



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:16 PM UTC

PDB ID : 3H8G / pdb_00003h8g
Title : Bestatin complex structure of leucine aminopeptidase from *Pseudomonas putida*
Authors : Kale, A.; Dijkstra, B.W.; Sonke, T.; Thunnissen, A.M.W.H.
Deposited on : 2009-04-29
Resolution : 1.50 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

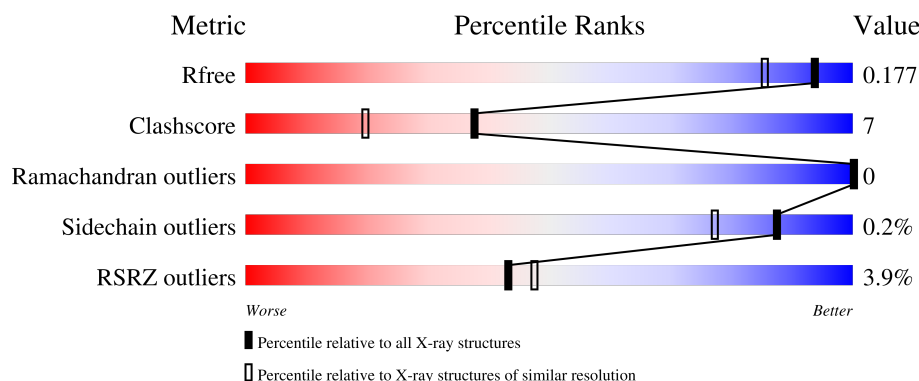
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	497	4% 86% 12% .
1	B	497	4% 87% 12% .
1	C	497	4% 88% 10% .
1	D	497	4% 87% 11% .
1	E	497	4% 89% 10% .

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Mol	Chain	Length	Quality of chain
1	F	497	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a small red segment at the beginning labeled '4%', a large green segment in the middle labeled '88%', and a small yellow segment at the end labeled '9%'. A small black dot is located at the far right end of the bar.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25232 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 Cytosol aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	497	Total	C	N	O	S	0	0	0
			3682	2324	644	696	18			
1	A	497	Total	C	N	O	S	0	0	0
			3682	2324	644	696	18			
1	B	497	Total	C	N	O	S	0	0	0
			3678	2322	644	694	18			
1	C	497	Total	C	N	O	S	0	0	0
			3678	2322	644	694	18			
1	D	497	Total	C	N	O	S	0	0	0
			3682	2324	644	696	18			
1	E	497	Total	C	N	O	S	0	0	0
			3682	2324	644	696	18			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

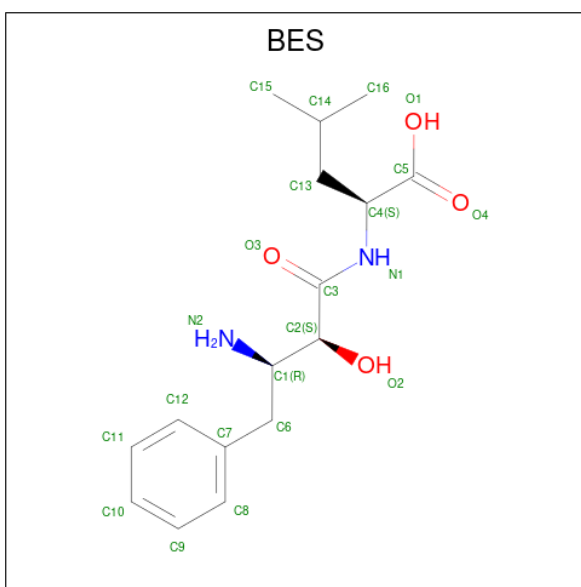
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total K 1 1	0	0
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0
4	E	1	Total K 1 1	0	0

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 6 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (CCD ID: BES) (formula: C₁₆H₂₄N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	N	O	0	0
			22	16	2	4		
6	A	1	Total	C	N	O	0	0
			22	16	2	4		
6	B	1	Total	C	N	O	0	0
			22	16	2	4		
6	C	1	Total	C	N	O	0	0
			22	16	2	4		
6	D	1	Total	C	N	O	0	0
			22	16	2	4		
6	E	1	Total	C	N	O	0	0
			22	16	2	4		

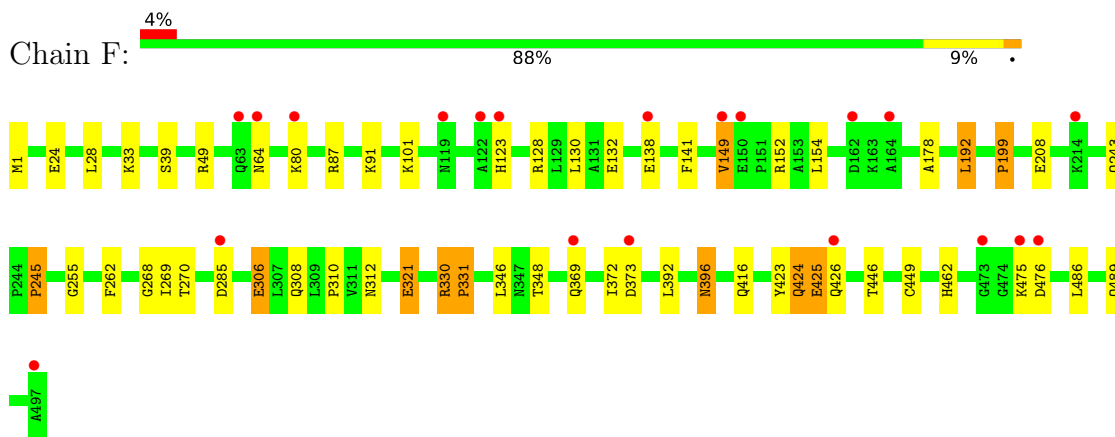
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	523	Total	O	0	0
			523	523		
7	A	480	Total	O	0	0
			480	480		
7	B	511	Total	O	0	0
			511	511		
7	C	488	Total	O	0	0
			488	488		
7	D	481	Total	O	0	0
			481	481		
7	E	491	Total	O	0	0
			491	491		

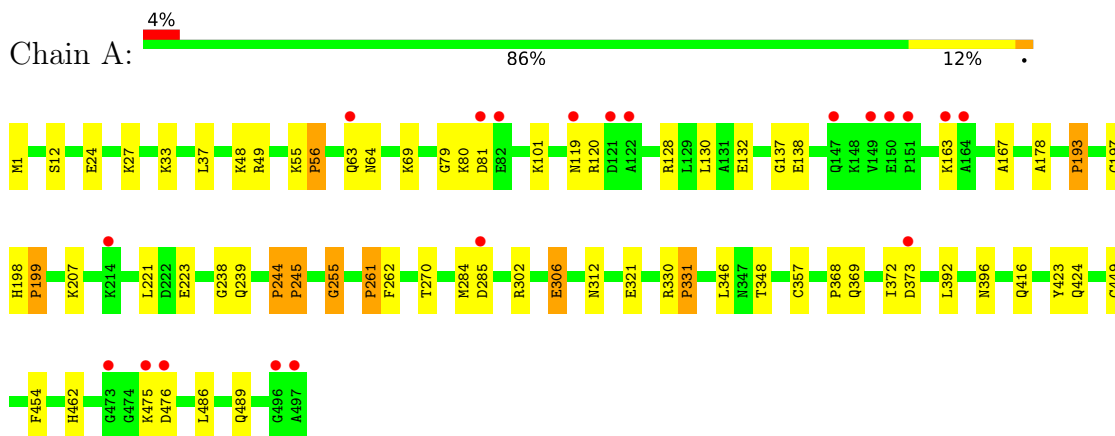
3 Residue-property plots [i](#)

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.

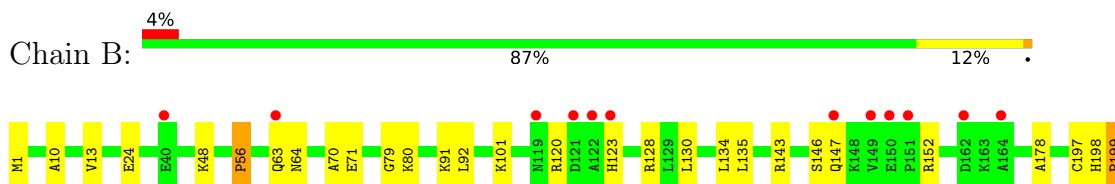
- Molecule 1: Cytosol aminopeptidase

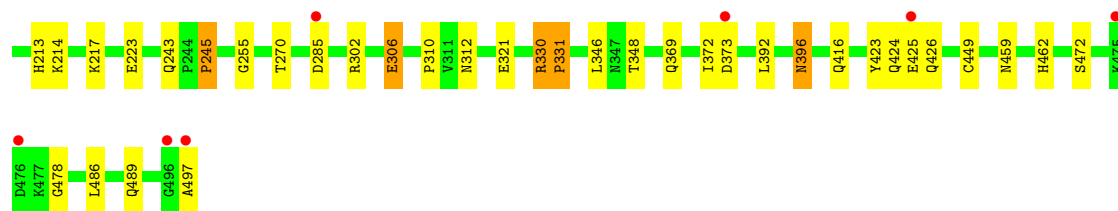


- Molecule 1: Cytosol aminopeptidase

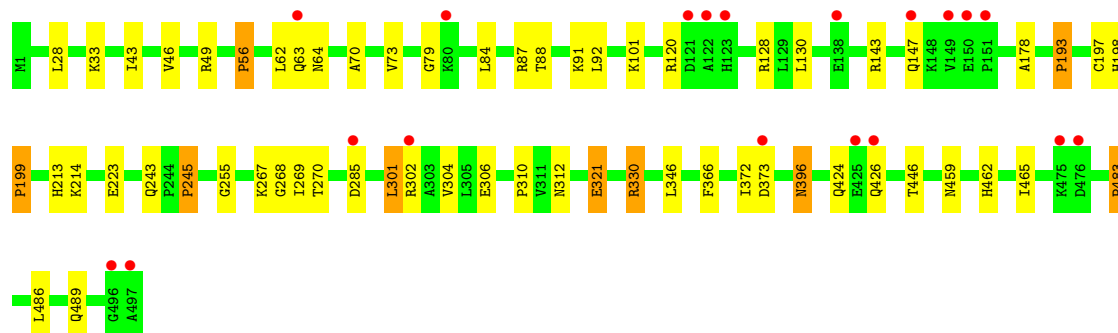
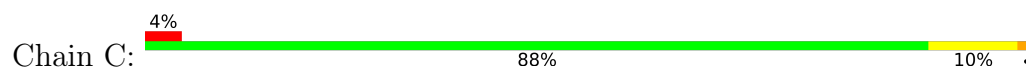


- Molecule 1: Cytosol aminopeptidase

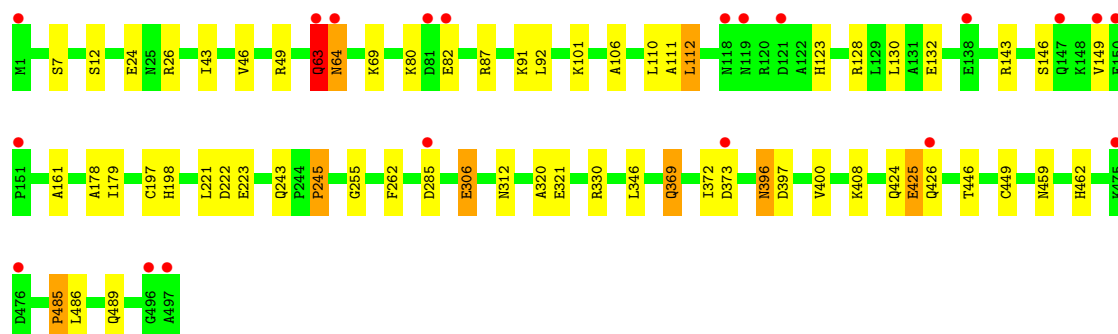
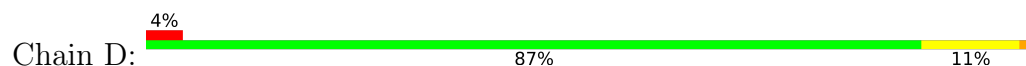




