



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:20 PM UTC

PDB ID : 5NTD / pdb_00005ntd
Title : Structure of Leucyl aminopeptidase from Trypanosoma brucei in complex with Bestatin
Authors : Timm, J.; Wilson, K.
Deposited on : 2017-04-27
Resolution : 2.30 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

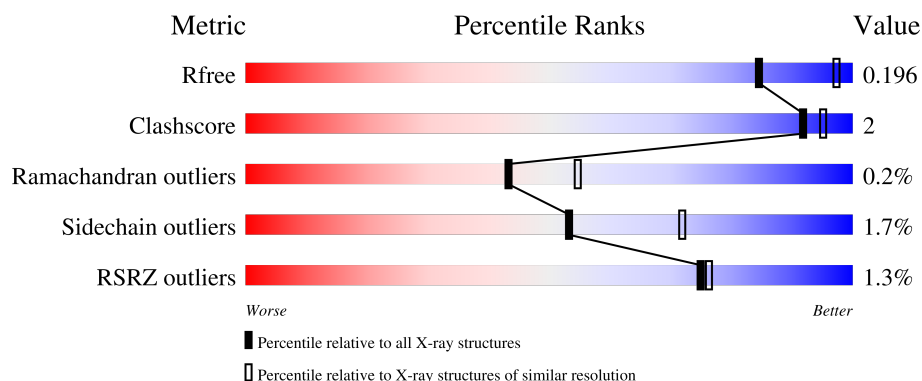
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	521	2% 93% 6%
1	B	521	0% 95% 5%
1	C	521	2% 95% 3%
1	D	521	2% 96% 2%
1	E	521	0% 95% 5%

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Mol	Chain	Length	Quality of chain
1	F	521	% 96% .
1	G	521	% 95% 5% .
1	H	521	% 96% .
1	I	521	2% 95% .
1	J	521	% 95% .
1	K	521	2% 94% 5% .
1	L	521	% 96% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 48865 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 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	2	0
			3833	2427	647	737	22			
1	B	519	Total	C	N	O	S	0	2	0
			3805	2407	643	733	22			
1	D	519	Total	C	N	O	S	0	0	0
			3809	2412	645	730	22			
1	C	518	Total	C	N	O	S	0	1	0
			3807	2408	646	731	22			
1	E	519	Total	C	N	O	S	0	1	0
			3809	2411	646	730	22			
1	F	519	Total	C	N	O	S	0	0	0
			3808	2408	647	731	22			
1	G	520	Total	C	N	O	S	0	2	0
			3812	2411	642	737	22			
1	H	519	Total	C	N	O	S	0	0	0
			3790	2397	642	729	22			
1	I	519	Total	C	N	O	S	0	1	0
			3785	2397	646	720	22			
1	J	519	Total	C	N	O	S	0	0	0
			3811	2412	645	732	22			
1	K	519	Total	C	N	O	S	0	0	0
			3781	2395	642	722	22			
1	L	519	Total	C	N	O	S	0	0	0
			3781	2393	637	729	22			

There are 24 discrepancies between the modelled and reference sequences:

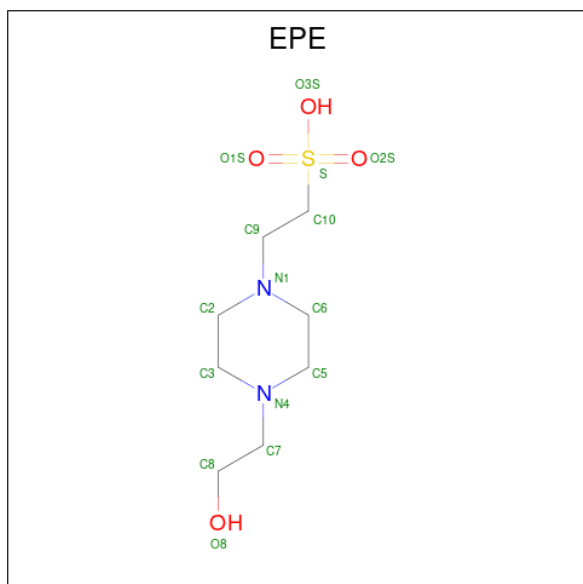
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	THR	conflict	UNP Q385B0
A	139	THR	ALA	conflict	UNP Q385B0
B	32	ALA	THR	conflict	UNP Q385B0
B	139	THR	ALA	conflict	UNP Q385B0
D	32	ALA	THR	conflict	UNP Q385B0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	139	THR	ALA	conflict	UNP Q385B0
C	32	ALA	THR	conflict	UNP Q385B0
C	139	THR	ALA	conflict	UNP Q385B0
E	32	ALA	THR	conflict	UNP Q385B0
E	139	THR	ALA	conflict	UNP Q385B0
F	32	ALA	THR	conflict	UNP Q385B0
F	139	THR	ALA	conflict	UNP Q385B0
G	32	ALA	THR	conflict	UNP Q385B0
G	139	THR	ALA	conflict	UNP Q385B0
H	32	ALA	THR	conflict	UNP Q385B0
H	139	THR	ALA	conflict	UNP Q385B0
I	32	ALA	THR	conflict	UNP Q385B0
I	139	THR	ALA	conflict	UNP Q385B0
J	32	ALA	THR	conflict	UNP Q385B0
J	139	THR	ALA	conflict	UNP Q385B0
K	32	ALA	THR	conflict	UNP Q385B0
K	139	THR	ALA	conflict	UNP Q385B0
L	32	ALA	THR	conflict	UNP Q385B0
L	139	THR	ALA	conflict	UNP Q385B0

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



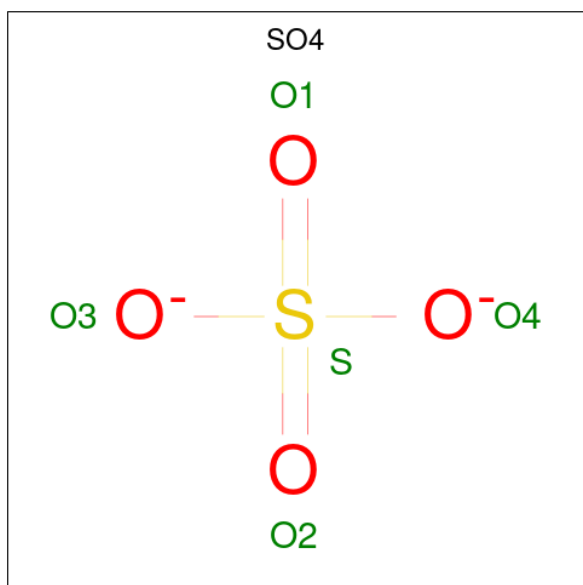
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		

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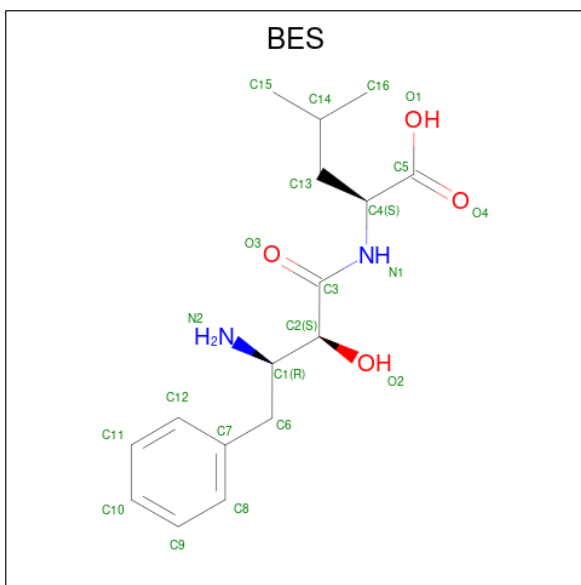
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

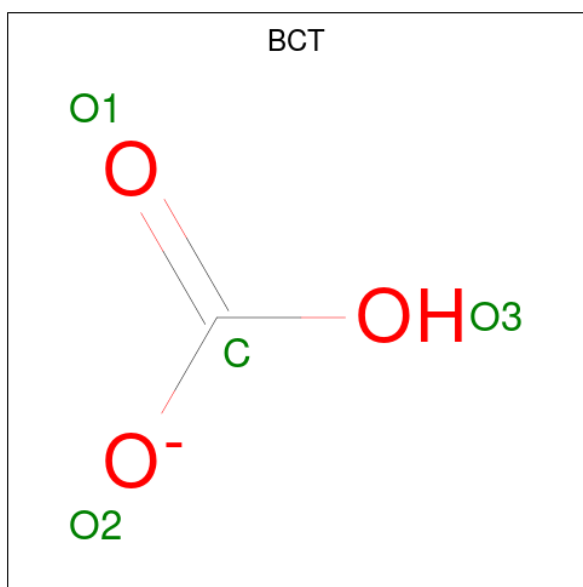
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		
4	B	2	Total	Mn	0	0
			2	2		
4	D	2	Total	Mn	0	0
			2	2		
4	C	2	Total	Mn	0	0
			2	2		
4	E	2	Total	Mn	0	0
			2	2		
4	F	2	Total	Mn	0	0
			2	2		
4	G	2	Total	Mn	0	0
			2	2		
4	H	2	Total	Mn	0	0
			2	2		
4	I	2	Total	Mn	0	0
			2	2		
4	J	2	Total	Mn	0	0
			2	2		
4	K	2	Total	Mn	0	0
			2	2		
4	L	2	Total	Mn	0	0
			2	2		

- Molecule 5 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (CCD ID: BES) (formula: C₁₆H₂₄N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 22	C 16	N 2	O 4	0	0
5	B	1	Total 22	C 16	N 2	O 4	0	0
5	D	1	Total 22	C 16	N 2	O 4	0	0
5	C	1	Total 22	C 16	N 2	O 4	0	0
5	E	1	Total 22	C 16	N 2	O 4	0	0
5	F	1	Total 22	C 16	N 2	O 4	0	0
5	G	1	Total 22	C 16	N 2	O 4	0	0
5	H	1	Total 22	C 16	N 2	O 4	0	0
5	I	1	Total 22	C 16	N 2	O 4	0	0
5	J	1	Total 22	C 16	N 2	O 4	0	0
5	K	1	Total 22	C 16	N 2	O 4	0	0
5	L	1	Total 22	C 16	N 2	O 4	0	0

- Molecule 6 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	B	1	Total	C	O	0	0
			4	1	3		
6	D	1	Total	C	O	0	0
			4	1	3		
6	C	1	Total	C	O	0	0
			4	1	3		
6	E	1	Total	C	O	0	0
			4	1	3		
6	F	1	Total	C	O	0	0
			4	1	3		
6	G	1	Total	C	O	0	0
			4	1	3		
6	H	1	Total	C	O	0	0
			4	1	3		
6	I	1	Total	C	O	0	0
			4	1	3		
6	J	1	Total	C	O	0	0
			4	1	3		
6	K	1	Total	C	O	0	0
			4	1	3		
6	L	1	Total	C	O	0	0
			4	1	3		

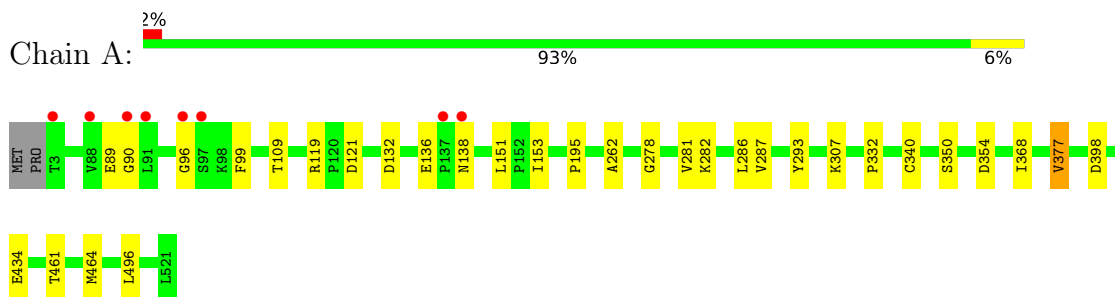
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	294	Total 294	O 294	0	0
7	B	222	Total 222	O 222	0	0
7	D	321	Total 321	O 321	0	0
7	C	235	Total 235	O 235	0	0
7	E	248	Total 248	O 248	0	0
7	F	220	Total 220	O 220	0	0
7	G	231	Total 231	O 231	0	0
7	H	212	Total 212	O 212	0	0
7	I	130	Total 130	O 130	0	0
7	J	251	Total 251	O 251	0	0
7	K	217	Total 217	O 217	0	0
7	L	217	Total 217	O 217	0	0

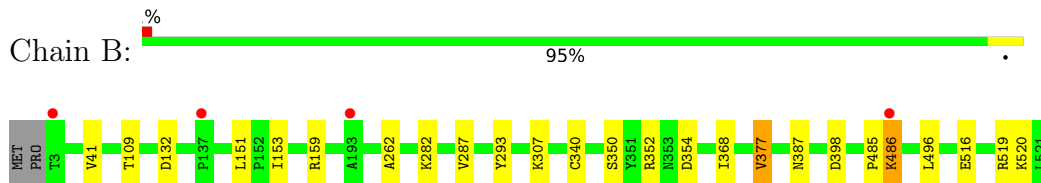
3 Residue-property plots

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.

