:HB	3:I:197:ILE:HD11	2.00	0.43
1:G:90:HIS:HA	1:G:91:PRO:HD2	1.82	0.42
1:A:318:ILE:HD11	3:I:610:MET:HE2	2.01	0.42
1:C:22:GLN:HG3	1:C:28:PHE:HA	2.01	0.42
1:E:230:LEU:HB2	1:E:263:THR:HG22	2.01	0.42
1:G:42:CYS:HA	1:G:43:PRO:HD3	1.84	0.42
1:G:248:ARG:CZ	1:G:286:TYR:HB3	2.50	0.42
3:J:527:MET:HE2	3:J:601:LEU:HD22	2.00	0.42
3:X:602:GLU:O	3:X:605:VAL:HG22	2.19	0.42
1:C:6:LEU:HD12	1:C:6:LEU:HA	1.82	0.42
1:C:27:ALA:O	1:C:31:GLN:HG2	2.19	0.42
1:A:26:LEU:HG	1:A:30:MET:HE3	2.02	0.42
1:E:26:LEU:HB3	3:X:599:THR:OG1	2.19	0.42
1:E:101:THR:HG23	1:E:136:SER:HB2	2.00	0.42
2:F:136:ASP:HA	2:F:139:ILE:HG12	2.00	0.42
1:G:68:LYS:HE3	1:G:177:ASN:HA	2.02	0.42
1:G:182:TYR:OH	7:G:2033:HOH:O	2.22	0.42
3:I:548:LEU:HD11	3:I:553:ALA:HB2	2.01	0.42
3:J:166:GLN:NE2	3:J:195:LEU:O	2.48	0.42
1:A:100:ASP:OD2	1:A:137:SER:OG	2.29	0.42
1:C:18:LYS:HD3	3:X:146:SER:HB3	2.00	0.42
1:C:39:LEU:HD13	1:C:53:LEU:HD12	2.00	0.42
3:I:352:TYR:CZ	6:I:1631:B12:H361	2.54	0.42
3:J:259:ASP:CG	3:J:263:LYS:HD2	2.44	0.42
4:K:169:ASP:O	4:K:173:ILE:HG12	2.20	0.42
4:K:596:ARG:NH2	7:K:2114:HOH:O	2.52	0.42
3:X:309:ASP:HA	3:X:310:PRO:HD3	1.85	0.42
2:B:68:PRO:HB2	2:B:295:PRO:HG2	2.02	0.42
2:F:99:HIS:HA	2:F:100:PRO:HD3	1.87	0.42
1:G:51:GLU:CD	1:G:51:GLU:N	2.72	0.42
3:I:630:VAL:HA	7:I:2154:HOH:O	2.20	0.42
1:C:269:ASP:O	1:C:275:ALA:HB2	2.19	0.42
1:C:278:GLU:HG3	7:C:2073:HOH:O	2.19	0.42
2:D:24:LYS:O	2:D:124:PRO:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:LYS:HE3	2:D:254:LYS:HB2	1.83	0.42
2:H:139:ILE:O	2:H:143:ILE:HG12	2.19	0.42
2:H:303:GLU:O	2:H:306:LYS:HB2	2.19	0.42
4:K:128:GLU:N	7:K:2011:HOH:O	2.38	0.42
4:K:569:TYR:CZ	4:K:571:GLY:HA2	2.55	0.42
1:A:94:LEU:HD22	1:A:292:LEU:HD21	2.01	0.42
2:D:294:HIS:HA	2:D:295:PRO:HD3	1.92	0.42
2:F:67:GLU:O	2:F:70:LYS:HG3	2.20	0.42
1:G:26:LEU:HB3	4:K:599:THR:OG1	2.19	0.42
1:G:281:VAL:O	1:G:285:LYS:HB2	2.19	0.42
3:X:346:MET:HE2	3:X:578:ALA:HA	2.02	0.42
3:X:619:ILE:HA	3:X:620:PRO:HA	1.76	0.42
1:A:439:ILE:HG23	1:A:443:TRP:HB3	2.02	0.42
2:B:28:LEU:HD21	2:B:289:LEU:HB2	2.01	0.42
1:E:401:HIS:O	1:E:402:ARG:NH1	2.47	0.42
2:F:71:ASP:O	7:F:2018:HOH:O	2.21	0.42
2:F:246:ILE:HD12	2:F:278:THR:HG22	2.02	0.42
2:B:34:LEU:HB2	2:B:37:LEU:HD12	2.02	0.42
1:C:70:GLU:H	1:C:70:GLU:CD	2.27	0.42
1:C:83:ARG:O	1:C:314:PRO:HG3	2.20	0.42
6:C:1444:B12:H473	6:C:1444:B12:H481	1.92	0.42
1:G:182:TYR:CG	1:G:183:ALA:HB2	2.54	0.42
2:H:34:LEU:HB2	2:H:37:LEU:HD12	2.02	0.42
3:J:569:TYR:CZ	3:J:571:GLY:HA2	2.55	0.42
4:K:203:SER:C	4:K:205:ARG:H	2.27	0.42
6:C:1444:B12:H361	3:J:352:TYR:CZ	2.55	0.41
1:E:299:ASP:OD1	2:F:273:HIS:NE2	2.43	0.41
3:X:441:PRO:HD2	3:X:493:GLU:O	2.20	0.41
1:C:339:THR:OG1	1:C:340:THR:N	2.52	0.41
2:D:240:MET:HG3	7:D:2042:HOH:O	2.20	0.41
1:E:182:TYR:CD2	1:E:183:ALA:HB2	2.55	0.41
3:J:123:ASP:O	3:J:585:ARG:HG3	2.20	0.41
1:A:227:ASN:O	1:A:228:LEU:HD23	2.20	0.41
1:A:363:LEU:HB3	1:A:389:PHE:CE1	2.54	0.41
2:D:200:ALA:HA	2:D:201:PRO:HD3	1.94	0.41
2:F:72:VAL:HG21	2:F:79:TRP:HA	2.02	0.41
1:G:9:TYR:HE1	1:G:25:CYS:HB2	1.84	0.41
1:G:340:THR:OG1	1:G:345:THR:HG21	2.20	0.41
4:K:209:LEU:HG	4:K:290:ILE:HG21	2.02	0.41
1:A:167:LEU:HD13	1:A:181:LEU:HD22	2.02	0.41
1:A:167:LEU:HD12	1:A:192:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:ILE:HG22	1:C:343:SER:OG	2.19	0.41
2:F:166:VAL:HG12	2:F:170:MET:HE3	2.03	0.41
1:G:241:LEU:HD22	2:H:308:ILE:HD11	2.01	0.41
2:H:98:ALA:O	2:H:135:LYS:NZ	2.41	0.41
3:I:164:TYR:CE1	4:K:306:LEU:HB3	2.55	0.41
3:J:362:LEU:HG	3:J:580:LYS:HD3	2.03	0.41
4:K:353:VAL:HG11	4:K:394:THR:HG21	2.03	0.41
2:B:210:ILE:HG22	2:B:220:SER:HB3	2.02	0.41
1:C:247:ILE:HG23	1:C:259:PHE:HB3	2.02	0.41
2:F:147:LEU:HD23	2:F:152:CYS:SG	2.61	0.41
1:G:58:ALA:HA	1:G:59:PRO:HD3	1.94	0.41
1:G:241:LEU:CD1	1:G:285:LYS:HG2	2.51	0.41
3:J:346:MET:HE2	3:J:578:ALA:HA	2.03	0.41
3:J:430:LYS:HA	7:J:2093:HOH:O	2.19	0.41
3:J:551:LYS:HE3	3:J:551:LYS:HB3	1.76	0.41
1:C:148:ALA:O	1:C:152:GLU:HG2	2.20	0.41
1:C:208:LYS:HA	1:C:233:GLN:HB2	2.02	0.41
1:E:18:LYS:O	3:J:142:ARG:NH1	2.53	0.41
1:A:86:LYS:HB3	1:A:87:ARG:H	1.67	0.41
1:A:134:LYS:HE3	1:A:136:SER:HB3	2.03	0.41
2:B:248:GLN:O	2:B:252:LYS:HE2	2.20	0.41
1:C:329:ASN:OD1	7:C:2088:HOH:O	2.21	0.41
1:C:436:ASN:O	1:C:440:LYS:HG3	2.21	0.41
2:D:99:HIS:HA	2:D:100:PRO:HD3	1.85	0.41
2:F:115:LYS:HE2	2:F:150:ARG:HH22	1.85	0.41
1:G:185:THR:HG23	7:G:2042:HOH:O	2.21	0.41
1:G:273:TYR:O	1:G:277:MET:HE2	2.21	0.41
1:C:3:LEU:HD23	1:C:3:LEU:HA	1.83	0.41
1:G:28:PHE:O	1:G:32:ILE:HG12	2.20	0.41
2:H:166:VAL:HG13	2:H:199:LEU:HD22	2.02	0.41
4:K:349:VAL:HG21	4:K:598:MET:SD	2.60	0.41
4:K:485:GLU:HB3	4:K:503:THR:HG22	2.03	0.41
4:K:619:ILE:HA	4:K:620:PRO:HA	1.84	0.41
1:A:28:PHE:O	1:A:32:ILE:HG12	2.21	0.41
1:A:84:HIS:ND1	7:A:2031:HOH:O	2.05	0.41
1:A:134:LYS:HA	1:A:161:ILE:HB	2.03	0.41
1:A:182:TYR:HA	1:A:183:ALA:HA	1.77	0.41
1:A:321:GLU:HA	1:A:322:PRO:HD3	1.80	0.41
1:A:357:ARG:NH1	1:A:357:ARG:HG2	2.34	0.41
1:C:230:LEU:HG	1:C:261:TYR:HB2	2.03	0.41
1:C:318:ILE:N	1:C:318:ILE:CD1	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:GLY:N	7:E:2102:HOH:O	2.23	0.41
2:H:20:GLY:HA3	2:H:124:PRO:HB3	2.03	0.41
3:I:152:PHE:CD2	3:I:160:LEU:HB2	2.56	0.41
3:I:257:ASN:HA	3:I:258:PRO:HD3	1.88	0.41
3:X:211:ILE:HG23	3:X:220:VAL:HG22	2.03	0.41
3:X:378:ILE:HG12	3:X:544:PHE:CD2	2.56	0.41
2:B:56:THR:HG21	2:B:103:GLN:HE22	1.86	0.41
1:C:26:LEU:O	1:C:30:MET:HG2	2.21	0.41
2:D:205:ILE:HG12	2:D:241:PRO:HG2	2.03	0.41
1:G:60:PRO:HB3	1:G:251:ALA:O	2.20	0.41
2:H:33:THR:HB	2:H:41:GLY:HA3	2.03	0.41
3:I:229:LYS:HE2	3:I:229:LYS:HB3	1.93	0.41
6:I:1631:B12:H473	6:I:1631:B12:H481	1.89	0.41
3:X:413:ARG:HB2	7:X:2087:HOH:O	2.20	0.41
6:X:1631:B12:H552	6:X:1631:B12:H531	2.02	0.41
2:D:21:THR:HG22	2:D:22:GLY:H	1.85	0.40
1:E:22:GLN:HG3	1:E:28:PHE:HA	2.03	0.40
2:H:164:PRO:HG2	2:H:165:ILE:HD12	2.02	0.40
4:K:337:MET:O	7:K:2049:HOH:O	2.22	0.40
4:K:412:MET:HE2	4:K:418:ALA:HB2	2.03	0.40
1:A:407:PRO:HB3	6:I:1631:B12:C9B	2.51	0.40
2:B:24:LYS:HG3	2:B:122:ASP:C	2.46	0.40
1:C:330:PRO:HB2	1:C:361:TYR:CZ	2.56	0.40
1:E:42:CYS:HA	1:E:43:PRO:HD3	1.83	0.40
2:H:99:HIS:HA	2:H:100:PRO:HD3	1.93	0.40
3:I:330:ALA:HB3	3:I:339:PRO:HA	2.03	0.40
4:K:286:GLU:HG2	4:K:288:LYS:NZ	2.37	0.40
1:A:26:LEU:HB3	3:I:599:THR:OG1	2.21	0.40
1:A:416:LYS:O	1:A:420:LEU:HB2	2.21	0.40
1:G:53:LEU:HD12	1:G:53:LEU:HA	1.84	0.40
1:G:205:VAL:HG22	1:G:220:ILE:HD12	2.03	0.40
3:I:126:PHE:CD1	3:I:126:PHE:C	2.99	0.40
2:B:55:ASP:OD2	2:B:97:SER:OG	2.27	0.40
1:E:48:GLU:CD	1:E:48:GLU:H	2.29	0.40
2:H:52:GLU:HA	2:H:92:ALA:HB3	2.03	0.40
3:J:135:VAL:HA	3:J:136:PRO:HD3	1.98	0.40
3:J:171:PRO:HG2	3:X:309:ASP:HB3	2.02	0.40
3:J:177:GLU:HG2	3:J:199:SER:HB3	2.03	0.40
3:J:346:MET:HA	3:J:347:PRO:HD3	1.85	0.40
3:X:446:GLY:HA3	3:X:544:PHE:CE1	2.55	0.40
1:A:140:ALA:HA	1:A:166:GLN:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:ILE:HD13	1:G:278:GLU:HG2	2.02	0.40
2:H:173:GLY:HA2	2:H:203:ARG:NH2	2.36	0.40
6:I:1631:B12:H552	6:I:1631:B12:H531	2.02	0.40
3:J:140:ASP:O	3:J:147:ARG:NH2	2.41	0.40
4:K:452:LEU:HD21	4:K:502:ILE:HG21	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)
7:G:2071:HOH:O	7:X:2105:HOH:O[1_645]	1.99	0.21

