



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:56 PM UTC

PDB ID : 1LQF / pdb_00001lqf
Title : Structure of PTP1b in Complex with a Peptidic Bisphosphonate Inhibitor
Authors : Asante-Appiah, E.; Patel, S.; Dufresne, C.; Scapin, G.
Deposited on : 2002-05-10
Resolution : 2.50 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

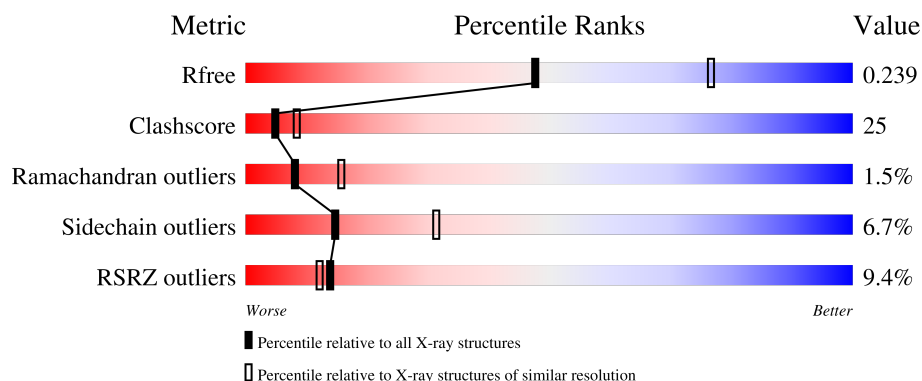
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	295	5% 55% 37% 5%
1	B	295	2% 58% 33% 6%
1	C	295	9% 56% 34% 7%
1	D	295	20% 55% 36% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10076 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 protein-tyrosine phosphatase, non-receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2336	1483	402	435	16			
1	B	287	Total	C	N	O	S	0	0	0
			2335	1483	401	435	16			
1	C	287	Total	C	N	O	S	0	0	0
			2322	1472	401	433	16			
1	D	287	Total	C	N	O	S	0	0	0
			2339	1486	402	435	16			

There are 48 discrepancies between the modelled and reference sequences:

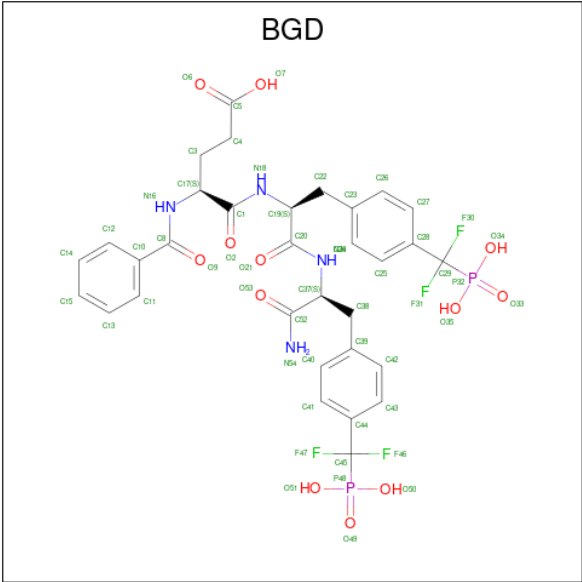
Chain	Residue	Modelled	Actual	Comment	Reference
A	489	MET	-	see remark 999	UNP P18031
A	490	ASP	-	see remark 999	UNP P18031
A	491	TYR	-	see remark 999	UNP P18031
A	492	LYS	-	see remark 999	UNP P18031
A	493	ASP	-	see remark 999	UNP P18031
A	494	ASP	-	see remark 999	UNP P18031
A	495	ASP	-	see remark 999	UNP P18031
A	496	ASP	-	see remark 999	UNP P18031
A	497	LYS	-	see remark 999	UNP P18031
A	498	LEU	-	see remark 999	UNP P18031
A	499	GLU	-	see remark 999	UNP P18031
A	500	PHE	-	see remark 999	UNP P18031
B	489	MET	-	see remark 999	UNP P18031
B	490	ASP	-	see remark 999	UNP P18031
B	491	TYR	-	see remark 999	UNP P18031
B	492	LYS	-	see remark 999	UNP P18031
B	493	ASP	-	see remark 999	UNP P18031
B	494	ASP	-	see remark 999	UNP P18031
B	495	ASP	-	see remark 999	UNP P18031
B	496	ASP	-	see remark 999	UNP P18031
B	497	LYS	-	see remark 999	UNP P18031