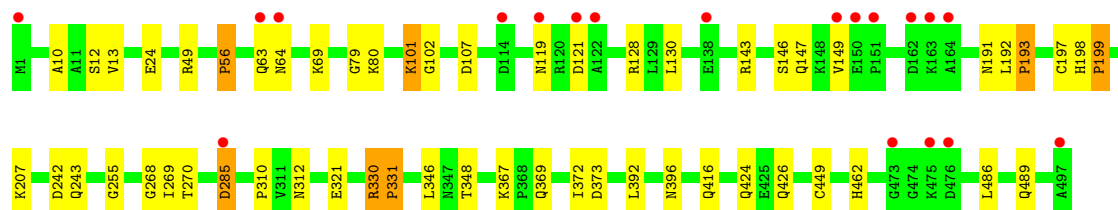
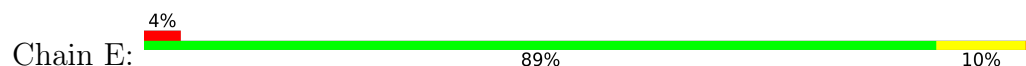
● Molecule 1: Cytosol aminopeptidase



● Molecule 1: Cytosol aminopeptidase



● Molecule 1: Cytosol aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.98Å 95.99Å 96.00Å 100.82° 107.78° 93.23°	Depositor
Resolution (Å)	38.63 – 1.50 38.63 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (38.63-1.50) 95.2 (38.63-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.3.0022	Depositor
R, R_{free}	0.149 , 0.173 0.160 , 0.177	Depositor DCC
R_{free} test set	24264 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.1	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	0.96	EDS
Total number of atoms	25232	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, K, ZN, BES, MN

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	1.01	16/3737 (0.4%)	1.02	11/5054 (0.2%)
1	B	1.04	15/3733 (0.4%)	0.98	9/5049 (0.2%)
1	C	1.07	21/3733 (0.6%)	1.00	10/5049 (0.2%)
1	D	0.98	11/3737 (0.3%)	0.95	5/5054 (0.1%)
1	E	1.03	18/3737 (0.5%)	1.01	14/5054 (0.3%)
1	F	1.01	13/3737 (0.3%)	1.01	12/5054 (0.2%)
All	All	1.02	94/22414 (0.4%)	0.99	61/30314 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
All	All	0	5

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	ARG	C-N	15.38	1.53	1.33
1	C	120	ARG	C-N	11.09	1.48	1.33
1	A	475	LYS	C-N	-10.17	1.20	1.33
1	F	423	TYR	C-N	9.81	1.46	1.33
1	C	396	ASN	C-N	9.80	1.47	1.34
1	A	476	ASP	C-N	-9.71	1.20	1.33
1	C	245	PRO	N-CD	-9.65	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	372	ILE	C-N	-9.02	1.20	1.33
1	F	268	GLY	C-O	-8.85	1.11	1.23
1	E	285	ASP	C-N	-8.82	1.21	1.33
1	B	147	GLN	C-N	-8.57	1.21	1.33
1	C	372	ILE	C-N	-8.50	1.21	1.33
1	D	197	CYS	C-O	-8.19	1.13	1.23
1	C	301	LEU	C-N	-8.16	1.22	1.33
1	C	268	GLY	C-O	-8.11	1.12	1.23
1	D	425	GLU	C-N	-8.10	1.23	1.34
1	D	82	GLU	C-N	-8.02	1.22	1.33
1	C	424	GLN	C-O	-7.81	1.15	1.24
1	E	146	SER	C-N	-7.75	1.20	1.33
1	D	372	ILE	C-N	-7.73	1.23	1.33
1	C	483	PRO	N-CD	-7.72	1.37	1.47
1	C	366	PHE	C-N	-7.47	1.25	1.33
1	C	223	GLU	C-O	-7.46	1.15	1.24
1	C	197	CYS	C-O	-7.45	1.13	1.23
1	A	238	GLY	C-N	7.43	1.44	1.34
1	D	146	SER	C-N	-7.34	1.22	1.33
1	F	396	ASN	C-N	-7.31	1.24	1.33
1	B	197	CYS	C-O	-7.30	1.14	1.23
1	A	197	CYS	C-O	-7.22	1.14	1.23
1	F	306	GLU	C-N	-7.13	1.23	1.33
1	B	213	HIS	C-O	-7.08	1.16	1.24
1	E	147	GLN	C-N	-7.05	1.23	1.33
1	A	423	TYR	C-N	7.02	1.43	1.33
1	C	73	VAL	C-O	-7.02	1.16	1.24
1	F	476	ASP	C-N	-6.98	1.24	1.33
1	A	132	GLU	C-N	-6.96	1.25	1.33
1	A	163	LYS	C-O	-6.71	1.16	1.24
1	C	56	PRO	N-CD	-6.58	1.38	1.47
1	E	268	GLY	C-O	-6.58	1.15	1.23
1	F	425	GLU	C-N	-6.55	1.25	1.34
1	D	222	ASP	C-N	-6.45	1.25	1.33
1	C	269	ILE	C-O	-6.39	1.16	1.23
1	C	199	PRO	N-CD	-6.37	1.38	1.47
1	D	106	ALA	C-N	6.30	1.42	1.33
1	B	70	ALA	C-N	-6.30	1.25	1.34
1	E	101	LYS	C-O	-6.30	1.16	1.24
1	E	372	ILE	C-O	-6.28	1.17	1.24
1	D	198	HIS	C-O	-6.27	1.16	1.24
1	D	369	GLN	C-O	-6.24	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	PRO	N-CD	-6.13	1.39	1.47
1	C	213	HIS	C-O	-6.06	1.16	1.24
1	C	62	LEU	C-O	-6.01	1.16	1.23
1	C	70	ALA	C-N	-6.01	1.25	1.34
1	F	425	GLU	C-O	-5.97	1.16	1.24
1	F	475	LYS	C-N	-5.96	1.26	1.33
1	B	369	GLN	C-O	-5.86	1.16	1.24
1	B	306	GLU	C-N	-5.83	1.25	1.33
1	B	245	PRO	N-CD	-5.82	1.39	1.47
1	E	369	GLN	C-O	-5.80	1.16	1.24
1	E	119	ASN	C-N	-5.77	1.26	1.33
1	A	198	HIS	C-O	-5.76	1.16	1.24
1	F	39	SER	C-O	-5.75	1.16	1.24
1	B	423	TYR	C-N	5.74	1.41	1.33
1	F	132	GLU	C-N	-5.59	1.26	1.33
1	E	197	CYS	C-O	-5.55	1.16	1.23
1	C	198	HIS	C-O	-5.54	1.17	1.24
1	F	372	ILE	C-N	-5.51	1.25	1.33
1	A	199	PRO	N-CD	-5.51	1.40	1.47
1	E	426	GLN	C-O	-5.49	1.17	1.24
1	B	478	GLY	C-O	-5.47	1.16	1.23
1	B	198	HIS	C-O	-5.42	1.17	1.24
1	E	121	ASP	C-N	-5.42	1.26	1.33
1	A	207	LYS	C-N	-5.41	1.26	1.33
1	B	331	PRO	N-CD	-5.40	1.40	1.47
1	C	267	LYS	C-O	-5.40	1.17	1.23
1	E	367	LYS	CA-CB	5.39	1.56	1.52
1	A	167	ALA	C-O	-5.38	1.17	1.24
1	E	269	ILE	C-O	-5.33	1.18	1.23
1	F	269	ILE	C-O	-5.30	1.18	1.23
1	E	191	ASN	C-N	5.29	1.41	1.33
1	E	198	HIS	C-O	-5.29	1.17	1.24
1	A	255	GLY	N-CA	5.28	1.49	1.44
1	A	306	GLU	C-N	-5.27	1.25	1.33
1	E	199	PRO	N-CD	-5.26	1.40	1.47
1	A	284	MET	C-N	-5.24	1.26	1.33
1	D	306	GLU	C-N	-5.22	1.25	1.33
1	C	302	ARG	C-N	-5.16	1.27	1.33
1	B	426	GLN	C-O	-5.16	1.17	1.24
1	B	214	LYS	C-O	-5.16	1.18	1.24
1	E	102	GLY	C-O	-5.15	1.16	1.23
1	F	149	VAL	CA-C	5.14	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	207	LYS	C-N	-5.12	1.26	1.33
1	D	396	ASN	C-N	5.10	1.41	1.34
1	A	372	ILE	C-N	-5.01	1.26	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	192	LEU	O-C-N	14.46	135.29	121.27
1	E	192	LEU	O-C-N	12.57	133.47	121.27
1	E	243	GLN	O-C-N	10.59	130.31	121.31
1	B	245	PRO	CA-N-CD	-9.45	98.77	112.00
1	A	119	ASN	CA-C-N	9.38	136.23	123.00
1	A	119	ASN	C-N-CA	9.38	136.23	123.00
1	F	310	PRO	CA-N-CD	-9.33	98.94	112.00
1	D	485	PRO	CA-N-CD	-9.25	99.05	112.00
1	A	244	PRO	CA-N-CD	-9.13	99.22	112.00
1	C	56	PRO	CA-N-CD	-9.08	99.28	112.00
1	C	245	PRO	CA-N-CD	-9.08	99.29	112.00
1	E	310	PRO	CA-N-CD	-9.03	99.36	112.00
1	A	261	PRO	CA-N-CD	-8.99	99.42	112.00
1	C	396	ASN	O-C-N	8.84	135.45	123.34
1	D	245	PRO	CA-N-CD	-8.79	99.69	112.00
1	B	310	PRO	CA-N-CD	-8.77	99.72	112.00
1	E	56	PRO	CA-N-CD	-8.77	99.73	112.00
1	A	331	PRO	CA-N-CD	-8.73	99.77	112.00
1	A	245	PRO	CA-N-CD	-8.72	99.79	112.00
1	A	120	ARG	O-C-N	-8.72	113.16	123.27
1	B	56	PRO	CA-N-CD	-8.71	99.80	112.00
1	F	245	PRO	CA-N-CD	-8.71	99.81	112.00
1	B	331	PRO	CA-N-CD	-8.70	99.83	112.00
1	F	199	PRO	CA-N-CD	-8.65	99.89	112.00
1	C	193	PRO	CA-N-CD	-8.64	99.90	112.00
1	C	199	PRO	CA-N-CD	-8.63	99.92	112.00
1	E	193	PRO	CA-N-CD	-8.60	99.96	112.00
1	A	193	PRO	CA-N-CD	-8.55	100.03	112.00
1	F	331	PRO	CA-N-CD	-8.49	100.11	112.00
1	C	310	PRO	CA-N-CD	-8.47	100.14	112.00
1	A	199	PRO	CA-N-CD	-8.42	100.22	112.00
1	A	56	PRO	CA-N-CD	-8.32	100.35	112.00
1	E	331	PRO	CA-N-CD	-8.32	100.36	112.00
1	E	199	PRO	CA-N-CD	-8.18	100.55	112.00
1	E	192	LEU	CA-C-N	-8.12	112.02	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	192	LEU	C-N-CA	-8.12	112.02	120.38
1	B	199	PRO	CA-N-CD	-8.00	100.80	112.00
1	C	483	PRO	CA-N-CD	-7.80	100.59	111.50
1	F	192	LEU	CA-C-N	-6.99	113.18	120.38
1	F	192	LEU	C-N-CA	-6.99	113.18	120.38
1	F	321	GLU	O-C-N	-6.87	115.23	123.27
1	E	243	GLN	CA-C-N	-6.85	113.33	120.38
1	E	243	GLN	C-N-CA	-6.85	113.33	120.38
1	D	396	ASN	O-C-N	6.63	132.42	123.34
1	C	64	ASN	CB-CA-C	-6.28	102.08	109.80
1	B	396	ASN	O-C-N	6.20	131.83	123.34
1	D	320	ALA	CA-C-N	-6.01	114.53	123.00
1	D	320	ALA	C-N-CA	-6.01	114.53	123.00
1	F	475	LYS	O-C-N	5.85	128.32	122.12
1	F	396	ASN	O-C-N	-5.78	116.51	123.27
1	F	64	ASN	CB-CA-C	-5.76	102.72	109.80
1	B	146	SER	CA-C-N	5.72	130.28	122.84
1	B	146	SER	C-N-CA	5.72	130.28	122.84
1	C	214	LYS	N-CA-C	5.62	117.41	111.28
1	F	424	GLN	O-C-N	-5.48	116.31	122.12
1	A	132	GLU	O-C-N	-5.16	116.65	122.12
1	E	330	ARG	CG-CD-NE	-5.15	100.68	112.00
1	E	242	ASP	CA-C-N	5.14	128.40	121.20
1	E	242	ASP	C-N-CA	5.14	128.40	121.20
1	C	321	GLU	O-C-N	-5.10	117.30	123.27
1	B	472	SER	N-CA-C	5.04	116.86	111.36