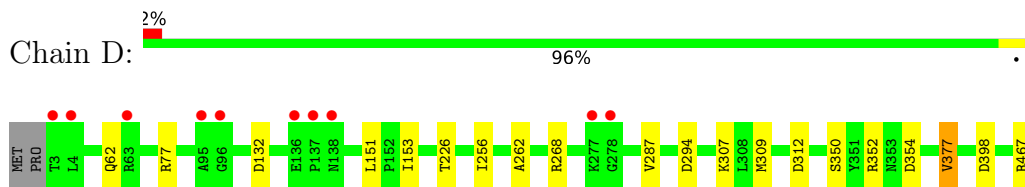
- Molecule 1: leucyl aminopeptidase



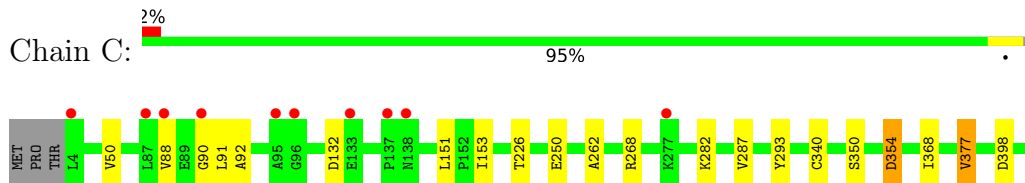
- Molecule 1: leucyl aminopeptidase



- Molecule 1: leucyl aminopeptidase



- Molecule 1: leucyl aminopeptidase



- Molecule 1: leucyl aminopeptidase





- Molecule 1: leucyl aminopeptidase



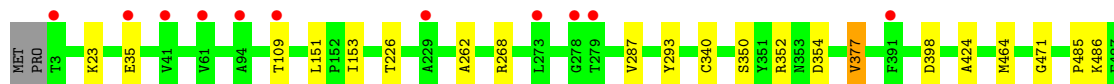
- Molecule 1: leucyl aminopeptidase



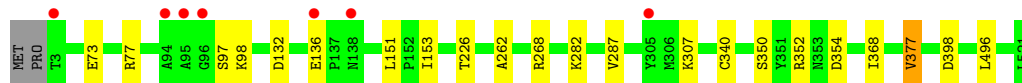
- Molecule 1: leucyl aminopeptidase



- Molecule 1: leucyl aminopeptidase

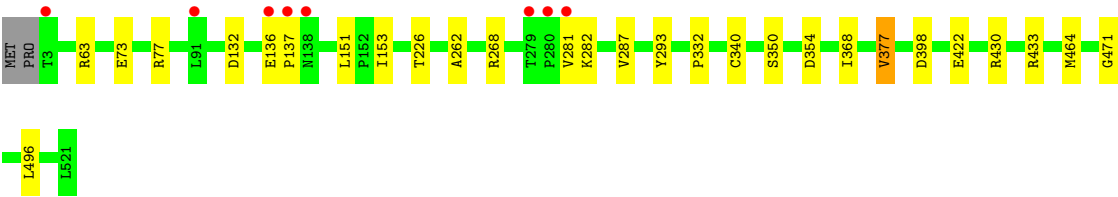


- Molecule 1: leucyl aminopeptidase



- Molecule 1: leucyl aminopeptidase





• Molecule 1: leucyl aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.26Å 143.45Å 268.03Å 90.00° 95.54° 90.00°	Depositor
Resolution (Å)	80.33 – 2.30 80.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (80.33-2.30) 99.7 (80.33-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.189 , 0.214 (Not available) , 0.196	Depositor DCC
R_{free} test set	14322 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	48865	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: SO4, BCT, EPE, MN, BES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.11	3/3913 (0.1%)	0.98	2/5337 (0.0%)
1	B	1.05	0/3889	0.95	1/5313 (0.0%)
1	C	1.06	2/3888 (0.1%)	0.93	1/5307 (0.0%)
1	D	1.10	0/3887	0.94	1/5305 (0.0%)
1	E	1.05	0/3890	0.95	1/5311 (0.0%)
1	F	1.07	1/3886 (0.0%)	0.93	0/5306
1	G	1.06	3/3896 (0.1%)	0.93	1/5322 (0.0%)
1	H	1.10	1/3868 (0.0%)	0.93	0/5285
1	I	1.05	1/3866 (0.0%)	0.92	0/5282
1	J	1.08	2/3889 (0.1%)	0.93	0/5308
1	K	1.07	1/3859 (0.0%)	0.94	2/5272 (0.0%)
1	L	1.09	2/3859 (0.1%)	0.92	0/5275
All	All	1.07	16/46590 (0.0%)	0.94	9/63623 (0.0%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	137	PRO	CA-C	7.33	1.61	1.53
1	L	234	LYS	N-CA	6.18	1.53	1.46
1	J	136	GLU	N-CA	5.55	1.49	1.46
1	A	282	LYS	N-CA	5.48	1.53	1.46
1	A	138	ASN	N-CA	5.41	1.53	1.46
1	C	354	ASP	N-CA	5.35	1.53	1.46
1	G	250	GLU	N-CA	5.33	1.52	1.46
1	F	250	GLU	N-CA	5.29	1.52	1.46
1	J	98	LYS	C-O	-5.29	1.18	1.24
1	I	35	GLU	N-CA	5.21	1.52	1.46
1	A	195	PRO	CA-C	5.20	1.54	1.51
1	C	250	GLU	N-CA	5.19	1.52	1.46
1	L	35	GLU	N-CA	5.19	1.52	1.46
1	G	354	ASP	N-CA	5.18	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	354	ASP	N-CA	5.12	1.52	1.46
1	G	136	GLU	N-CA	5.07	1.50	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	486	LYS	CB-CG-CD	7.48	128.50	111.30
1	K	136	GLU	CA-C-N	-7.29	113.18	120.98
1	K	136	GLU	C-N-CA	-7.29	113.18	120.98
1	A	278	GLY	N-CA-C	6.11	120.34	111.24
1	A	136	GLU	CB-CA-C	6.00	118.16	108.87
1	D	377	VAL	N-CA-CB	5.51	118.03	110.54
1	E	63	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	C	50	VAL	N-CA-C	5.23	115.65	108.12
1	G	2	PRO	N-CA-CB	5.07	108.58	103.00

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	3833	0	3758	21	0
1	B	3805	0	3695	14	0
1	C	3807	0	3717	17	0
1	D	3809	0	3726	16	0
1	E	3809	0	3717	15	0
1	F	3808	0	3715	8	0
1	G	3812	0	3703	13	0
1	H	3790	0	3681	13	0
1	I	3785	0	3680	18	0
1	J	3811	0	3726	11	0
1	K	3781	0	3677	15	0
1	L	3781	0	3655	11	0
2	A	15	0	17	1	0
2	E	15	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	15	0	18	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	22	0	21	0	0
5	B	22	0	21	0	0
5	C	22	0	21	0	0
5	D	22	0	21	0	0
5	E	22	0	21	0	0
5	F	22	0	21	0	0
5	G	22	0	21	0	0
5	H	22	0	21	0	0
5	I	22	0	21	0	0
5	J	22	0	21	0	0
5	K	22	0	21	0	0
5	L	22	0	21	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
6	E	4	0	1	0	0
6	F	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	4	0	0	0	0
6	H	4	0	0	0	0
6	I	4	0	0	0	0
6	J	4	0	0	0	0
6	K	4	0	0	0	0
6	L	4	0	0	0	0
7	A	294	0	0	4	0
7	B	222	0	0	1	0
7	C	235	0	0	1	0
7	D	321	0	0	1	0
7	E	248	0	0	2	0
7	F	220	0	0	0	0
7	G	231	0	0	5	0
7	H	212	0	0	3	0
7	I	130	0	0	2	0
7	J	251	0	0	0	0
7	K	217	0	0	4	0
7	L	217	0	0	0	0
All	All	48865	0	44755	147	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 2.

All (147) 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:K:422:GLU:CB	7:K:896:HOH:O	2.11	0.98
1:C:92:ALA:CB	1:I:485:PRO:HB2	2.02	0.89
1:A:119:ARG:NH1	1:A:121:ASP:OD2	2.15	0.79
1:C:92:ALA:HB2	1:I:485:PRO:HB2	1.63	0.78
1:D:294:ASP:HB3	1:D:309:MET:HE2	1.65	0.77
1:E:88:VAL:HG21	1:E:91:LEU:HD22	1.65	0.76
1:J:73:GLU:OE2	1:J:77:ARG:NH1	2.17	0.76
1:K:281:VAL:HG12	1:K:332:PRO:O	1.87	0.75
1:A:281:VAL:HG21	1:A:332:PRO:O	1.88	0.74
1:A:90:GLY:N	7:A:701:HOH:O	2.19	0.72
1:H:4:LEU:HD11	1:H:264:PHE:HE2	1.55	0.70
1:H:279:THR:HG22	7:H:911:HOH:O	1.89	0.70
1:C:92:ALA:HB1	1:I:485:PRO:HB2	1.73	0.69
1:K:433:ARG:NH1	7:K:701:HOH:O	2.19	0.69
1:C:90:GLY:O	1:I:486:LYS:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:CYS:HB3	1:C:377:VAL:HG13	1.78	0.66
1:D:309:MET:HE3	1:D:312:ASP:HB2	1.78	0.65
1:G:330:GLN:HG2	7:G:783:HOH:O	1.96	0.65
1:I:340:CYS:HB3	1:I:377:VAL:HG13	1.79	0.65
1:B:340:CYS:HB3	1:B:377:VAL:HG13	1.79	0.65
1:F:340:CYS:HB3	1:F:377:VAL:HG13	1.79	0.65
1:K:340:CYS:HB3	1:K:377:VAL:HG13	1.79	0.65
1:E:340:CYS:HB3	1:E:377:VAL:HG13	1.78	0.64
1:B:516:GLU:OE1	1:B:519:ARG:HD3	1.98	0.63
1:L:340:CYS:HB3	1:L:377:VAL:HG13	1.79	0.63
1:D:77:ARG:NH2	1:E:135:LYS:HE2	2.12	0.63
1:G:340:CYS:HB3	1:G:377:VAL:HG13	1.81	0.63
1:A:434:GLU:HG3	7:A:716:HOH:O	1.98	0.62
1:H:4:LEU:HD11	1:H:264:PHE:CE2	2.34	0.62
1:H:340:CYS:HB3	1:H:377:VAL:HG13	1.80	0.62
1:J:340:CYS:HB3	1:J:377:VAL:HG13	1.81	0.61
1:A:340:CYS:HB3	1:A:377:VAL:HG13	1.81	0.61
1:B:520:LYS:HE2	7:B:908:HOH:O	2.02	0.60
1:A:119:ARG:NH2	7:A:704:HOH:O	2.34	0.59
1:D:309:MET:CE	1:D:312:ASP:HB2	2.32	0.59
1:I:488:THR:O	1:I:488:THR:HG22	2.02	0.59
1:E:63:ARG:NH2	7:E:703:HOH:O	2.37	0.58
1:H:279:THR:CG2	7:H:911:HOH:O	2.51	0.58
1:E:88:VAL:CG2	1:E:91:LEU:HD22	2.35	0.56
1:D:309:MET:HE3	1:D:309:MET:HA	1.88	0.55
1:C:88:VAL:CG1	1:C:91:LEU:HG	2.36	0.55
1:D:294:ASP:CB	1:D:309:MET:HE2	2.34	0.55
1:C:88:VAL:HG12	1:C:91:LEU:HG	1.90	0.54
1:D:309:MET:HE1	1:D:312:ASP:CG	2.35	0.52
1:K:73:GLU:OE1	1:K:77:ARG:NH1	2.41	0.51
1:B:387:ASN:OD1	1:B:486:LYS:HD3	2.11	0.51
1:D:262:ALA:HB2	1:D:350:SER:HA	1.93	0.51
1:B:262:ALA:HB2	1:B:350:SER:HA	1.92	0.51
1:D:256:ILE:HA	1:D:377:VAL:HG12	1.91	0.51
1:A:119:ARG:NH1	1:A:121:ASP:CG	2.69	0.50
1:B:516:GLU:O	1:B:519:ARG:HG2	2.12	0.50
1:H:4:LEU:CD1	1:H:4:LEU:N	2.74	0.50
1:D:309:MET:CE	1:D:312:ASP:CG	2.84	0.50
1:G:79:LYS:NZ	7:G:705:HOH:O	2.45	0.50
1:A:262:ALA:HB2	1:A:350:SER:HA	1.94	0.49
1:G:135:LYS:HG2	7:G:906:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:293:TYR:CD2	1:I:352:ARG:HD3	2.48	0.49
1:I:488:THR:O	1:I:488:THR:CG2	2.59	0.49
1:E:101:ARG:HG2	1:E:133:GLU:OE1	2.13	0.48
1:I:262:ALA:HB2	1:I:350:SER:HA	1.95	0.48
1:J:262:ALA:HB2	1:J:350:SER:HA	1.96	0.48
1:C:90:GLY:O	1:I:486:LYS:CG	2.61	0.48
1:G:4:LEU:HD12	1:G:4:LEU:N	2.28	0.48
1:H:4:LEU:N	1:H:4:LEU:HD12	2.29	0.48
1:H:262:ALA:HB2	1:H:350:SER:HA	1.94	0.48
1:K:262:ALA:HB2	1:K:350:SER:HA	1.95	0.48
1:C:262:ALA:HB2	1:C:350:SER:HA	1.95	0.48
1:G:103:VAL:CG2	1:G:133:GLU:OE1	2.62	0.48
2:A:601:EPE:O2S	2:L:601:EPE:H81	2.14	0.48
1:F:262:ALA:HB2	1:F:350:SER:HA	1.96	0.47
1:E:340:CYS:CB	1:E:377:VAL:HG13	2.45	0.47
1:J:307:LYS:HE3	1:K:368:ILE:HD13	1.97	0.47
1:L:262:ALA:HB2	1:L:350:SER:HA	1.96	0.47
1:B:340:CYS:CB	1:B:377:VAL:HG13	2.45	0.47
1:C:92:ALA:HB1	1:I:485:PRO:CB	2.42	0.47
1:G:262:ALA:HB2	1:G:350:SER:HA	1.96	0.46
1:H:89:GLU:CB	7:H:912:HOH:O	2.63	0.46
1:J:307:LYS:HE3	1:K:368:ILE:CD1	2.45	0.46
1:L:340:CYS:CB	1:L:377:VAL:HG13	2.46	0.46
1:A:119:ARG:HH11	1:A:121:ASP:CG	2.24	0.46
1:E:262:ALA:HB2	1:E:350:SER:HA	1.96	0.46
1:G:352:ARG:HD3	1:I:293:TYR:CD2	2.51	0.46
1:G:103:VAL:HG22	1:G:133:GLU:OE1	2.16	0.45
1:A:293:TYR:CD2	1:B:352:ARG:HD3	2.52	0.45
1:A:368:ILE:HD13	1:D:307:LYS:HE3	1.98	0.45
1:F:287:VAL:O	1:F:398:ASP:HA	2.17	0.45
1:A:89:GLU:HG3	1:A:99:PHE:CE2	2.51	0.45
1:C:340:CYS:CB	1:C:377:VAL:HG13	2.46	0.45
1:H:340:CYS:CB	1:H:377:VAL:HG13	2.47	0.45
1:K:293:TYR:CD2	1:L:352:ARG:HD3	2.51	0.45
1:A:307:LYS:HE3	1:B:368:ILE:HD13	1.98	0.45
1:B:293:TYR:CD2	1:D:352:ARG:HD3	2.52	0.45
1:I:287:VAL:O	1:I:398:ASP:HA	2.16	0.45
1:A:368:ILE:CD1	1:D:307:LYS:HE3	2.47	0.44
1:D:287:VAL:O	1:D:398:ASP:HA	2.17	0.44
1:C:467:ARG:NH1	7:C:709:HOH:O	2.50	0.44
1:J:352:ARG:HD3	1:L:293:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:287:VAL:O	1:J:398:ASP:HA	2.17	0.44
1:L:287:VAL:O	1:L:398:ASP:HA	2.18	0.44
1:B:287:VAL:O	1:B:398:ASP:HA	2.17	0.44
1:C:287:VAL:O	1:C:398:ASP:HA	2.17	0.44
1:E:412:ARG:HD2	7:E:884:HOH:O	2.18	0.44
1:K:63:ARG:NH1	7:K:703:HOH:O	2.48	0.44
1:I:23:LYS:HA	7:I:820:HOH:O	2.17	0.43
1:E:293:TYR:CD2	1:F:352:ARG:HD3	2.53	0.43
1:A:307:LYS:HE3	1:B:368:ILE:CD1	2.48	0.43
1:G:287:VAL:O	1:G:398:ASP:HA	2.18	0.43
1:C:293:TYR:CD2	1:E:352:ARG:HD3	2.54	0.43
1:F:340:CYS:CB	1:F:377:VAL:HG13	2.46	0.43
1:G:226:THR:OG1	1:G:268:ARG:HD3	2.19	0.43
1:K:287:VAL:O	1:K:398:ASP:HA	2.17	0.43
1:J:340:CYS:CB	1:J:377:VAL:HG13	2.48	0.43
1:G:467:ARG:HD2	7:G:754:HOH:O	2.18	0.43
1:H:287:VAL:O	1:H:398:ASP:HA	2.18	0.43
1:A:287:VAL:O	1:A:398:ASP:HA	2.19	0.43
1:J:368:ILE:HD13	1:L:307:LYS:HE3	2.00	0.43
1:E:287:VAL:O	1:E:398:ASP:HA	2.18	0.43
1:I:226:THR:OG1	1:I:268:ARG:HD3	2.19	0.43
1:I:424:ALA:N	7:I:706:HOH:O	2.47	0.42
1:K:340:CYS:CB	1:K:377:VAL:HG13	2.46	0.42
1:J:368:ILE:CD1	1:L:307:LYS:HE3	2.49	0.42
1:C:368:ILE:CD1	1:F:307:LYS:HE3	2.50	0.42
1:F:226:THR:OG1	1:F:268:ARG:HD3	2.19	0.42
1:A:96:GLY:O	2:L:601:EPE:H51	2.20	0.42
1:I:340:CYS:CB	1:I:377:VAL:HG13	2.47	0.42
1:A:281:VAL:CG2	1:A:332:PRO:O	2.64	0.42
1:L:226:THR:OG1	1:L:268:ARG:HD3	2.20	0.41
1:A:340:CYS:CB	1:A:377:VAL:HG13	2.50	0.41
1:B:485:PRO:HB2	1:L:41:VAL:CG2	2.50	0.41
1:D:226:THR:OG1	1:D:268:ARG:HD3	2.21	0.41
1:B:307:LYS:CB	7:D:967:HOH:O	2.69	0.41
1:D:309:MET:CE	1:D:312:ASP:CB	2.98	0.41
1:G:412:ARG:HD2	7:G:832:HOH:O	2.20	0.41
1:I:464:MET:HE1	1:I:471:GLY:HA2	2.02	0.41
1:K:430:ARG:NH2	7:K:709:HOH:O	2.54	0.41
1:L:68:ASN:OD1	1:L:68:ASN:C	2.64	0.41
1:C:368:ILE:HD13	1:F:307:LYS:HE3	2.03	0.40
1:E:68:ASN:OD1	1:E:68:ASN:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:ILE:HG12	1:E:461:THR:HB	2.04	0.40
1:A:368:ILE:HG12	1:A:461:THR:HB	2.03	0.40
1:A:464:MET:HE1	7:A:873:HOH:O	2.21	0.40
1:J:226:THR:OG1	1:J:268:ARG:HD3	2.21	0.40
1:K:464:MET:HE1	1:K:471:GLY:HA2	2.03	0.40
1:C:226:THR:OG1	1:C:268:ARG:HD3	2.21	0.40
1:H:368:ILE:HG12	1:H:461:THR:HB	2.04	0.40
1:E:226:THR:OG1	1:E:268:ARG:HD3	2.21	0.40
1:K:226:THR:OG1	1:K:268:ARG:HD3	2.22	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	518/521 (99%)	509 (98%)	8 (2%)	1 (0%)	43	55
1	B	519/521 (100%)	509 (98%)	9 (2%)	1 (0%)	43	55
1	C	517/521 (99%)	508 (98%)	8 (2%)	1 (0%)	43	55
1	D	517/521 (99%)	507 (98%)	9 (2%)	1 (0%)	43	55
1	E	518/521 (99%)	509 (98%)	8 (2%)	1 (0%)	43	55
1	F	517/521 (99%)	508 (98%)	8 (2%)	1 (0%)	43	55
1	G	520/521 (100%)	510 (98%)	9 (2%)	1 (0%)	43	55
1	H	517/521 (99%)	508 (98%)	8 (2%)	1 (0%)	43	55
1	I	518/521 (99%)	507 (98%)	10 (2%)	1 (0%)	43	55
1	J	517/521 (99%)	508 (98%)	8 (2%)	1 (0%)	43	55
1	K	517/521 (99%)	508 (98%)	8 (2%)	1 (0%)	43	55
1	L	517/521 (99%)	508 (98%)	8 (2%)	1 (0%)	43	55
All	All	6212/6252 (99%)	6099 (98%)	101 (2%)	12 (0%)	43	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ASP
1	B	354	ASP
1	D	354	ASP
1	C	354	ASP
1	E	354	ASP
1	F	354	ASP
1	G	354	ASP
1	H	354	ASP
1	I	354	ASP
1	J	354	ASP
1	K	354	ASP
1	L	354	ASP