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Chain	Residue	Modelled	Actual	Comment	Reference
B	498	LEU	-	see remark 999	UNP P18031
B	499	GLU	-	see remark 999	UNP P18031
B	500	PHE	-	see remark 999	UNP P18031
C	489	MET	-	see remark 999	UNP P18031
C	490	ASP	-	see remark 999	UNP P18031
C	491	TYR	-	see remark 999	UNP P18031
C	492	LYS	-	see remark 999	UNP P18031
C	493	ASP	-	see remark 999	UNP P18031
C	494	ASP	-	see remark 999	UNP P18031
C	495	ASP	-	see remark 999	UNP P18031
C	496	ASP	-	see remark 999	UNP P18031
C	497	LYS	-	see remark 999	UNP P18031
C	498	LEU	-	see remark 999	UNP P18031
C	499	GLU	-	see remark 999	UNP P18031
C	500	PHE	-	see remark 999	UNP P18031
D	489	MET	-	see remark 999	UNP P18031
D	490	ASP	-	see remark 999	UNP P18031
D	491	TYR	-	see remark 999	UNP P18031
D	492	LYS	-	see remark 999	UNP P18031
D	493	ASP	-	see remark 999	UNP P18031
D	494	ASP	-	see remark 999	UNP P18031
D	495	ASP	-	see remark 999	UNP P18031
D	496	ASP	-	see remark 999	UNP P18031
D	497	LYS	-	see remark 999	UNP P18031
D	498	LEU	-	see remark 999	UNP P18031
D	499	GLU	-	see remark 999	UNP P18031
D	500	PHE	-	see remark 999	UNP P18031

- Molecule 2 is N-BENZOYL-L-GLUTAMYL-[4-PHOSPHONO(DIFLUOROMETHYL)]-L-PHENYLALANINE-[4-PHOSPHONO(DIFLUORO-METHYL)]-L-PHENYLALANINEAMIDE (CCD ID: BGD) (formula: C₃₂H₃₄F₄N₄O₁₂P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 54	C 32	F 4	N 4	O 12	P 2	0	0
2	B	1	Total 54	C 32	F 4	N 4	O 12	P 2	0	0
2	C	1	Total 54	C 32	F 4	N 4	O 12	P 2	0	0
2	D	1	Total 54	C 32	F 4	N 4	O 12	P 2	0	0

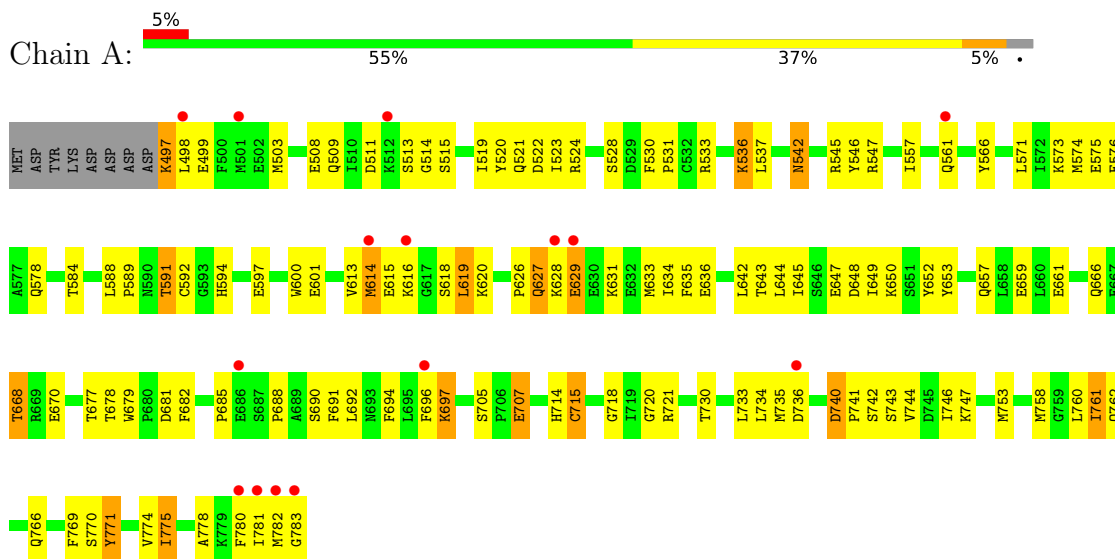
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total	O	0	0
			129	129		
3	B	176	Total	O	0	0
			176	176		
3	C	126	Total	O	0	0
			126	126		
3	D	97	Total	O	0	0
			97	97		