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	440/442 (100%)	422 (96%)	18 (4%)	0	100	100
1	C	440/442 (100%)	424 (96%)	16 (4%)	0	100	100
1	E	440/442 (100%)	425 (97%)	15 (3%)	0	100	100
1	G	439/442 (99%)	411 (94%)	28 (6%)	0	100	100
2	B	307/309 (99%)	294 (96%)	13 (4%)	0	100	100
2	D	307/309 (99%)	298 (97%)	9 (3%)	0	100	100
2	F	307/309 (99%)	297 (97%)	10 (3%)	0	100	100
2	H	307/309 (99%)	296 (96%)	11 (4%)	0	100	100
3	I	507/509 (100%)	492 (97%)	15 (3%)	0	100	100
3	J	507/509 (100%)	493 (97%)	14 (3%)	0	100	100
3	X	507/509 (100%)	490 (97%)	17 (3%)	0	100	100
4	K	508/510 (100%)	485 (96%)	23 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5016/5041 (100%)	4827 (96%)	189 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	361/361 (100%)	357 (99%)	4 (1%)	65 83
1	C	361/361 (100%)	349 (97%)	12 (3%)	33 58
1	E	361/361 (100%)	355 (98%)	6 (2%)	53 77
1	G	361/361 (100%)	353 (98%)	8 (2%)	45 71
2	B	256/256 (100%)	256 (100%)	0	100 100
2	D	256/256 (100%)	252 (98%)	4 (2%)	55 78
2	F	256/256 (100%)	252 (98%)	4 (2%)	55 78
2	H	256/256 (100%)	252 (98%)	4 (2%)	55 78
3	I	422/422 (100%)	415 (98%)	7 (2%)	53 77
3	J	422/422 (100%)	416 (99%)	6 (1%)	59 80
3	X	422/422 (100%)	411 (97%)	11 (3%)	40 66
4	K	423/423 (100%)	416 (98%)	7 (2%)	53 77
All	All	4157/4157 (100%)	4084 (98%)	73 (2%)	51 75