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	398/411 (97%)	391 (98%)	7 (2%)	51	70
1	B	391/411 (95%)	382 (98%)	9 (2%)	44	63
1	C	393/411 (96%)	387 (98%)	6 (2%)	57	75
1	D	393/411 (96%)	387 (98%)	6 (2%)	57	75
1	E	392/411 (95%)	384 (98%)	8 (2%)	48	67
1	F	393/411 (96%)	387 (98%)	6 (2%)	57	75
1	G	393/411 (96%)	387 (98%)	6 (2%)	57	75
1	H	389/411 (95%)	383 (98%)	6 (2%)	57	75
1	I	385/411 (94%)	380 (99%)	5 (1%)	61	77
1	J	394/411 (96%)	387 (98%)	7 (2%)	51	70
1	K	386/411 (94%)	380 (98%)	6 (2%)	55	73
1	L	386/411 (94%)	380 (98%)	6 (2%)	55	73
All	All	4693/4932 (95%)	4615 (98%)	78 (2%)	53	72

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	THR
1	A	132	ASP
1	A	151	LEU
1	A	153	ILE
1	A	286	LEU
1	A	377	VAL
1	A	496	LEU
1	B	41	VAL
1	B	109	THR
1	B	132	ASP
1	B	151	LEU
1	B	153	ILE
1	B	159	ARG
1	B	282	LYS
1	B	377	VAL
1	B	496	LEU
1	D	62	GLN
1	D	132	ASP
1	D	151	LEU
1	D	153	ILE
1	D	467	ARG
1	D	496	LEU
1	C	132	ASP
1	C	151	LEU
1	C	153	ILE
1	C	282	LYS
1	C	377	VAL
1	C	496	LEU
1	E	88	VAL
1	E	132	ASP
1	E	135	LYS
1	E	151	LEU
1	E	153	ILE
1	E	282	LYS
1	E	377	VAL
1	E	496	LEU
1	F	54	LYS
1	F	132	ASP
1	F	151	LEU
1	F	153	ILE
1	F	377	VAL
1	F	496	LEU

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Mol	Chain	Res	Type
1	G	132	ASP
1	G	151	LEU
1	G	153	ILE
1	G	282	LYS
1	G	377	VAL
1	G	496	LEU
1	H	132	ASP
1	H	151	LEU
1	H	153	ILE
1	H	282	LYS
1	H	377	VAL
1	H	496	LEU
1	I	109	THR
1	I	151	LEU
1	I	153	ILE
1	I	377	VAL
1	I	496	LEU
1	J	97	SER
1	J	132	ASP
1	J	151	LEU
1	J	153	ILE
1	J	282	LYS
1	J	377	VAL
1	J	496	LEU
1	K	132	ASP
1	K	151	LEU
1	K	153	ILE
1	K	282	LYS
1	K	377	VAL
1	K	496	LEU
1	L	109	THR
1	L	132	ASP
1	L	151	LEU
1	L	153	ILE
1	L	377	VAL
1	L	496	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	ASN
1	D	387	ASN

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Mol	Chain	Res	Type
1	C	387	ASN
1	E	387	ASN
1	F	185	GLN
1	F	387	ASN
1	G	387	ASN
1	H	185	GLN
1	H	387	ASN
1	I	185	GLN
1	I	387	ASN
1	J	185	GLN
1	J	387	ASN
1	J	504	ASN
1	K	185	GLN
1	K	387	ASN
1	L	148	ASN
1	L	185	GLN
1	L	504	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](#)

Of 62 ligands modelled in this entry, 24 are monoatomic - leaving 38 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
6	BCT	I	605	-	3,3,3	0.87	0	2,3,3	2.27	1 (50%)
2	EPE	L	601	-	15,15,15	1.81	1 (6%)	19,20,20	2.09	6 (31%)
6	BCT	L	606	-	3,3,3	1.63	1 (33%)	2,3,3	1.98	1 (50%)
3	SO4	G	601	-	4,4,4	0.39	0	6,6,6	0.35	0
6	BCT	B	605	-	3,3,3	0.96	0	2,3,3	1.33	0
3	SO4	L	602	-	4,4,4	0.38	0	6,6,6	0.16	0
5	BES	G	604	4	22,22,22	0.94	2 (9%)	26,29,29	1.62	3 (11%)
5	BES	J	604	4	22,22,22	1.28	4 (18%)	26,29,29	1.52	4 (15%)
3	SO4	C	601	-	4,4,4	0.46	0	6,6,6	0.88	0
6	BCT	C	605	-	3,3,3	1.20	0	2,3,3	1.58	1 (50%)
5	BES	H	604	4	22,22,22	0.99	1 (4%)	26,29,29	1.64	5 (19%)
6	BCT	E	605	-	3,3,3	0.75	0	2,3,3	1.25	0
3	SO4	D	601	-	4,4,4	0.31	0	6,6,6	0.40	0
6	BCT	J	605	-	3,3,3	0.75	0	2,3,3	1.69	0
3	SO4	B	601	-	4,4,4	0.39	0	6,6,6	0.35	0
3	SO4	I	601	-	4,4,4	0.21	0	6,6,6	0.45	0
5	BES	L	605	4	22,22,22	0.82	1 (4%)	26,29,29	1.73	7 (26%)
2	EPE	E	601	-	15,15,15	2.15	1 (6%)	19,20,20	1.69	3 (15%)
3	SO4	A	602	-	4,4,4	0.42	0	6,6,6	0.43	0
5	BES	F	604	4	22,22,22	0.97	0	26,29,29	1.72	5 (19%)
6	BCT	K	605	-	3,3,3	0.41	0	2,3,3	2.95	2 (100%)
6	BCT	F	605	-	3,3,3	2.03	1 (33%)	2,3,3	1.18	0
3	SO4	H	601	-	4,4,4	0.58	0	6,6,6	0.62	0
5	BES	B	604	4	22,22,22	0.79	0	26,29,29	1.65	6 (23%)
5	BES	C	604	4	22,22,22	0.78	1 (4%)	26,29,29	1.59	4 (15%)
5	BES	A	605	4	22,22,22	0.88	1 (4%)	26,29,29	1.76	5 (19%)
5	BES	E	604	4	22,22,22	1.00	2 (9%)	26,29,29	1.59	5 (19%)
5	BES	I	604	4	22,22,22	1.21	3 (13%)	26,29,29	1.74	5 (19%)
6	BCT	D	605	-	3,3,3	1.06	0	2,3,3	4.60	2 (100%)
6	BCT	H	605	-	3,3,3	0.87	0	2,3,3	0.43	0
5	BES	K	604	4	22,22,22	1.04	2 (9%)	26,29,29	1.70	6 (23%)
6	BCT	G	605	-	3,3,3	1.86	1 (33%)	2,3,3	1.08	0
3	SO4	J	601	-	4,4,4	0.43	0	6,6,6	0.53	0
5	BES	D	604	4	22,22,22	0.93	2 (9%)	26,29,29	1.83	5 (19%)
3	SO4	K	601	-	4,4,4	0.22	0	6,6,6	0.25	0
2	EPE	A	601	-	15,15,15	1.95	1 (6%)	19,20,20	1.58	2 (10%)
6	BCT	A	606	-	3,3,3	1.07	0	2,3,3	1.74	0
3	SO4	F	601	-	4,4,4	0.30	0	6,6,6	0.36	0

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
5	BES	C	604	4	-	11/24/24/24	0/1/1/1
5	BES	L	605	4	-	9/24/24/24	0/1/1/1
5	BES	A	605	4	-	6/24/24/24	0/1/1/1
2	EPE	E	601	-	-	1/9/19/19	0/1/1/1
5	BES	G	604	4	-	7/24/24/24	0/1/1/1
5	BES	F	604	4	-	6/24/24/24	0/1/1/1
2	EPE	L	601	-	-	4/9/19/19	0/1/1/1
5	BES	E	604	4	-	8/24/24/24	0/1/1/1
5	BES	H	604	4	-	8/24/24/24	0/1/1/1
5	BES	I	604	4	-	8/24/24/24	0/1/1/1
5	BES	J	604	4	-	8/24/24/24	0/1/1/1
5	BES	K	604	4	-	8/24/24/24	0/1/1/1
5	BES	D	604	4	-	10/24/24/24	0/1/1/1
2	EPE	A	601	-	-	1/9/19/19	0/1/1/1
5	BES	B	604	4	-	7/24/24/24	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	EPE	C10-S	-7.91	1.66	1.77
2	A	601	EPE	C10-S	-7.04	1.67	1.77
2	L	601	EPE	C10-S	-6.58	1.68	1.77
5	I	604	BES	C2-C1	-3.85	1.49	1.54
5	J	604	BES	O2-C2	3.12	1.48	1.42
6	F	605	BCT	O1-C	3.09	1.36	1.25
6	G	605	BCT	O1-C	2.87	1.35	1.25
5	H	604	BES	O2-C2	2.59	1.47	1.42
5	J	604	BES	C9-C8	2.57	1.43	1.38
6	L	606	BCT	O1-C	2.54	1.34	1.25
5	I	604	BES	C2-C3	-2.43	1.47	1.52
5	D	604	BES	O1-C5	-2.39	1.23	1.30
5	K	604	BES	O2-C2	2.35	1.46	1.42
5	E	604	BES	O2-C2	2.23	1.46	1.42
5	G	604	BES	O1-C5	-2.23	1.23	1.30
5	G	604	BES	O2-C2	2.23	1.46	1.42
5	C	604	BES	O1-C5	-2.22	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	604	BES	O1-C5	-2.22	1.23	1.30
5	D	604	BES	O2-C2	2.21	1.46	1.42
5	E	604	BES	O1-C5	-2.14	1.23	1.30
5	J	604	BES	O1-C5	-2.13	1.23	1.30
5	A	605	BES	O1-C5	-2.13	1.23	1.30
5	I	604	BES	O1-C5	-2.08	1.24	1.30
5	J	604	BES	C11-C12	2.04	1.42	1.38
5	L	605	BES	O1-C5	-2.00	1.24	1.30