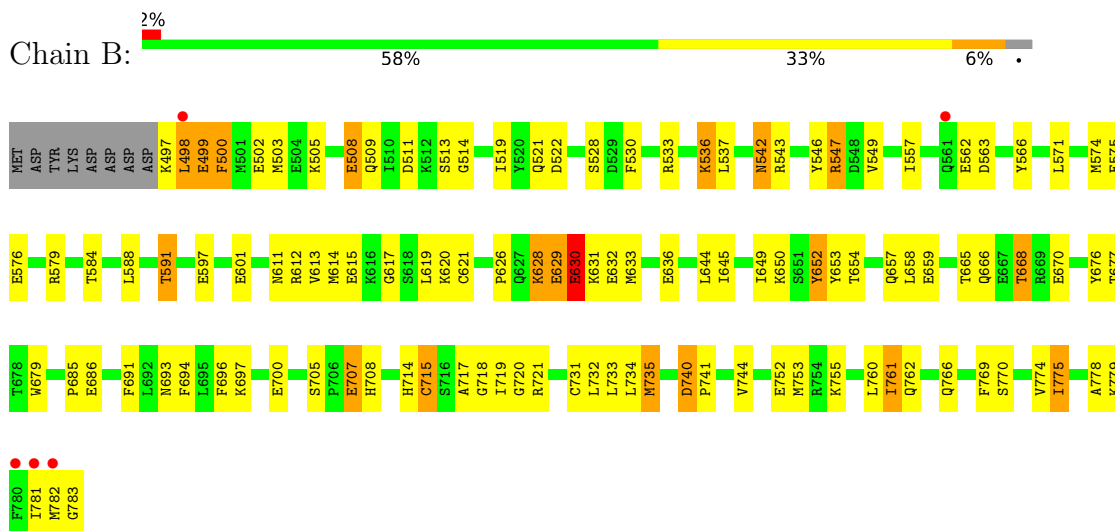
3 Residue-property plots [i](#)

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: protein-tyrosine phosphatase, non-receptor type 1