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LYS
1	A	138	GLN
1	A	200	ASN
1	A	235	GLU
1	C	10	LYS
1	C	39	LEU

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Mol	Chain	Res	Type
1	C	52	LEU
1	C	54	GLU
1	C	55	SER
1	C	187	ASP
1	C	190	GLU
1	C	270	GLU
1	C	318	ILE
1	C	323	LYS
1	C	391	LYS
1	C	440	LYS
2	D	13	LYS
2	D	184	ILE
2	D	296	LYS
2	D	306	LYS
1	E	174	GLU
1	E	269	ASP
1	E	321	GLU
1	E	380	LYS
1	E	418	GLN
1	E	421	SER
2	F	70	LYS
2	F	71	ASP
2	F	237	ILE
2	F	263	GLU
1	G	4	THR
1	G	50	LYS
1	G	71	LYS
1	G	75	ILE
1	G	104	GLU
1	G	173	THR
1	G	215	GLU
1	G	333	ASP
2	H	28	LEU
2	H	31	ASP
2	H	237	ILE
2	H	260	GLU
3	I	127	LYS
3	I	170	LEU
3	I	429	LEU
3	I	455	ASN
3	I	501	VAL
3	I	564	ILE

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Mol	Chain	Res	Type
3	I	630	VAL
3	J	153	SER
3	J	422	VAL
3	J	472	VAL
3	J	514	LYS
3	J	565	ASN
3	J	593	GLU
4	K	290	ILE
4	K	310	PRO
4	K	420	GLU
4	K	475	GLU
4	K	482	ASP
4	K	628	PRO
4	K	629	SER
3	X	157	ASN
3	X	163	GLU
3	X	165	GLU
3	X	169	ASP
3	X	193	LYS
3	X	206	VAL
3	X	247	VAL
3	X	430	LYS
3	X	432	LYS
3	X	502	ILE
3	X	514	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	274	GLN
1	A	315	GLN
1	A	329	ASN
1	A	400	ASN
2	B	172	HIS
2	B	189	GLN
1	C	315	GLN
1	C	436	ASN
2	D	198	ASN
1	E	11	HIS
1	E	77	HIS
1	E	400	ASN

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Mol	Chain	Res	Type
1	E	418	GLN
2	H	273	HIS
3	I	166	GLN
3	I	257	ASN
3	I	625	HIS
3	J	159	ASN
4	K	159	ASN
4	K	257	ASN
3	X	240	GLN
3	X	381	ASN

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)