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	605	BCT	O3-C-O1	-6.04	104.22	119.68
2	E	601	EPE	O1S-S-C10	5.18	114.56	106.73
5	G	604	BES	O3-C3-N1	5.10	132.08	122.96
5	D	604	BES	O3-C3-N1	4.85	131.63	122.96
5	H	604	BES	O3-C3-N1	4.70	131.38	122.96
5	A	605	BES	O3-C3-N1	4.68	131.33	122.96
5	D	604	BES	C2-C1-N2	-4.52	99.88	111.38
5	C	604	BES	O3-C3-N1	4.47	130.97	122.96
5	J	604	BES	O3-C3-N1	4.24	130.55	122.96
5	F	604	BES	O3-C3-N1	4.21	130.49	122.96
5	E	604	BES	O3-C3-N1	4.18	130.45	122.96
5	L	605	BES	O3-C3-N1	4.17	130.42	122.96
5	I	604	BES	O3-C3-N1	4.16	130.40	122.96
2	A	601	EPE	O3S-S-O2S	-4.12	101.08	111.40
5	I	604	BES	O3-C3-C2	-4.08	112.80	119.99
5	K	604	BES	O3-C3-N1	4.02	130.16	122.96
5	A	605	BES	O3-C3-C2	-4.00	112.93	119.99
2	A	601	EPE	O2S-S-C10	3.99	112.76	106.73
2	L	601	EPE	C5-C6-N1	-3.92	102.75	110.65
5	B	604	BES	O3-C3-N1	3.90	129.94	122.96
5	I	604	BES	O2-C2-C3	-3.86	102.55	110.63
5	I	604	BES	C2-C1-N2	-3.66	102.08	111.38
2	L	601	EPE	O2S-S-C10	3.65	112.25	106.73
5	F	604	BES	O3-C3-C2	-3.55	113.74	119.99
5	G	604	BES	O3-C3-C2	-3.48	113.87	119.99
5	A	605	BES	C2-C1-N2	-3.46	102.58	111.38
5	L	605	BES	O2-C2-C3	-3.46	103.39	110.63
6	K	605	BCT	O2-C-O1	3.45	128.51	119.68
5	C	604	BES	O3-C3-C2	-3.35	114.08	119.99
5	L	605	BES	O3-C3-C2	-3.34	114.11	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	604	BES	C2-C1-N2	-3.31	102.98	111.38
2	L	601	EPE	C3-C2-N1	-3.25	104.09	110.65
5	A	605	BES	C7-C6-C1	3.24	120.37	113.48
2	L	601	EPE	C5-N4-C3	3.23	115.79	108.84
5	D	604	BES	C4-N1-C3	3.22	128.57	121.65
5	K	604	BES	O3-C3-C2	-3.21	114.33	119.99
5	K	604	BES	C2-C1-N2	-3.12	103.46	111.38
5	D	604	BES	O3-C3-C2	-3.09	114.54	119.99
5	E	604	BES	O3-C3-C2	-3.08	114.56	119.99
5	L	605	BES	C7-C6-C1	3.06	119.99	113.48
5	B	604	BES	O3-C3-C2	-3.03	114.66	119.99
5	F	604	BES	C2-C1-N2	-3.02	103.70	111.38
5	L	605	BES	C2-C1-N2	-2.98	103.80	111.38
5	H	604	BES	O3-C3-C2	-2.98	114.73	119.99
5	C	604	BES	C4-N1-C3	2.97	128.03	121.65
6	I	605	BCT	O2-C-O1	2.94	127.20	119.68
5	E	604	BES	C7-C6-C1	2.80	119.44	113.48
5	B	604	BES	C4-N1-C3	2.76	127.58	121.65
2	L	601	EPE	C2-C3-N4	2.76	116.21	110.65
5	K	604	BES	C4-N1-C3	2.73	127.51	121.65
5	F	604	BES	C7-C6-C1	2.68	119.18	113.48
5	E	604	BES	C2-C1-N2	-2.63	104.68	111.38
5	B	604	BES	O2-C2-C3	-2.62	105.15	110.63
5	C	604	BES	C2-C1-N2	-2.59	104.80	111.38
5	K	604	BES	C7-C6-C1	2.58	118.96	113.48
6	L	606	BCT	O2-C-O1	-2.58	113.08	119.68
5	D	604	BES	C7-C6-C1	2.56	118.92	113.48
5	F	604	BES	O2-C2-C3	-2.53	105.33	110.63
5	H	604	BES	O2-C2-C1	2.51	114.80	109.64
5	J	604	BES	C4-N1-C3	2.49	127.00	121.65
5	J	604	BES	O3-C3-C2	-2.47	115.64	119.99
6	D	605	BCT	O2-C-O1	2.40	125.81	119.68
6	K	605	BCT	O3-C-O1	-2.33	113.72	119.68
5	B	604	BES	O1-C5-O4	-2.31	118.83	124.08
5	E	604	BES	O2-C2-C3	-2.27	105.89	110.63
5	G	604	BES	O2-C2-C1	2.23	114.23	109.64
5	H	604	BES	C7-C6-C1	2.23	118.22	113.48
5	L	605	BES	C4-N1-C3	2.23	126.43	121.65
2	E	601	EPE	O3S-S-O1S	-2.19	105.92	111.40
6	C	605	BCT	O2-C-O1	-2.17	114.14	119.68
2	E	601	EPE	C6-N1-C2	2.12	113.42	108.84
5	H	604	BES	C2-C1-N2	-2.12	105.99	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	604	BES	O1-C5-O4	-2.11	119.30	124.08
2	L	601	EPE	C6-C5-N4	2.09	114.87	110.65
5	A	605	BES	C10-C9-C8	2.06	122.78	120.24
5	L	605	BES	O1-C5-C4	2.04	120.42	113.51
5	I	604	BES	C4-N1-C3	2.04	126.03	121.65
5	J	604	BES	C15-C14-C13	2.02	118.35	111.08

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	EPE	C8-C7-N4-C3
5	A	605	BES	N2-C1-C2-C3
5	B	604	BES	N2-C1-C2-C3
5	D	604	BES	N2-C1-C2-O2
5	D	604	BES	N2-C1-C2-C3
5	D	604	BES	C6-C1-C2-O2
5	D	604	BES	C6-C1-C2-C3
5	C	604	BES	N2-C1-C2-O2
5	C	604	BES	N2-C1-C2-C3
5	C	604	BES	C6-C1-C2-O2
5	C	604	BES	C6-C1-C2-C3
5	E	604	BES	N2-C1-C2-C3
5	F	604	BES	N2-C1-C2-O2
5	F	604	BES	N2-C1-C2-C3
5	G	604	BES	N2-C1-C2-O2
5	G	604	BES	N2-C1-C2-C3
5	H	604	BES	N2-C1-C2-O2
5	H	604	BES	N2-C1-C2-C3
5	I	604	BES	N2-C1-C2-C3
5	J	604	BES	N2-C1-C2-O2
5	J	604	BES	N2-C1-C2-C3
5	J	604	BES	C6-C1-C2-O2
5	K	604	BES	N2-C1-C2-O2
5	K	604	BES	N2-C1-C2-C3
5	L	605	BES	N2-C1-C2-C3
5	L	605	BES	C6-C1-C2-C3
2	L	601	EPE	C9-C10-S-O3S
2	L	601	EPE	N4-C7-C8-O8
5	A	605	BES	N2-C1-C6-C7
5	B	604	BES	N2-C1-C6-C7
5	D	604	BES	N2-C1-C6-C7

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Mol	Chain	Res	Type	Atoms
5	C	604	BES	N2-C1-C6-C7
5	E	604	BES	N2-C1-C6-C7
5	I	604	BES	N2-C1-C6-C7
5	L	605	BES	N2-C1-C6-C7
5	D	604	BES	C4-C13-C14-C15
5	C	604	BES	C4-C13-C14-C15
5	I	604	BES	C4-C13-C14-C15
5	G	604	BES	O2-C2-C3-N1
5	H	604	BES	O2-C2-C3-N1
5	J	604	BES	O2-C2-C3-N1
5	K	604	BES	C4-C13-C14-C15
5	E	604	BES	C4-C13-C14-C15
2	L	601	EPE	C9-C10-S-O1S
2	L	601	EPE	C9-C10-S-O2S
5	G	604	BES	N2-C1-C6-C7
5	H	604	BES	N2-C1-C6-C7
5	J	604	BES	N2-C1-C6-C7
5	K	604	BES	N2-C1-C6-C7
5	C	604	BES	C2-C1-C6-C7
5	L	605	BES	C4-C13-C14-C15
5	A	605	BES	C6-C1-C2-C3
5	B	604	BES	C6-C1-C2-C3
5	E	604	BES	C6-C1-C2-C3
5	F	604	BES	C6-C1-C2-C3
5	G	604	BES	C6-C1-C2-C3
5	H	604	BES	C6-C1-C2-C3
5	I	604	BES	C6-C1-C2-C3
5	J	604	BES	C6-C1-C2-C3
5	K	604	BES	C6-C1-C2-C3
5	B	604	BES	C6-C1-C2-O2
5	G	604	BES	C6-C1-C2-O2
5	H	604	BES	C6-C1-C2-O2
5	I	604	BES	C14-C13-C4-C5
5	L	605	BES	C14-C13-C4-N1
5	C	604	BES	C14-C13-C4-N1
5	I	604	BES	C14-C13-C4-N1
5	L	605	BES	C14-C13-C4-C5
5	C	604	BES	C14-C13-C4-C5
5	G	604	BES	O2-C2-C3-O3
5	H	604	BES	O2-C2-C3-O3
5	J	604	BES	O2-C2-C3-O3
5	L	605	BES	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	D	604	BES	C14-C13-C4-C5
5	A	605	BES	O2-C2-C3-N1
5	B	604	BES	O2-C2-C3-N1
5	D	604	BES	O2-C2-C3-N1
5	C	604	BES	O2-C2-C3-N1
5	E	604	BES	O2-C2-C3-N1
5	K	604	BES	O2-C2-C3-N1
5	L	605	BES	O2-C2-C3-N1
5	D	604	BES	C14-C13-C4-N1
2	E	601	EPE	C10-C9-N1-C2
5	A	605	BES	O2-C2-C3-O3
5	B	604	BES	N2-C1-C2-O2
5	B	604	BES	O2-C2-C3-O3
5	D	604	BES	O2-C2-C3-O3
5	C	604	BES	O2-C2-C3-O3
5	E	604	BES	N2-C1-C2-O2
5	E	604	BES	O2-C2-C3-O3
5	F	604	BES	O2-C2-C3-O3
5	I	604	BES	O2-C2-C3-O3
5	K	604	BES	O2-C2-C3-O3
5	F	604	BES	O2-C2-C3-N1
5	I	604	BES	O2-C2-C3-N1
5	J	604	BES	C4-C13-C14-C15
5	A	605	BES	C6-C1-C2-O2
5	E	604	BES	C6-C1-C2-O2
5	F	604	BES	C6-C1-C2-O2
5	K	604	BES	C6-C1-C2-O2
5	L	605	BES	C6-C1-C2-O2
5	H	604	BES	C4-C13-C14-C15

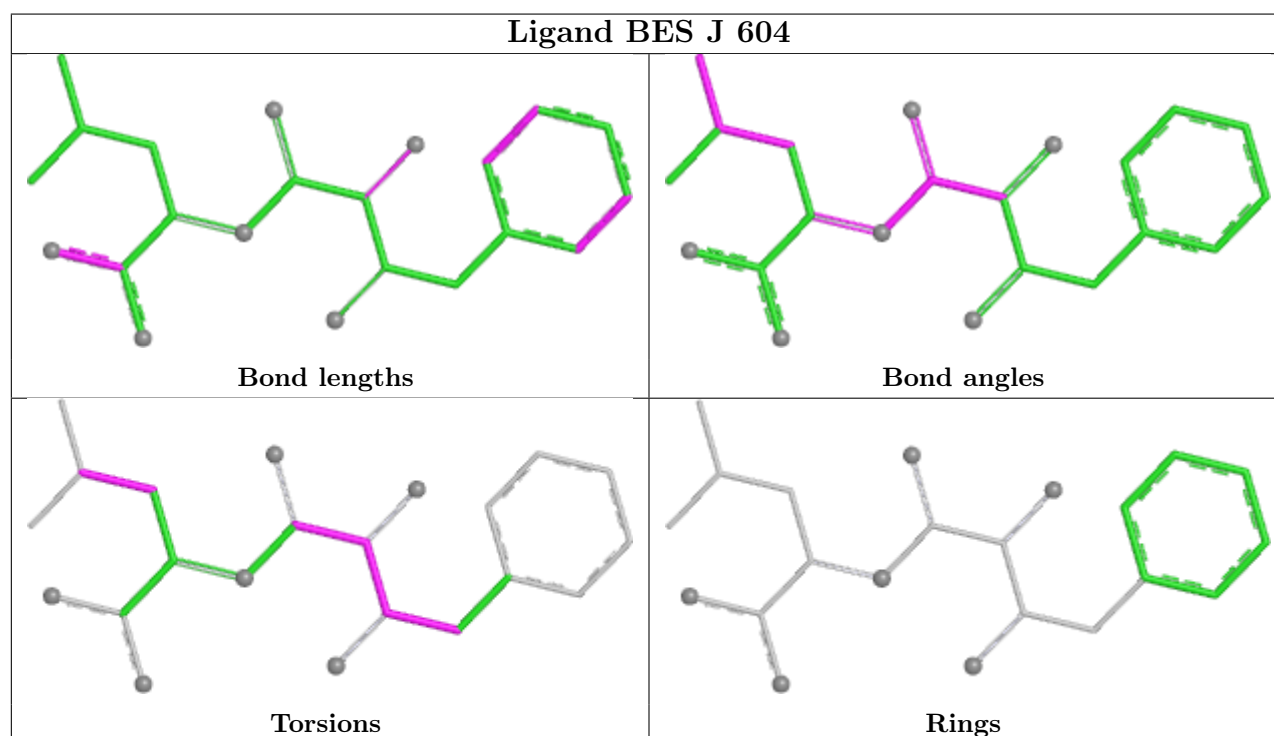
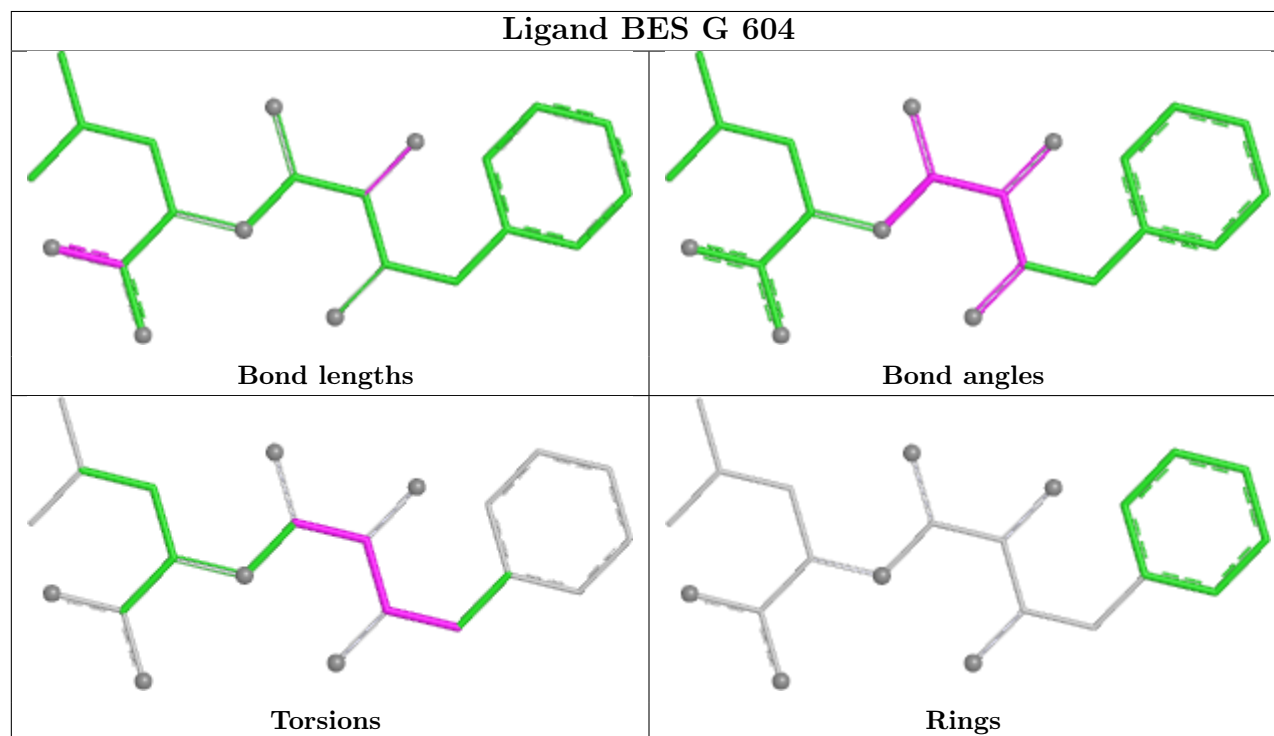
There are no ring outliers.