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	GLN	Sidechain
1	B	330	ARG	Sidechain
1	C	330	ARG	Sidechain
1	D	63	GLN	Peptide
1	F	330	ARG	Sidechain

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	3682	0	3777	68	1
1	B	3678	0	3773	65	0
1	C	3678	0	3773	51	0
1	D	3682	0	3777	58	0
1	E	3682	0	3777	49	0
1	F	3682	0	3777	53	1
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
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
5	E	4	0	0	0	0
5	F	4	0	0	0	0
6	A	22	0	22	0	0
6	B	22	0	22	0	0
6	C	22	0	22	0	0
6	D	22	0	22	0	0
6	E	22	0	22	0	0
6	F	22	0	22	0	0
7	A	480	0	0	15	0
7	B	511	0	0	14	0
7	C	488	0	0	3	0
7	D	481	0	0	7	0
7	E	491	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	523	0	0	8	0
All	All	25232	0	22786	316	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (316) 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:D:101:LYS:HG2	7:D:2782:HOH:O	1.35	1.22
1:E:101:LYS:HG2	7:E:2756:HOH:O	1.36	1.22
1:F:373:ASP:OD1	1:F:462:HIS:HA	1.52	1.09
1:B:373:ASP:OD1	1:B:462:HIS:HA	1.51	1.09
1:D:373:ASP:OD1	1:D:462:HIS:HA	1.54	1.07
1:E:24:GLU:OE1	1:E:80:LYS:HG3	1.54	1.05
1:A:262:PHE:CZ	1:A:369:GLN:NE2	2.24	1.05
1:E:331:PRO:HD3	1:E:348:THR:HG23	1.38	1.04
1:C:373:ASP:OD1	1:C:462:HIS:HA	1.58	1.03
1:D:24:GLU:OE1	1:D:80:LYS:HG3	1.59	1.02
1:F:331:PRO:HD3	1:F:348:THR:HG23	1.42	1.02
1:B:302:ARG:HD2	7:B:3190:HOH:O	1.58	1.02
1:E:101:LYS:HG3	7:E:3011:HOH:O	1.58	1.02
1:A:331:PRO:HD3	1:A:348:THR:HG23	1.38	1.01
1:A:373:ASP:OD1	1:A:462:HIS:HA	1.60	1.01
1:F:262:PHE:CZ	1:F:369:GLN:NE2	2.30	0.99
1:B:331:PRO:HD3	1:B:348:THR:HG23	1.44	0.98
1:B:178:ALA:HA	1:B:306:GLU:OE1	1.64	0.97
1:D:262:PHE:CZ	1:D:369:GLN:NE2	2.31	0.96
1:A:101:LYS:HG2	7:A:2736:HOH:O	1.64	0.95
1:C:178:ALA:HA	1:C:306:GLU:OE1	1.67	0.95
1:D:178:ALA:HA	1:D:306:GLU:OE1	1.72	0.90
1:F:49:ARG:HH21	1:B:63:GLN:HE21	1.18	0.89
1:A:128:ARG:HH12	1:A:489:GLN:HE22	1.19	0.89
1:A:261:PRO:HD2	1:A:368:PRO:HA	1.55	0.89
1:F:128:ARG:HH12	1:F:489:GLN:HE22	1.19	0.88
1:B:1:MET:HE1	1:B:134:LEU:HG	1.53	0.87
1:B:199:PRO:HD3	1:B:270:THR:HG21	1.57	0.87
1:E:128:ARG:HH12	1:E:489:GLN:HE22	1.23	0.87
1:C:128:ARG:HH12	1:C:489:GLN:HE22	1.22	0.86
1:B:1:MET:CE	1:B:135:LEU:HD23	2.06	0.86
1:C:199:PRO:HD3	1:C:270:THR:HG21	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ARG:HH21	1:E:63:GLN:HE21	1.24	0.85
1:A:24:GLU:OE2	7:A:2939:HOH:O	1.97	0.83
1:E:373:ASP:OD1	1:E:462:HIS:HD2	1.61	0.83
1:A:101:LYS:HE2	1:A:138:GLU:OE2	1.79	0.83
1:A:199:PRO:HD3	1:A:270:THR:HG21	1.59	0.83
1:D:128:ARG:HH12	1:D:489:GLN:HE22	1.23	0.82
1:F:199:PRO:HD3	1:F:270:THR:HG21	1.61	0.82
1:F:178:ALA:HA	1:F:306:GLU:OE1	1.79	0.82
1:F:285:ASP:OD2	1:C:346:LEU:HD22	1.79	0.81
1:E:107:ASP:CG	7:E:3323:HOH:O	2.23	0.80
1:A:178:ALA:HA	1:A:306:GLU:OE1	1.82	0.80
1:E:24:GLU:OE1	1:E:80:LYS:CG	2.31	0.79
1:B:199:PRO:HD3	1:B:270:THR:CG2	2.12	0.78
1:F:199:PRO:HD3	1:F:270:THR:CG2	2.13	0.78
1:A:101:LYS:HG3	7:A:3082:HOH:O	1.84	0.78
1:E:193:PRO:HD2	1:E:193:PRO:O	1.83	0.78
1:B:48:LYS:HE2	7:B:2904:HOH:O	1.84	0.77
1:E:199:PRO:HD3	1:E:270:THR:HG21	1.65	0.77
1:C:101:LYS:HG3	7:C:2728:HOH:O	1.85	0.77
1:C:193:PRO:HD2	1:C:193:PRO:O	1.85	0.76
1:C:199:PRO:HD3	1:C:270:THR:CG2	2.15	0.76
1:B:128:ARG:HH12	1:B:489:GLN:HE22	1.29	0.76
1:D:285:ASP:OD2	1:E:346:LEU:HD22	1.85	0.76
1:B:346:LEU:HD22	1:E:285:ASP:OD2	1.85	0.75
1:D:24:GLU:OE1	1:D:80:LYS:CG	2.33	0.75
1:A:193:PRO:HD2	1:A:193:PRO:O	1.86	0.75
1:A:199:PRO:HD3	1:A:270:THR:CG2	2.16	0.75
1:B:424:GLN:NE2	1:B:449:CYS:SG	2.60	0.74
1:B:1:MET:HE2	1:B:135:LEU:HD23	1.68	0.74
1:A:346:LEU:HD22	1:C:285:ASP:OD2	1.88	0.74
1:B:24:GLU:OE1	1:B:80:LYS:CG	2.37	0.73
1:B:56:PRO:HD3	1:B:79:GLY:CA	2.19	0.72
1:F:346:LEU:HD22	1:A:285:ASP:OD2	1.89	0.72
1:C:245:PRO:HD2	1:C:245:PRO:O	1.88	0.72
1:E:199:PRO:HD3	1:E:270:THR:CG2	2.20	0.72
1:D:424:GLN:NE2	1:D:449:CYS:SG	2.63	0.72
1:A:331:PRO:HD3	1:A:348:THR:CG2	2.18	0.72
1:C:143:ARG:HD3	7:C:2667:HOH:O	1.89	0.71
1:F:91:LYS:HG3	7:F:3076:HOH:O	1.88	0.71
1:D:426:GLN:OE1	1:D:446:THR:CG2	2.39	0.70
1:B:285:ASP:OD2	1:D:346:LEU:HD22	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:PRO:HD3	1:E:79:GLY:N	2.07	0.70
1:A:244:PRO:HD2	7:A:519:HOH:O	1.92	0.70
1:F:1:MET:HE3	1:F:138:GLU:OE2	1.92	0.69
1:C:56:PRO:HD3	1:C:79:GLY:CA	2.21	0.69
1:B:24:GLU:OE1	1:B:80:LYS:HG2	1.91	0.69
1:B:424:GLN:HE22	1:B:449:CYS:CB	2.04	0.69
1:C:301:LEU:O	1:C:304:VAL:HG12	1.93	0.69
1:A:245:PRO:HD2	1:A:245:PRO:O	1.92	0.69
1:F:331:PRO:HD3	1:F:348:THR:CG2	2.22	0.69
1:A:244:PRO:HD2	1:A:244:PRO:O	1.91	0.69
1:C:49:ARG:HH21	1:E:63:GLN:NE2	1.89	0.69
1:D:245:PRO:HD2	1:D:245:PRO:O	1.93	0.68
1:F:49:ARG:HH21	1:B:63:GLN:NE2	1.88	0.68
1:B:245:PRO:HD2	1:B:245:PRO:O	1.91	0.68
1:B:302:ARG:CD	7:B:3190:HOH:O	2.30	0.68
1:C:301:LEU:HA	1:C:304:VAL:HG12	1.74	0.68
1:C:63:GLN:HE21	1:E:49:ARG:HH21	1.39	0.68
1:F:426:GLN:OE1	1:F:446:THR:CG2	2.43	0.67
1:A:101:LYS:NZ	1:A:137:GLY:O	2.28	0.67
1:E:396:ASN:ND2	7:E:891:HOH:O	2.27	0.67
1:B:425:GLU:HG3	7:B:3122:HOH:O	1.95	0.67
1:C:33:LYS:HE3	7:C:3312:HOH:O	1.93	0.67
1:D:462:HIS:HE1	7:D:509:HOH:O	1.78	0.67
1:F:1:MET:CE	1:F:138:GLU:OE2	2.43	0.66
1:A:24:GLU:OE1	1:A:80:LYS:HG3	1.96	0.66
1:A:56:PRO:HD3	1:A:79:GLY:N	2.10	0.66
1:C:56:PRO:HD3	1:C:79:GLY:N	2.11	0.66
1:C:373:ASP:OD1	1:C:462:HIS:CA	2.42	0.66
1:D:397:ASP:HA	1:D:400:VAL:HG22	1.76	0.66
1:A:49:ARG:CZ	7:A:3199:HOH:O	2.44	0.65
1:B:331:PRO:HD3	1:B:348:THR:CG2	2.22	0.65
1:B:462:HIS:HE1	7:B:514:HOH:O	1.80	0.65
1:F:396:ASN:ND2	7:F:780:HOH:O	2.27	0.65
1:B:424:GLN:NE2	1:B:449:CYS:HB3	2.12	0.65
1:F:285:ASP:OD2	1:C:346:LEU:CD2	2.45	0.64
1:B:424:GLN:NE2	1:B:449:CYS:CB	2.60	0.64
1:A:462:HIS:HE1	7:A:528:HOH:O	1.81	0.64
1:E:462:HIS:HE1	7:E:537:HOH:O	1.81	0.64
1:A:396:ASN:ND2	7:A:1195:HOH:O	2.30	0.63
1:B:373:ASP:OD1	1:B:462:HIS:CA	2.39	0.63
7:A:976:HOH:O	1:C:147:GLN:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:PRO:HD3	1:E:79:GLY:CA	2.30	0.62
1:A:261:PRO:HD2	1:A:261:PRO:O	1.98	0.62
1:B:91:LYS:HG3	7:B:3363:HOH:O	1.98	0.62
1:A:49:ARG:HH21	1:D:63:GLN:HE21	1.47	0.62
1:F:245:PRO:HD2	1:F:245:PRO:O	1.98	0.62
1:D:179:ILE:HG23	1:D:485:PRO:HD3	1.82	0.62
1:F:24:GLU:OE1	1:F:80:LYS:HG3	2.00	0.61
1:A:424:GLN:NE2	1:A:449:CYS:SG	2.72	0.61
1:E:24:GLU:CD	1:E:80:LYS:HG3	2.24	0.61
1:E:331:PRO:HD3	1:E:348:THR:CG2	2.21	0.60
1:D:132:GLU:OE2	1:D:485:PRO:HG3	2.00	0.60
1:E:24:GLU:OE1	1:E:80:LYS:HE3	2.02	0.60
1:D:426:GLN:OE1	1:D:446:THR:HG21	2.01	0.60
1:D:373:ASP:OD1	1:D:462:HIS:CA	2.42	0.60
1:D:424:GLN:HE22	1:D:449:CYS:CB	2.15	0.59
1:A:56:PRO:HD3	1:A:79:GLY:CA	2.32	0.59
1:A:424:GLN:NE2	1:A:449:CYS:HB3	2.16	0.59
1:B:424:GLN:HE22	1:B:449:CYS:HB3	1.66	0.59
1:B:321:GLU:OE2	1:D:330:ARG:HD3	2.01	0.59
1:C:49:ARG:NH2	1:E:63:GLN:HE21	1.96	0.59
1:C:301:LEU:O	1:C:304:VAL:CG1	2.50	0.59
1:D:24:GLU:CD	1:D:80:LYS:HG3	2.28	0.59
1:D:285:ASP:OD2	1:E:346:LEU:CD2	2.50	0.59
1:F:346:LEU:CD2	1:A:285:ASP:OD2	2.51	0.58
1:B:1:MET:HE3	1:B:135:LEU:CD2	2.34	0.58
1:D:424:GLN:NE2	1:D:449:CYS:CB	2.67	0.58
1:D:424:GLN:NE2	1:D:449:CYS:HB3	2.18	0.58
1:F:255:GLY:H	1:F:312:ASN:ND2	2.02	0.58
1:B:101:LYS:HG3	1:B:152:ARG:HD3	1.86	0.58
1:D:425:GLU:HG3	7:D:2857:HOH:O	2.04	0.58
1:B:56:PRO:HD3	1:B:79:GLY:N	2.19	0.58
1:C:465:ILE:HG21	1:C:483:PRO:HG3	1.86	0.58
1:E:255:GLY:H	1:E:312:ASN:ND2	2.01	0.58
1:F:24:GLU:OE1	1:F:80:LYS:CG	2.52	0.58