8 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
6	B12	C	1444	3	93,101,101	0.73	3 (3%)	146,166,166	0.99	9 (6%)
6	B12	I	1631	3	93,101,101	0.69	3 (3%)	146,166,166	0.99	9 (6%)
6	B12	K	1631	4	93,101,101	0.75	2 (2%)	146,166,166	0.99	10 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	B12	X	1631	3	93,101,101	0.71	4 (4%)	146,166,166	1.00	9 (6%)
5	SF4	C	1445	1	0,12,12	-	-	-		
5	SF4	G	1444	1	0,12,12	-	-	-		
5	SF4	E	1444	1	0,12,12	-	-	-		
5	SF4	A	1444	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
6	B12	C	1444	3	-	6/56/223/223	0/3/11/11
6	B12	I	1631	3	-	7/56/223/223	0/3/11/11
6	B12	X	1631	3	-	6/56/223/223	0/3/11/11
6	B12	K	1631	4	-	9/56/223/223	0/3/11/11
5	SF4	C	1445	1	-	-	0/6/5/5
5	SF4	G	1444	1	-	-	0/6/5/5
5	SF4	E	1444	1	-	-	0/6/5/5
5	SF4	A	1444	1	-	-	0/6/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	1631	B12	C14-N23	4.32	1.40	1.35
6	C	1444	B12	C14-N23	3.84	1.40	1.35
6	X	1631	B12	C14-N23	3.79	1.39	1.35
6	I	1631	B12	C14-N23	3.72	1.39	1.35
6	C	1444	B12	C16-C15	3.21	1.53	1.44
6	K	1631	B12	C16-C15	3.11	1.53	1.44
6	X	1631	B12	C16-C15	3.08	1.53	1.44
6	I	1631	B12	C16-C15	2.95	1.52	1.44
6	C	1444	B12	C1P-C2P	2.06	1.56	1.51
6	X	1631	B12	C9-N22	2.04	1.35	1.30
6	I	1631	B12	C1P-C2P	2.01	1.56	1.51
6	X	1631	B12	C1P-C2P	2.00	1.56	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1444	B12	C10-C9-N22	3.30	129.51	125.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	1631	B12	C10-C9-N22	3.29	129.51	125.73
6	K	1631	B12	C10-C9-N22	3.27	129.48	125.73
6	X	1631	B12	C10-C9-N22	3.22	129.42	125.73
6	X	1631	B12	C35-C5-C4	-3.06	110.56	116.79
6	X	1631	B12	C35-C5-C6	3.02	127.23	122.43
6	K	1631	B12	C35-C5-C4	-2.91	110.86	116.79
6	K	1631	B12	C35-C5-C6	2.86	126.99	122.43
6	X	1631	B12	C15-C16-N24	-2.81	118.37	122.42
6	C	1444	B12	C35-C5-C4	-2.80	111.08	116.79
6	C	1444	B12	C35-C5-C6	2.80	126.88	122.43
6	C	1444	B12	C15-C16-N24	-2.77	118.43	122.42
6	C	1444	B12	C17-C18-C19	2.72	106.52	102.36
6	I	1631	B12	C35-C5-C6	2.69	126.72	122.43
6	I	1631	B12	C35-C5-C4	-2.64	111.41	116.79
6	K	1631	B12	C55-C17-C18	-2.60	106.13	111.15
6	K	1631	B12	C15-C16-N24	-2.57	118.72	122.42
6	K	1631	B12	C17-C18-C19	2.48	106.15	102.36
6	X	1631	B12	C17-C18-C19	2.47	106.14	102.36
6	I	1631	B12	C15-C16-N24	-2.45	118.90	122.42
6	I	1631	B12	C17-C18-C19	2.39	106.01	102.36
6	I	1631	B12	C55-C17-C18	-2.38	106.54	111.15
6	I	1631	B12	C5-C6-N22	-2.29	120.38	123.88
6	C	1444	B12	C55-C17-C18	-2.25	106.81	111.15
6	I	1631	B12	C55-C56-C57	-2.24	106.34	111.23
6	C	1444	B12	C55-C56-C57	-2.23	106.36	111.23
6	C	1444	B12	O3-P-O4	2.23	117.83	109.47
6	K	1631	B12	C7-C8-C9	-2.16	98.14	100.90
6	C	1444	B12	C7-C8-C9	-2.15	98.16	100.90
6	X	1631	B12	C55-C17-C18	-2.13	107.02	111.15
6	X	1631	B12	C20-C1-C19	-2.12	107.31	109.36
6	I	1631	B12	C7-C8-C9	-2.12	98.19	100.90
6	X	1631	B12	C20-C1-C2	2.12	116.82	113.28
6	K	1631	B12	C55-C56-C57	-2.04	106.78	111.23
6	X	1631	B12	C55-C56-C57	-2.03	106.79	111.23
6	K	1631	B12	P-O2-C3R	2.01	126.72	119.41
6	K	1631	B12	C36-C7-C37	2.00	114.10	110.80

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	1631	B12	C1P-C2P-O3-P

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Mol	Chain	Res	Type	Atoms
6	K	1631	B12	C14-C13-C48-C49
6	C	1444	B12	C2R-C1R-N1B-C8B
6	C	1444	B12	O6R-C1R-N1B-C8B
6	I	1631	B12	C2R-C1R-N1B-C8B
6	K	1631	B12	C2R-C1R-N1B-C8B
6	K	1631	B12	O6R-C1R-N1B-C8B
6	X	1631	B12	C2R-C1R-N1B-C8B
6	X	1631	B12	O6R-C1R-N1B-C8B
6	I	1631	B12	C3P-C2P-O3-P
6	K	1631	B12	C1P-C2P-O3-P
6	K	1631	B12	C3P-C2P-O3-P
6	C	1444	B12	C14-C13-C48-C49
6	I	1631	B12	C14-C13-C48-C49
6	X	1631	B12	C2P-O3-P-O2
6	K	1631	B12	C48-C49-C50-N52
6	C	1444	B12	C2P-O3-P-O2
6	I	1631	B12	O6R-C1R-N1B-C8B
6	K	1631	B12	C48-C49-C50-O51
6	C	1444	B12	C1P-C2P-O3-P
6	X	1631	B12	C1P-C2P-O3-P
6	C	1444	B12	C42-C41-C8-C9
6	I	1631	B12	C42-C41-C8-C9
6	K	1631	B12	C42-C41-C8-C9
6	X	1631	B12	C14-C13-C48-C49
6	X	1631	B12	C42-C41-C8-C9
6	I	1631	B12	C2P-O3-P-O2
6	K	1631	B12	C2P-O3-P-O2

There are no ring outliers.

