Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2021 – 10:53 AM EDT

PDB ID	:	3INL
Title	:	Human Mitochondrial Aldehyde Dehydrogenase Asian Variant, ALDH2*2, complexed with agonist Alda-1
Authors	:	Perez-Miller, S.; Hurley, T.D.
Deposited on	:	2009-08-12
Resolution	:	1.86 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 following versions of software and data (see references ⓘ) were used in the production of this report:

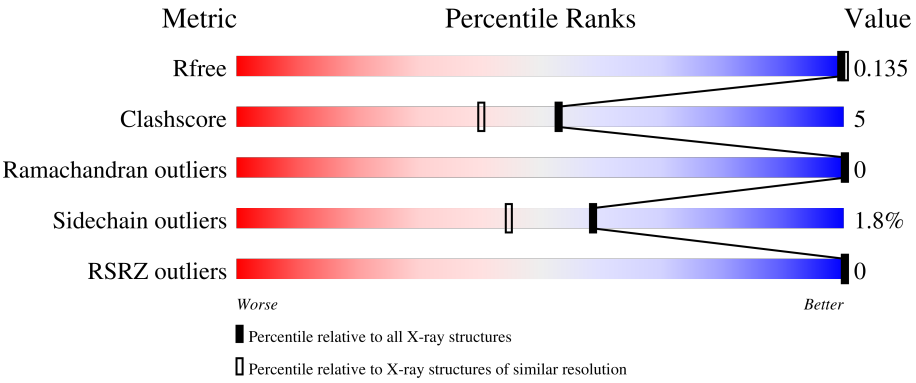
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	500	88% 11% •
1	B	500	87% 12% •
1	C	500	86% 12% ••
1	D	500	88% 10% ••
1	E	500	88% 10% ••

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Mol	Chain	Length	Quality of chain
1	F	500	
1	G	500	
1	H	500	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 34144 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 Aldehyde dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	1	0
			3812	2424	652	719	17			
1	B	494	Total	C	N	O	S	0	1	0
			3803	2419	650	717	17			
1	C	494	Total	C	N	O	S	0	1	0
			3800	2417	649	717	17			
1	D	494	Total	C	N	O	S	0	1	0
			3803	2419	650	717	17			
1	E	494	Total	C	N	O	S	0	1	0
			3805	2420	652	716	17			
1	F	494	Total	C	N	O	S	0	0	0
			3798	2416	649	716	17			
1	G	494	Total	C	N	O	S	0	1	0
			3803	2419	650	717	17			
1	H	495	Total	C	N	O	S	0	1	0
			3812	2424	652	719	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	SER	CYS	engineered mutation	UNP P05091
A	487	LYS	GLU	engineered mutation	UNP P05091
B	302	SER	CYS	engineered mutation	UNP P05091
B	487	LYS	GLU	engineered mutation	UNP P05091
C	302	SER	CYS	engineered mutation	UNP P05091
C	487	LYS	GLU	engineered mutation	UNP P05091
D	302	SER	CYS	engineered mutation	UNP P05091
D	487	LYS	GLU	engineered mutation	UNP P05091
E	302	SER	CYS	engineered mutation	UNP P05091
E	487	LYS	GLU	engineered mutation	UNP P05091
F	302	SER	CYS	engineered mutation	UNP P05091
F	487	LYS	GLU	engineered mutation	UNP P05091
G	302	SER	CYS	engineered mutation	UNP P05091

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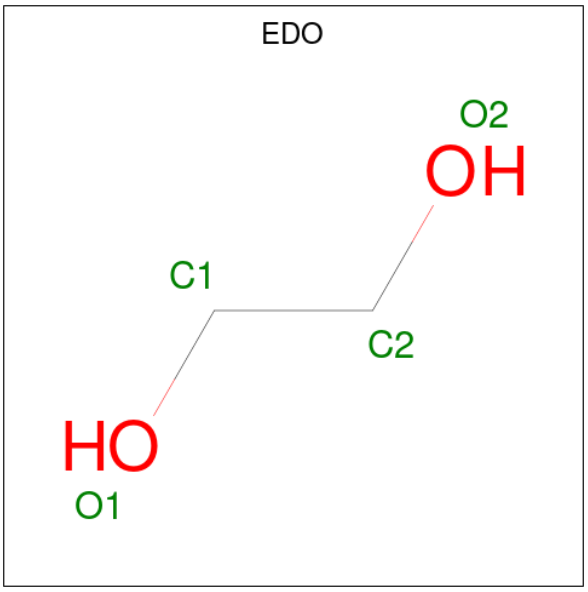
Chain	Residue	Modelled	Actual	Comment	Reference
G	487	LYS	GLU	engineered mutation	UNP P05091
H	302	SER	CYS	engineered mutation	UNP P05091
H	487	LYS	GLU	engineered mutation	UNP P05091

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0
2	G	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

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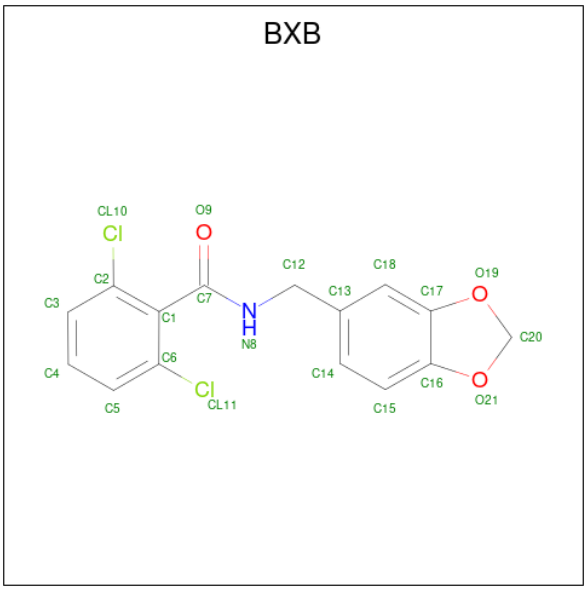
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is N-(1,3-benzodioxol-5-ylmethyl)-2,6-dichlorobenzamide (three-letter code: BXB) (formula: $C_{15}H_{11}Cl_2NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl N O 21 15 2 1 3	0	0
4	B	1	Total C Cl N O 21 15 2 1 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	Cl	N	O	0	0
			21	15	2	1	3		
4	D	1	Total	C	Cl	N	O	0	0
			21	15	2	1	3		
4	E	1	Total	C	Cl	N	O	0	0
			21	15	2	1	3		
4	F	1	Total	C	Cl	N	O	0	0
			21	15	2	1	3		
4	G	1	Total	C	Cl	N	O	0	0
			21	15	2	1	3		
4	H	1	Total	C	Cl	N	O	0	0
			21	15	2	1	3		

- Molecule 5 is water.

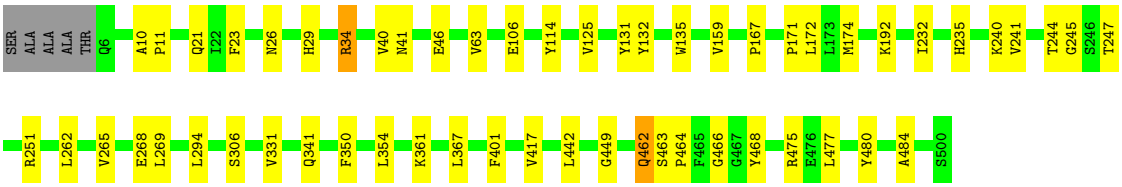
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	409	Total	O	0	0
			409	409		
5	B	429	Total	O	0	0
			429	429		
5	C	427	Total	O	0	0
			427	427		
5	D	416	Total	O	0	0
			416	416		
5	E	440	Total	O	0	0
			440	440		
5	F	444	Total	O	0	0
			444	444		
5	G	457	Total	O	0	0
			457	457		
5	H	386	Total	O	0	0
			386	386		

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.

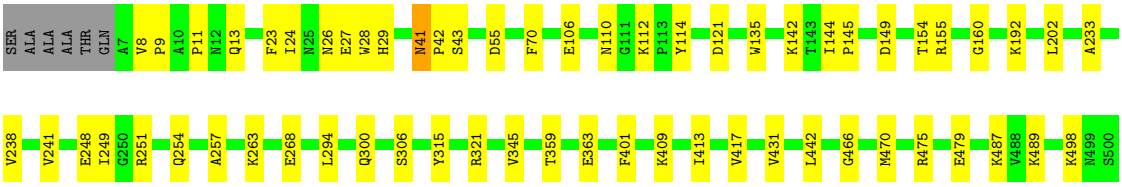
• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain A:



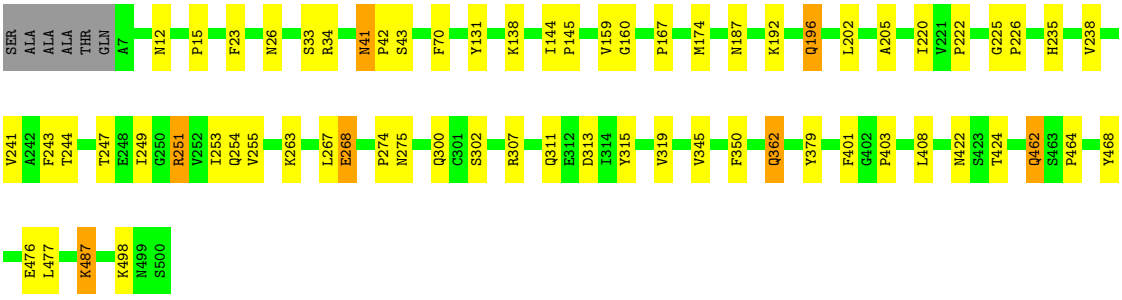
• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain B:



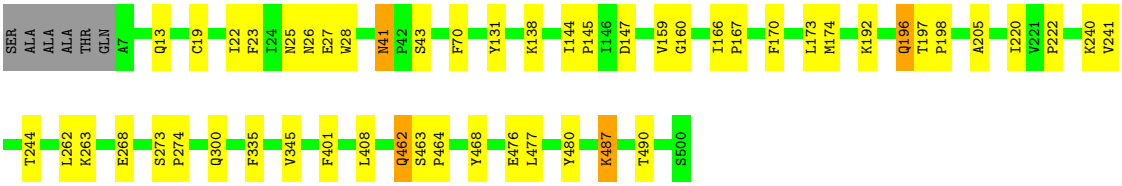
• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain C:



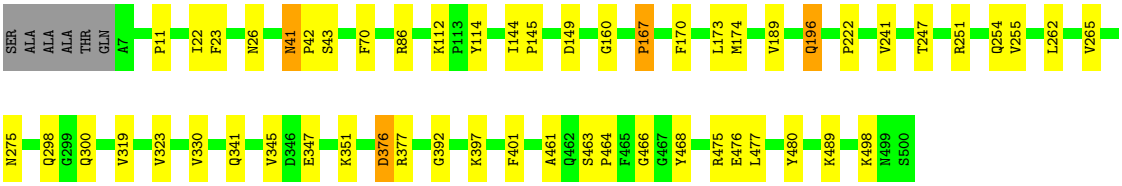
• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain D:



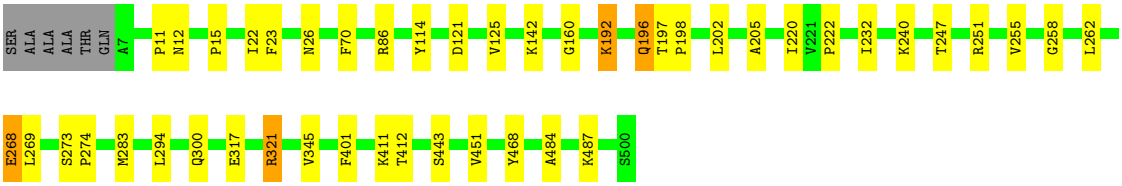
• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain E:



• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain F:

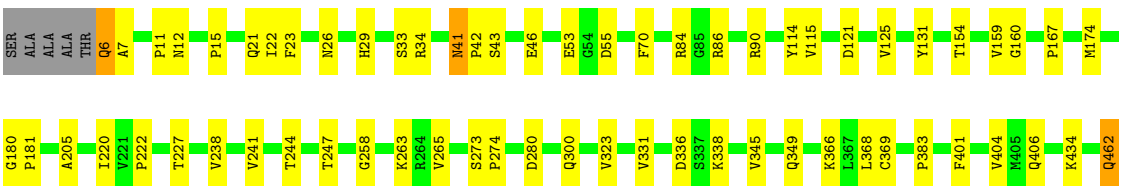


• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain G:

• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain H:




S463
P464
F465
G466
G467
Y468
K469
M470
R475
E476
Y480
K487
V488
K489
S500

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.12Å 176.90Å 102.32Å 90.00° 94.57° 90.00°	Depositor
Resolution (Å)	49.00 – 1.86 49.00 – 1.86	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.00-1.86) 98.8 (49.00-1.86)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.4_4	Depositor
R, R_{free}	0.136 , 0.168 0.137 , 0.135	Depositor DCC
R_{free} test set	15105 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.367 for l,-k,h	Xtriage
Reported twinning fraction	0.378 for l,-k,h	Depositor
Outliers	0 of 299102 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	34144	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, EDO, BXB

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	0.28	0/3900	0.45	0/5290
1	B	0.28	0/3891	0.44	0/5278
1	C	0.28	0/3888	0.44	0/5274
1	D	0.27	0/3891	0.43	0/5278
1	E	0.27	0/3893	0.44	0/5280
1	F	0.28	0/3882	0.44	0/5266
1	G	0.28	0/3891	0.44	0/5278
1	H	0.27	0/3900	0.44	0/5290
All	All	0.28	0/31136	0.44	0/42234

There are no bond length outliers.

There are no bond angle outliers.