1:B:1:MET:CE	1:B:135:LEU:CD2	2.80	0.58
1:F:87:ARG:HG3	1:F:91:LYS:HE2	1.86	0.58
1:B:24:GLU:OE1	1:B:80:LYS:HG3	2.02	0.57
1:F:123:HIS:HE1	7:F:2725:HOH:O	1.87	0.57
1:B:396:ASN:HD22	1:B:459:ASN:ND2	2.02	0.57
1:C:301:LEU:HA	1:C:304:VAL:CG1	2.34	0.57
1:D:87:ARG:HG3	1:D:91:LYS:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:LYS:HG3	1:F:152:ARG:CD	2.35	0.57
1:F:373:ASP:OD1	1:F:462:HIS:CA	2.39	0.57
1:F:425:GLU:HG3	7:F:3119:HOH:O	2.04	0.57
1:A:261:PRO:CD	1:A:368:PRO:HA	2.32	0.57
1:C:199:PRO:CD	1:C:270:THR:HG21	2.34	0.57
1:C:28:LEU:O	1:C:33:LYS:HE2	2.05	0.57
1:E:424:GLN:NE2	1:E:449:CYS:SG	2.78	0.57
1:F:128:ARG:HH12	1:F:489:GLN:NE2	1.98	0.57
1:D:123:HIS:HE1	7:D:2762:HOH:O	1.87	0.57
1:A:424:GLN:HE22	1:A:449:CYS:CB	2.18	0.56
1:A:346:LEU:CD2	1:C:285:ASP:OD2	2.53	0.56
1:B:396:ASN:HD22	1:B:459:ASN:CG	2.13	0.56
1:F:308:GLN:HG2	7:F:2739:HOH:O	2.06	0.56
1:F:426:GLN:OE1	1:F:446:THR:HG21	2.06	0.56
1:A:424:GLN:NE2	1:A:449:CYS:CB	2.69	0.56
1:E:373:ASP:OD1	1:E:462:HIS:CD2	2.51	0.56
1:A:255:GLY:H	1:A:312:ASN:ND2	2.04	0.55
1:A:24:GLU:OE1	1:A:80:LYS:CG	2.55	0.55
1:A:373:ASP:OD1	1:A:462:HIS:CA	2.47	0.55
1:C:301:LEU:CA	1:C:304:VAL:HG12	2.37	0.55
1:B:1:MET:HE3	1:B:135:LEU:HD23	1.89	0.54
1:C:63:GLN:NE2	1:E:49:ARG:HH21	2.05	0.54
1:C:396:ASN:HD22	1:C:459:ASN:ND2	2.05	0.54
1:F:33:LYS:HE3	7:F:3133:HOH:O	2.07	0.54
1:C:63:GLN:HE21	1:E:49:ARG:NH2	2.06	0.54
1:E:424:GLN:NE2	1:E:449:CYS:HB3	2.23	0.54
1:D:321:GLU:OE2	1:E:330:ARG:HD3	2.08	0.53
1:C:396:ASN:HD22	1:C:459:ASN:CG	2.16	0.53
1:B:285:ASP:OD2	1:D:346:LEU:CD2	2.56	0.53
1:D:397:ASP:HA	1:D:400:VAL:CG2	2.38	0.53
1:C:301:LEU:C	1:C:304:VAL:HG12	2.33	0.53
1:C:426:GLN:OE1	1:C:446:THR:HG21	2.09	0.53
1:B:255:GLY:H	1:B:312:ASN:ND2	2.07	0.53
1:B:48:LYS:CE	7:B:2904:HOH:O	2.50	0.52
1:A:424:GLN:HE22	1:A:449:CYS:HB3	1.75	0.52
1:D:43:ILE:O	1:D:46:VAL:HG22	2.10	0.52
1:E:424:GLN:NE2	1:E:449:CYS:CB	2.73	0.52
1:F:199:PRO:CD	1:F:270:THR:HG21	2.36	0.52
1:D:396:ASN:HD22	1:D:459:ASN:CG	2.16	0.52
1:A:27:LYS:NZ	1:A:81:ASP:OD2	2.43	0.52
1:D:110:LEU:HB3	1:D:112:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:LYS:HG3	1:F:152:ARG:HD3	1.92	0.52
1:B:346:LEU:CD2	1:E:285:ASP:OD2	2.56	0.52
1:C:193:PRO:O	1:C:193:PRO:CD	2.57	0.52
1:D:396:ASN:HD22	1:D:459:ASN:ND2	2.08	0.52
1:C:56:PRO:CD	1:C:79:GLY:CA	2.87	0.51
1:F:24:GLU:CD	1:F:80:LYS:HG3	2.34	0.51
1:F:330:ARG:HD3	1:A:321:GLU:OE2	2.10	0.51
1:F:424:GLN:NE2	1:F:449:CYS:SG	2.83	0.51
1:A:331:PRO:CD	1:A:348:THR:HG23	2.26	0.51
1:F:128:ARG:NH1	1:F:489:GLN:HE22	2.00	0.51
1:A:199:PRO:CD	1:A:270:THR:HG21	2.37	0.51
1:A:49:ARG:NE	7:A:3199:HOH:O	2.43	0.51
1:E:331:PRO:CD	1:E:348:THR:HG23	2.25	0.50
1:F:152:ARG:CZ	7:F:2813:HOH:O	2.59	0.50
1:D:486:LEU:C	1:D:486:LEU:HD23	2.37	0.50
1:F:28:LEU:O	1:F:33:LYS:HE2	2.12	0.50
1:B:101:LYS:HG3	1:B:152:ARG:CD	2.42	0.50
1:D:255:GLY:H	1:D:312:ASN:ND2	2.09	0.50
1:A:55:LYS:HE2	7:A:575:HOH:O	2.10	0.49
1:D:64:ASN:OD1	1:D:64:ASN:N	2.44	0.49
1:B:143:ARG:HD3	7:B:2662:HOH:O	2.12	0.49
1:D:408:LYS:NZ	7:D:2542:HOH:O	2.44	0.49
1:A:101:LYS:NZ	1:A:137:GLY:C	2.71	0.49
1:B:71:GLU:OE1	7:B:607:HOH:O	2.20	0.49
1:C:255:GLY:H	1:C:312:ASN:ND2	2.11	0.49
1:D:221:LEU:HD12	1:D:221:LEU:N	2.28	0.49
1:D:149:VAL:O	1:D:149:VAL:HG23	2.12	0.48
1:B:64:ASN:OD1	7:B:1278:HOH:O	2.20	0.48
1:D:143:ARG:HD3	7:D:2695:HOH:O	2.12	0.48
1:F:101:LYS:HG3	1:F:152:ARG:HD2	1.95	0.48
1:A:330:ARG:HD3	1:C:321:GLU:OE2	2.12	0.48
1:E:10:ALA:O	1:E:13:VAL:HG22	2.12	0.48
1:F:424:GLN:NE2	1:F:449:CYS:HB3	2.29	0.48
1:D:128:ARG:HH12	1:D:489:GLN:NE2	2.02	0.48
1:B:199:PRO:CD	1:B:270:THR:HG21	2.37	0.48
1:E:128:ARG:HH12	1:E:489:GLN:NE2	2.03	0.48
1:A:486:LEU:HD23	1:A:486:LEU:C	2.40	0.47
1:A:128:ARG:HH12	1:A:489:GLN:NE2	2.01	0.47
1:B:392:LEU:O	1:B:416:GLN:HA	2.15	0.47
1:E:424:GLN:HE22	1:E:449:CYS:CB	2.27	0.47
1:F:308:GLN:HG2	7:F:2901:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:C	1:A:130:LEU:HD23	2.40	0.47
1:D:223:GLU:HB2	1:D:245:PRO:CD	2.45	0.47
1:B:24:GLU:CD	1:B:80:LYS:HG3	2.40	0.47
1:B:1:MET:CE	1:B:134:LEU:HG	2.36	0.47
1:D:130:LEU:C	1:D:130:LEU:HD23	2.40	0.47
1:E:486:LEU:C	1:E:486:LEU:HD23	2.40	0.46
1:B:223:GLU:HB2	1:B:245:PRO:CD	2.44	0.46
1:E:101:LYS:CG	7:E:2756:HOH:O	2.19	0.46
1:B:10:ALA:O	1:B:13:VAL:HG12	2.15	0.46
1:B:486:LEU:C	1:B:486:LEU:HD23	2.40	0.46
1:D:424:GLN:HE22	1:D:449:CYS:HB3	1.76	0.46
1:B:130:LEU:C	1:B:130:LEU:HD23	2.40	0.46
1:C:63:GLN:HG2	7:E:1354:HOH:O	2.14	0.46
1:D:397:ASP:CA	1:D:400:VAL:HG22	2.45	0.46
1:B:123:HIS:HE1	7:B:2817:HOH:O	1.99	0.46
1:B:48:LYS:HE3	7:B:3233:HOH:O	2.16	0.46
1:B:128:ARG:HH12	1:B:489:GLN:NE2	2.06	0.46
1:E:101:LYS:HE2	7:E:3011:HOH:O	2.16	0.45
1:A:12:SER:O	1:A:69:LYS:HD3	2.17	0.45
1:C:130:LEU:HD23	1:C:130:LEU:C	2.41	0.45
1:A:101:LYS:CG	7:A:3082:HOH:O	2.55	0.45
1:A:193:PRO:O	1:A:193:PRO:CD	2.60	0.45
1:B:56:PRO:CD	1:B:79:GLY:CA	2.93	0.45
1:E:56:PRO:CD	1:E:79:GLY:CA	2.94	0.45
1:A:244:PRO:O	1:A:244:PRO:CD	2.63	0.45
1:A:37:LEU:HD23	7:A:2835:HOH:O	2.18	0.44
1:D:149:VAL:O	1:D:149:VAL:CG2	2.66	0.44
1:F:424:GLN:NE2	1:F:449:CYS:CB	2.80	0.44
1:C:128:ARG:HH12	1:C:489:GLN:NE2	2.02	0.44
1:D:12:SER:O	1:D:69:LYS:HD3	2.18	0.44
1:C:426:GLN:OE1	1:C:446:THR:CG2	2.65	0.44
1:C:486:LEU:HD23	1:C:486:LEU:C	2.43	0.44
1:A:302:ARG:HG3	7:A:2987:HOH:O	2.18	0.44
1:F:243:GLN:HB2	1:F:321:GLU:OE1	2.17	0.43
1:A:48:LYS:HE2	7:A:3158:HOH:O	2.18	0.43
1:C:43:ILE:O	1:C:46:VAL:HG22	2.18	0.43
1:F:141:PHE:HZ	1:F:192:LEU:HD23	1.83	0.43
1:C:92:LEU:C	1:C:92:LEU:HD23	2.43	0.43
1:B:92:LEU:C	1:B:92:LEU:HD23	2.44	0.43
1:C:87:ARG:HG3	1:C:91:LYS:HE3	2.00	0.43
1:C:84:LEU:HD22	1:C:88:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:GLN:HB2	1:C:321:GLU:OE1	2.18	0.43
1:D:243:GLN:HB2	1:D:321:GLU:OE1	2.19	0.43
1:E:143:ARG:HE	1:E:143:ARG:HB2	1.43	0.43
1:B:330:ARG:HD3	1:E:321:GLU:OE2	2.19	0.43
1:D:245:PRO:O	1:D:245:PRO:CD	2.65	0.43
1:F:130:LEU:C	1:F:130:LEU:HD23	2.44	0.43
1:A:101:LYS:HE3	7:A:3082:HOH:O	2.19	0.43
1:A:128:ARG:NH1	1:A:489:GLN:HE22	2.01	0.43
1:B:497:ALA:HB2	7:B:3407:HOH:O	2.19	0.42
1:A:223:GLU:HB2	1:A:245:PRO:CD	2.49	0.42
1:D:111:ALA:C	1:D:112:LEU:HD12	2.45	0.42
1:F:1:MET:HE3	1:F:138:GLU:CD	2.44	0.42
1:A:1:MET:HE3	1:A:138:GLU:CD	2.45	0.42
1:D:92:LEU:HD23	1:D:92:LEU:C	2.44	0.42
1:F:486:LEU:HD23	1:F:486:LEU:C	2.45	0.42
1:E:12:SER:O	1:E:69:LYS:HD3	2.19	0.42
1:F:1:MET:HE2	1:F:154:LEU:HD23	2.01	0.42
1:A:392:LEU:O	1:A:416:GLN:HA	2.20	0.42
1:B:1:MET:HE3	1:B:135:LEU:HD21	2.02	0.42
1:A:221:LEU:HD12	1:A:221:LEU:N	2.35	0.41
1:B:217:LYS:HD3	7:B:671:HOH:O	2.19	0.41
1:B:243:GLN:HB2	1:B:321:GLU:OE1	2.20	0.41
1:A:63:GLN:O	1:A:64:ASN:C	2.63	0.41
1:E:130:LEU:C	1:E:130:LEU:HD23	2.45	0.41
1:A:63:GLN:NE2	1:D:49:ARG:NH2	2.69	0.41
1:F:321:GLU:OE2	1:C:330:ARG:HD3	2.20	0.41
1:D:7:SER:HA	1:D:161:ALA:O	2.21	0.41
1:F:392:LEU:O	1:F:416:GLN:HA	2.20	0.41
1:D:223:GLU:HB2	1:D:245:PRO:HD2	2.03	0.41
1:D:112:LEU:HD12	1:D:112:LEU:N	2.35	0.41
1:D:26:ARG:HD3	7:D:2720:HOH:O	2.20	0.41
1:A:331:PRO:CD	1:A:348:THR:CG2	2.95	0.40
1:A:262:PHE:HZ	1:A:369:GLN:NE2	2.06	0.40
1:E:392:LEU:O	1:E:416:GLN:HA	2.20	0.40
1:E:199:PRO:CD	1:E:270:THR:HG21	2.44	0.40
1:F:24:GLU:OE1	1:F:80:LYS:HG2	2.21	0.40
1:A:357:CYS:HB2	1:A:454:PHE:CG	2.56	0.40
1:E:63:GLN:O	1:E:64:ASN:C	2.65	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:GLU:OE2	1:A:33:LYS:NZ[1_655]	1.81	0.39