2 monomers are involved in 2 short contacts:

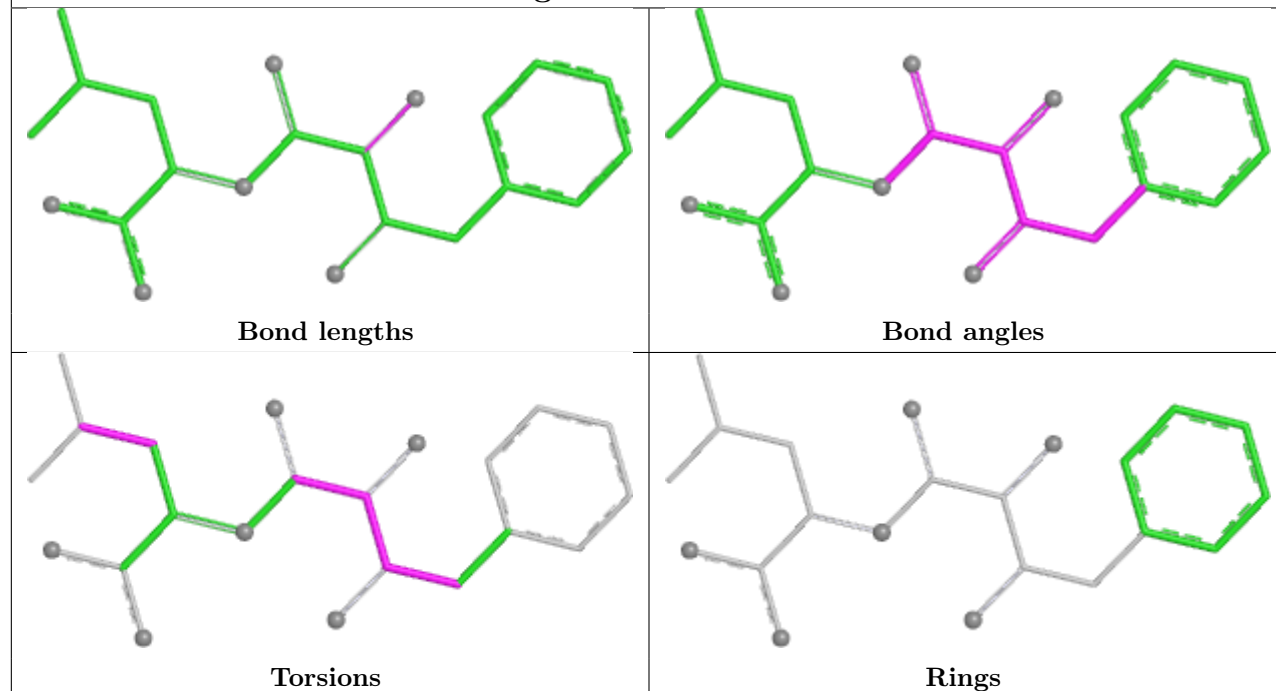
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	601	EPE	2	0
2	A	601	EPE	1	0

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.

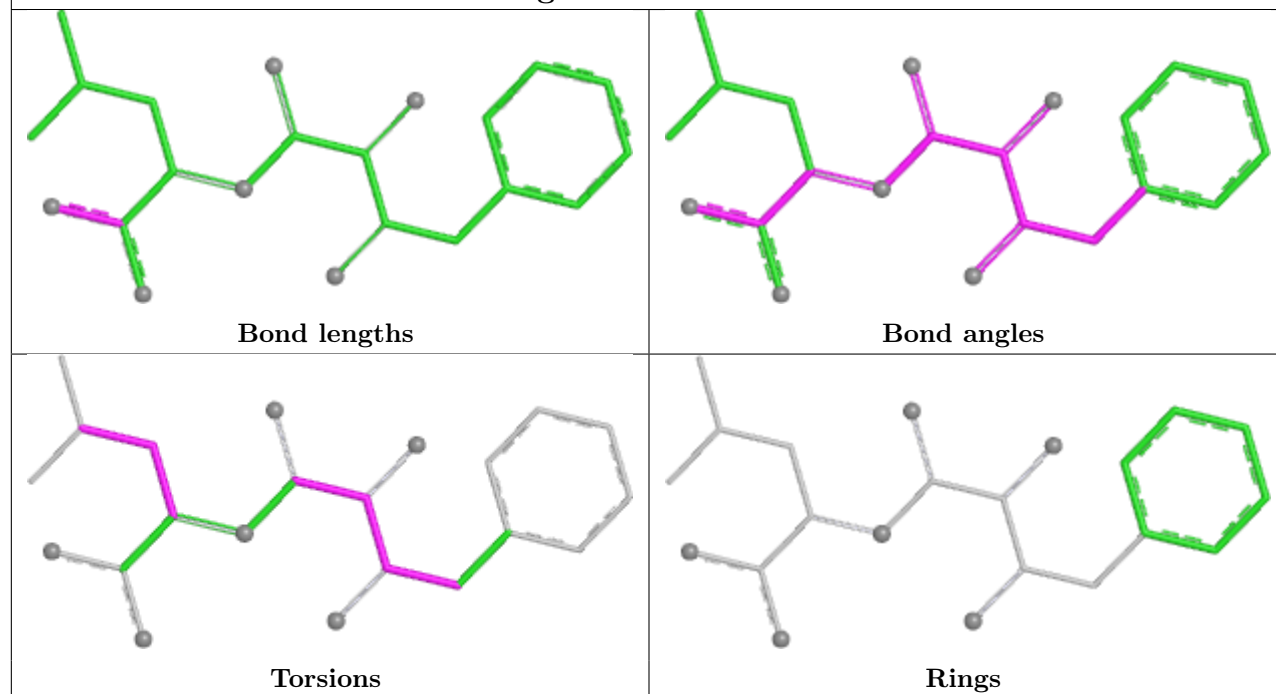
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