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	3812	0	3764	43	0
1	B	3803	0	3756	45	0
1	C	3800	0	3753	52	0
1	D	3803	0	3756	42	0
1	E	3805	0	3761	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3798	0	3752	35	0
1	G	3803	0	3756	50	0
1	H	3812	0	3764	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	24	0	36	1	0
3	B	16	0	24	1	0
3	C	12	0	18	3	0
3	D	8	0	12	0	0
3	E	20	0	30	1	0
3	F	12	0	18	0	0
3	G	20	0	30	0	0
3	H	12	0	18	1	0
4	A	21	0	11	0	0
4	B	21	0	11	0	0
4	C	21	0	11	0	0
4	D	21	0	11	0	0
4	E	21	0	11	0	0
4	F	21	0	11	0	0
4	G	21	0	11	1	0
4	H	21	0	11	0	0
5	A	409	0	0	0	0
5	B	429	0	0	4	0
5	C	427	0	0	4	0
5	D	416	0	0	0	0
5	E	440	0	0	2	0
5	F	444	0	0	2	0
5	G	457	0	0	3	0
5	H	386	0	0	5	0
All	All	34144	0	30336	330	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 5.

All (330) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:HH11	1:A:34:ARG:HG3	1.03	1.12
1:F:196:GLN:H	1:F:196:GLN:HE21	1.14	0.95
1:G:196:GLN:H	1:G:196:GLN:HE21	1.17	0.89
1:A:34:ARG:HG3	1:A:34:ARG:NH1	1.84	0.87
1:C:196:GLN:HE21	1:C:196:GLN:H	1.24	0.86
1:H:366:LYS:HE2	1:H:368:LEU:HD21	1.59	0.85
1:E:262:LEU:HD21	1:F:251:ARG:HD2	1.57	0.84
1:D:196:GLN:H	1:D:196:GLN:HE21	1.31	0.79
1:D:41:ASN:C	1:D:41:ASN:HD22	1.88	0.75
1:D:41:ASN:ND2	1:D:43:SER:H	1.85	0.74
1:F:247:THR:O	1:F:251:ARG:HG2	1.88	0.74
1:G:241:VAL:CG1	1:G:265:VAL:HG22	2.18	0.73
1:F:196:GLN:H	1:F:196:GLN:NE2	1.88	0.71
1:D:464:PRO:HG3	1:D:480:TYR:CD1	2.26	0.71
1:B:241:VAL:HG23	1:B:263:LYS:HD3	1.70	0.71
1:D:41:ASN:HD22	1:D:43:SER:H	1.36	0.71
1:C:244:THR:HG23	1:C:268:GLU:HB3	1.74	0.70
1:G:241:VAL:HG12	1:G:265:VAL:HG22	1.74	0.70
1:E:464:PRO:HG3	1:E:480:TYR:CD1	2.27	0.69
1:A:34:ARG:HH11	1:A:34:ARG:CG	1.93	0.68
1:H:41:ASN:ND2	1:H:43:SER:H	1.92	0.67
1:H:41:ASN:C	1:H:41:ASN:HD22	1.97	0.67
1:C:487:LYS:HD2	1:D:468:TYR:CZ	2.30	0.67
1:H:46:GLU:HB2	3:H:703:EDO:H21	1.76	0.67
1:G:251:ARG:HH21	1:G:470:MET:HE1	1.60	0.66
1:G:262:LEU:HD13	1:H:470:MET:HG2	1.78	0.66
1:B:248:GLU:HG3	1:B:249:ILE:N	2.11	0.65
1:H:12:ASN:O	1:H:15:PRO:HD3	1.97	0.64
1:E:196:GLN:H	1:E:196:GLN:HE21	1.44	0.64
1:E:461:ALA:HA	1:E:477:LEU:HD22	1.80	0.64
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.33	0.63
1:D:159:VAL:HG11	1:D:240:LYS:HB2	1.80	0.63
1:G:41:ASN:C	1:G:41:ASN:HD22	2.02	0.62
1:H:41:ASN:HD22	1:H:43:SER:H	1.48	0.62
1:D:22:ILE:HG12	1:D:222:PRO:HD2	1.82	0.62
1:C:41:ASN:C	1:C:41:ASN:HD22	2.03	0.62
1:F:196:GLN:HE21	1:F:196:GLN:N	1.93	0.62
1:B:41:ASN:C	1:B:41:ASN:HD22	2.03	0.62
1:E:41:ASN:C	1:E:41:ASN:HD22	2.02	0.61
1:G:462:GLN:H	1:G:462:GLN:NE2	1.98	0.61
1:F:247:THR:HA	1:F:269:LEU:HD13	1.83	0.61
1:A:167:PRO:HD2	1:A:174:MET:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:PRO:HG3	1:A:480:TYR:CD1	2.36	0.60
1:C:41:ASN:HB2	3:C:703:EDO:H11	1.84	0.60
1:G:196:GLN:HE21	1:G:196:GLN:N	1.94	0.60
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.37	0.60
1:H:167:PRO:HD2	1:H:174:MET:HG3	1.84	0.60
1:B:251:ARG:HH11	1:B:251:ARG:HB3	1.66	0.60
1:C:41:ASN:ND2	1:C:43:SER:H	2.00	0.59
1:E:475:ARG:HB2	5:E:3107:HOH:O	2.01	0.59
1:D:462:GLN:NE2	1:D:462:GLN:H	2.00	0.59
1:E:41:ASN:ND2	1:E:43:SER:H	1.98	0.59
1:A:247:THR:O	1:A:251:ARG:HG2	2.03	0.59
1:B:41:ASN:ND2	1:B:43:SER:H	2.01	0.58
1:F:268:GLU:HG3	5:F:2967:HOH:O	2.02	0.58
1:G:41:ASN:ND2	1:G:43:SER:H	2.00	0.58
1:G:254:GLN:HG2	1:H:258:GLY:CA	2.33	0.58
1:C:241:VAL:HG23	1:C:263:LYS:HD3	1.86	0.58
1:H:159:VAL:HA	1:H:487:LYS:HE2	1.85	0.58
1:D:244:THR:HG23	1:D:268:GLU:HB3	1.85	0.58
1:E:167:PRO:HD2	1:E:174:MET:HG3	1.86	0.58
1:G:41:ASN:HD22	1:G:43:SER:H	1.51	0.57
1:A:262:LEU:HD12	1:B:470:MET:HG3	1.86	0.57
1:A:462:GLN:H	1:A:462:GLN:NE2	2.02	0.57
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.87	0.57
1:C:487:LYS:HD2	1:D:468:TYR:CE1	2.40	0.57
1:G:13:GLN:HG3	1:G:335:PHE:CG	2.40	0.57
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.39	0.56
1:D:41:ASN:HD21	1:D:43:SER:HB2	1.68	0.56
1:E:300:GLN:HE22	1:E:345:VAL:H	1.53	0.56
1:A:466:GLY:HA3	1:A:475:ARG:HD3	1.86	0.56
1:G:251:ARG:HH21	1:G:470:MET:CE	2.19	0.56
1:C:462:GLN:H	1:C:462:GLN:NE2	2.04	0.56
1:G:254:GLN:HG2	1:H:258:GLY:HA2	1.88	0.56
1:B:24:ILE:O	1:B:27:GLU:HB2	2.06	0.55
1:H:466:GLY:HA3	1:H:475:ARG:HD3	1.88	0.55
1:A:361:LYS:HD2	1:A:367:LEU:HD22	1.89	0.55
1:C:247:THR:O	1:C:251:ARG:HG2	2.06	0.55
1:E:241:VAL:CG1	1:E:265:VAL:HG22	2.37	0.55
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.42	0.55
1:C:205:ALA:HB2	1:C:220:ILE:HD12	1.88	0.54
1:G:424:THR:HB	1:G:470:MET:HG3	1.89	0.54
1:E:298:GLN:HG3	1:E:341:GLN:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:366:LYS:HD2	1:G:388:ASP:OD2	2.08	0.54
1:B:149:ASP:HA	1:B:498:LYS:HB2	1.90	0.54
1:H:300:GLN:HE22	1:H:345:VAL:H	1.56	0.54
1:A:262:LEU:HD23	1:B:254:GLN:OE1	2.07	0.54
1:D:300:GLN:HE22	1:D:345:VAL:H	1.55	0.54
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.42	0.54
1:A:167:PRO:HG3	1:A:244:THR:HG22	1.90	0.54
1:E:468:TYR:CZ	1:F:487:LYS:HE3	2.43	0.53
1:A:63:VAL:HG11	1:A:235:HIS:CE1	2.43	0.53
1:D:241:VAL:HG23	1:D:263:LYS:HD3	1.89	0.53
1:F:300:GLN:HE22	1:F:345:VAL:H	1.56	0.53
1:C:254:GLN:OE1	1:D:262:LEU:HD23	2.08	0.53
1:C:41:ASN:HD22	1:C:42:PRO:N	2.07	0.53
1:E:41:ASN:HD22	1:E:43:SER:H	1.56	0.53
1:E:254:GLN:HE22	1:F:262:LEU:HA	1.74	0.53
1:B:70:PHE:CZ	1:B:160:GLY:HA2	2.44	0.53
1:E:392:GLY:HA2	1:E:397:LYS:HE3	1.91	0.52
1:H:55:ASP:OD1	1:H:227:THR:HB	2.10	0.52
1:H:238:VAL:O	1:H:263:LYS:HE3	2.10	0.52
1:H:336:ASP:OD1	1:H:338:LYS:HG2	2.10	0.52
1:E:251:ARG:O	1:E:255:VAL:HG23	2.10	0.52
1:E:254:GLN:OE1	1:F:262:LEU:HG	2.10	0.52
1:G:359:THR:O	1:G:363:GLU:HG3	2.09	0.52
1:D:41:ASN:C	1:D:41:ASN:ND2	2.61	0.51
1:G:487:LYS:HG2	1:H:468:TYR:CE1	2.45	0.51
1:A:21:GLN:HB3	1:A:29:HIS:O	2.10	0.51
1:A:417:VAL:CG2	1:A:442:LEU:HD23	2.40	0.51
1:B:413:ILE:O	1:B:417:VAL:HG23	2.11	0.51
1:G:422:ASN:HB3	5:G:1455:HOH:O	2.11	0.51
1:G:468:TYR:CE1	1:H:487:LYS:HD2	2.45	0.51
1:D:197:THR:N	1:D:198:PRO:HD3	2.27	0.50
1:E:196:GLN:H	1:E:196:GLN:NE2	2.08	0.50
1:B:321:ARG:HD3	5:B:3223:HOH:O	2.11	0.50
1:H:70:PHE:CZ	1:H:160:GLY:HA2	2.47	0.50
1:G:11:PRO:HG3	1:G:114:TYR:CD2	2.46	0.50
1:B:41:ASN:HD22	1:B:42:PRO:N	2.09	0.50
1:H:464:PRO:HA	1:H:476:GLU:O	2.12	0.50
1:G:13:GLN:HG2	5:G:985:HOH:O	2.12	0.50
1:H:22:ILE:HG12	1:H:222:PRO:HD2	1.92	0.50
1:H:131:TYR:CE1	1:H:462:GLN:HG3	2.46	0.50
1:G:159:VAL:HG11	1:G:240:LYS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:487:LYS:HE3	1:H:468:TYR:CZ	2.47	0.49
1:D:131:TYR:CE1	1:D:462:GLN:HG3	2.48	0.49
1:A:468:TYR:CZ	1:B:487:LYS:HE3	2.47	0.49
1:G:196:GLN:H	1:G:196:GLN:NE2	1.99	0.49
1:A:245:GLY:O	1:A:269:LEU:HA	2.13	0.49
1:A:331:VAL:HG22	1:A:341:GLN:HB3	1.94	0.49
1:B:294:LEU:HD23	1:B:306:SER:HA	1.95	0.49
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.48	0.49
5:C:1910:HOH:O	1:D:147:ASP:HB2	2.13	0.49
1:C:196:GLN:H	1:C:196:GLN:NE2	2.03	0.48
1:B:135:TRP:CE2	1:D:138:LYS:HD3	2.48	0.48
1:H:462:GLN:H	1:H:462:GLN:NE2	2.11	0.48
1:F:240:LYS:HE2	1:F:484:ALA:O	2.13	0.48
1:B:315:TYR:CD1	1:B:409:LYS:HE2	2.48	0.48
1:B:359:THR:O	1:B:363:GLU:HG3	2.13	0.48
1:E:330:VAL:HA	3:E:702:EDO:H11	1.95	0.48
1:C:41:ASN:HD22	1:C:43:SER:H	1.60	0.48
1:E:86[A]:ARG:HD3	5:E:654:HOH:O	2.14	0.48
1:C:362:GLN:HG2	5:C:2741:HOH:O	2.13	0.48
1:D:170:PHE:HB2	1:D:174:MET:HG2	1.96	0.48
1:F:205:ALA:HB2	1:F:220:ILE:HD12	1.96	0.48
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.95	0.47
1:H:154:THR:HA	1:H:489:LYS:O	2.14	0.47
1:B:55:ASP:HB3	5:B:3400:HOH:O	2.13	0.47
1:E:489:LYS:HB2	1:F:468:TYR:OH	2.14	0.47
1:H:33:SER:O	1:H:34:ARG:HB2	2.14	0.47
1:E:41:ASN:HD22	1:E:42:PRO:N	2.12	0.47
1:D:196:GLN:H	1:D:196:GLN:NE2	2.06	0.47
1:C:487:LYS:HD2	1:D:468:TYR:CE2	2.49	0.47
1:E:241:VAL:HG12	1:E:265:VAL:HG22	1.96	0.47
1:F:22:ILE:HG12	1:F:222:PRO:HD2	1.97	0.47
1:F:294:LEU:HD13	1:F:294:LEU:C	2.35	0.47
1:D:159:VAL:HA	1:D:487:LYS:HE2	1.96	0.47
1:G:22:ILE:HG12	1:G:222:PRO:HD2	1.97	0.47
1:G:350:PHE:CD1	1:G:379:TYR:HB3	2.50	0.47
1:G:498:LYS:HE2	1:G:498:LYS:HB3	1.75	0.47
1:A:449:GLY:HA3	1:A:466:GLY:O	2.15	0.46
1:E:347:GLU:HG2	1:E:351:LYS:HE2	1.97	0.46
1:B:300:GLN:HE22	1:B:345:VAL:H	1.64	0.46
1:C:33:SER:O	1:C:34:ARG:HB2	2.16	0.46
1:C:302[B]:SER:HG	3:C:701:EDO:H22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HA	1:B:254:GLN:HE22	1.80	0.46