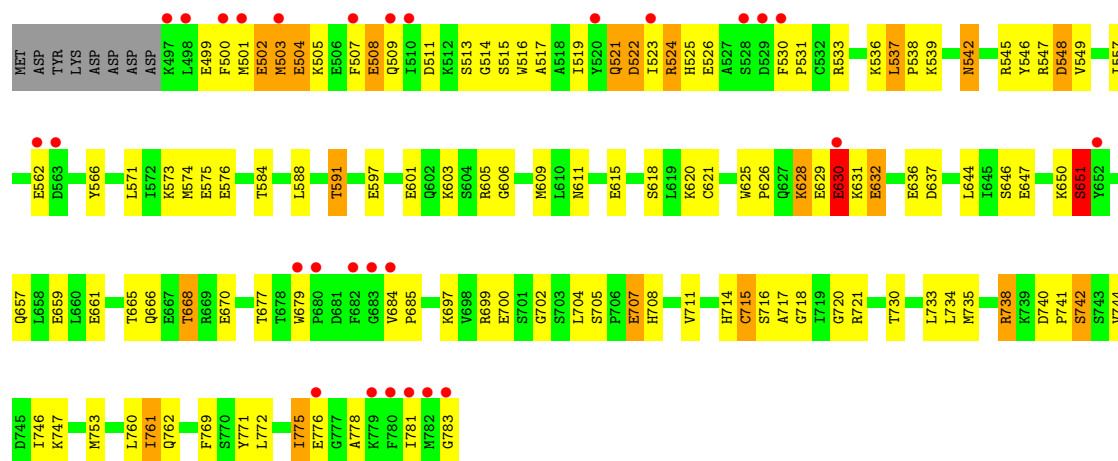


- Molecule 1: protein-tyrosine phosphatase, non-receptor type 1

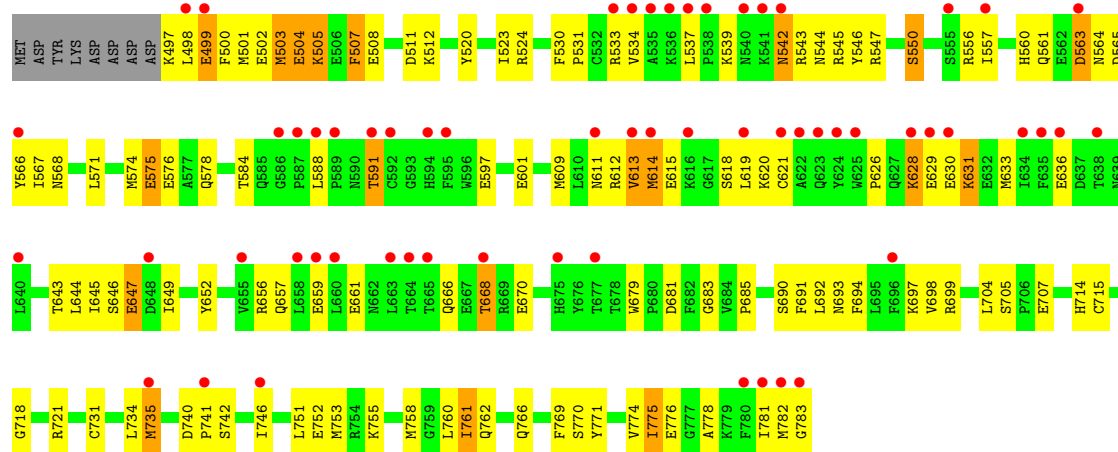


- Molecule 1: protein-tyrosine phosphatase, non-receptor type 1





- Molecule 1: protein-tyrosine phosphatase, non-receptor type 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.87Å 154.42Å 64.60Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	29.00 – 2.50 29.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.4 (29.00-2.50) 96.9 (29.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.286 0.241 , 0.239	Depositor DCC
R_{free} test set	3230 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10076	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: BGD

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	0.70	1/2389 (0.0%)	1.06	12/3218 (0.4%)
1	B	0.78	0/2388	1.08	10/3218 (0.3%)
1	C	0.68	0/2374	1.07	11/3200 (0.3%)
1	D	0.64	0/2392	1.07	11/3222 (0.3%)
All	All	0.70	1/9543 (0.0%)	1.07	44/12858 (0.3%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	758	MET	SD-CE	5.04	1.92	1.79

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	504	GLU	N-CA-C	-8.82	100.46	111.75
1	A	740	ASP	CA-C-N	8.09	128.18	119.28
1	A	740	ASP	C-N-CA	8.09	128.18	119.28
1	B	499	GLU	N-CA-C	-7.86	103.79	113.15
1	D	628	LYS	N-CA-C	-7.31	99.46	110.28
1	D	499	GLU	N-CA-C	-7.25	104.17	112.87
1	A	697	LYS	N-CA-C	-7.09	103.48	111.07