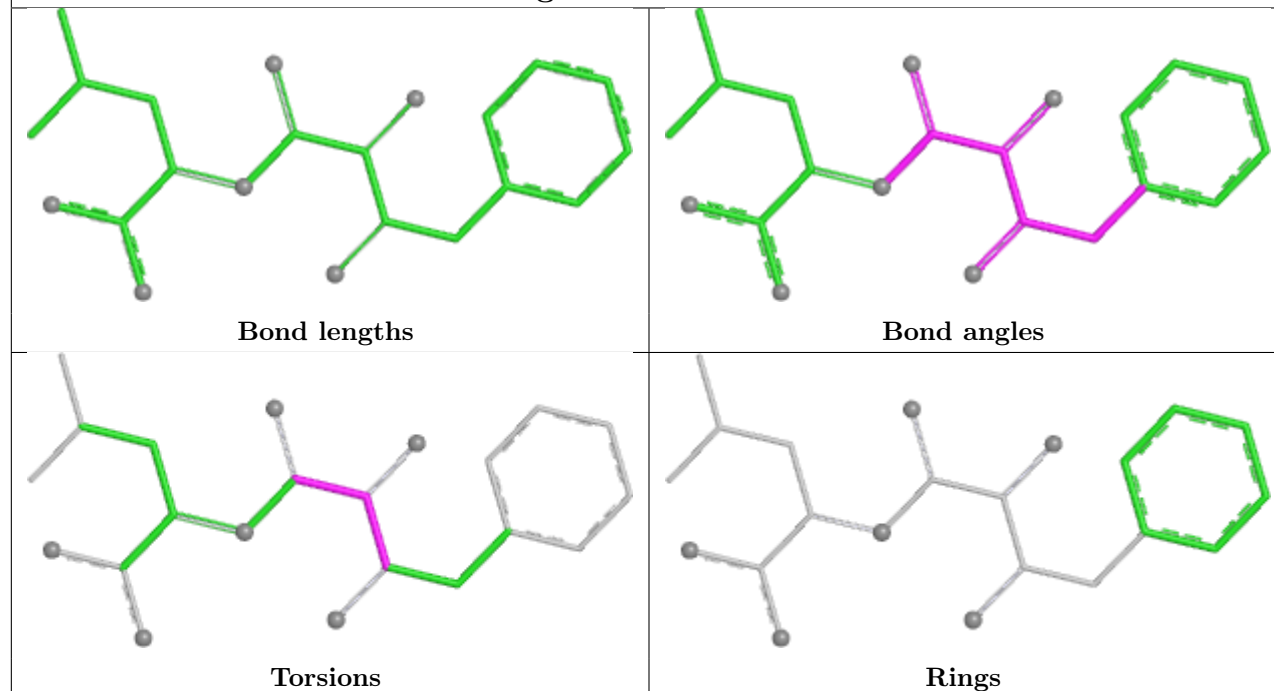
Ligand BES H 604



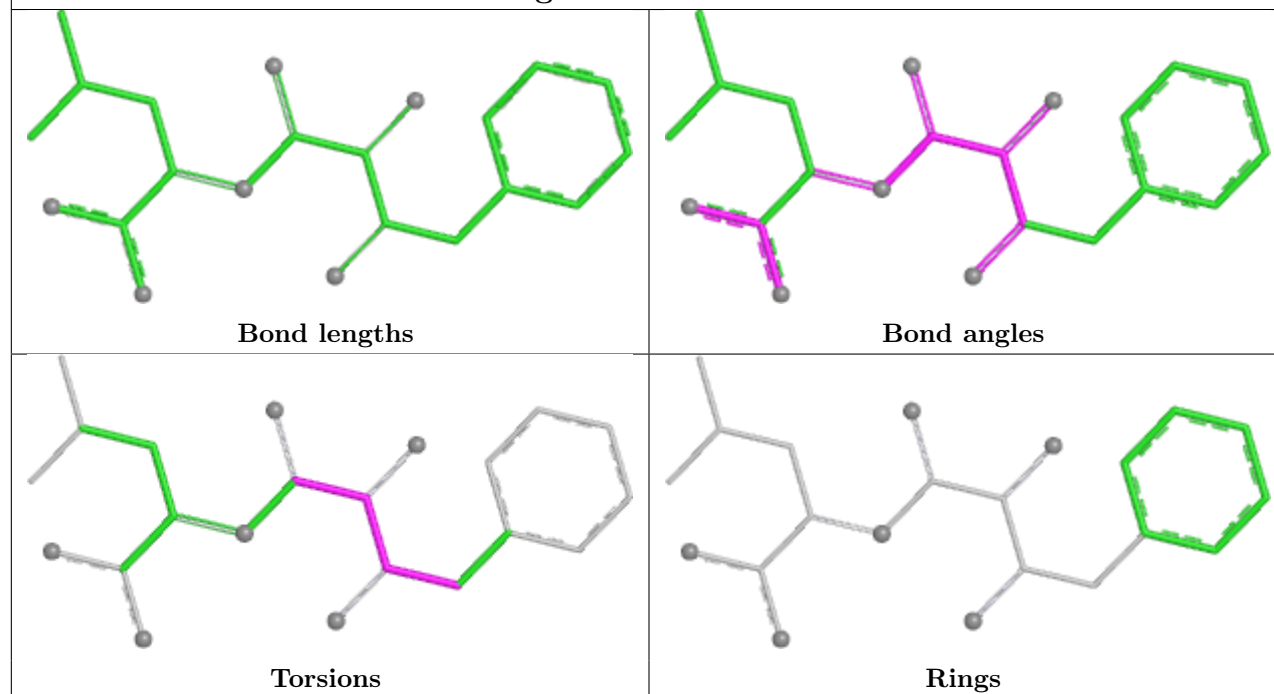
Ligand BES L 605



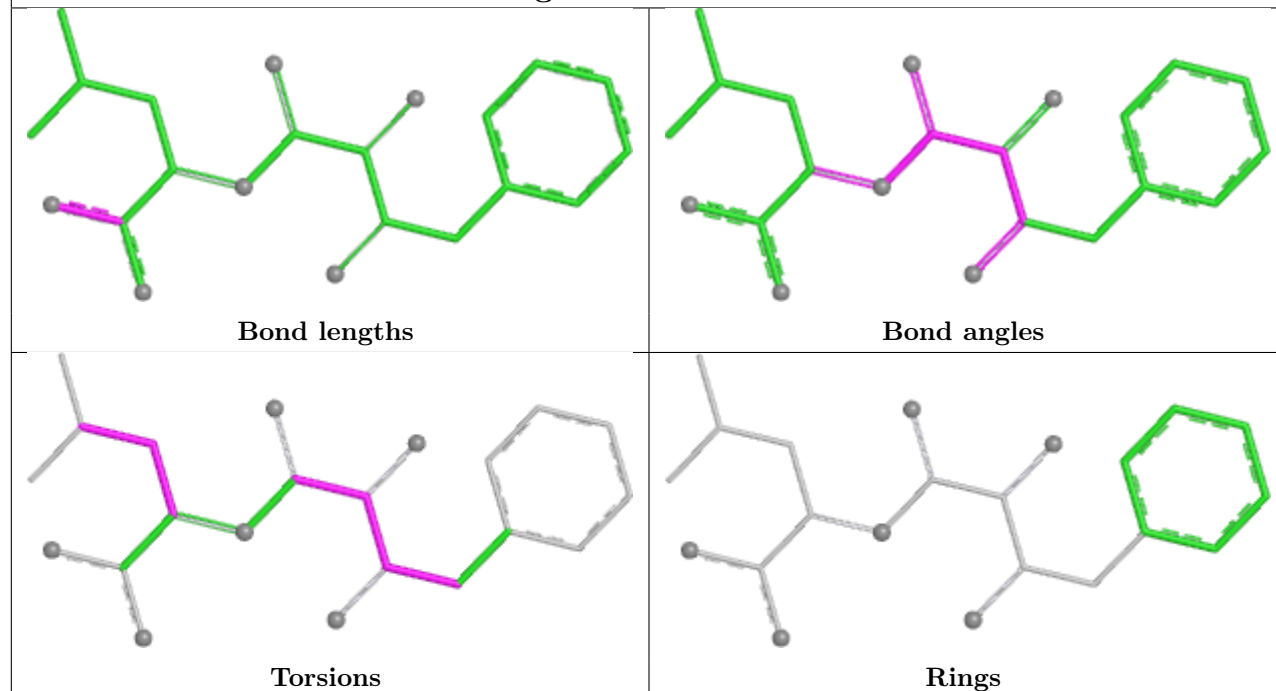
Ligand BES F 604



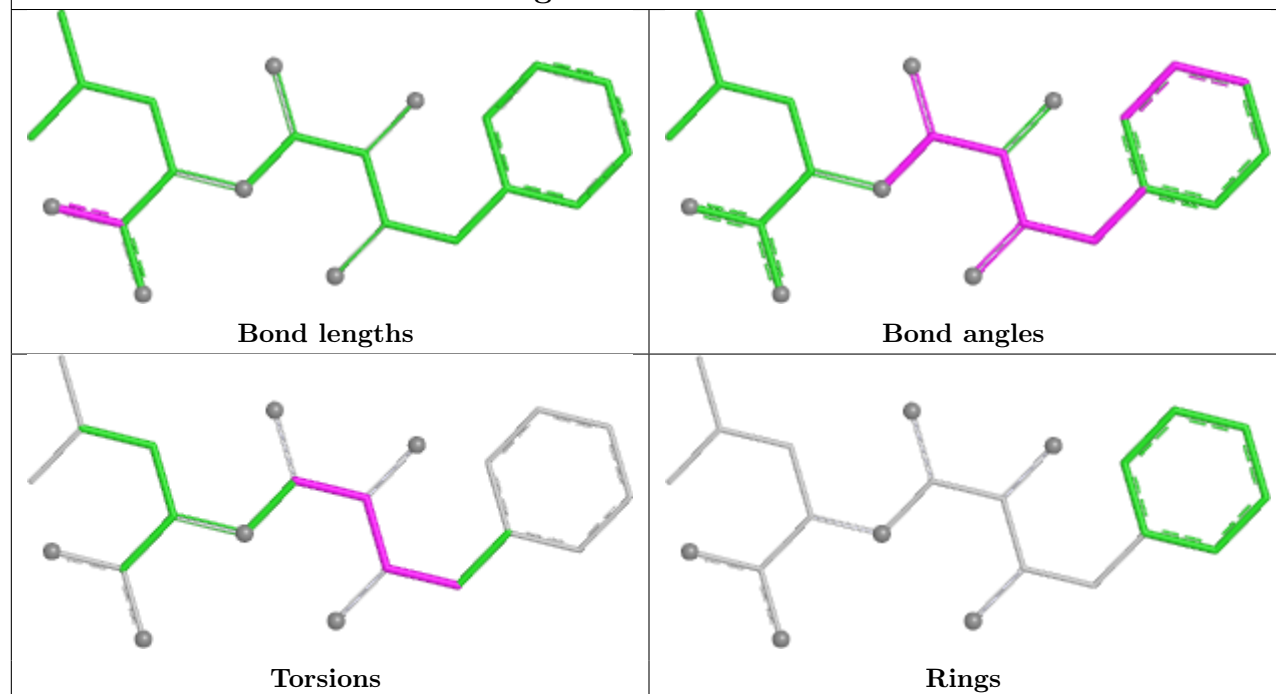
Ligand BES B 604



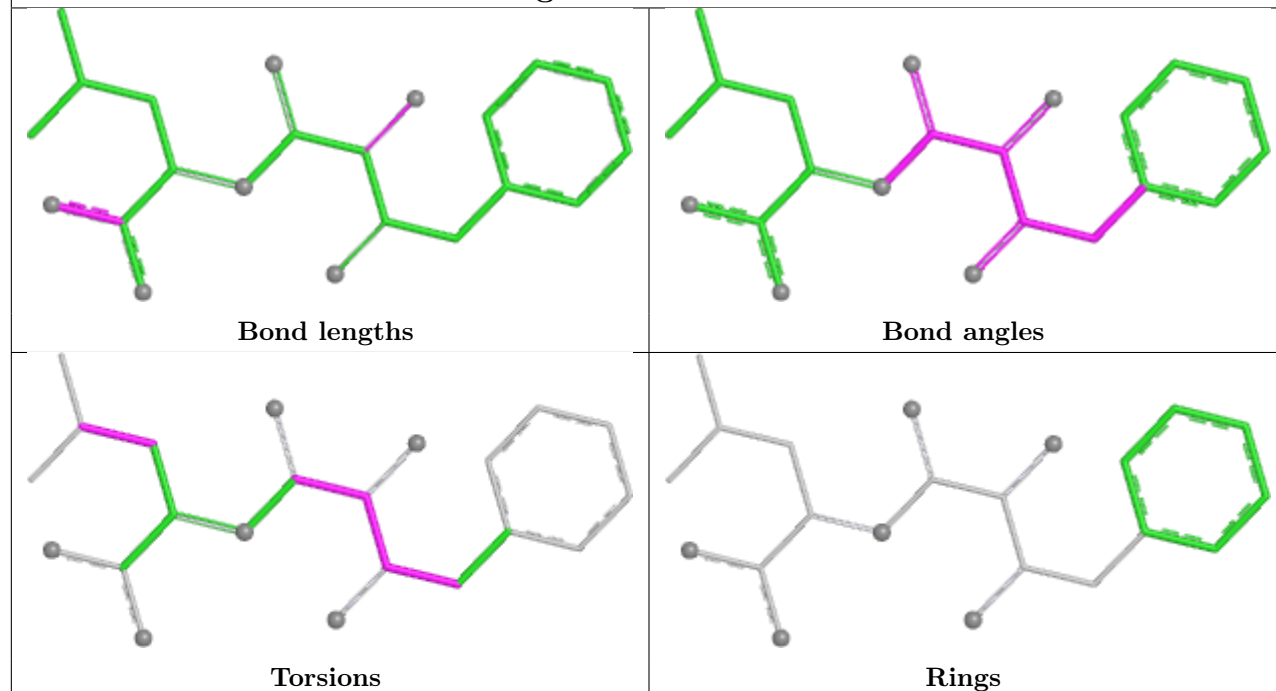
Ligand BES C 604



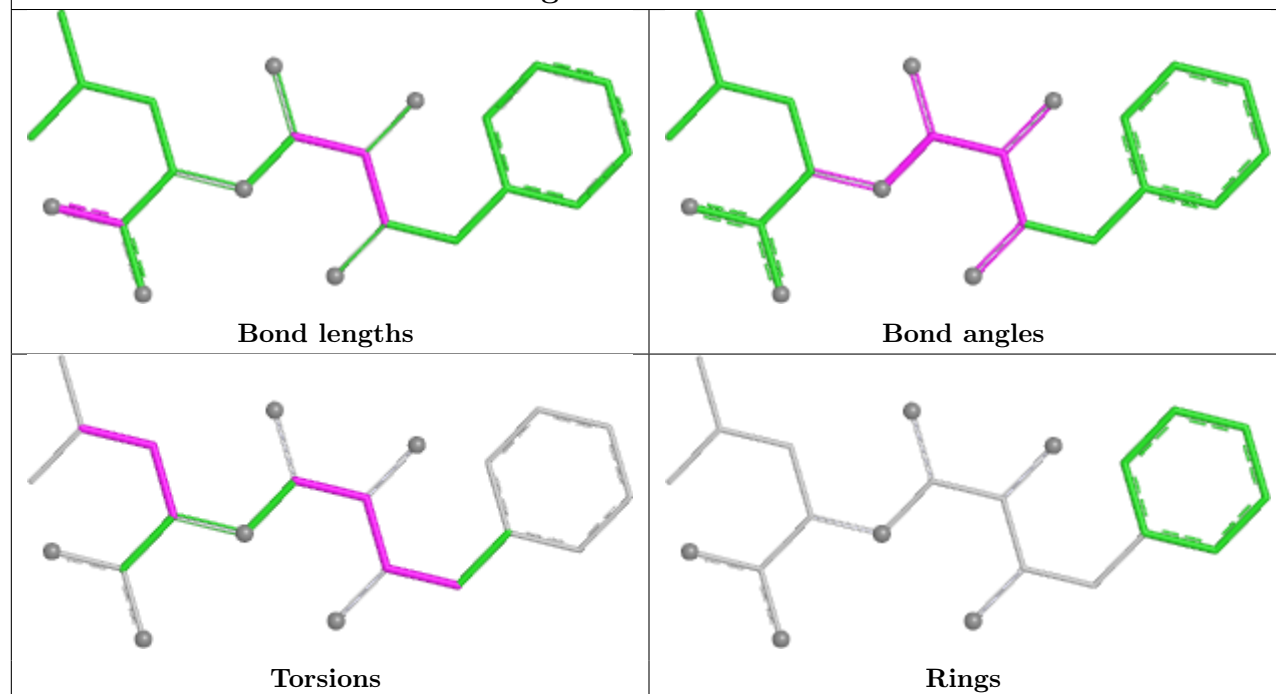
Ligand BES A 605

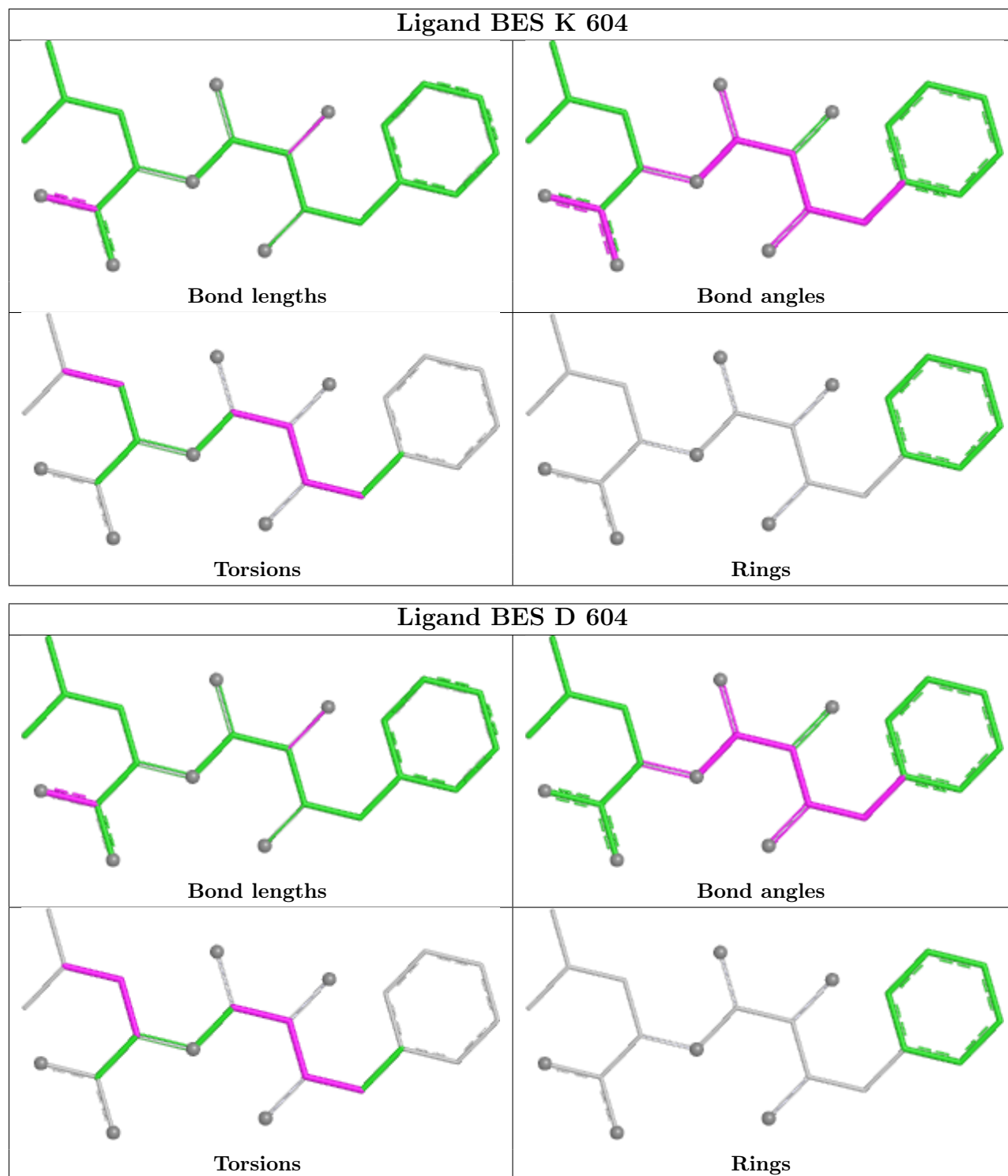


Ligand BES E 604



Ligand BES I 604





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	519/521 (99%)	-0.16	8 (1%) 72 73	16, 27, 46, 78	2 (0%)
1	B	519/521 (99%)	-0.02	4 (0%) 82 83	22, 30, 49, 71	2 (0%)
1	C	518/521 (99%)	0.07	10 (1%) 66 68	20, 32, 49, 76	1 (0%)
1	D	519/521 (99%)	-0.19	10 (1%) 66 68	21, 29, 46, 72	0
1	E	519/521 (99%)	-0.08	2 (0%) 88 89	17, 31, 46, 70	1 (0%)
1	F	519/521 (99%)	-0.03	5 (0%) 79 80	22, 31, 47, 80	0
1	G	520/521 (99%)	-0.05	5 (0%) 79 80	17, 30, 47, 81	2 (0%)
1	H	519/521 (99%)	0.15	6 (1%) 76 77	23, 32, 49, 80	0
1	I	519/521 (99%)	0.54	12 (2%) 61 63	25, 38, 53, 70	1 (0%)
1	J	519/521 (99%)	-0.11	7 (1%) 75 76	23, 30, 49, 71	0
1	K	519/521 (99%)	0.06	8 (1%) 72 73	24, 32, 51, 92	0
1	L	519/521 (99%)	0.10	6 (1%) 76 77	23, 30, 45, 65	0
All	All	6228/6252 (99%)	0.02	83 (1%) 75 76	16, 31, 49, 92	9 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	2	PRO	6.0
1	C	90	GLY	5.7
1	B	3	THR	5.0
1	K	138	ASN	4.7
1	J	3	THR	4.6
1	E	3	THR	4.6
1	A	3	THR	4.4
1	I	3	THR	4.3
1	K	279	THR	4.0
1	K	3	THR	3.9
1	F	3	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	K	137	PRO	3.7
1	D	3	THR	3.7
1	D	137	PRO	3.7
1	L	90	GLY	3.6
1	C	88	VAL	3.6
1	A	90	GLY	3.5
1	A	91	LEU	3.5
1	H	138	ASN	3.5
1	C	137	PRO	3.3
1	A	138	ASN	3.3
1	K	136	GLU	3.2
1	H	137	PRO	3.2
1	F	137	PRO	3.1
1	D	136	GLU	3.1
1	L	3	THR	3.0
1	D	63	ARG	3.0
1	L	279	THR	3.0
1	C	138	ASN	2.9
1	G	133	GLU	2.8
1	G	3	THR	2.7
1	I	279	THR	2.6
1	F	96	GLY	2.6
1	I	94	ALA	2.6
1	J	136	GLU	2.6
1	H	3	THR	2.6
1	L	137	PRO	2.6
1	C	95	ALA	2.5
1	A	96	GLY	2.5
1	J	96	GLY	2.5
1	K	280	PRO	2.5
1	C	277	LYS	2.5
1	J	138	ASN	2.5
1	G	136	GLU	2.5
1	I	391	PHE	2.5
1	K	281	VAL	2.4
1	H	136	GLU	2.4
1	I	109	THR	2.4
1	I	273	LEU	2.4
1	D	95	ALA	2.4
1	G	90	GLY	2.4
1	D	96	GLY	2.3
1	E	279	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	137	PRO	2.3
1	I	278	GLY	2.3
1	K	91	LEU	2.3
1	A	88	VAL	2.3
1	H	273	LEU	2.3
1	C	96	GLY	2.2
1	I	35	GLU	2.2
1	B	486	LYS	2.2
1	A	137	PRO	2.2
1	F	135	LYS	2.2
1	D	4	LEU	2.2
1	I	61	VAL	2.2
1	D	278	GLY	2.2
1	F	136	GLU	2.2
1	J	94	ALA	2.2
1	C	87	LEU	2.2
1	I	510	GLY	2.2
1	A	97	SER	2.2
1	J	305	TYR	2.1
1	L	59	PRO	2.1
1	H	90	GLY	2.1
1	C	4	LEU	2.1
1	D	138	ASN	2.1
1	L	278	GLY	2.1
1	B	193	ALA	2.1
1	I	229	ALA	2.1
1	C	133	GLU	2.0
1	I	41	VAL	2.0
1	D	277	LYS	2.0
1	J	95	ALA	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