1:B:13:GLN:NE2	5:B:1588:HOH:O	2.49	0.46
1:C:144:ILE:HA	1:C:145:PRO:HD3	1.78	0.46
1:B:257:ALA:HB1	1:B:263:LYS:HG3	1.96	0.46
1:C:41:ASN:CB	3:C:703:EDO:H11	2.45	0.46
1:C:249:ILE:O	1:C:253:ILE:HG12	2.15	0.46
1:D:25:ASN:O	1:D:27:GLU:HG2	2.16	0.46
1:F:443:SER:HA	1:F:451:VAL:HG11	1.98	0.46
1:H:273:SER:HA	1:H:274:PRO:HD3	1.71	0.46
1:C:196:GLN:HE21	1:C:196:GLN:N	2.03	0.46
1:D:476:GLU:O	1:D:477:LEU:HB2	2.16	0.46
1:E:70:PHE:CZ	1:E:160:GLY:HA2	2.50	0.46
1:E:498:LYS:HB3	1:E:498:LYS:HE2	1.69	0.46
1:A:46:GLU:HB2	3:A:705:EDO:H21	1.98	0.45
1:G:41:ASN:HD21	1:G:43:SER:HB2	1.81	0.45
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.52	0.45
1:G:106:GLU:O	1:G:110:ASN:HB3	2.17	0.45
1:B:28:TRP:HZ3	1:B:202:LEU:HD22	1.81	0.45
1:A:11:PRO:HG3	1:A:114:TYR:CD2	2.51	0.45
1:B:11:PRO:HG3	1:B:114:TYR:CD2	2.52	0.45
1:C:167:PRO:HD2	1:C:174:MET:HG3	1.98	0.45
1:A:135:TRP:CE2	1:C:138:LYS:HD3	2.51	0.45
1:C:476:GLU:O	1:C:477:LEU:HB2	2.17	0.45
1:H:41:ASN:ND2	1:H:41:ASN:C	2.68	0.45
1:B:41:ASN:HD22	1:B:43:SER:H	1.65	0.45
1:C:225:GLY:N	1:C:226:PRO:HD2	2.30	0.45
1:D:462:GLN:H	1:D:462:GLN:HE21	1.65	0.45
1:E:144:ILE:HA	1:E:145:PRO:HD3	1.73	0.45
1:G:142:LYS:HE2	1:H:480:TYR:CZ	2.52	0.45
1:C:408:LEU:HD12	1:C:408:LEU:N	2.32	0.45
1:G:202:LEU:HD21	1:G:222:PRO:HG3	1.99	0.45
1:G:247:THR:HA	1:G:269:LEU:HD13	1.99	0.45
1:F:251:ARG:O	1:F:255:VAL:HG23	2.17	0.44
1:C:315:TYR:O	1:C:319:VAL:HG23	2.18	0.44
1:F:317:GLU:O	1:F:321:ARG:HG2	2.16	0.44
1:G:167:PRO:HD2	1:G:174:MET:HG3	1.99	0.44
1:H:121:ASP:O	1:H:125:VAL:HG23	2.17	0.44
1:A:294:LEU:HD13	1:A:294:LEU:C	2.38	0.44
1:C:131:TYR:CE1	1:C:462:GLN:HG3	2.52	0.44
1:D:144:ILE:HA	1:D:145:PRO:HD3	1.78	0.44
1:E:22:ILE:HG12	1:E:222:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:THR:HG23	1:F:269:LEU:HD13	1.99	0.44
1:H:323:VAL:HG13	1:H:369:CYS:HB3	2.00	0.44
1:C:311:GLN:OE1	1:C:313:ASP:HB2	2.18	0.44
1:C:468:TYR:CD1	1:D:487:LYS:HD2	2.53	0.44
1:D:70:PHE:CZ	1:D:160:GLY:HA2	2.53	0.44
1:G:468:TYR:CD1	1:H:487:LYS:HD2	2.52	0.44
1:A:294:LEU:HD23	1:A:306:SER:HA	2.00	0.44
1:D:170:PHE:HB3	1:D:173:LEU:HB3	2.00	0.44
1:F:192:LYS:HB2	1:F:232:ILE:HD12	2.00	0.44
1:F:273:SER:HA	1:F:274:PRO:HD3	1.77	0.44
1:G:464:PRO:HG3	1:G:480:TYR:CD1	2.52	0.44
1:B:238:VAL:O	1:B:263:LYS:HE3	2.17	0.44
1:B:251:ARG:HB3	1:B:251:ARG:NH1	2.32	0.43
1:E:170:PHE:HB3	1:E:173:LEU:HB3	1.99	0.43
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.53	0.43
1:A:480:TYR:CZ	1:B:142:LYS:HE2	2.54	0.43
1:C:235:HIS:HB3	1:C:238:VAL:HG23	2.00	0.43
1:C:300:GLN:HE22	1:C:345:VAL:H	1.66	0.43
1:D:167:PRO:HG3	1:D:244:THR:O	2.18	0.43
1:G:249:ILE:O	1:G:253:ILE:HG12	2.18	0.43
1:D:273:SER:HA	1:D:274:PRO:HD3	1.81	0.43
1:A:192:LYS:HB2	1:A:232:ILE:CD1	2.49	0.43
1:B:294:LEU:C	1:B:294:LEU:HD13	2.39	0.43
1:B:487:LYS:HB2	1:B:487:LYS:HE2	1.78	0.43
1:C:243:PHE:HB3	1:C:267:LEU:CD2	2.48	0.43
1:F:411:LYS:HG2	1:F:412:THR:HG23	2.01	0.43
1:G:273:SER:HA	1:G:274:PRO:HD3	1.76	0.43
1:F:197:THR:N	1:F:198:PRO:HD3	2.33	0.43
1:G:413:ILE:O	1:G:417:VAL:HG23	2.19	0.43
1:G:487:LYS:HE3	1:H:468:TYR:CE2	2.54	0.43
1:H:7:ALA:HB3	5:H:3308:HOH:O	2.17	0.43
1:B:106:GLU:O	1:B:110:ASN:HB3	2.19	0.43
1:B:233:ALA:HA	1:B:241:VAL:HG21	2.00	0.43
1:B:321:ARG:CZ	5:B:3174:HOH:O	2.66	0.43
1:C:12:ASN:O	1:C:15:PRO:HD3	2.19	0.43
1:G:166:ILE:HD11	5:G:594:HOH:O	2.19	0.43
1:A:241:VAL:CG1	1:A:265:VAL:HG22	2.48	0.43
1:B:27:GLU:HB2	1:B:29:HIS:NE2	2.33	0.43
1:B:135:TRP:CZ2	1:B:479:GLU:HB2	2.53	0.43
1:E:11:PRO:HB3	1:E:114:TYR:CZ	2.54	0.43
1:A:132:TYR:OH	1:A:477:LEU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:VAL:HG21	1:B:442:LEU:HB3	2.00	0.43
1:H:21:GLN:HB3	1:H:29:HIS:O	2.18	0.43
1:H:180:GLY:N	1:H:181:PRO:HD2	2.34	0.43
1:F:487:LYS:HD3	5:F:2507:HOH:O	2.19	0.42
1:G:254:GLN:HG2	1:H:258:GLY:HA3	2.00	0.42
1:C:422:ASN:HB3	5:C:2799:HOH:O	2.20	0.42
1:B:144:ILE:HA	1:B:145:PRO:HD3	1.79	0.42
1:H:115:VAL:HG23	5:H:554:HOH:O	2.19	0.42
1:G:144:ILE:CG2	1:H:462:GLN:HB3	2.49	0.42
1:H:86:ARG:HD2	1:H:86:ARG:HA	1.84	0.42
1:C:350:PHE:CD1	1:C:379:TYR:HB3	2.55	0.42
1:E:254:GLN:CD	1:F:258:GLY:HA2	2.40	0.42
1:E:480:TYR:CZ	1:F:142:LYS:HE2	2.54	0.42
1:B:8:VAL:HA	1:B:9:PRO:HD3	1.89	0.42
1:C:468:TYR:CE1	1:D:487:LYS:HD2	2.55	0.42
1:H:6:GLN:HE21	1:H:6:GLN:HB3	1.60	0.42
1:B:466:GLY:HA3	1:B:475:ARG:HD3	2.01	0.42
1:F:202:LEU:HD21	1:F:222:PRO:HG3	2.01	0.42
1:F:283:MET:CG	1:F:321:ARG:HH21	2.33	0.42
1:A:125:VAL:HG21	1:A:172:LEU:HB3	2.02	0.42
1:C:70:PHE:CZ	1:C:160:GLY:HA2	2.55	0.42
1:C:251:ARG:HG2	1:C:251:ARG:H	1.63	0.42
1:G:170:PHE:HB3	1:G:173:LEU:HB3	2.02	0.42
1:H:241:VAL:HG13	1:H:241:VAL:O	2.19	0.42
1:H:41:ASN:HD22	1:H:42:PRO:N	2.17	0.42
1:A:463:SER:HA	1:A:464:PRO:HD3	1.92	0.41
1:C:464:PRO:HG2	1:D:490:THR:OG1	2.19	0.41
1:B:155:ARG:HD2	3:B:703:EDO:O1	2.20	0.41
1:D:19:CYS:HB3	1:D:28:TRP:CH2	2.55	0.41
1:E:149:ASP:HA	1:E:498:LYS:HB2	2.02	0.41
1:F:121:ASP:O	1:F:125:VAL:HG23	2.20	0.41
1:G:154:THR:HA	1:G:489:LYS:O	2.20	0.41
1:H:331:VAL:HG21	1:H:383:PRO:HD3	2.02	0.41
1:B:112:LYS:NZ	1:B:121:ASP:OD1	2.45	0.41
1:C:274:PRO:HG3	1:C:307:ARG:NH2	2.35	0.41
1:C:498:LYS:HE2	1:C:498:LYS:HB3	1.94	0.41
1:E:247:THR:O	1:E:251:ARG:HG3	2.20	0.41
1:E:351:LYS:HB2	1:E:351:LYS:HE3	1.83	0.41
1:E:466:GLY:HA3	1:E:475:ARG:HD3	2.02	0.41
1:F:86:ARG:HA	1:F:86:ARG:HD2	1.87	0.41
1:G:70:PHE:CZ	1:G:160:GLY:HA2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:SER:HA	1:D:464:PRO:HD3	1.87	0.41
1:A:10:ALA:HA	1:A:11:PRO:HD3	1.97	0.41
1:B:154:THR:HA	1:B:489:LYS:O	2.21	0.41
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.55	0.41
1:D:166:ILE:HA	1:D:167:PRO:HD3	1.90	0.41
1:G:124:MET:SD	4:G:1001:BXB:CL11	3.16	0.41
1:G:312:GLU:OE1	1:G:411:LYS:HG3	2.21	0.41
1:H:167:PRO:HG3	1:H:244:THR:HG22	2.03	0.41
1:A:240:LYS:HE2	1:A:484:ALA:O	2.20	0.41
1:H:404:VAL:HG12	1:H:406:GLN:OE1	2.19	0.41
1:C:251:ARG:O	1:C:255:VAL:HG23	2.21	0.41
1:D:408:LEU:N	1:D:408:LEU:HD12	2.36	0.41
1:E:319:VAL:O	1:E:323:VAL:HG23	2.21	0.41
1:A:131:TYR:CE1	1:A:462:GLN:HG3	2.56	0.41
1:A:247:THR:HA	1:A:269:LEU:HB3	2.03	0.41
1:A:350:PHE:O	1:A:354:LEU:HG	2.21	0.41
1:A:417:VAL:HG23	1:A:442:LEU:CD2	2.51	0.41
1:D:13:GLN:HG2	1:D:335:PHE:CG	2.56	0.41
1:F:12:ASN:O	1:F:15:PRO:HD3	2.21	0.41
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.56	0.41
1:H:280:ASP:O	1:H:434:LYS:HG3	2.20	0.41
1:A:34:ARG:HA	1:A:34:ARG:HD2	1.81	0.41
1:A:468:TYR:CE2	1:B:487:LYS:HE3	2.56	0.41
1:C:41:ASN:HD22	1:C:42:PRO:HD2	1.86	0.41
1:C:41:ASN:C	1:C:41:ASN:ND2	2.73	0.40
1:H:84:ARG:HD3	5:H:2380:HOH:O	2.20	0.40
1:A:106:GLU:OE1	1:A:171:PRO:HD2	2.20	0.40
1:A:192:LYS:HB2	1:A:232:ILE:HD11	2.03	0.40
1:G:464:PRO:HA	1:G:476:GLU:O	2.21	0.40
1:A:40:VAL:HG12	1:A:41:ASN:N	2.37	0.40
1:C:41:ASN:HD22	1:C:42:PRO:CD	2.32	0.40
1:E:463:SER:HA	1:E:464:PRO:HD3	1.85	0.40
1:H:241:VAL:HG12	1:H:265:VAL:HG22	2.03	0.40
1:H:349:GLN:NE2	5:H:2750:HOH:O	2.49	0.40
1:C:202:LEU:HD21	1:C:222:PRO:HG3	2.04	0.40
1:C:268:GLU:HG2	5:C:2350:HOH:O	2.21	0.40
1:E:476:GLU:O	1:E:477:LEU:HB2	2.20	0.40
1:F:70:PHE:CZ	1:F:160:GLY:HA2	2.56	0.40
1:C:159:VAL:HG12	1:C:187:ASN:OD1	2.20	0.40
1:E:112:LYS:HE2	1:E:112:LYS:HB3	1.91	0.40
1:E:376:ASP:OD2	1:E:376:ASP:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:ARG:NH1	5:H:2425:HOH:O	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/500 (99%)	479 (97%)	15 (3%)	0	100	100
1	B	493/500 (99%)	477 (97%)	16 (3%)	0	100	100
1	C	493/500 (99%)	474 (96%)	19 (4%)	0	100	100
1	D	493/500 (99%)	480 (97%)	13 (3%)	0	100	100
1	E	493/500 (99%)	479 (97%)	14 (3%)	0	100	100
1	F	492/500 (98%)	479 (97%)	13 (3%)	0	100	100
1	G	493/500 (99%)	477 (97%)	16 (3%)	0	100	100
1	H	494/500 (99%)	478 (97%)	16 (3%)	0	100	100
All	All	3945/4000 (99%)	3823 (97%)	122 (3%)	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	401/402 (100%)	396 (99%)	5 (1%)	71	62
1	B	400/402 (100%)	396 (99%)	4 (1%)	76	69
1	C	400/402 (100%)	388 (97%)	12 (3%)	41	24
1	D	400/402 (100%)	394 (98%)	6 (2%)	65	53
1	E	400/402 (100%)	392 (98%)	8 (2%)	55	40
1	F	399/402 (99%)	394 (99%)	5 (1%)	69	58
1	G	400/402 (100%)	391 (98%)	9 (2%)	50	34
1	H	401/402 (100%)	392 (98%)	9 (2%)	52	36
All	All	3201/3216 (100%)	3143 (98%)	58 (2%)	59	45