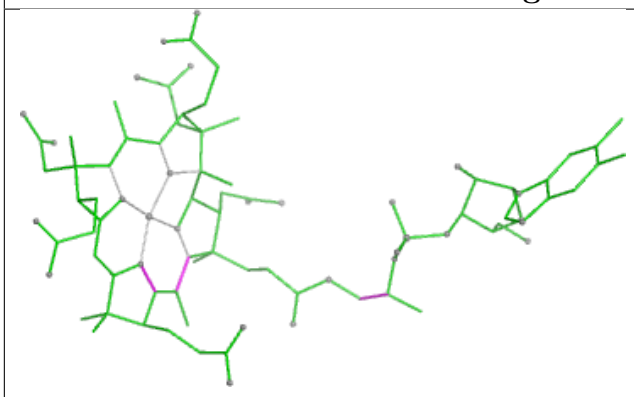
6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1444	B12	9	0
6	I	1631	B12	10	0
6	K	1631	B12	5	0
6	X	1631	B12	5	0
5	G	1444	SF4	1	0
5	A	1444	SF4	1	0

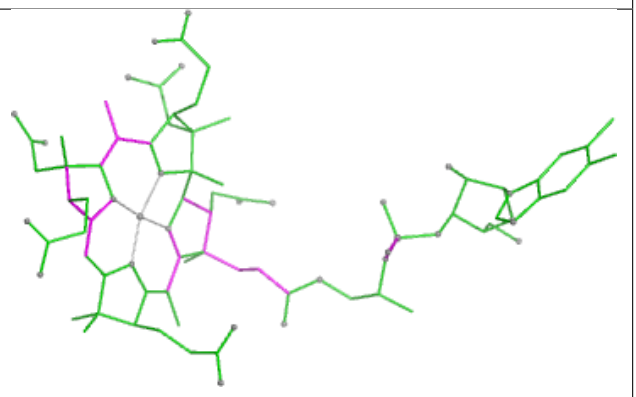
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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.