1	C	738	ARG	N-CA-C	6.55	119.01	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	677	THR	N-CA-C	6.45	120.86	112.92
1	B	740	ASP	N-CA-C	-6.38	100.38	109.24
1	D	766	GLN	N-CA-C	-6.35	104.45	111.82
1	A	627	GLN	N-CA-C	6.30	121.06	112.68
1	D	504	GLU	N-CA-C	-6.23	105.81	113.41
1	D	550	SER	CA-C-N	6.22	126.71	119.99
1	D	550	SER	C-N-CA	6.22	126.71	119.99
1	D	505	LYS	N-CA-C	-6.20	104.44	111.07
1	C	651	SER	N-CA-C	6.18	123.97	110.80
1	D	762	GLN	N-CA-C	6.12	120.75	113.28
1	B	566	TYR	N-CA-C	6.09	119.30	110.28
1	B	500	PHE	N-CA-C	-6.06	104.23	111.69
1	A	762	GLN	N-CA-C	6.05	120.82	113.38
1	A	766	GLN	N-CA-C	-6.03	104.78	111.36
1	A	771	TYR	N-CA-C	-5.85	104.82	111.14
1	D	643	THR	N-CA-C	5.82	117.89	108.34
1	D	683	GLY	N-CA-C	-5.69	105.96	112.79
1	B	762	GLN	N-CA-C	5.66	120.25	113.23
1	B	707	GLU	N-CA-C	-5.65	106.36	113.20
1	C	575	GLU	N-CA-C	5.63	117.11	110.97
1	A	566	TYR	N-CA-C	5.55	118.98	110.20
1	B	766	GLN	N-CA-C	-5.48	105.39	111.36
1	C	707	GLU	N-CA-C	-5.40	106.66	113.20
1	B	536	LYS	N-CA-C	5.39	119.86	113.28
1	C	762	GLN	N-CA-C	5.39	120.01	113.38
1	C	637	ASP	N-CA-C	5.37	117.13	111.28
1	D	507	PHE	N-CA-C	-5.32	105.40	111.14
1	C	566	TYR	N-CA-C	5.31	118.59	110.20
1	A	707	GLU	N-CA-C	-5.26	106.83	113.20
1	B	677	THR	N-CA-C	5.26	119.39	112.92
1	A	643	THR	N-CA-C	5.25	117.64	108.76
1	A	677	THR	N-CA-C	5.25	119.78	113.17
1	A	536	LYS	N-CA-C	5.15	119.54	113.16
1	B	645	ILE	CB-CA-C	-5.08	106.62	111.44
1	C	625	TRP	CA-C-N	5.05	124.98	119.78
1	C	625	TRP	C-N-CA	5.05	124.98	119.78