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	159	VAL
1	A	268	GLU
1	A	401	PHE
1	A	462	GLN
1	B	41	ASN
1	B	192	LYS
1	B	268	GLU
1	B	401	PHE
1	C	41	ASN
1	C	192	LYS
1	C	196	GLN
1	C	251	ARG
1	C	268	GLU
1	C	275	ASN
1	C	362	GLN
1	C	401	PHE
1	C	403	PRO
1	C	424	THR
1	C	462	GLN
1	C	487	LYS
1	D	41	ASN
1	D	192	LYS
1	D	196	GLN
1	D	401	PHE
1	D	462	GLN
1	D	487	LYS

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Mol	Chain	Res	Type
1	E	41	ASN
1	E	167	PRO
1	E	189	VAL
1	E	196	GLN
1	E	275	ASN
1	E	376	ASP
1	E	377	ARG
1	E	401	PHE
1	F	192	LYS
1	F	196	GLN
1	F	268	GLU
1	F	321	ARG
1	F	401	PHE
1	G	41	ASN
1	G	121	ASP
1	G	192	LYS
1	G	196	GLN
1	G	268	GLU
1	G	275	ASN
1	G	362	GLN
1	G	401	PHE
1	G	462	GLN
1	H	6	GLN
1	H	41	ASN
1	H	53	GLU
1	H	90	ARG
1	H	247	THR
1	H	401	PHE
1	H	462	GLN
1	H	470	MET
1	H	487	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	26	ASN
1	A	275	ASN
1	A	297	ASN
1	A	358	ASN
1	A	462	GLN
1	B	13	GLN

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Mol	Chain	Res	Type
1	B	26	ASN
1	B	41	ASN
1	B	175	GLN
1	C	14	GLN
1	C	41	ASN
1	C	196	GLN
1	C	275	ASN
1	C	362	GLN
1	C	462	GLN
1	D	26	ASN
1	D	41	ASN
1	D	175	GLN
1	D	196	GLN
1	D	275	ASN
1	D	300	GLN
1	D	344	GLN
1	D	362	GLN
1	D	462	GLN
1	E	26	ASN
1	E	41	ASN
1	E	164	GLN
1	E	196	GLN
1	E	275	ASN
1	F	13	GLN
1	F	26	ASN
1	F	71	GLN
1	F	196	GLN
1	F	300	GLN
1	F	362	GLN
1	G	13	GLN
1	G	14	GLN
1	G	26	ASN
1	G	41	ASN
1	G	196	GLN
1	G	275	ASN
1	G	462	GLN
1	H	6	GLN
1	H	26	ASN
1	H	41	ASN
1	H	175	GLN
1	H	275	ASN
1	H	462	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 47 ligands modelled in this entry, 8 are monoatomic - leaving 39 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	A	703	-	3,3,3	0.35	0	2,2,2	0.40	0
3	EDO	D	702	-	3,3,3	0.37	0	2,2,2	0.38	0
3	EDO	B	702	-	3,3,3	0.41	0	2,2,2	0.34	0
3	EDO	A	701	-	3,3,3	0.42	0	2,2,2	0.34	0
3	EDO	F	701	-	3,3,3	0.38	0	2,2,2	0.56	0
3	EDO	E	703	-	3,3,3	0.42	0	2,2,2	0.21	0
3	EDO	A	706	-	3,3,3	0.35	0	2,2,2	0.55	0
3	EDO	C	703	-	3,3,3	0.38	0	2,2,2	0.31	0
3	EDO	G	704	-	3,3,3	0.42	0	2,2,2	0.27	0
3	EDO	D	701	-	3,3,3	0.42	0	2,2,2	0.33	0
4	BXB	A	1001	-	23,23,23	2.04	5 (21%)	32,32,32	1.43	6 (18%)
4	BXB	F	1001	-	23,23,23	2.11	5 (21%)	32,32,32	1.40	5 (15%)
3	EDO	H	701	-	3,3,3	0.37	0	2,2,2	0.40	0
3	EDO	B	701	-	3,3,3	0.44	0	2,2,2	0.23	0
3	EDO	F	501	-	3,3,3	0.41	0	2,2,2	0.16	0
4	BXB	D	1001	-	23,23,23	2.01	5 (21%)	32,32,32	1.51	7 (21%)
3	EDO	B	703	-	3,3,3	0.38	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	B	704	-	3,3,3	0.39	0	2,2,2	0.33	0
3	EDO	H	703	-	3,3,3	0.40	0	2,2,2	0.34	0
3	EDO	H	704	-	3,3,3	0.40	0	2,2,2	0.20	0
3	EDO	G	702	-	3,3,3	0.40	0	2,2,2	0.37	0
3	EDO	E	704	-	3,3,3	0.36	0	2,2,2	0.46	0
3	EDO	F	703	-	3,3,3	0.39	0	2,2,2	0.35	0
4	BXB	C	1001	-	23,23,23	1.99	5 (21%)	32,32,32	1.48	8 (25%)
4	BXB	H	1001	-	23,23,23	2.01	5 (21%)	32,32,32	1.44	4 (12%)
3	EDO	G	701	-	3,3,3	0.36	0	2,2,2	0.51	0
3	EDO	G	705	-	3,3,3	0.41	0	2,2,2	0.35	0
3	EDO	A	702	-	3,3,3	0.43	0	2,2,2	0.21	0
3	EDO	E	702	-	3,3,3	0.38	0	2,2,2	0.32	0
3	EDO	E	501	-	3,3,3	0.41	0	2,2,2	0.35	0
4	BXB	G	1001	-	23,23,23	2.01	5 (21%)	32,32,32	1.41	6 (18%)
3	EDO	A	705	-	3,3,3	0.40	0	2,2,2	0.27	0
3	EDO	C	702	-	3,3,3	0.36	0	2,2,2	0.51	0
4	BXB	B	1001	-	23,23,23	2.00	5 (21%)	32,32,32	1.51	6 (18%)
3	EDO	A	704	-	3,3,3	0.38	0	2,2,2	0.52	0
3	EDO	G	501	-	3,3,3	0.35	0	2,2,2	0.64	0
4	BXB	E	1001	-	23,23,23	2.04	5 (21%)	32,32,32	1.38	5 (15%)
3	EDO	E	701	-	3,3,3	0.38	0	2,2,2	0.32	0
3	EDO	C	701	-	3,3,3	0.40	0	2,2,2	0.46	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
3	EDO	A	703	-	-	0/1/1/1	-
3	EDO	D	702	-	-	0/1/1/1	-
3	EDO	B	702	-	-	1/1/1/1	-
3	EDO	A	701	-	-	1/1/1/1	-
3	EDO	F	701	-	-	0/1/1/1	-
3	EDO	E	703	-	-	0/1/1/1	-
3	EDO	A	706	-	-	1/1/1/1	-
3	EDO	C	703	-	-	0/1/1/1	-
3	EDO	G	704	-	-	0/1/1/1	-
3	EDO	D	701	-	-	0/1/1/1	-
4	BXB	A	1001	-	-	0/9/15/15	0/3/3/3
4	BXB	F	1001	-	-	0/9/15/15	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	H	701	-	-	0/1/1/1	-
3	EDO	B	701	-	-	0/1/1/1	-
3	EDO	F	501	-	-	0/1/1/1	-
4	BXB	D	1001	-	-	0/9/15/15	0/3/3/3
3	EDO	B	703	-	-	0/1/1/1	-
3	EDO	B	704	-	-	0/1/1/1	-
3	EDO	H	703	-	-	1/1/1/1	-
3	EDO	H	704	-	-	0/1/1/1	-
3	EDO	G	702	-	-	0/1/1/1	-
3	EDO	E	704	-	-	0/1/1/1	-
3	EDO	F	703	-	-	0/1/1/1	-
4	BXB	C	1001	-	-	0/9/15/15	0/3/3/3
4	BXB	H	1001	-	-	0/9/15/15	0/3/3/3
3	EDO	G	701	-	-	1/1/1/1	-
3	EDO	G	705	-	-	0/1/1/1	-
3	EDO	A	702	-	-	0/1/1/1	-
3	EDO	E	702	-	-	1/1/1/1	-
3	EDO	E	501	-	-	0/1/1/1	-
4	BXB	G	1001	-	-	0/9/15/15	0/3/3/3
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	C	702	-	-	0/1/1/1	-
4	BXB	B	1001	-	-	0/9/15/15	0/3/3/3
3	EDO	A	704	-	-	0/1/1/1	-
3	EDO	G	501	-	-	1/1/1/1	-
4	BXB	E	1001	-	-	0/9/15/15	0/3/3/3
3	EDO	E	701	-	-	0/1/1/1	-
3	EDO	C	701	-	-	1/1/1/1	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1001	BXB	C1-C2	6.29	1.49	1.39
4	B	1001	BXB	C1-C2	6.17	1.49	1.39
4	H	1001	BXB	C1-C2	6.04	1.48	1.39
4	A	1001	BXB	C1-C2	6.02	1.48	1.39
4	E	1001	BXB	C1-C2	6.02	1.48	1.39
4	F	1001	BXB	C1-C6	6.02	1.48	1.39
4	C	1001	BXB	C1-C2	5.92	1.48	1.39
4	E	1001	BXB	C1-C6	5.90	1.48	1.39
4	C	1001	BXB	C1-C6	5.86	1.48	1.39
4	D	1001	BXB	C1-C2	5.84	1.48	1.39
4	G	1001	BXB	C1-C2	5.81	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	BXB	C1-C6	5.80	1.48	1.39
4	H	1001	BXB	C1-C6	5.75	1.48	1.39
4	D	1001	BXB	C1-C6	5.72	1.48	1.39
4	G	1001	BXB	C1-C6	5.71	1.48	1.39
4	B	1001	BXB	C1-C6	5.46	1.48	1.39
4	E	1001	BXB	C17-C16	2.71	1.46	1.39
4	G	1001	BXB	C6-CL11	2.70	1.80	1.73
4	F	1001	BXB	C17-C16	2.70	1.46	1.39
4	B	1001	BXB	C2-CL10	2.69	1.80	1.73
4	D	1001	BXB	C17-C16	2.68	1.46	1.39
4	G	1001	BXB	C17-C16	2.66	1.46	1.39
4	G	1001	BXB	C2-CL10	2.65	1.79	1.73
4	A	1001	BXB	C2-CL10	2.62	1.79	1.73
4	D	1001	BXB	C6-CL11	2.59	1.79	1.73
4	F	1001	BXB	C2-CL10	2.57	1.79	1.73
4	D	1001	BXB	C2-CL10	2.55	1.79	1.73
4	A	1001	BXB	C17-C16	2.53	1.45	1.39
4	H	1001	BXB	C6-CL11	2.50	1.79	1.73
4	B	1001	BXB	C17-C16	2.50	1.45	1.39
4	C	1001	BXB	C17-C16	2.48	1.45	1.39
4	B	1001	BXB	C6-CL11	2.44	1.79	1.73
4	E	1001	BXB	C6-CL11	2.43	1.79	1.73
4	A	1001	BXB	C6-CL11	2.41	1.79	1.73
4	H	1001	BXB	C17-C16	2.39	1.45	1.39
4	F	1001	BXB	C6-CL11	2.38	1.79	1.73
4	H	1001	BXB	C2-CL10	2.37	1.79	1.73
4	E	1001	BXB	C2-CL10	2.26	1.79	1.73
4	C	1001	BXB	C6-CL11	2.24	1.79	1.73
4	C	1001	BXB	C2-CL10	2.24	1.79	1.73