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	495/497 (100%)	485 (98%)	10 (2%)	0	100	100
1	B	495/497 (100%)	485 (98%)	10 (2%)	0	100	100
1	C	495/497 (100%)	485 (98%)	10 (2%)	0	100	100
1	D	495/497 (100%)	485 (98%)	10 (2%)	0	100	100
1	E	495/497 (100%)	485 (98%)	10 (2%)	0	100	100
1	F	495/497 (100%)	482 (97%)	13 (3%)	0	100	100
All	All	2970/2982 (100%)	2907 (98%)	63 (2%)	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	378/378 (100%)	378 (100%)	0	100	100
1	B	377/378 (100%)	377 (100%)	0	100	100
1	C	377/378 (100%)	377 (100%)	0	100	100
1	D	378/378 (100%)	375 (99%)	3 (1%)	73	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	378/378 (100%)	377 (100%)	1 (0%)	86	75
1	F	378/378 (100%)	377 (100%)	1 (0%)	86	75
All	All	2266/2268 (100%)	2261 (100%)	5 (0%)	87	77

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	149	VAL
1	D	63	GLN
1	D	64	ASN
1	D	112	LEU
1	E	149	VAL

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

Mol	Chain	Res	Type
1	F	63	GLN
1	F	123	HIS
1	F	312	ASN
1	F	341	GLN
1	F	424	GLN
1	F	489	GLN
1	A	63	GLN
1	A	104	ASN
1	A	253	GLN
1	A	312	ASN
1	A	341	GLN
1	A	424	GLN
1	A	459	ASN
1	A	462	HIS
1	A	489	GLN
1	B	63	GLN
1	B	123	HIS
1	B	312	ASN
1	B	341	GLN
1	B	396	ASN
1	B	424	GLN
1	B	459	ASN
1	B	462	HIS
1	B	489	GLN

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Mol	Chain	Res	Type
1	C	63	GLN
1	C	123	HIS
1	C	253	GLN
1	C	308	GLN
1	C	312	ASN
1	C	396	ASN
1	C	459	ASN
1	C	489	GLN
1	D	63	GLN
1	D	123	HIS
1	D	312	ASN
1	D	424	GLN
1	D	459	ASN
1	D	462	HIS
1	D	489	GLN
1	E	63	GLN
1	E	147	GLN
1	E	243	GLN
1	E	308	GLN
1	E	312	ASN
1	E	341	GLN
1	E	424	GLN
1	E	459	ASN
1	E	462	HIS
1	E	489	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 18 are monoatomic - leaving 12 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$
5	BCT	D	504	-	3,3,3	0.56	0	2,3,3	0.32	0
5	BCT	E	504	-	3,3,3	0.72	0	2,3,3	0.99	0
5	BCT	A	504	-	3,3,3	1.00	0	2,3,3	1.14	0
5	BCT	C	504	-	3,3,3	0.60	0	2,3,3	0.88	0
6	BES	A	505	2,3	22,22,22	0.88	0	26,29,29	1.52	6 (23%)
5	BCT	F	504	-	3,3,3	0.39	0	2,3,3	0.48	0
5	BCT	B	504	-	3,3,3	0.39	0	2,3,3	0.31	0
6	BES	C	505	2,3	22,22,22	1.13	3 (13%)	26,29,29	1.28	3 (11%)
6	BES	F	505	2,3	22,22,22	1.02	0	26,29,29	1.54	4 (15%)
6	BES	E	505	2,3	22,22,22	1.09	2 (9%)	26,29,29	1.30	3 (11%)
6	BES	D	505	2,3	22,22,22	0.99	1 (4%)	26,29,29	1.29	4 (15%)
6	BES	B	505	2,3	22,22,22	1.02	2 (9%)	26,29,29	1.43	4 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BES	C	505	2,3	-	5/24/24/24	0/1/1/1
6	BES	A	505	2,3	-	4/24/24/24	0/1/1/1
6	BES	F	505	2,3	-	5/24/24/24	0/1/1/1
6	BES	E	505	2,3	-	4/24/24/24	0/1/1/1
6	BES	D	505	2,3	-	4/24/24/24	0/1/1/1
6	BES	B	505	2,3	-	4/24/24/24	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	505	BES	C2-C3	-2.75	1.47	1.52
6	C	505	BES	O2-C2	2.60	1.47	1.42
6	E	505	BES	O2-C2	2.57	1.47	1.42
6	E	505	BES	C2-C3	-2.55	1.47	1.52
6	C	505	BES	C9-C8	2.22	1.42	1.38
6	B	505	BES	O2-C2	2.19	1.46	1.42
6	D	505	BES	C2-C3	-2.17	1.48	1.52
6	B	505	BES	C2-C3	-2.10	1.48	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	505	BES	C12-C7-C8	3.55	123.51	118.23
6	B	505	BES	C13-C4-N1	-3.42	102.87	110.58
6	F	505	BES	C13-C4-N1	-3.12	103.55	110.58
6	A	505	BES	C13-C4-N1	-2.96	103.89	110.58
6	D	505	BES	C11-C10-C9	2.92	123.86	119.87
6	F	505	BES	C6-C7-C12	-2.90	115.51	120.90
6	A	505	BES	C6-C7-C12	-2.90	115.51	120.90
6	A	505	BES	C12-C7-C8	2.59	122.08	118.23
6	B	505	BES	O2-C2-C3	-2.59	105.22	110.63
6	A	505	BES	C11-C10-C9	2.54	123.34	119.87
6	D	505	BES	C13-C4-N1	-2.47	105.00	110.58
6	E	505	BES	C13-C4-N1	-2.47	105.02	110.58
6	C	505	BES	C6-C7-C12	-2.46	116.33	120.90
6	F	505	BES	C11-C12-C7	-2.45	117.17	120.61
6	B	505	BES	C12-C7-C8	2.35	121.73	118.23
6	E	505	BES	C6-C7-C12	-2.28	116.67	120.90
6	C	505	BES	C13-C4-N1	-2.25	105.51	110.58
6	E	505	BES	C12-C7-C8	2.20	121.51	118.23
6	B	505	BES	C11-C10-C9	2.18	122.86	119.87
6	C	505	BES	O2-C2-C3	-2.16	106.11	110.63
6	A	505	BES	C9-C8-C7	-2.16	117.57	120.61
6	D	505	BES	C10-C9-C8	-2.10	117.64	120.24
6	A	505	BES	C10-C11-C12	-2.08	117.68	120.24
6	D	505	BES	C12-C7-C8	2.03	121.25	118.23