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	SO4	H	601	5/5	0.82	0.15	53,67,76,84	0
3	SO4	I	601	5/5	0.85	0.12	63,68,71,76	0
2	EPE	E	601	15/15	0.86	0.20	52,81,93,94	0
3	SO4	L	602	5/5	0.86	0.11	76,77,80,88	0
6	BCT	G	605	4/4	0.86	0.17	32,40,42,55	0
6	BCT	J	605	4/4	0.86	0.17	28,34,34,49	0
6	BCT	I	605	4/4	0.87	0.15	39,44,46,53	0
2	EPE	L	601	15/15	0.87	0.15	58,71,91,95	0
5	BES	H	604	22/22	0.88	0.13	40,45,51,55	0
6	BCT	K	605	4/4	0.89	0.18	28,36,38,51	0
6	BCT	E	605	4/4	0.90	0.15	30,36,38,47	0
5	BES	G	604	22/22	0.90	0.12	35,41,49,54	0
5	BES	F	604	22/22	0.90	0.12	34,38,50,54	0
5	BES	J	604	22/22	0.90	0.13	37,38,46,52	0
6	BCT	B	605	4/4	0.90	0.15	30,36,37,45	0
6	BCT	F	605	4/4	0.91	0.13	31,37,42,47	0
5	BES	E	604	22/22	0.91	0.12	37,40,50,54	0
6	BCT	H	605	4/4	0.91	0.14	28,36,38,49	0
6	BCT	D	605	4/4	0.91	0.13	33,37,39,39	0
6	BCT	C	605	4/4	0.91	0.13	37,39,41,53	0
6	BCT	A	606	4/4	0.91	0.11	31,41,43,49	0
6	BCT	L	606	4/4	0.91	0.13	34,40,42,52	0
5	BES	K	604	22/22	0.92	0.11	34,40,46,49	0
5	BES	L	605	22/22	0.92	0.10	39,44,49,53	0
5	BES	A	605	22/22	0.92	0.10	30,36,42,44	0
5	BES	B	604	22/22	0.92	0.11	34,38,45,54	0
5	BES	C	604	22/22	0.92	0.11	37,43,47,53	0
5	BES	I	604	22/22	0.92	0.11	39,47,54,59	0
2	EPE	A	601	15/15	0.92	0.14	46,66,74,76	0
5	BES	D	604	22/22	0.93	0.10	32,34,42,44	0
3	SO4	C	601	5/5	0.93	0.11	50,57,64,65	0
3	SO4	G	601	5/5	0.94	0.12	52,62,67,73	0
3	SO4	D	601	5/5	0.94	0.15	56,56,66,67	0
3	SO4	B	601	5/5	0.94	0.08	63,63,67,71	0
3	SO4	F	601	5/5	0.94	0.12	54,65,72,73	0
3	SO4	J	601	5/5	0.95	0.11	54,54,63,64	0
3	SO4	K	601	5/5	0.95	0.12	56,62,67,68	0

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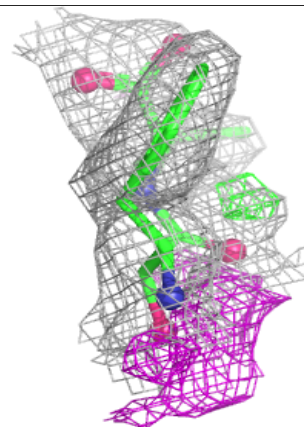
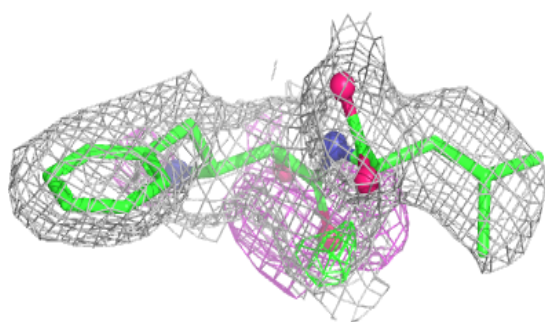
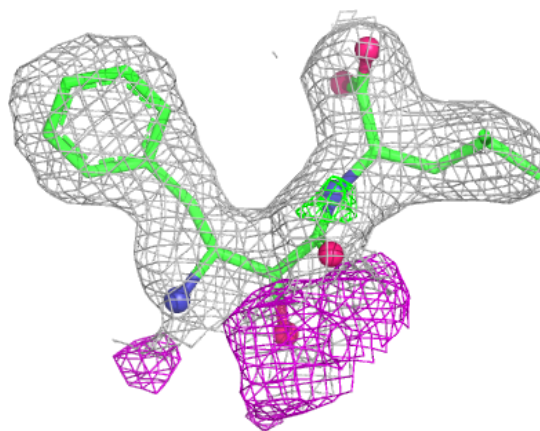
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	602	5/5	0.95	0.10	54,57,59,62	0
4	MN	I	603	1/1	0.98	0.07	43,43,43,43	0
4	MN	E	602	1/1	0.99	0.08	35,35,35,35	0
4	MN	E	603	1/1	0.99	0.04	32,32,32,32	0
4	MN	F	602	1/1	0.99	0.07	31,31,31,31	0
4	MN	F	603	1/1	0.99	0.05	31,31,31,31	0
4	MN	G	602	1/1	0.99	0.06	36,36,36,36	0
4	MN	H	602	1/1	0.99	0.09	36,36,36,36	0
4	MN	H	603	1/1	0.99	0.07	34,34,34,34	0
4	MN	I	602	1/1	0.99	0.06	43,43,43,43	0
4	MN	A	603	1/1	0.99	0.08	31,31,31,31	0
4	MN	J	602	1/1	0.99	0.07	32,32,32,32	0
4	MN	K	602	1/1	0.99	0.07	33,33,33,33	0
4	MN	K	603	1/1	0.99	0.04	30,30,30,30	0
4	MN	L	603	1/1	0.99	0.07	36,36,36,36	0
4	MN	L	604	1/1	0.99	0.03	33,33,33,33	0
4	MN	A	604	1/1	0.99	0.04	26,26,26,26	0
4	MN	D	602	1/1	0.99	0.08	31,31,31,31	0
4	MN	D	603	1/1	0.99	0.03	28,28,28,28	0
4	MN	C	602	1/1	0.99	0.09	39,39,39,39	0
4	MN	C	603	1/1	0.99	0.04	32,32,32,32	0
4	MN	G	603	1/1	1.00	0.05	30,30,30,30	0
4	MN	B	603	1/1	1.00	0.03	29,29,29,29	0
4	MN	B	602	1/1	1.00	0.06	33,33,33,33	0
4	MN	J	603	1/1	1.00	0.03	31,31,31,31	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.

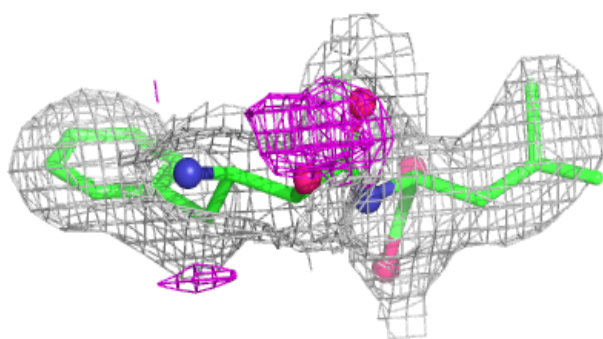
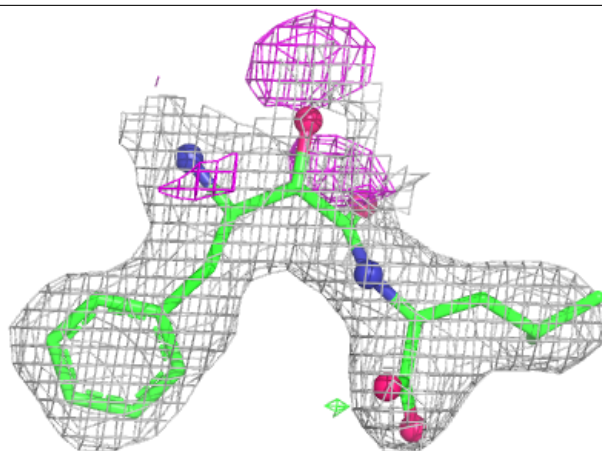
Electron density around BES H 604:

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

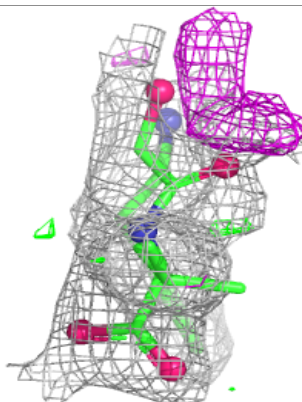
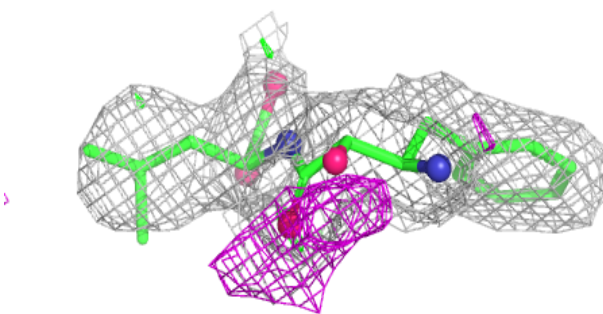
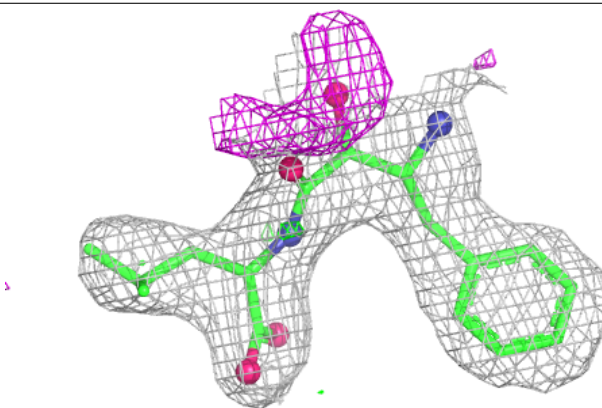


Electron density around BES G 604:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

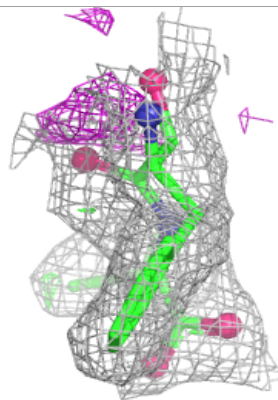
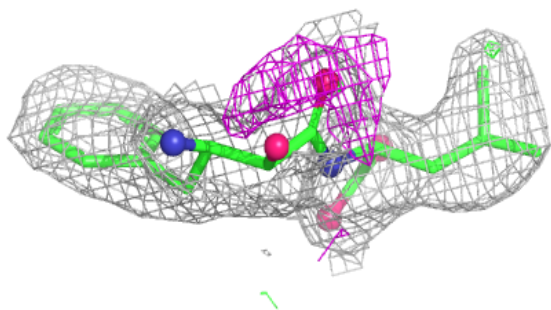
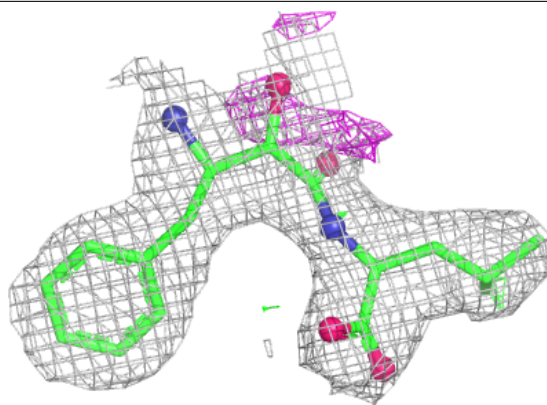
**Electron density around BES F 604:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



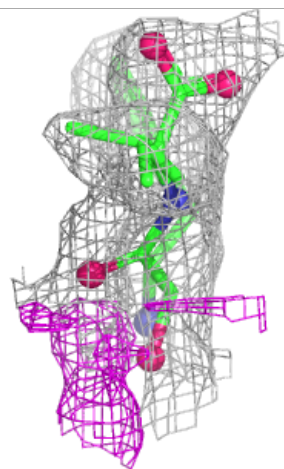
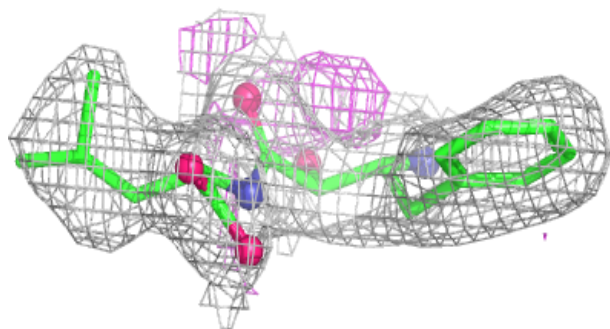
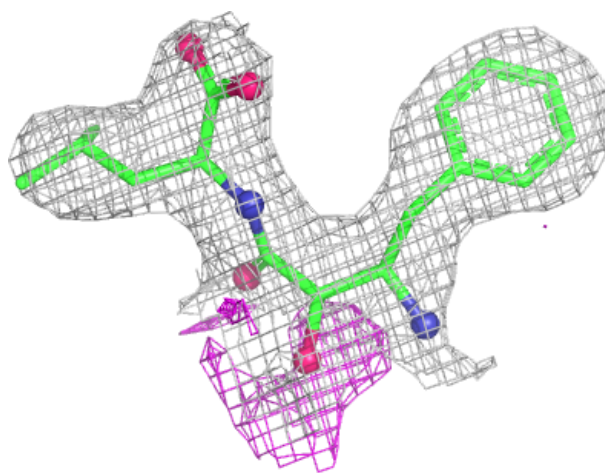
Electron density around BES J 604:

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and green (positive)



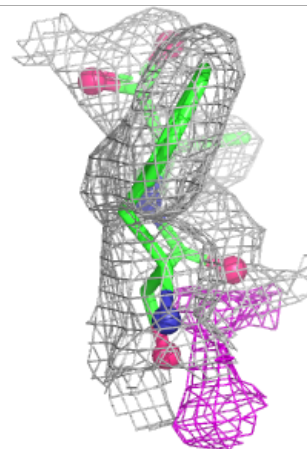
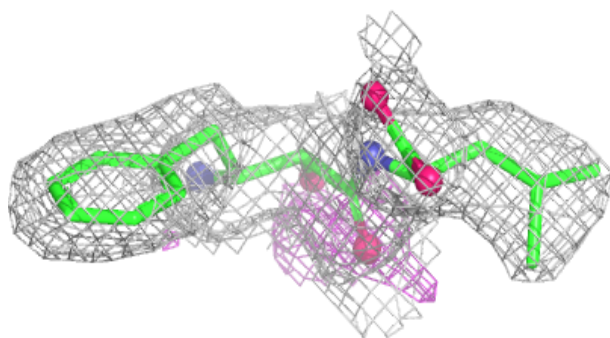
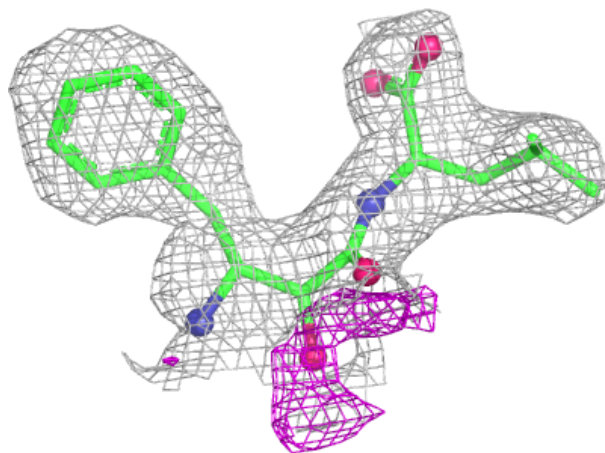
Electron density around BES E 604:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



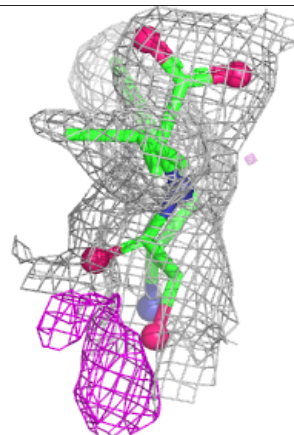
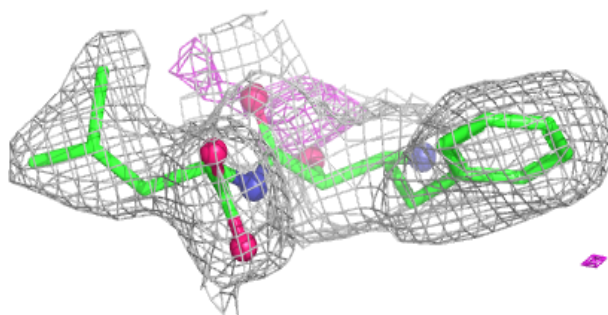
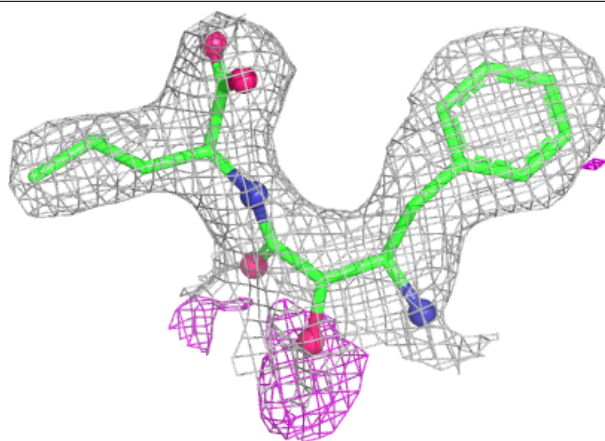
Electron density around BES K 604:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



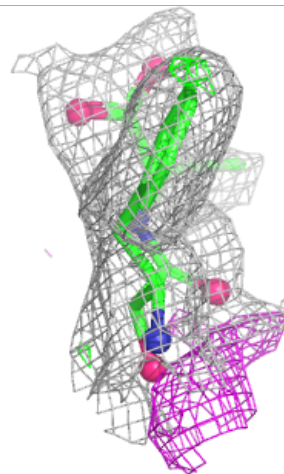
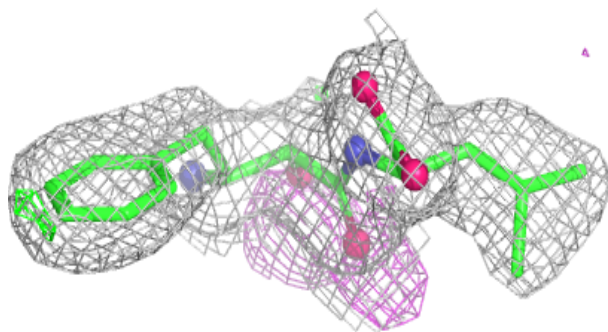
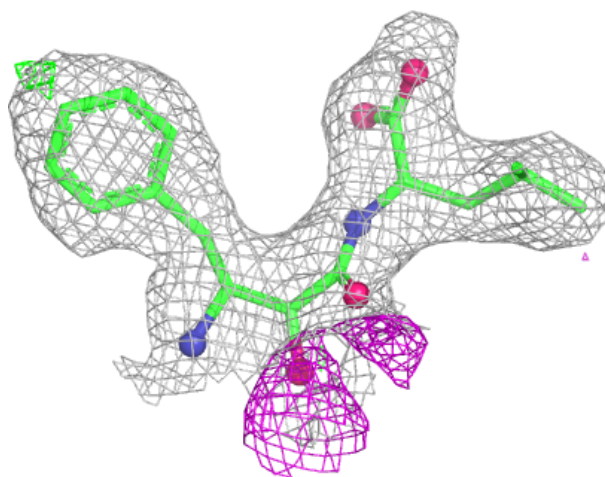
Electron density around BES L 605:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



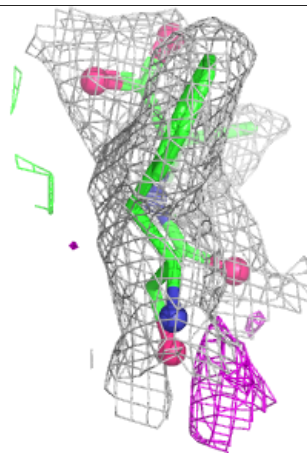
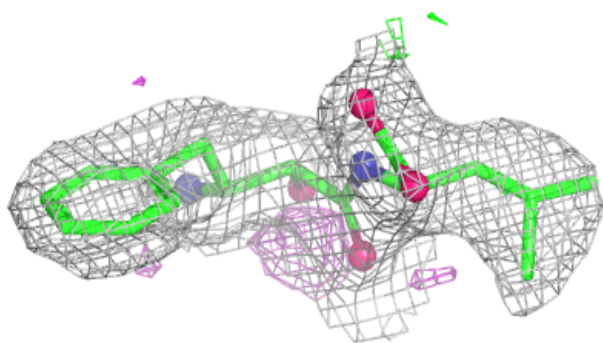
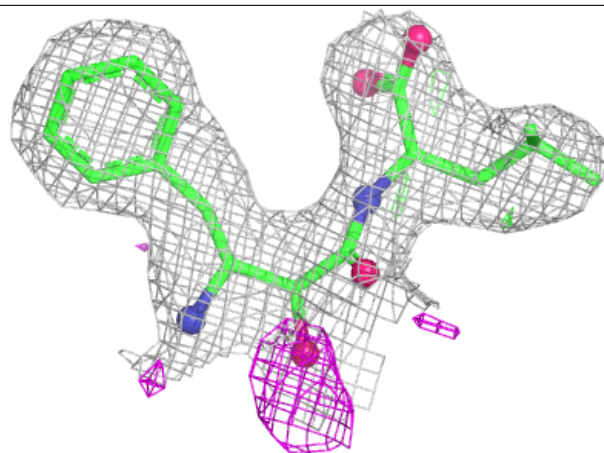
Electron density around BES A 605:

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and green (positive)



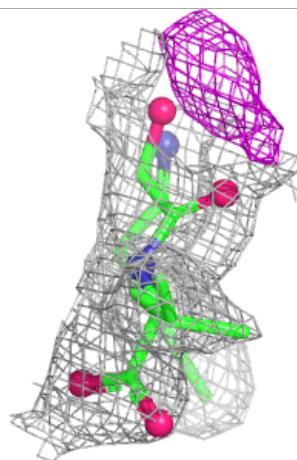
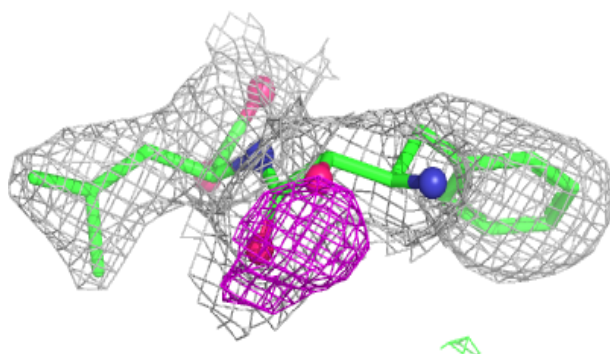
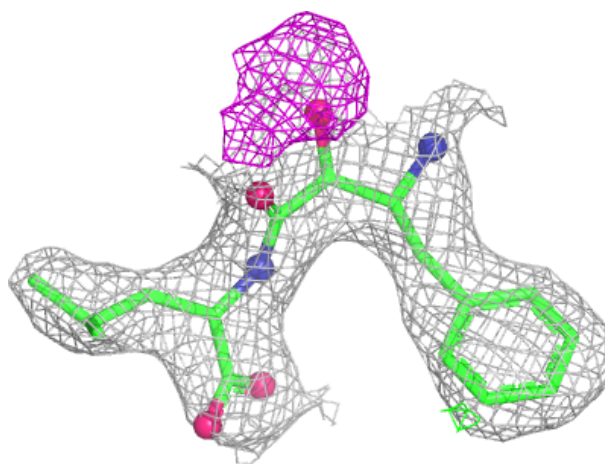
Electron density around BES B 604:

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and green (positive)



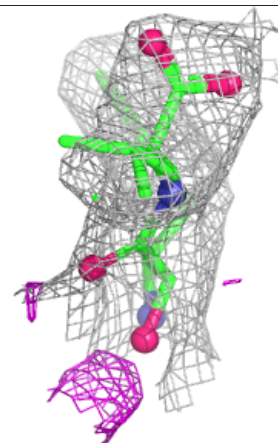
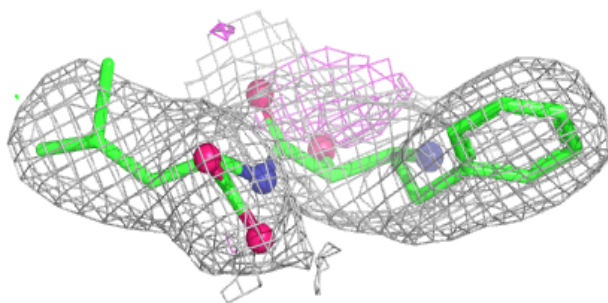
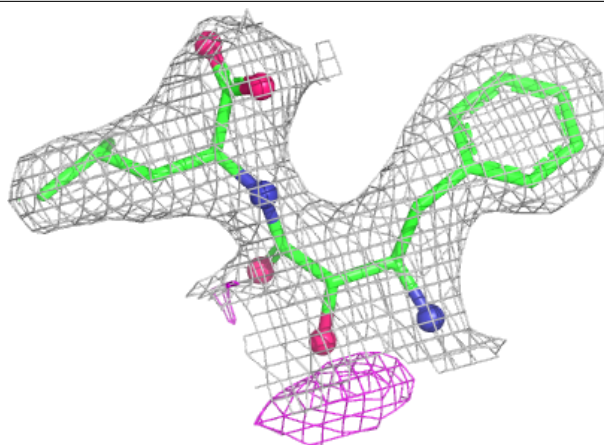
Electron density around BES C 604:

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



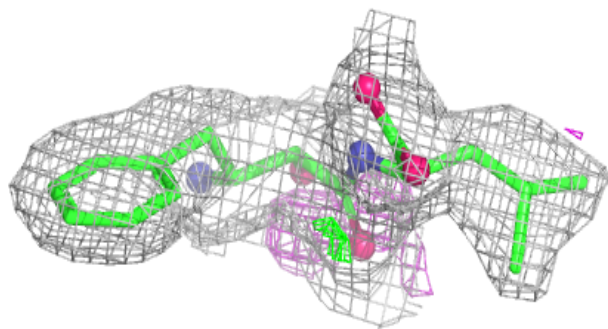
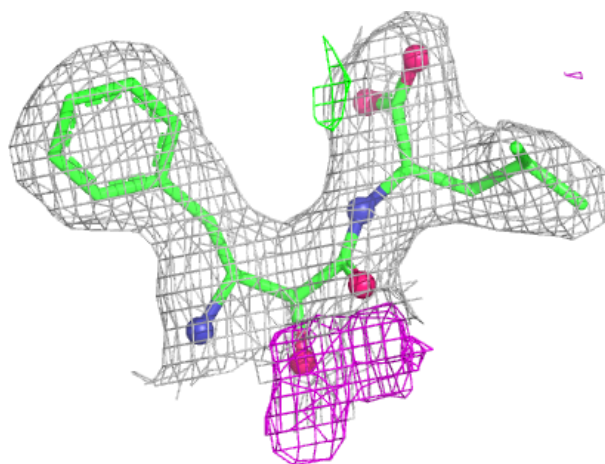
Electron density around BES I 604:

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



Electron density around BES D 604:

$2mF_o-DF_c$ (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.