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1001	BXB	C20-O19-C17	2.77	108.94	105.34
4	C	1001	BXB	C20-O19-C17	2.65	108.79	105.34
4	H	1001	BXB	C20-O19-C17	2.62	108.74	105.34
4	C	1001	BXB	C17-C18-C13	-2.59	116.17	120.05
4	H	1001	BXB	C20-O21-C16	2.59	108.70	105.34
4	B	1001	BXB	C20-O19-C17	2.55	108.66	105.34
4	C	1001	BXB	C14-C13-C18	2.55	122.11	118.54
4	D	1001	BXB	C14-C13-C18	2.46	121.98	118.54
4	F	1001	BXB	C20-O19-C17	2.44	108.50	105.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1001	BXB	C3-C2-C1	-2.42	118.64	121.86
4	F	1001	BXB	C17-C18-C13	-2.42	116.43	120.05
4	G	1001	BXB	C20-O19-C17	2.41	108.47	105.34
4	A	1001	BXB	C20-O19-C17	2.39	108.45	105.34
4	C	1001	BXB	C20-O21-C16	2.38	108.43	105.34
4	D	1001	BXB	C20-O19-C17	2.35	108.39	105.34
4	D	1001	BXB	C20-O21-C16	2.34	108.38	105.34
4	D	1001	BXB	O19-C17-C18	2.33	130.97	127.85
4	D	1001	BXB	C17-C18-C13	-2.33	116.56	120.05
4	B	1001	BXB	C20-O21-C16	2.32	108.36	105.34
4	A	1001	BXB	C3-C2-C1	-2.29	118.82	121.86
4	G	1001	BXB	C14-C13-C18	2.26	121.70	118.54
4	E	1001	BXB	C20-O21-C16	2.24	108.25	105.34
4	A	1001	BXB	C1-C7-N8	2.24	120.06	115.62
4	C	1001	BXB	C13-C12-N8	-2.23	108.27	113.05
4	G	1001	BXB	O19-C17-C18	2.23	130.83	127.85
4	B	1001	BXB	C13-C12-N8	-2.23	108.27	113.05
4	C	1001	BXB	O19-C17-C18	2.23	130.83	127.85
4	E	1001	BXB	O19-C17-C18	2.21	130.81	127.85
4	G	1001	BXB	C20-O21-C16	2.20	108.20	105.34
4	G	1001	BXB	C5-C6-C1	-2.20	118.93	121.86
4	F	1001	BXB	C3-C2-C1	-2.20	118.94	121.86
4	B	1001	BXB	C3-C2-C1	-2.19	118.94	121.86
4	A	1001	BXB	C20-O21-C16	2.18	108.18	105.34
4	E	1001	BXB	C17-C18-C13	-2.18	116.78	120.05
4	G	1001	BXB	C17-C18-C13	-2.16	116.81	120.05
4	B	1001	BXB	O19-C17-C18	2.12	130.69	127.85
4	A	1001	BXB	C14-C13-C18	2.12	121.50	118.54
4	H	1001	BXB	O19-C17-C18	2.12	130.68	127.85
4	H	1001	BXB	C14-C13-C18	2.11	121.49	118.54
4	B	1001	BXB	C14-C13-C18	2.10	121.47	118.54
4	C	1001	BXB	C1-C7-N8	2.07	119.72	115.62
4	A	1001	BXB	C17-C18-C13	-2.06	116.96	120.05
4	E	1001	BXB	O19-C17-C16	-2.06	107.44	109.78
4	D	1001	BXB	C13-C12-N8	-2.05	108.65	113.05
4	F	1001	BXB	C20-O21-C16	2.03	107.97	105.34
4	C	1001	BXB	C14-C15-C16	-2.02	116.21	120.06
4	F	1001	BXB	O19-C17-C18	2.02	130.55	127.85

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	701	EDO	O1-C1-C2-O2
3	G	701	EDO	O1-C1-C2-O2
3	A	701	EDO	O1-C1-C2-O2
3	A	706	EDO	O1-C1-C2-O2
3	G	501	EDO	O1-C1-C2-O2
3	H	703	EDO	O1-C1-C2-O2
3	B	702	EDO	O1-C1-C2-O2
3	E	702	EDO	O1-C1-C2-O2

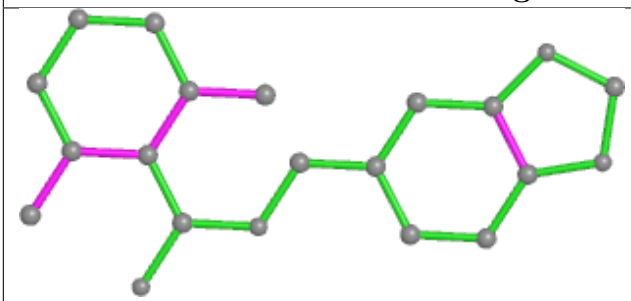
There are no ring outliers.

7 monomers are involved in 8 short contacts:

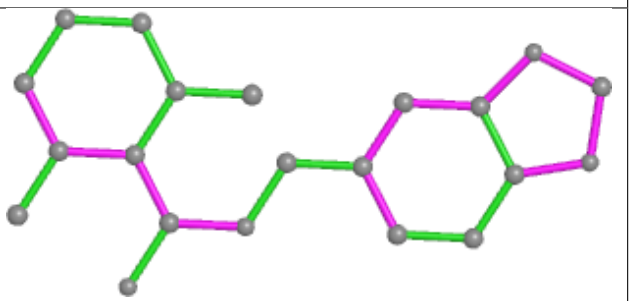
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	703	EDO	2	0
3	B	703	EDO	1	0
3	H	703	EDO	1	0
3	E	702	EDO	1	0
4	G	1001	BXB	1	0
3	A	705	EDO	1	0
3	C	701	EDO	1	0

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.