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	505	BES	O2-C2-C3-N1

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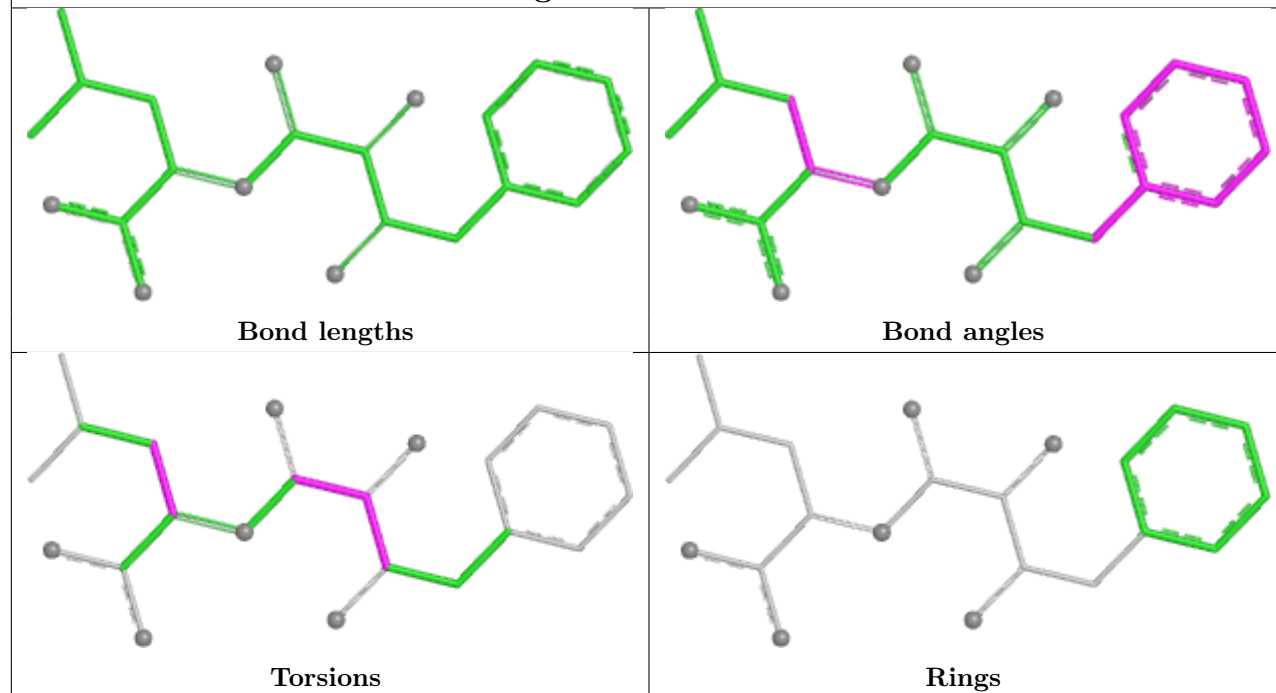
Mol	Chain	Res	Type	Atoms
6	B	505	BES	O2-C2-C3-O3
6	C	505	BES	O2-C2-C3-O3
6	D	505	BES	O2-C2-C3-O3
6	F	505	BES	O2-C2-C3-N1
6	A	505	BES	O2-C2-C3-N1
6	B	505	BES	O2-C2-C3-N1
6	C	505	BES	O2-C2-C3-N1
6	D	505	BES	O2-C2-C3-N1
6	F	505	BES	O2-C2-C3-O3
6	A	505	BES	O2-C2-C3-O3
6	E	505	BES	O2-C2-C3-O3
6	F	505	BES	C6-C1-C2-C3
6	C	505	BES	C6-C1-C2-C3
6	D	505	BES	C6-C1-C2-C3
6	E	505	BES	C6-C1-C2-C3
6	A	505	BES	C14-C13-C4-C5
6	B	505	BES	C14-C13-C4-C5
6	F	505	BES	N2-C1-C2-C3
6	A	505	BES	N2-C1-C2-C3
6	B	505	BES	N2-C1-C2-C3
6	C	505	BES	N2-C1-C2-C3
6	D	505	BES	C14-C13-C4-C5
6	F	505	BES	C14-C13-C4-C5
6	E	505	BES	C14-C13-C4-C5
6	C	505	BES	C6-C1-C2-O2

There are no ring outliers.

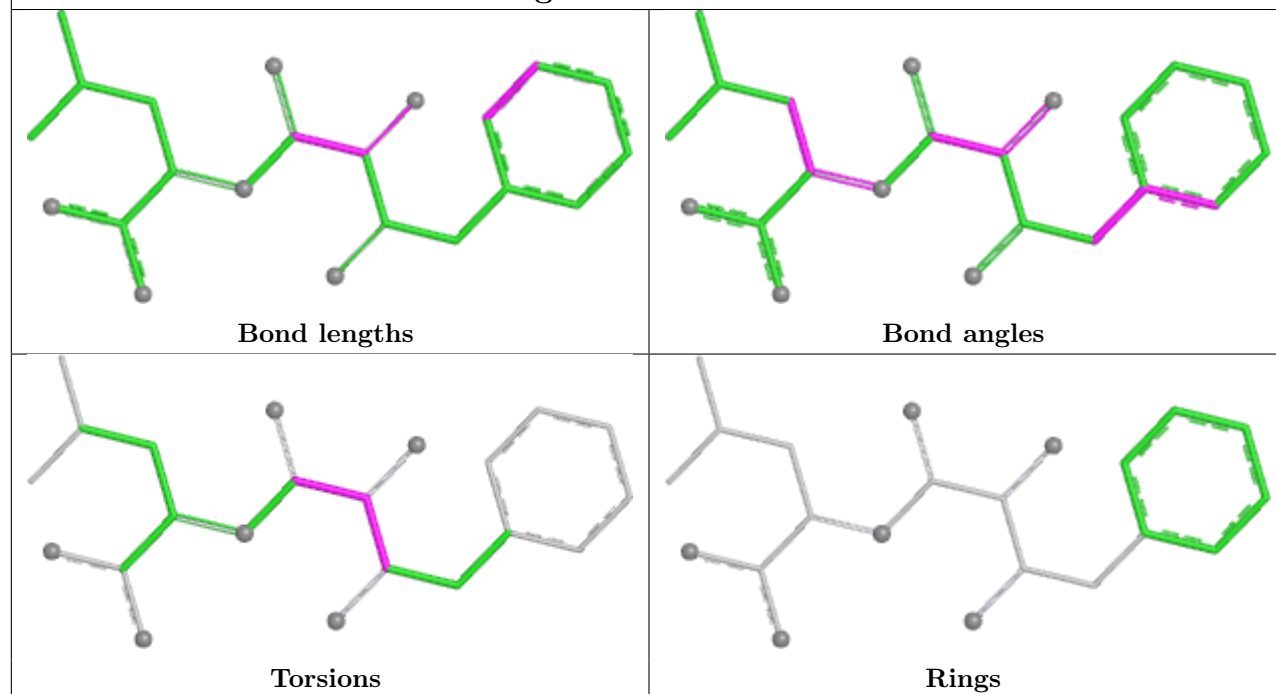
No monomer is involved in short contacts.

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.