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	652	TYR	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	2336	0	2297	122	0
1	B	2335	0	2295	102	0
1	C	2322	0	2275	133	0
1	D	2339	0	2306	130	0
2	A	54	0	27	6	0
2	B	54	0	29	2	0
2	C	54	0	27	5	0
2	D	54	0	29	3	0
3	A	129	0	0	17	0
3	B	176	0	0	10	0
3	C	126	0	0	20	0
3	D	97	0	0	11	0
All	All	10076	0	9285	477	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 25.

All (477) 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:B:498:LEU:HD12	1:B:498:LEU:H	1.29	0.98
1:B:563:ASP:HB3	3:B:3302:HOH:O	1.63	0.97
1:B:547:ARG:HB3	1:B:547:ARG:NH1	1.79	0.97
1:C:628:LYS:NZ	1:C:628:LYS:HB2	1.80	0.96
1:B:591:THR:HG21	3:B:3140:HOH:O	1.64	0.95
1:A:499:GLU:HG2	1:A:740:ASP:OD1	1.67	0.94
1:C:502:GLU:O	1:C:505:LYS:HB3	1.67	0.94
1:D:613:VAL:HG12	1:D:621:CYS:O	1.69	0.93
1:D:597:GLU:O	1:D:601:GLU:HG3	1.67	0.93
1:D:498:LEU:O	1:D:498:LEU:HD13	1.67	0.92
1:A:670:GLU:HG3	3:A:3013:HOH:O	1.69	0.92
1:D:539:LYS:HE2	1:D:564:ASN:HD22	1.35	0.90
1:A:770:SER:O	1:A:774:VAL:HG23	1.70	0.90
1:D:556:ARG:HB2	3:D:3237:HOH:O	1.71	0.89
1:B:693:ASN:HB2	3:B:3129:HOH:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3044:HOH:O	1:C:562:GLU:HB3	1.74	0.87
1:C:538:PRO:HD2	3:C:3175:HOH:O	1.73	0.86
1:C:597:GLU:O	1:C:601:GLU:HG3	1.75	0.86
1:B:770:SER:O	1:B:774:VAL:HG23	1.75	0.85
1:C:628:LYS:HB2	1:C:628:LYS:HZ2	1.40	0.85
1:D:693:ASN:O	1:D:697:LYS:HG2	1.78	0.84
1:A:597:GLU:O	1:A:601:GLU:HG3	1.79	0.83
1:D:626:PRO:HG3	1:D:633:MET:HG3	1.60	0.83
1:B:574:MET:HE2	1:B:753:MET:HE3	1.61	0.82
1:C:615:GLU:HB2	1:C:620:LYS:HG3	1.63	0.81
1:B:500:PHE:HZ	1:B:779:LYS:HZ2	1.28	0.81
1:C:500:PHE:HA	3:C:3403:HOH:O	1.79	0.81
1:A:627:GLN:H	1:A:631:LYS:HD3	1.47	0.80
1:B:707:GLU:OE2	1:C:708:HIS:CE1	2.34	0.80
1:B:659:GLU:OE2	1:B:668:THR:HB	1.81	0.79
1:A:521:GLN:HA	1:A:524:ARG:HD3	1.65	0.79
1:A:533:ARG:HG3	1:A:533:ARG:HH11	1.47	0.79
1:B:533:ARG:HG3	1:B:533:ARG:HH11	1.48	0.79
1:A:780:PHE:O	1:D:693:ASN:ND2	2.16	0.79
1:D:631:LYS:HE2	1:D:631:LYS:HA	1.64	0.79
1:B:497:LYS:C	1:B:499:GLU:H	1.86	0.79
1:C:533:ARG:HG3	1:C:533:ARG:HH11	1.49	0.78
1:A:659:GLU:OE2	1:A:668:THR:HB	1.80	0.78
1:B:497:LYS:O	1:B:782:MET:HE1	1.83	0.78
1:C:659:GLU:OE2	1:C:668:THR:HB	1.83	0.77
1:D:588:LEU:HB2	1:D:591:THR:HB	1.66	0.76
1:A:626:PRO:HB2	1:A:644:LEU:HB2	1.65	0.76
1:C:666:GLN:HG3	3:C:3292:HOH:O	1.84	0.76
1:B:708:HIS:NE2	1:C:707:GLU:OE1	2.19	0.75
1:C:697:LYS:HE2	3:C:3472:HOH:O	1.86	0.75
1:B:597:GLU:O	1:B:601:GLU:HG3	1.86	0.75
1:C:574:MET:HE2	1:C:753:MET:HE3	1.66	0.75
1:D:659:GLU:OE2	1:D:668:THR:HB	1.87	0.75
1:C:705:SER:OG	1:C:707:GLU:HG2	1.88	0.74
1:D:615:GLU:HB2	1:D:620:LYS:HG3	1.69	0.73
1:B:547:ARG:HB3	1:B:547:ARG:HH11	1.52	0.73
1:D:614:MET:HA	1:D:618:SER:O	1.87	0.73
1:A:705:SER:OG	1:A:707:GLU:HG2	1.88	0.73
1:D:533:ARG:HG3	1:D:533:ARG:HH11	1.54	0.72
1:A:746:ILE:HG13	1:A:771:TYR:CE2	2.25	0.72
1:C:628:LYS:HE3	1:C:631:LYS:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:THR:HG22	3:A:3017:HOH:O	1.89	0.72