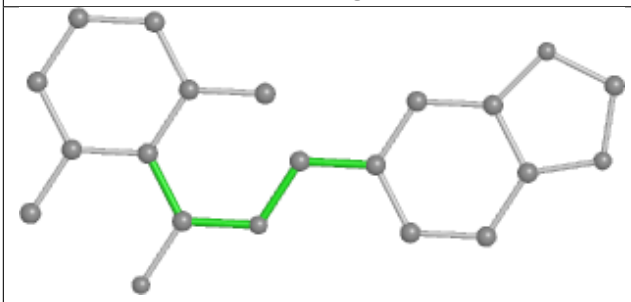
Ligand BXB A 1001



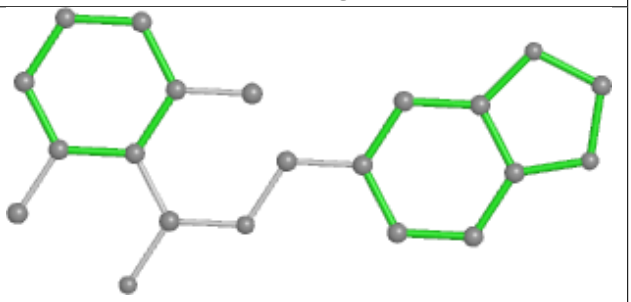
Bond lengths



Bond angles

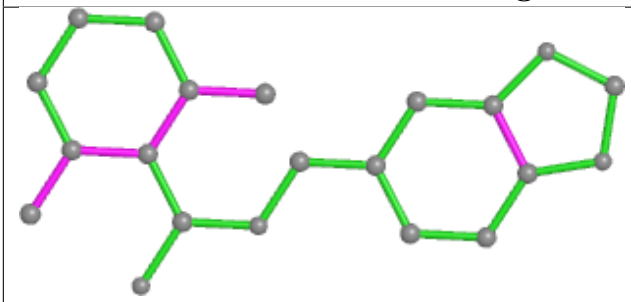


Torsions

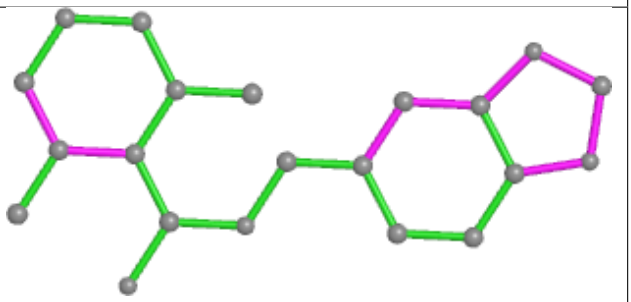


Rings

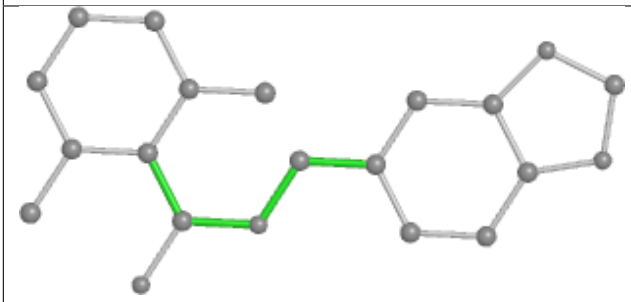
Ligand BXB F 1001



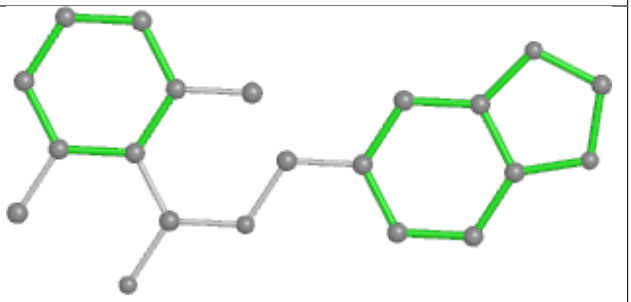
Bond lengths



Bond angles

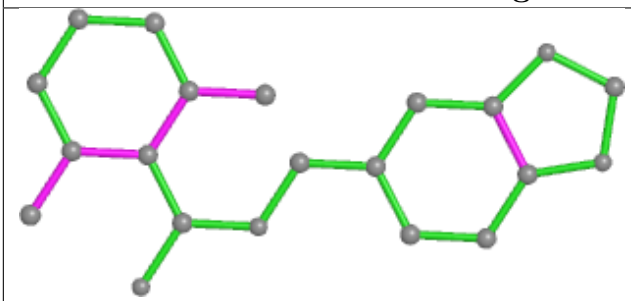


Torsions

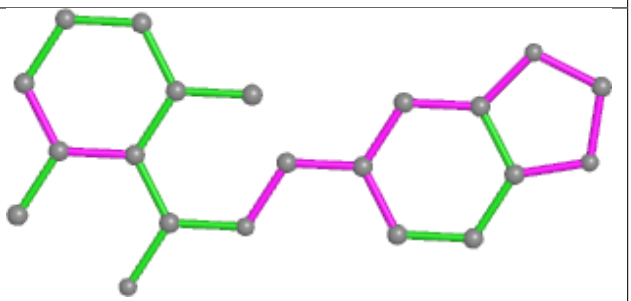


Rings

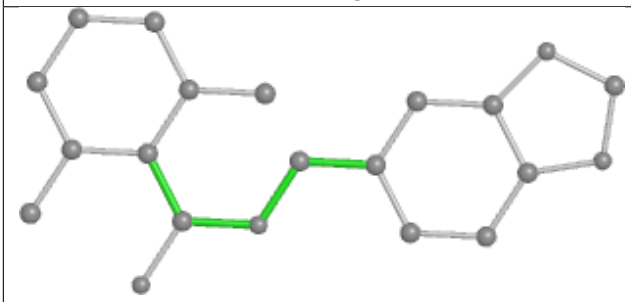
Ligand BXB D 1001



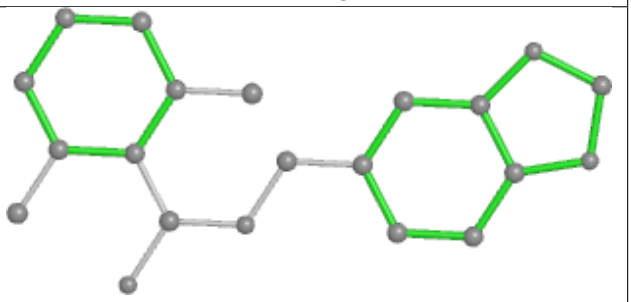
Bond lengths



Bond angles

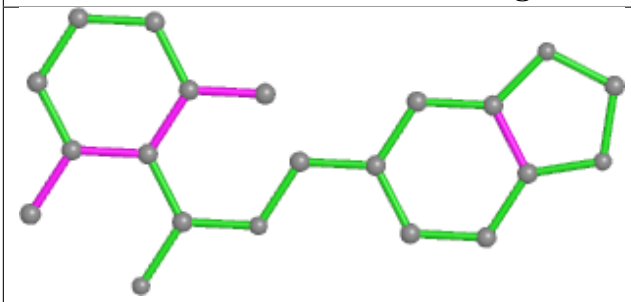


Torsions

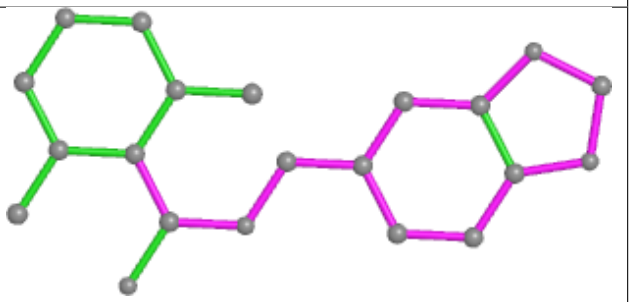


Rings

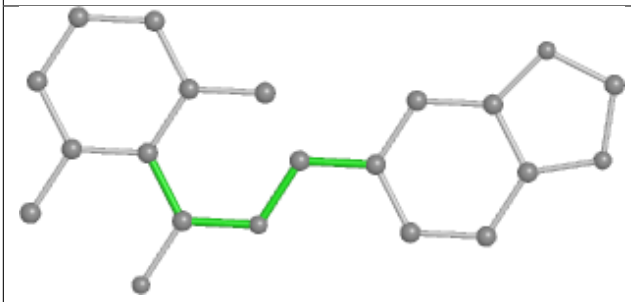
Ligand BXB C 1001



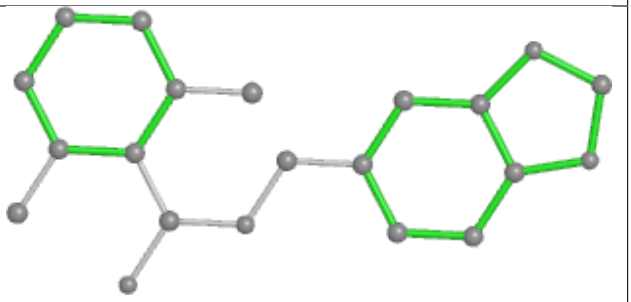
Bond lengths



Bond angles

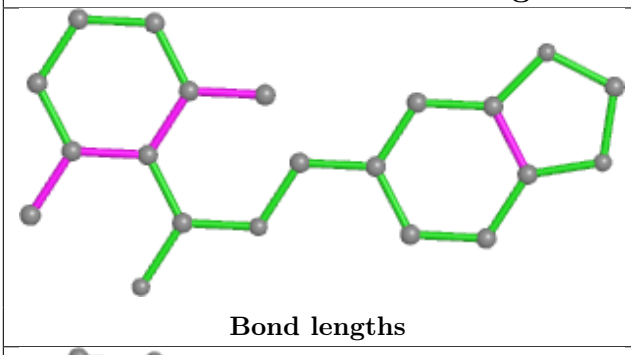


Torsions

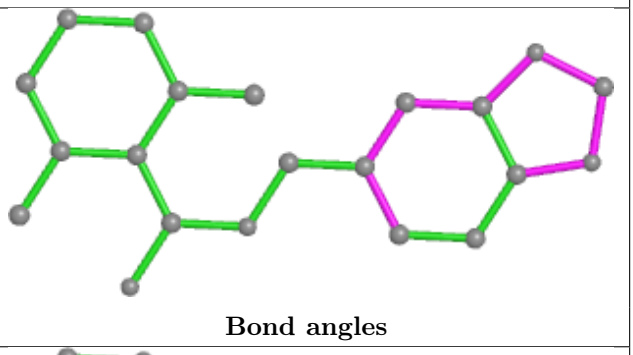


Rings

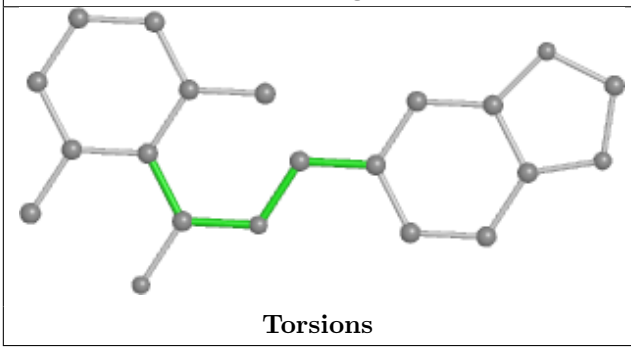
Ligand BXB H 1001



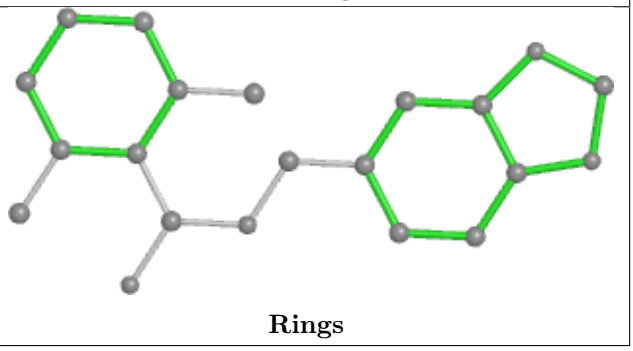
Bond lengths



Bond angles

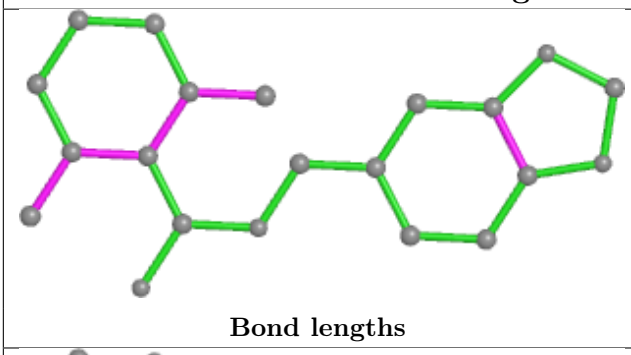


Torsions

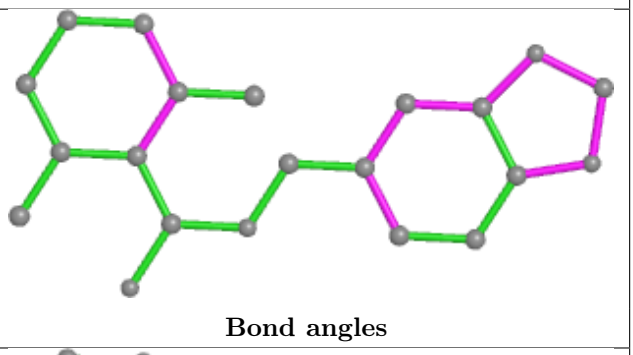


Rings

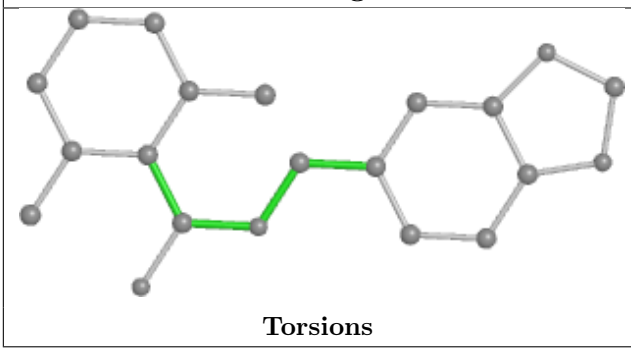
Ligand BXB G 1001



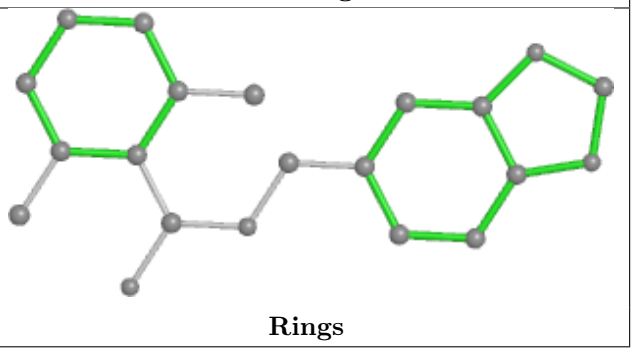
Bond lengths



Bond angles

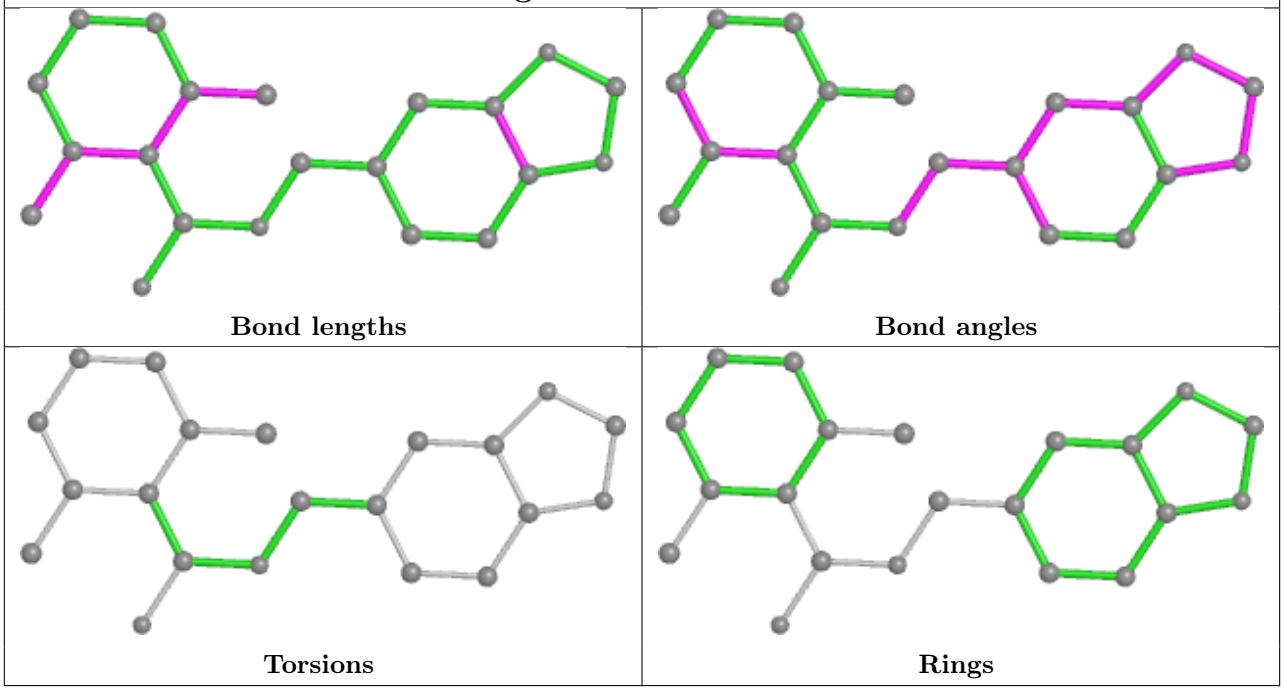


Torsions

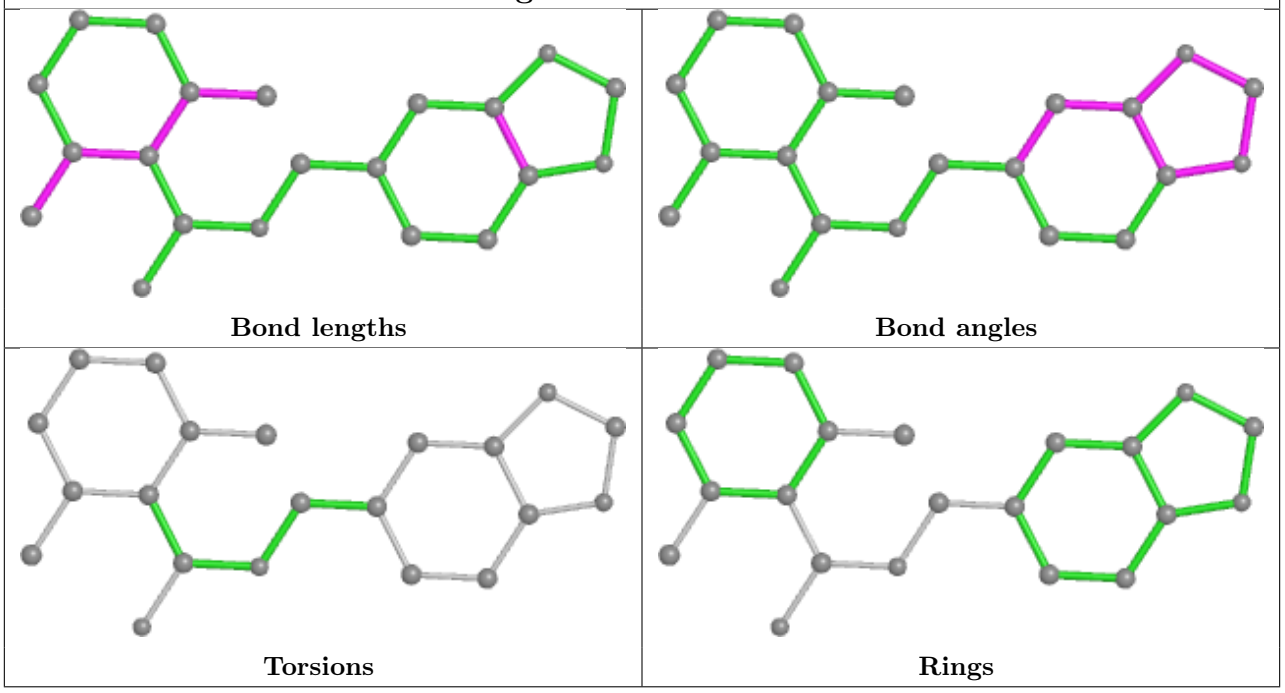


Rings

Ligand BXB B 1001



Ligand BXB E 1001



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	495/500 (99%)	-0.78	0	100	100	23, 31, 46, 60	1 (0%)
1	B	494/500 (98%)	-0.84	0	100	100	23, 29, 40, 56	0
1	C	494/500 (98%)	-0.78	0	100	100	24, 32, 46, 60	0
1	D	494/500 (98%)	-0.68	0	100	100	25, 34, 49, 70	0
1	E	494/500 (98%)	-0.78	0	100	100	23, 31, 43, 59	0
1	F	494/500 (98%)	-0.81	0	100	100	23, 30, 42, 58	0
1	G	494/500 (98%)	-0.86	0	100	100	22, 29, 38, 57	0
1	H	495/500 (99%)	-0.74	0	100	100	23, 31, 48, 66	1 (0%)
All	All	3954/4000 (98%)	-0.78	0	100	100	22, 31, 46, 70	2 (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 monosaccharides 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, 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
3	EDO	E	702	4/4	0.86	0.19	38,39,40,42	0
3	EDO	A	706	4/4	0.90	0.11	34,35,36,37	0
3	EDO	E	704	4/4	0.90	0.14	36,36,39,41	0
2	NA	G	601	1/1	0.93	0.09	30,30,30,30	0
3	EDO	H	703	4/4	0.93	0.11	41,41,41,43	0
3	EDO	H	704	4/4	0.93	0.09	36,36,38,40	0
4	BXB	A	1001	21/21	0.93	0.10	30,32,35,45	0
4	BXB	C	1001	21/21	0.93	0.11	31,33,36,41	0
4	BXB	D	1001	21/21	0.93	0.12	32,33,34,42	0
4	BXB	H	1001	21/21	0.93	0.11	29,31,33,43	0
3	EDO	A	703	4/4	0.94	0.10	30,31,33,34	0
4	BXB	B	1001	21/21	0.94	0.10	30,32,35,43	0
2	NA	D	601	1/1	0.94	0.06	34,34,34,34	0
3	EDO	C	702	4/4	0.94	0.09	29,30,30,32	0
4	BXB	E	1001	21/21	0.94	0.11	30,31,33,39	0
4	BXB	F	1001	21/21	0.94	0.10	29,31,35,43	0
4	BXB	G	1001	21/21	0.94	0.10	27,29,33,41	0
3	EDO	D	702	4/4	0.94	0.14	32,32,32,33	0
3	EDO	A	702	4/4	0.95	0.08	31,31,31,31	0
3	EDO	E	701	4/4	0.95	0.10	33,35,35,39	0
3	EDO	B	702	4/4	0.95	0.07	38,39,40,41	0
3	EDO	E	703	4/4	0.95	0.11	31,31,32,32	0
3	EDO	C	701	4/4	0.95	0.10	31,34,35,35	0
3	EDO	G	701	4/4	0.95	0.13	30,30,32,32	0
2	NA	E	601	1/1	0.95	0.07	32,32,32,32	0
3	EDO	D	701	4/4	0.95	0.09	33,34,35,35	0
3	EDO	A	705	4/4	0.96	0.11	37,37,38,39	0
3	EDO	E	501	4/4	0.96	0.10	28,28,28,30	0
3	EDO	F	703	4/4	0.96	0.07	34,37,37,37	0
3	EDO	F	501	4/4	0.96	0.09	26,28,28,30	0
3	EDO	B	701	4/4	0.96	0.08	30,31,32,32	0
3	EDO	F	701	4/4	0.97	0.09	31,32,33,33	0
3	EDO	C	703	4/4	0.97	0.07	37,37,37,38	0
3	EDO	B	703	4/4	0.97	0.11	30,30,32,33	0
3	EDO	G	702	4/4	0.97	0.06	29,29,29,30	0
2	NA	B	601	1/1	0.97	0.06	27,27,27,27	0
3	EDO	G	501	4/4	0.97	0.12	33,36,37,37	0
3	EDO	G	704	4/4	0.97	0.09	31,31,33,33	0
3	EDO	G	705	4/4	0.97	0.07	29,32,33,34	0
3	EDO	A	701	4/4	0.97	0.10	33,34,34,34	0
3	EDO	A	704	4/4	0.98	0.09	30,30,31,31	0
3	EDO	H	701	4/4	0.98	0.05	31,31,31,33	0
2	NA	C	601	1/1	0.98	0.04	30,30,30,30	0