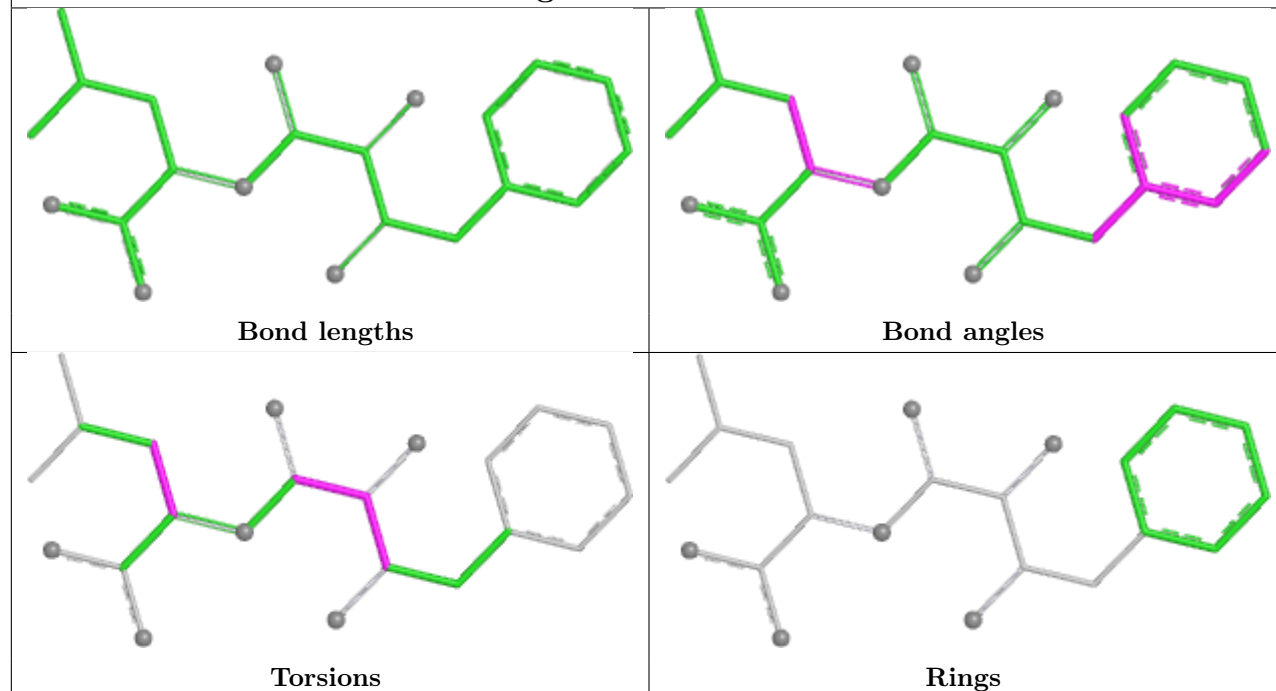
Ligand BES A 505



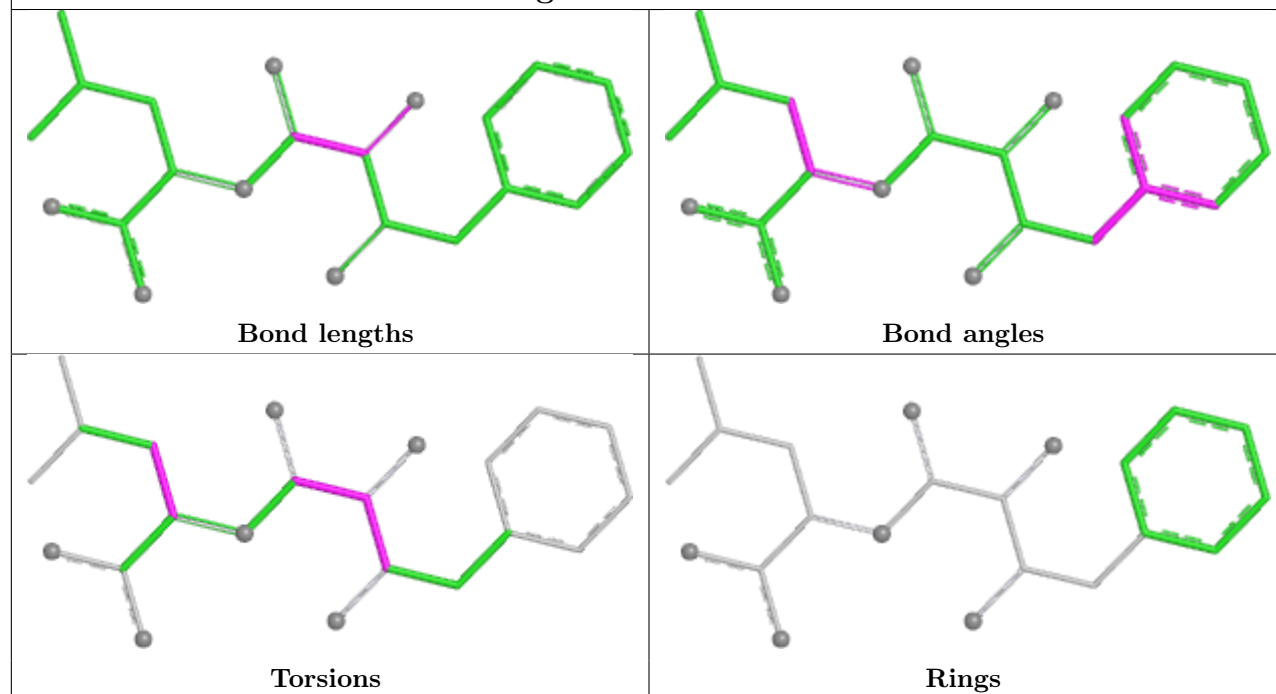
Ligand BES C 505

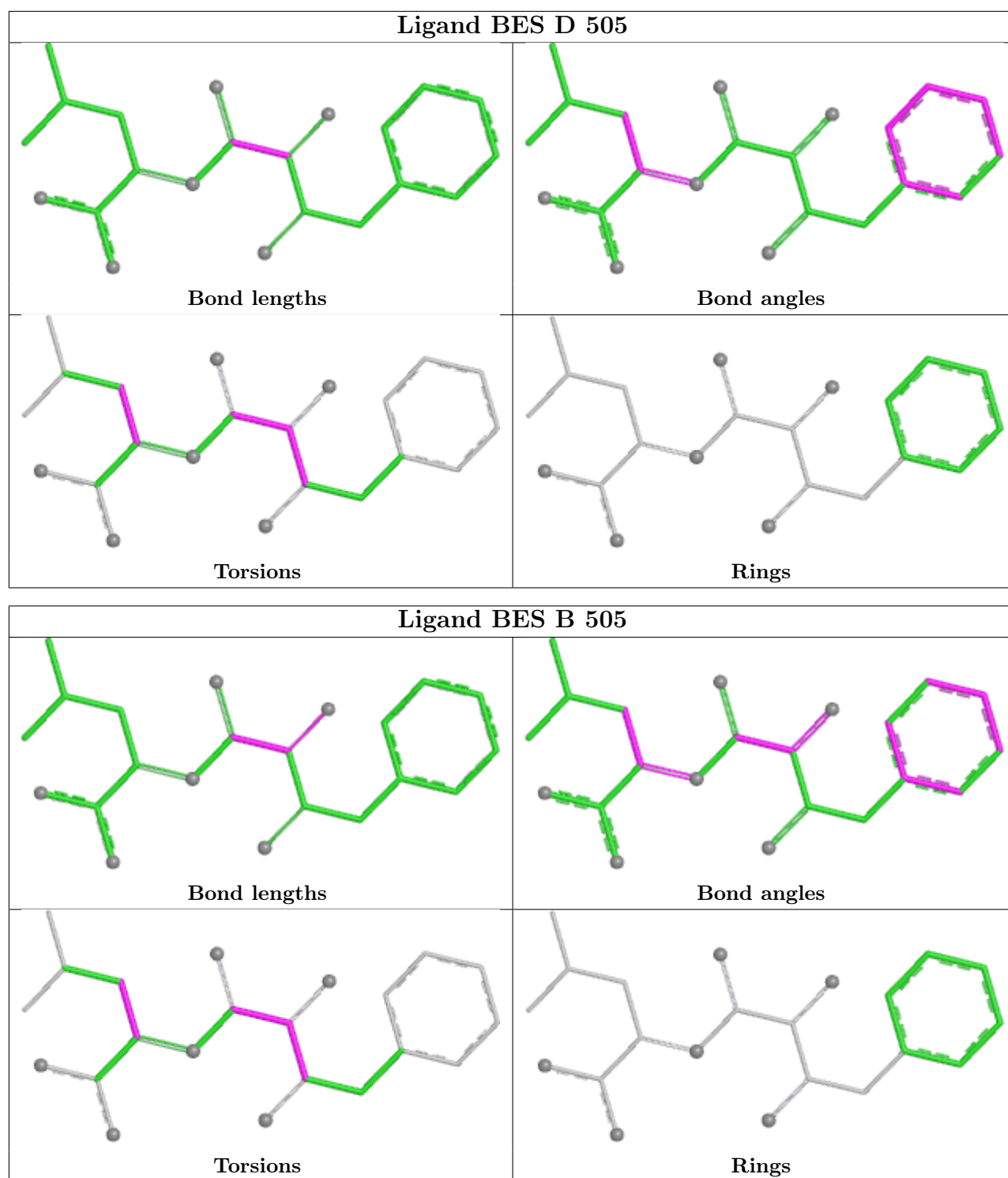


Ligand BES F 505



Ligand BES E 505





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	497/497 (100%)	-0.16	20 (4%)	42 46	4, 10, 25, 43	0
1	B	497/497 (100%)	-0.23	19 (3%)	44 48	5, 9, 23, 35	0
1	C	497/497 (100%)	-0.18	19 (3%)	44 48	5, 10, 23, 37	0
1	D	497/497 (100%)	-0.15	20 (4%)	42 46	5, 10, 25, 42	0
1	E	497/497 (100%)	-0.22	19 (3%)	44 48	5, 9, 23, 39	0
1	F	497/497 (100%)	-0.25	20 (4%)	42 46	4, 9, 22, 38	0
All	All	2982/2982 (100%)	-0.20	117 (3%)	43 47	4, 10, 24, 43	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	149	VAL	6.6
1	C	149	VAL	6.0
1	E	497	ALA	5.1
1	A	149	VAL	4.9
1	C	121	ASP	4.5
1	B	497	ALA	4.4
1	B	121	ASP	4.4
1	C	475	LYS	3.8
1	A	147	GLN	3.7
1	F	122	ALA	3.7
1	D	497	ALA	3.7
1	E	149	VAL	3.7
1	D	63	GLN	3.7
1	E	476	ASP	3.7
1	A	151	PRO	3.6
1	A	121	ASP	3.6
1	D	150	GLU	3.5
1	F	476	ASP	3.5
1	C	497	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	497	ALA	3.4
1	B	285	ASP	3.4
1	A	150	GLU	3.4
1	A	285	ASP	3.4
1	F	149	VAL	3.3
1	C	425	GLU	3.3
1	D	476	ASP	3.3
1	F	475	LYS	3.3
1	C	373	ASP	3.2
1	F	150	GLU	3.2
1	B	475	LYS	3.2
1	A	81	ASP	3.1
1	B	373	ASP	3.1
1	F	285	ASP	3.1
1	D	121	ASP	3.1
1	F	162	ASP	3.0
1	D	147	GLN	3.0
1	C	147	GLN	3.0
1	B	151	PRO	3.0
1	D	373	ASP	3.0
1	B	122	ALA	2.9
1	C	122	ALA	2.9
1	C	285	ASP	2.9
1	A	122	ALA	2.9
1	D	285	ASP	2.9
1	E	285	ASP	2.8
1	E	150	GLU	2.8
1	B	149	VAL	2.8
1	F	373	ASP	2.8
1	E	121	ASP	2.8
1	D	81	ASP	2.7
1	B	150	GLU	2.7
1	A	119	ASN	2.7
1	E	163	LYS	2.7
1	D	496	GLY	2.6
1	E	162	ASP	2.6
1	E	164	ALA	2.6
1	B	425	GLU	2.6
1	A	476	ASP	2.6
1	B	496	GLY	2.6
1	F	63	GLN	2.6
1	A	475	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	138	GLU	2.6
1	C	496	GLY	2.6
1	B	147	GLN	2.5
1	D	119	ASN	2.5
1	B	123	HIS	2.5
1	D	82	GLU	2.5
1	D	151	PRO	2.5
1	E	114	ASP	2.5
1	E	122	ALA	2.4
1	F	214	LYS	2.4
1	C	80	LYS	2.4
1	E	473	GLY	2.4
1	F	119	ASN	2.4
1	D	64	ASN	2.4
1	B	164	ALA	2.4
1	E	151	PRO	2.3
1	A	163	LYS	2.3
1	D	118	ASN	2.3
1	E	119	ASN	2.3
1	F	426	GLN	2.3
1	F	497	ALA	2.3
1	A	214	LYS	2.3
1	A	82	GLU	2.3
1	F	64	ASN	2.3
1	B	162	ASP	2.3
1	C	123	HIS	2.3
1	A	164	ALA	2.3
1	C	151	PRO	2.3
1	B	119	ASN	2.3
1	A	373	ASP	2.3
1	B	63	GLN	2.3
1	C	302	ARG	2.3
1	C	426	GLN	2.3
1	A	473	GLY	2.2
1	C	150	GLU	2.2
1	E	475	LYS	2.2
1	F	164	ALA	2.2
1	A	496	GLY	2.2
1	D	426	GLN	2.2
1	F	473	GLY	2.2
1	A	63	GLN	2.2
1	C	476	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	138	GLU	2.2
1	F	369	GLN	2.1
1	C	63	GLN	2.1
1	E	63	GLN	2.1
1	E	1	MET	2.1
1	F	80	LYS	2.1
1	D	475	LYS	2.1
1	F	123	HIS	2.1
1	D	138	GLU	2.1
1	B	40	GLU	2.0
1	D	1	MET	2.0
1	E	138	GLU	2.0
1	B	476	ASP	2.0
1	E	64	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BES	F	505	22/22	0.97	0.06	4,12,17,19	0
6	BES	A	505	22/22	0.97	0.06	4,11,18,22	0
6	BES	B	505	22/22	0.97	0.06	5,11,17,19	0
6	BES	C	505	22/22	0.97	0.06	5,12,17,19	0
6	BES	D	505	22/22	0.97	0.06	6,12,17,20	0
6	BES	E	505	22/22	0.97	0.06	5,13,17,20	0
5	BCT	A	504	4/4	0.98	0.04	6,6,7,8	0
5	BCT	B	504	4/4	0.99	0.03	7,7,7,8	0
5	BCT	C	504	4/4	0.99	0.04	6,7,7,7	0