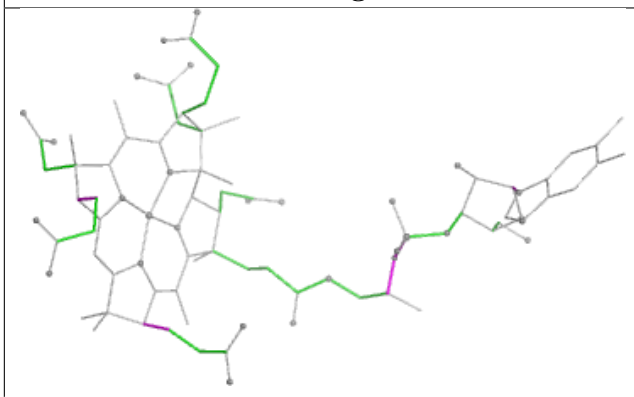
Ligand B12 C 1444



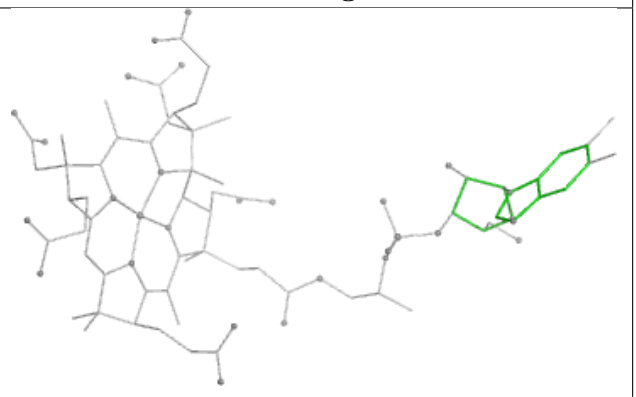
Bond lengths



Bond angles

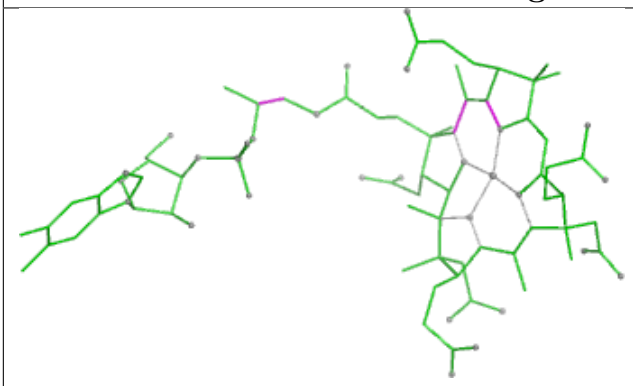


Torsions

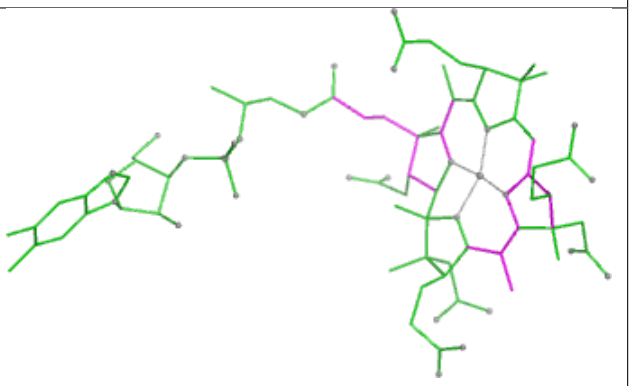


Rings

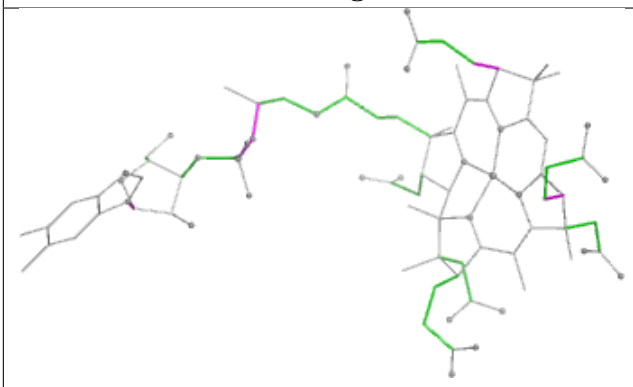
Ligand B12 I 1631



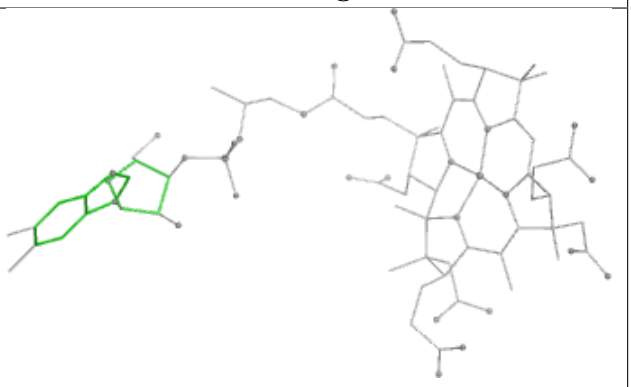
Bond lengths



Bond angles

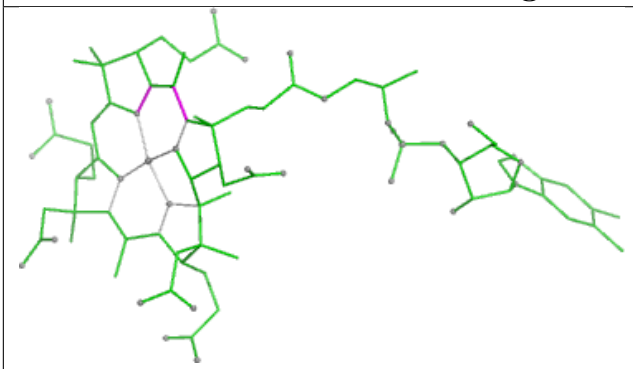


Torsions

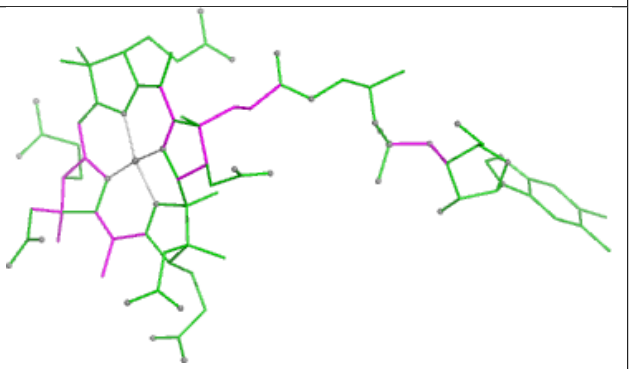


Rings

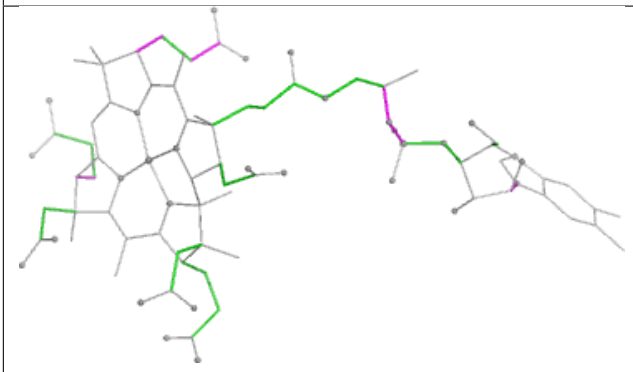
Ligand B12 K 1631



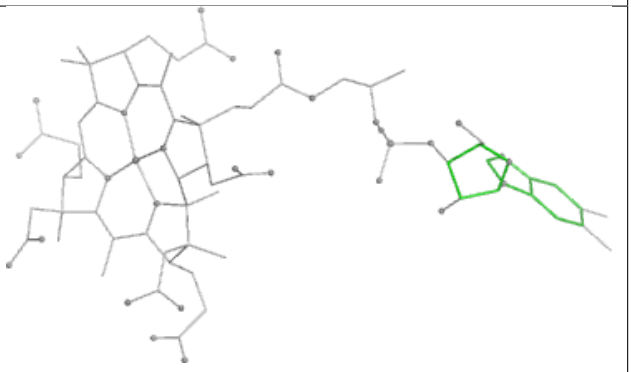
Bond lengths



Bond angles

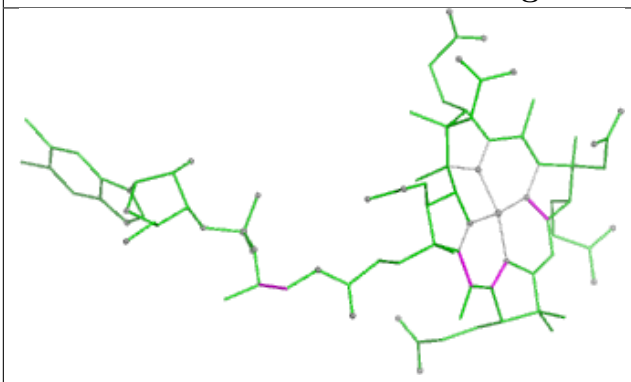


Torsions

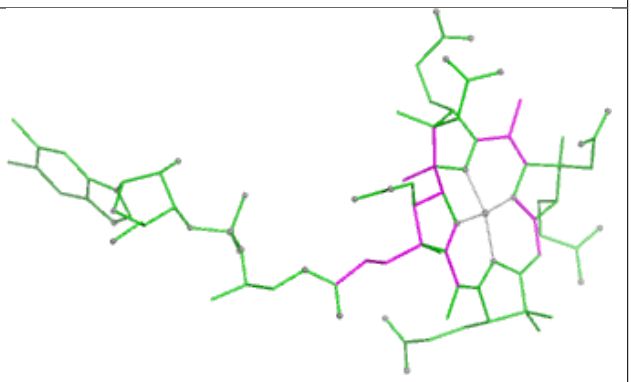


Rings

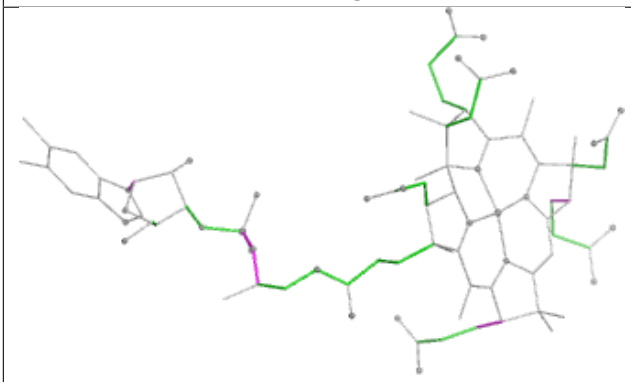
Ligand B12 X 1631



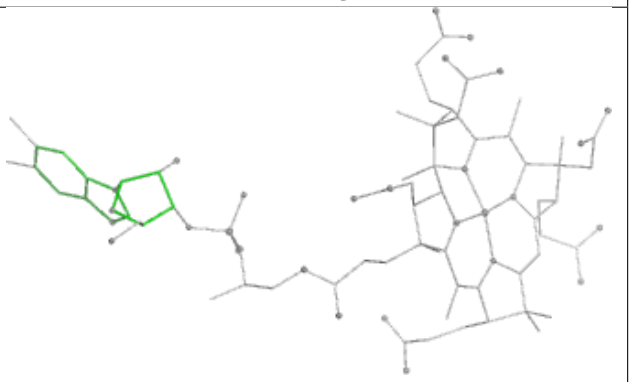
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	442/442 (100%)	-1.63	0	100	100	21, 40, 54, 66	2 (0%)
1	C	442/442 (100%)	-1.60	0	100	100	23, 39, 65, 86	1 (0%)
1	E	442/442 (100%)	-1.66	0	100	100	23, 37, 51, 58	1 (0%)
1	G	441/442 (99%)	-1.59	0	100	100	29, 47, 66, 82	0
2	B	309/309 (100%)	-1.66	0	100	100	23, 36, 50, 67	0
2	D	309/309 (100%)	-1.64	0	100	100	24, 38, 53, 74	0
2	F	309/309 (100%)	-1.63	0	100	100	24, 36, 51, 63	0