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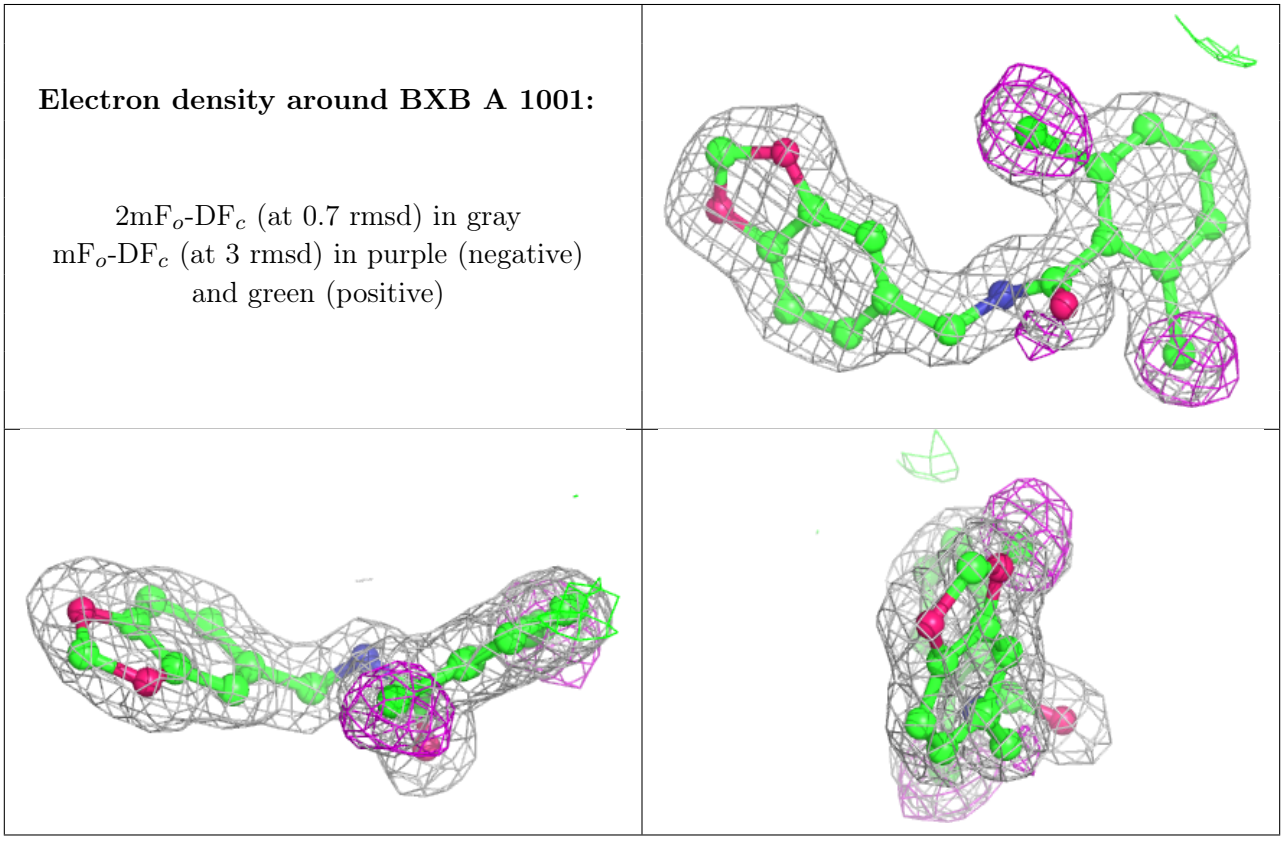
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	B	704	4/4	0.98	0.05	30,30,32,32	0
2	NA	A	601	1/1	0.98	0.05	33,33,33,33	0
2	NA	H	601	1/1	0.98	0.06	33,33,33,33	0
2	NA	F	601	1/1	0.99	0.07	29,29,29,29	0

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.

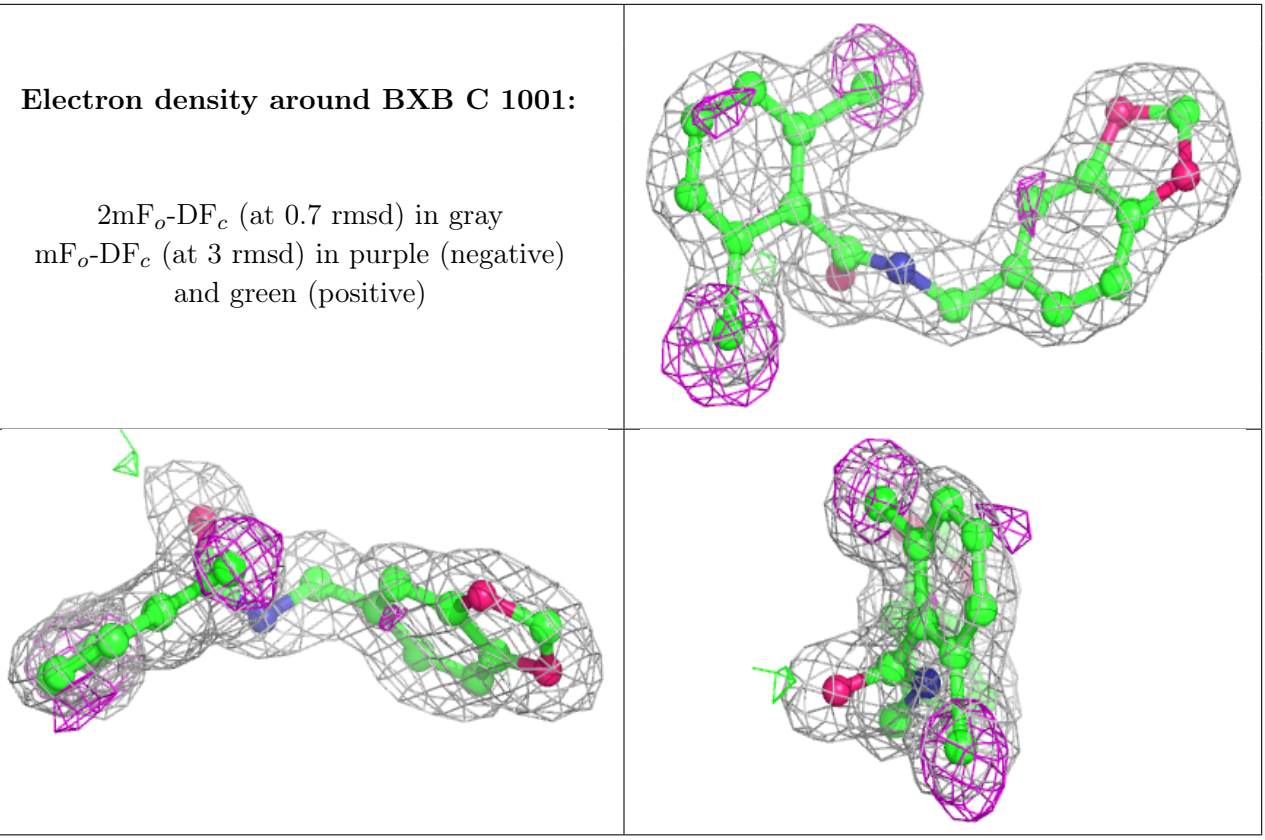
Electron density around BXB A 1001:

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



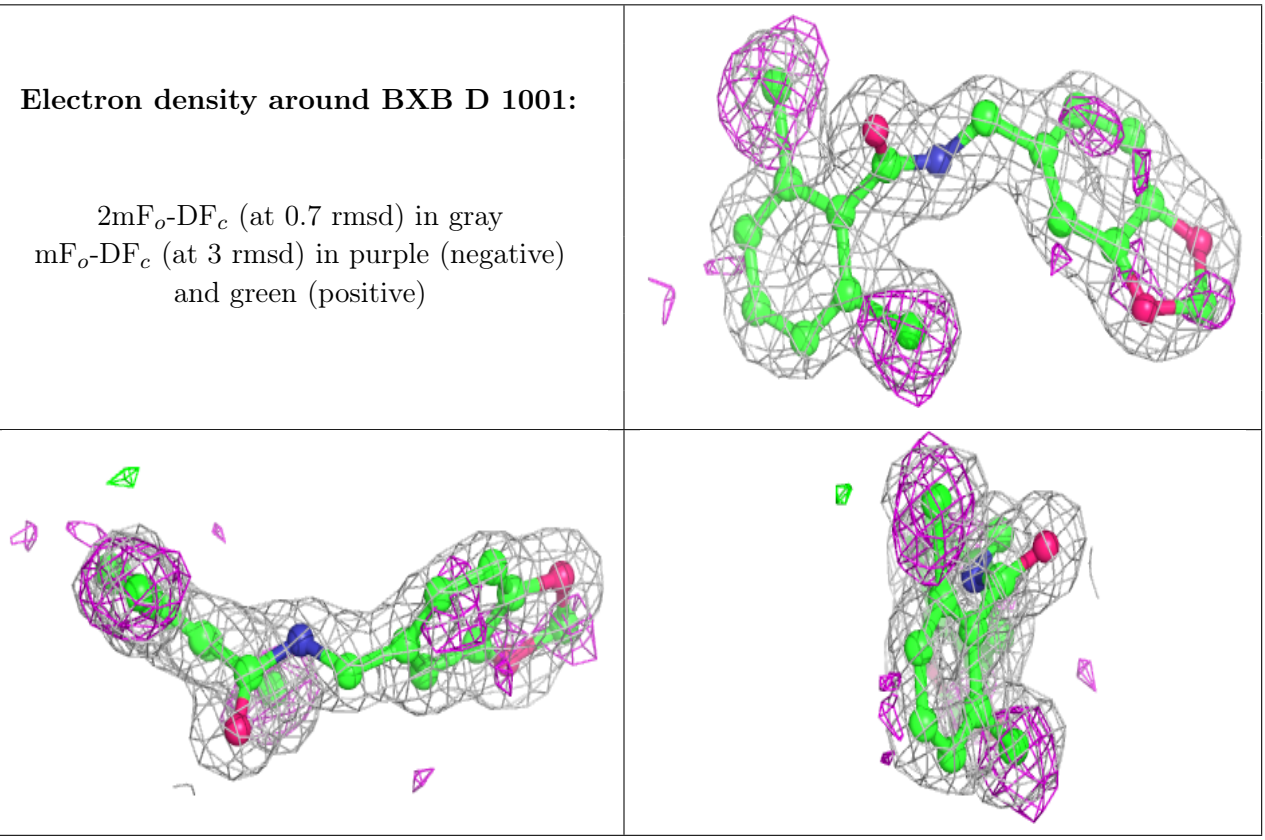
Electron density around BXB C 1001:

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



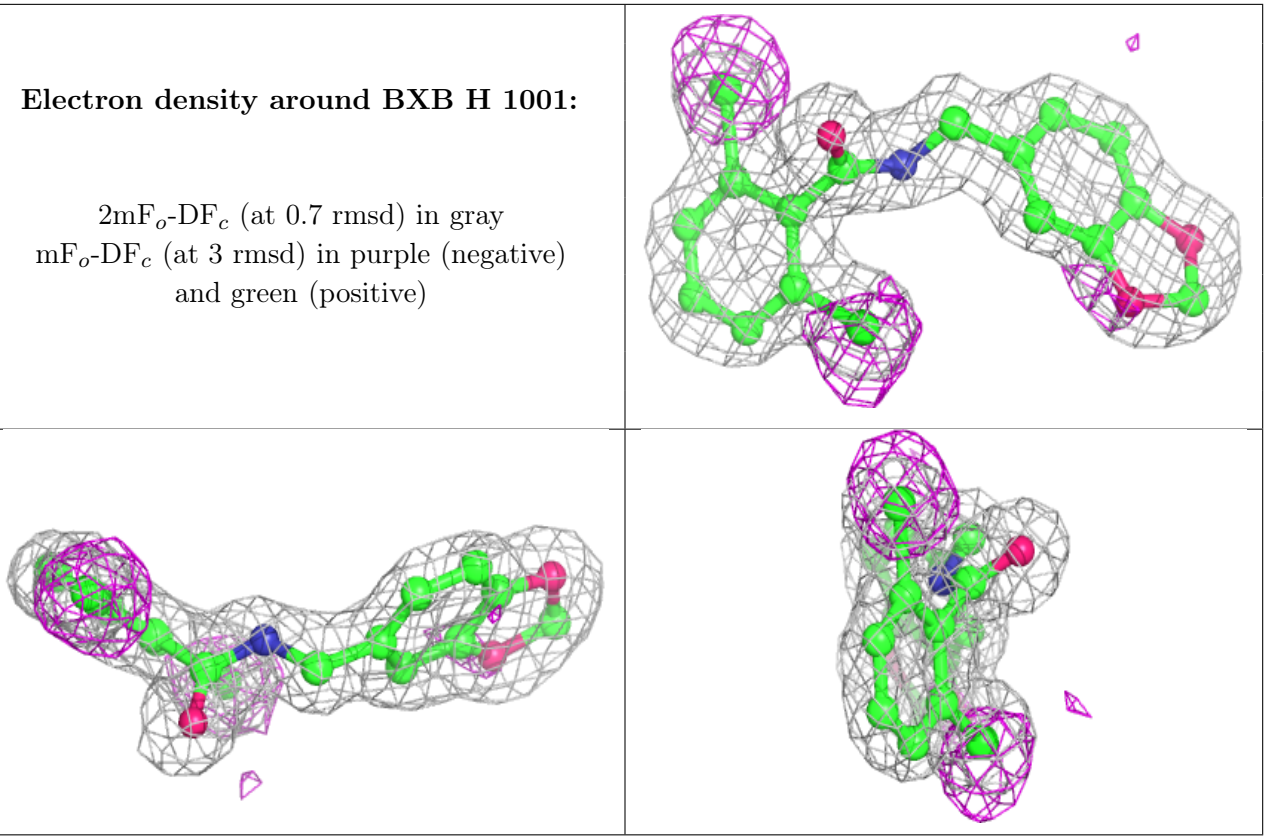
Electron density around BXB D 1001:

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



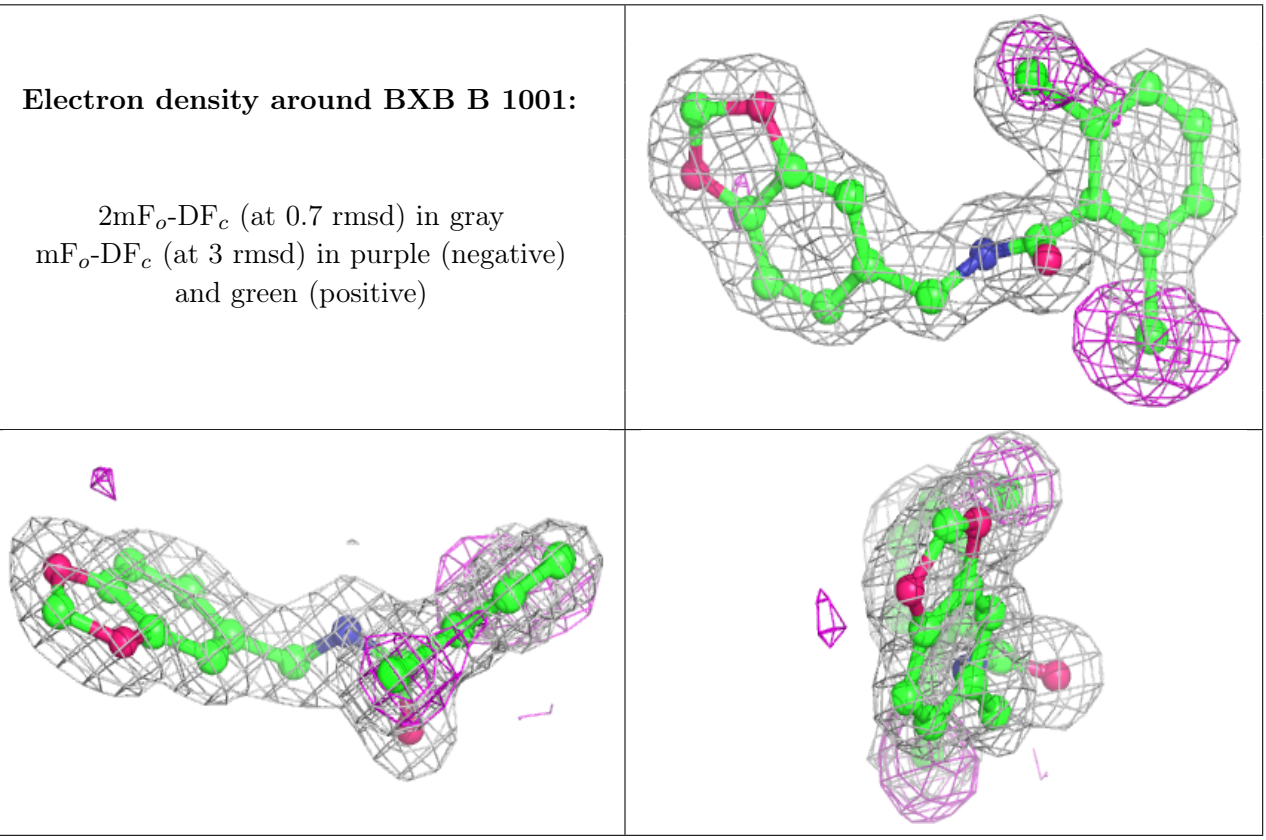
Electron density around BXB H 1001:

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



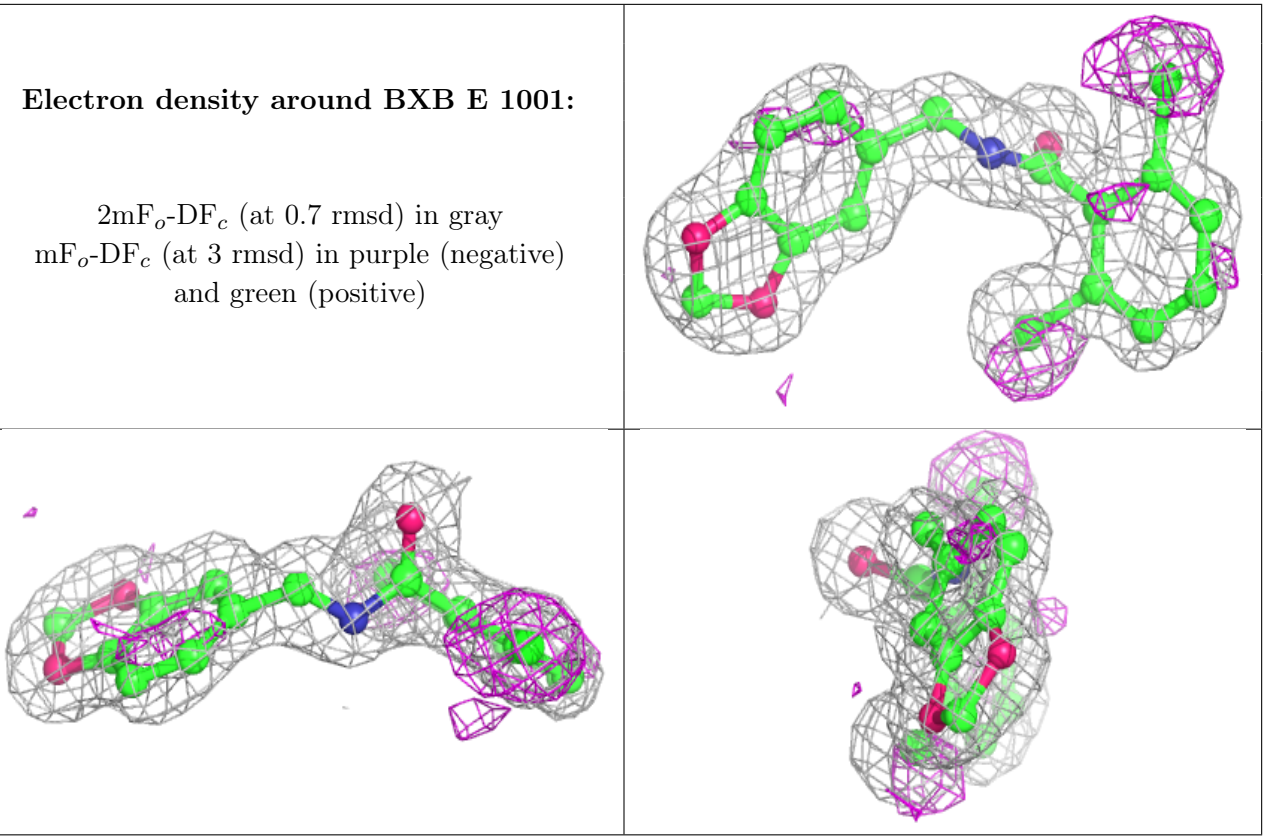
Electron density around BXB B 1001:

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



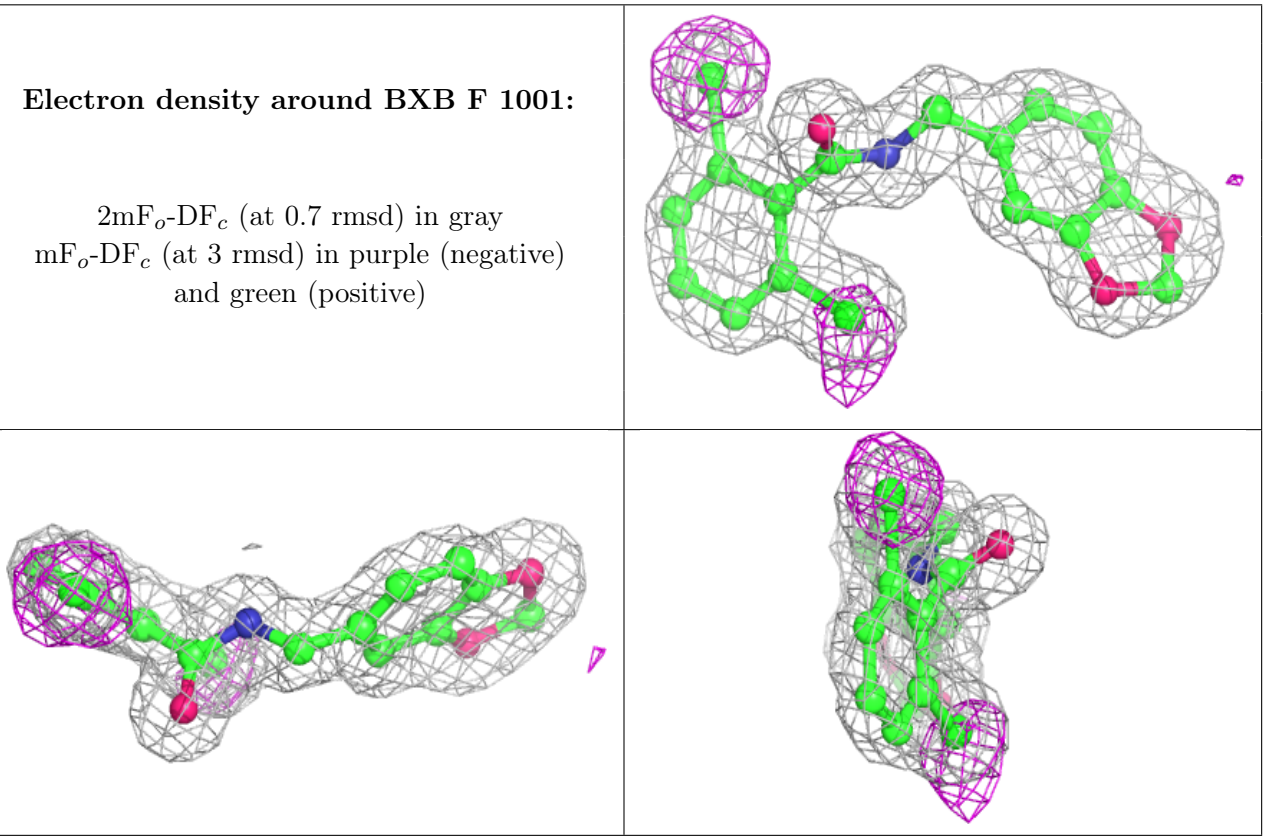
Electron density around BXB E 1001:

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



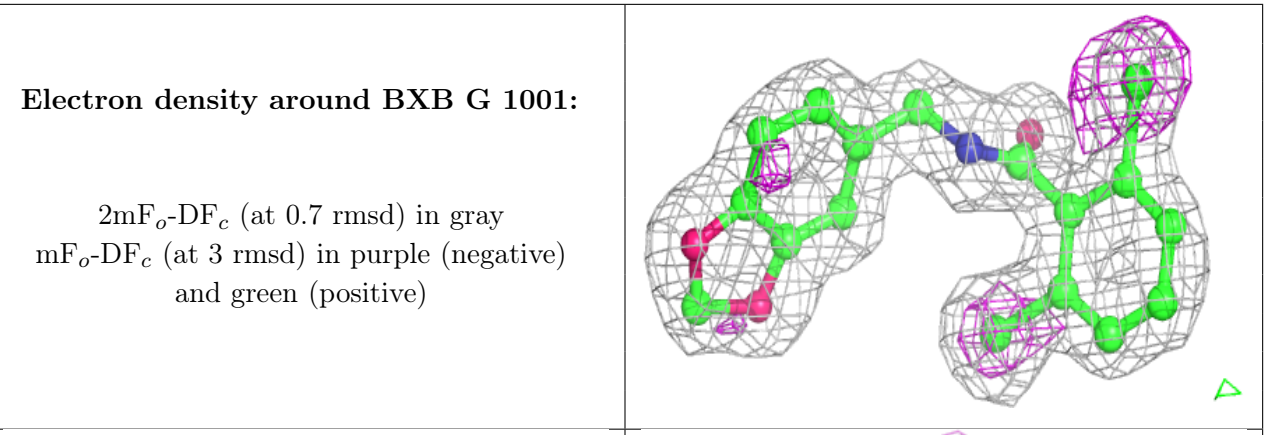
Electron density around BXB F 1001:

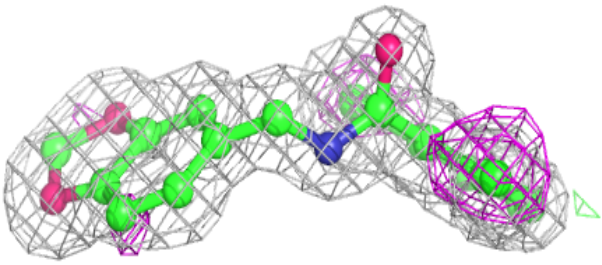
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

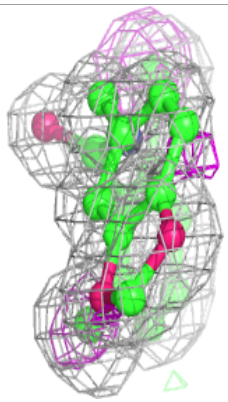


Electron density around BXB G 1001:

$2mF_o$-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.