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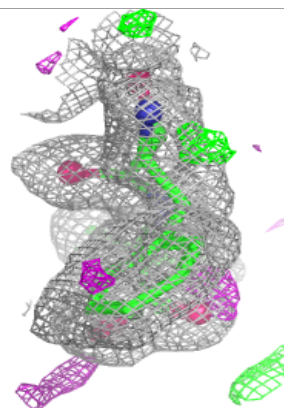
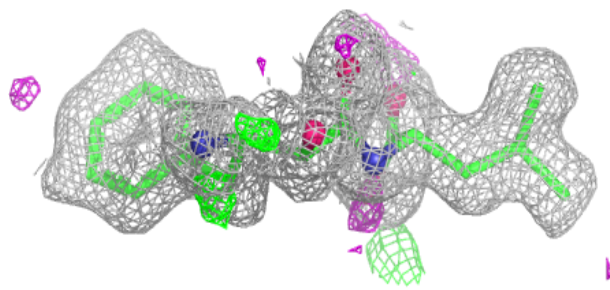
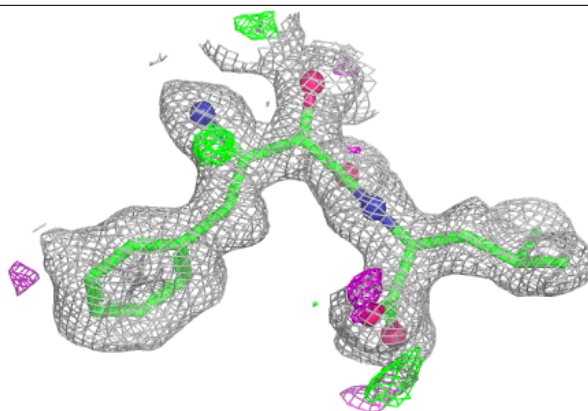
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BCT	D	504	4/4	0.99	0.03	6,6,7,8	0
5	BCT	E	504	4/4	0.99	0.04	5,6,7,7	0
5	BCT	F	504	4/4	0.99	0.03	6,7,7,8	0
4	K	F	503	1/1	1.00	0.04	6,6,6,6	0
4	K	A	503	1/1	1.00	0.02	6,6,6,6	0
4	K	B	503	1/1	1.00	0.04	6,6,6,6	0
4	K	C	503	1/1	1.00	0.02	6,6,6,6	0
4	K	D	503	1/1	1.00	0.02	6,6,6,6	0
4	K	E	503	1/1	1.00	0.04	6,6,6,6	0
2	ZN	F	501	1/1	1.00	0.02	6,6,6,6	1
2	ZN	A	501	1/1	1.00	0.01	5,5,5,5	1
2	ZN	B	501	1/1	1.00	0.02	6,6,6,6	1
2	ZN	C	501	1/1	1.00	0.03	6,6,6,6	1
2	ZN	D	501	1/1	1.00	0.02	6,6,6,6	1
2	ZN	E	501	1/1	1.00	0.02	6,6,6,6	1
3	MN	F	502	1/1	1.00	0.02	5,5,5,5	0
3	MN	A	502	1/1	1.00	0.01	5,5,5,5	0
3	MN	B	502	1/1	1.00	0.01	6,6,6,6	0
3	MN	C	502	1/1	1.00	0.01	5,5,5,5	0
3	MN	D	502	1/1	1.00	0.02	5,5,5,5	0
3	MN	E	502	1/1	1.00	0.02	5,5,5,5	0

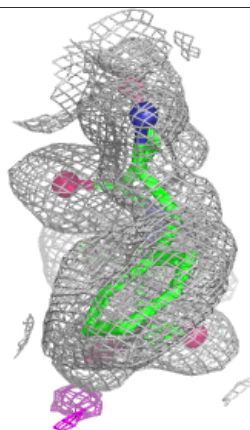
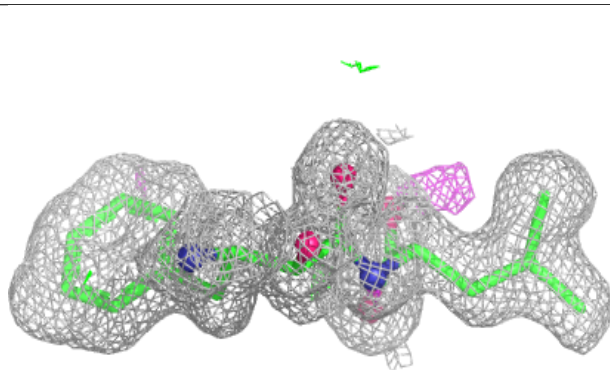
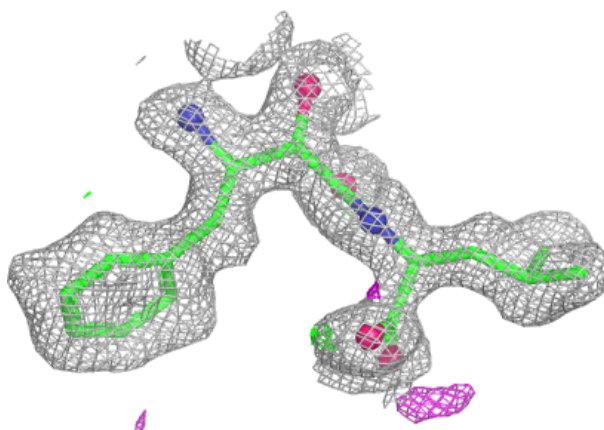
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BES F 505:

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

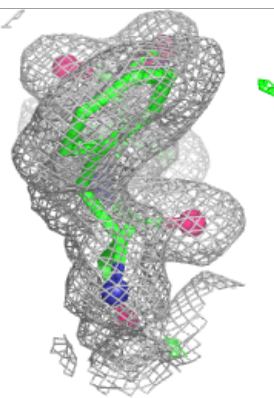
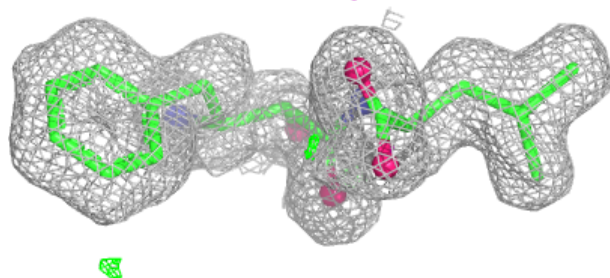
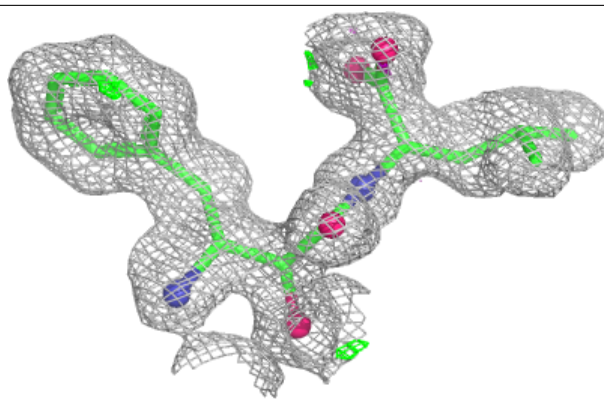
**Electron density around BES A 505:**

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

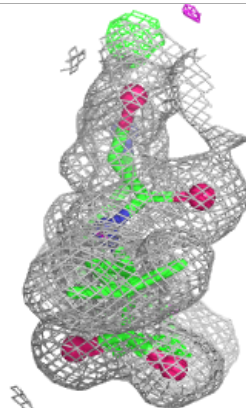
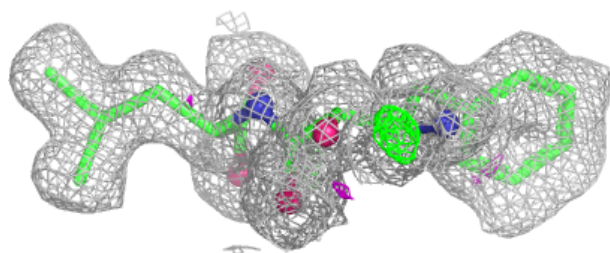
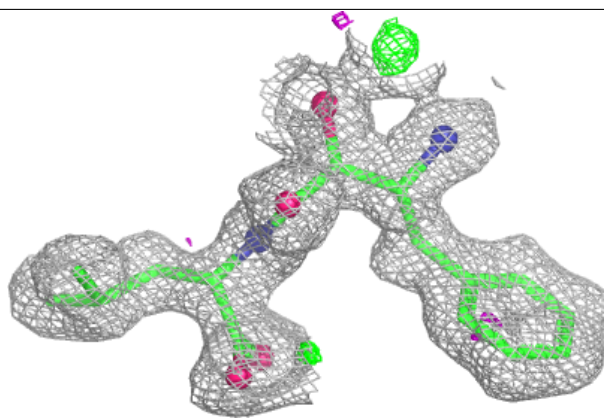


Electron density around BES B 505:

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

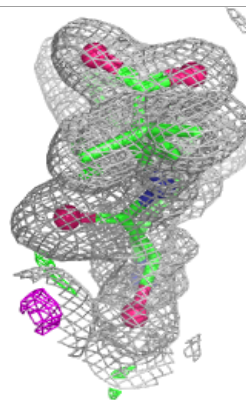
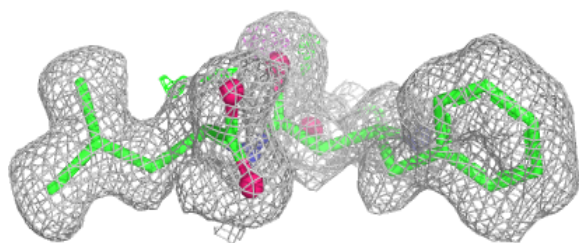
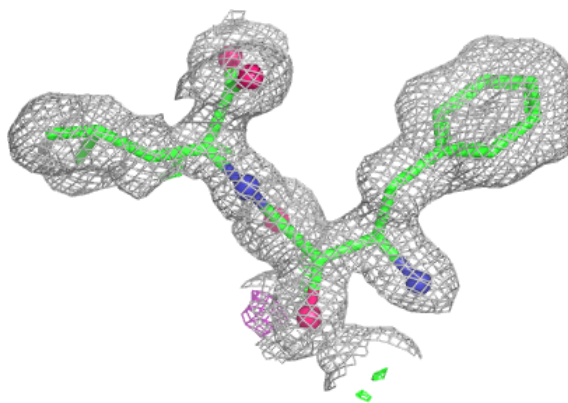
**Electron density around BES C 505:**

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

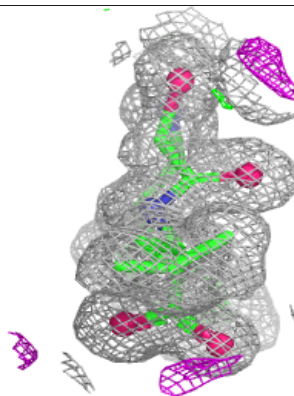
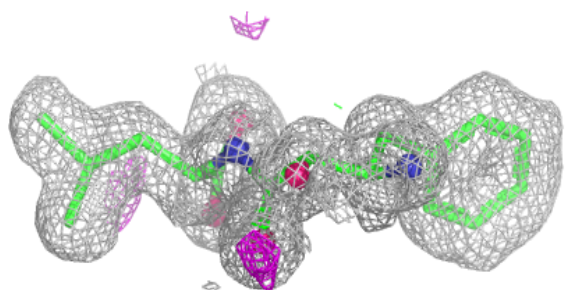
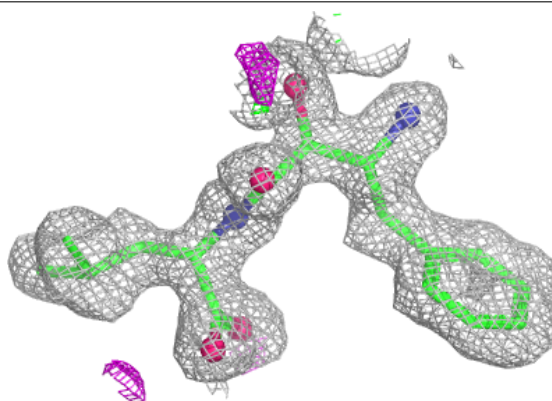


Electron density around BES D 505:

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

**Electron density around BES E 505:**

$2mF_o-DF_c$ (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.