2	H	309/309 (100%)	-1.61	0	100	100	29, 43, 60, 68	0
3	I	509/509 (100%)	-1.67	0	100	100	24, 33, 45, 61	5 (0%)
3	J	509/509 (100%)	-1.66	0	100	100	21, 34, 47, 65	3 (0%)
3	X	509/509 (100%)	-1.67	0	100	100	23, 34, 47, 60	3 (0%)
4	K	510/510 (100%)	-1.64	0	100	100	25, 37, 52, 72	3 (0%)
All	All	5040/5041 (99%)	-1.64	0	100	100	21, 37, 56, 86	18 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

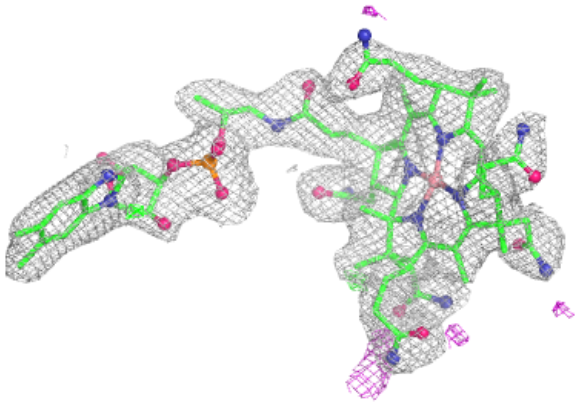
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

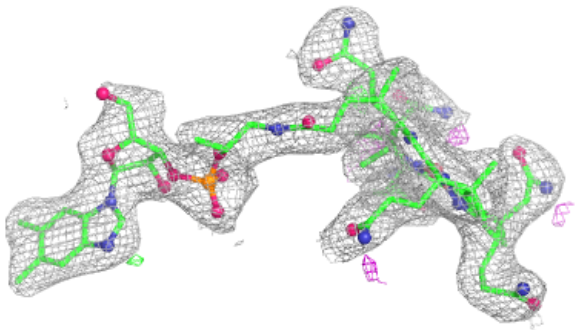
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SF4	A	1444	8/8	1.00	0.02	30,33,38,39	0
5	SF4	C	1445	8/8	1.00	0.01	43,47,58,61	0
5	SF4	E	1444	8/8	1.00	0.03	29,38,41,43	0
5	SF4	G	1444	8/8	1.00	0.02	36,42,46,47	0
6	B12	C	1444	91/91	1.00	0.03	21,29,38,46	0
6	B12	I	1631	91/91	1.00	0.02	17,24,31,41	0
6	B12	K	1631	91/91	1.00	0.03	24,32,38,52	0
6	B12	X	1631	91/91	1.00	0.03	20,26,35,47	0

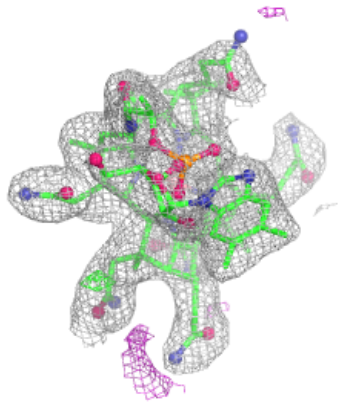
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B12 C 1444:

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

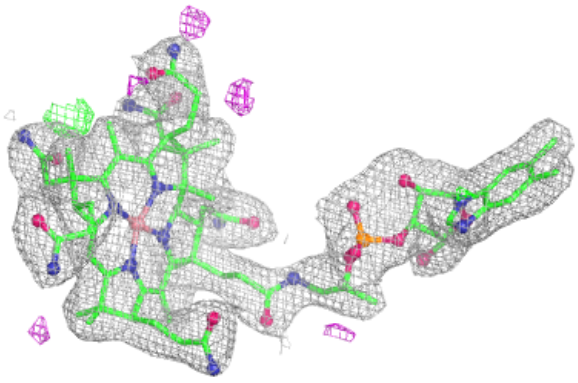


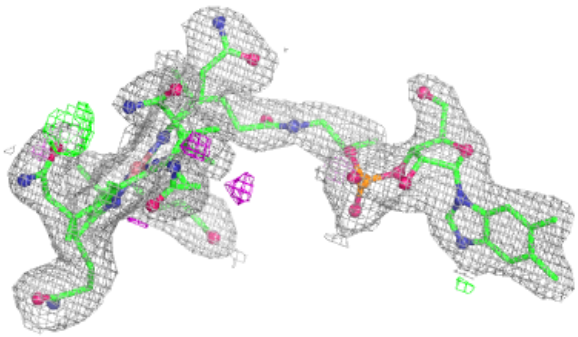


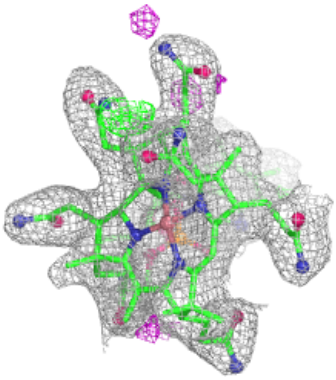


Electron density around B12 I 1631:

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

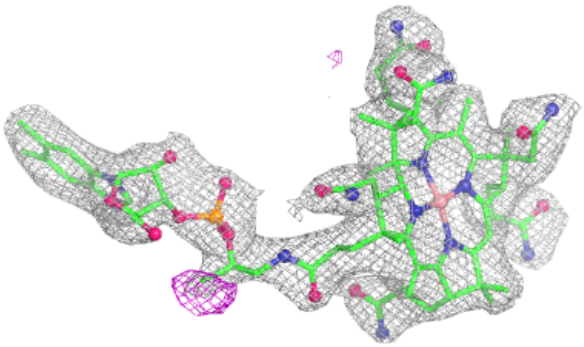


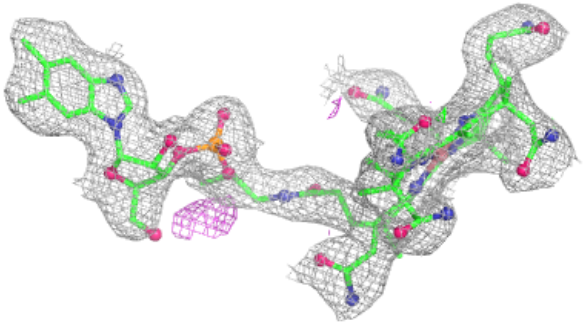


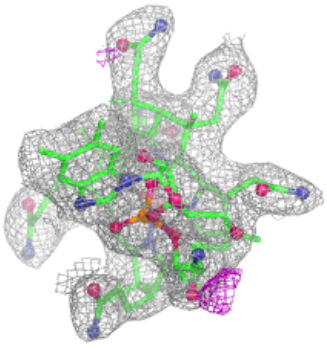


Electron density around B12 K 1631:

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

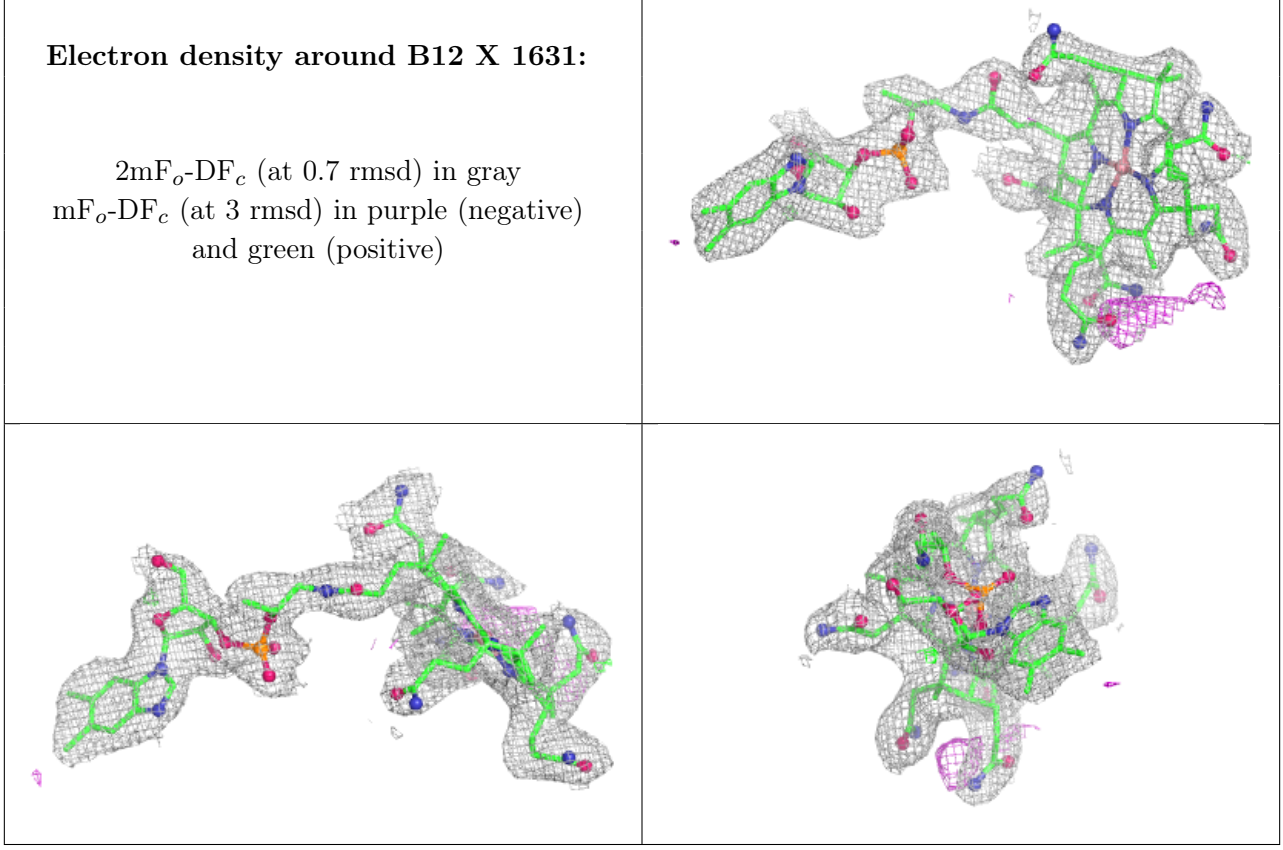






Electron density around B12 X 1631:

$2mF_o$-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.