1:B:499:GLU:OE1	1:B:741:PRO:HD2	1.90	0.72
1:D:705:SER:OG	1:D:707:GLU:HG2	1.90	0.71
1:C:628:LYS:CE	1:C:631:LYS:HD3	2.21	0.71
1:C:521:GLN:HG3	1:C:524:ARG:HH22	1.57	0.70
1:B:752:GLU:O	1:B:755:LYS:HB2	1.92	0.70
1:D:770:SER:O	1:D:774:VAL:HG23	1.92	0.69
1:D:539:LYS:CE	1:D:564:ASN:HD22	2.05	0.69
1:B:611:ASN:HB2	1:B:615:GLU:OE2	1.92	0.69
1:A:647:GLU:O	1:A:649:ILE:HD12	1.92	0.69
1:A:497:LYS:HE2	1:A:499:GLU:OE1	1.92	0.69
1:C:628:LYS:HA	3:C:3295:HOH:O	1.93	0.69
1:D:694:PHE:O	1:D:698:VAL:HG23	1.92	0.69
1:B:497:LYS:O	1:B:499:GLU:N	2.26	0.69
1:D:543:ARG:NH2	1:D:564:ASN:HB3	2.07	0.69
1:D:539:LYS:HE2	1:D:564:ASN:ND2	2.05	0.68
1:B:652:TYR:CE1	1:B:686:GLU:HG3	2.28	0.68
1:C:629:GLU:O	1:C:630:GLU:HB2	1.93	0.68
1:D:497:LYS:HE3	3:D:3244:HOH:O	1.94	0.68
1:D:631:LYS:HA	1:D:631:LYS:CE	2.23	0.68
1:C:685:PRO:HD2	1:C:769:PHE:CE2	2.29	0.67
1:A:594:HIS:CD2	3:A:3511:HOH:O	2.47	0.67
1:D:545:ARG:HH21	1:D:620:LYS:C	2.02	0.67
1:C:628:LYS:NZ	1:C:631:LYS:HD3	2.10	0.66
1:A:653:TYR:OH	1:A:697:LYS:NZ	2.29	0.66
1:A:574:MET:HE2	1:A:753:MET:HE3	1.78	0.66
1:D:752:GLU:HA	1:D:755:LYS:HE2	1.77	0.65
1:B:696:PHE:HE2	1:B:700:GLU:OE1	1.80	0.65
1:B:502:GLU:O	1:B:505:LYS:HB3	1.96	0.65
1:C:605:ARG:HG3	1:C:708:HIS:CE1	2.32	0.65
1:D:629:GLU:HG2	1:D:630:GLU:H	1.60	0.65
1:D:584:THR:O	1:D:714:HIS:HB2	1.97	0.65
1:C:523:ILE:HD11	1:C:747:LYS:HD2	1.77	0.65
1:B:528:SER:OG	1:B:755:LYS:HD2	1.97	0.65
1:B:629:GLU:C	1:B:631:LYS:H	2.05	0.65
1:C:525:HIS:O	3:C:3160:HOH:O	2.15	0.64
1:C:626:PRO:HB2	1:C:644:LEU:HB2	1.79	0.64
1:A:515:SER:HB3	3:A:3361:HOH:O	1.96	0.64
1:A:666:GLN:HG2	3:A:3434:HOH:O	1.96	0.64
1:B:500:PHE:HA	1:B:503:MET:HE3	1.80	0.64
1:D:647:GLU:OE1	1:D:649:ILE:HD11	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:TRP:CE2	1:C:721:ARG:HG2	2.32	0.63
1:D:499:GLU:HB3	1:D:742:SER:OG	1.98	0.63
1:B:696:PHE:CE2	1:B:700:GLU:OE1	2.51	0.63
1:A:645:ILE:HD11	1:A:659:GLU:HB2	1.80	0.63
1:C:533:ARG:HD3	3:D:3483:HOH:O	1.97	0.63
1:A:688:PRO:HG3	1:A:769:PHE:HE1	1.63	0.62
1:D:534:VAL:HG21	3:D:3456:HOH:O	1.98	0.62
1:A:627:GLN:N	1:A:631:LYS:HD3	2.14	0.62
1:D:500:PHE:HA	1:D:503:MET:HG2	1.80	0.62
1:A:545:ARG:HG2	1:A:546:TYR:CE1	2.35	0.62
1:A:679:TRP:CE2	1:A:721:ARG:HG2	2.34	0.62
1:D:626:PRO:HB2	1:D:644:LEU:HB2	1.82	0.62
1:A:588:LEU:HB2	1:A:591:THR:HB	1.80	0.62
1:A:575:GLU:OE2	1:A:575:GLU:N	2.26	0.62
1:C:501:MET:HA	1:C:504:GLU:OE2	1.99	0.62
1:A:742:SER:HB2	3:A:3443:HOH:O	2.00	0.62
1:C:523:ILE:CD1	1:C:747:LYS:HD2	2.29	0.62
1:A:503:MET:HE2	1:A:742:SER:HA	1.82	0.61
1:C:521:GLN:HG3	1:C:524:ARG:NH2	2.15	0.61
1:D:545:ARG:HD3	1:D:546:TYR:CE1	2.34	0.61
1:A:573:LYS:HE2	3:A:3069:HOH:O	2.00	0.61
1:C:537:LEU:HD12	3:C:3226:HOH:O	2.00	0.61
1:B:497:LYS:O	1:B:782:MET:CE	2.48	0.61
1:D:679:TRP:CE2	1:D:721:ARG:HG2	2.36	0.61
1:A:615:GLU:HB2	1:A:620:LYS:CG	2.30	0.61
1:C:545:ARG:HH11	1:C:545:ARG:HG3	1.65	0.61
1:B:509:GLN:HE21	1:B:509:GLN:HA	1.66	0.60
1:A:509:GLN:HA	1:A:509:GLN:HE21	1.67	0.60
1:C:588:LEU:HB2	1:C:591:THR:HB	1.82	0.60
1:D:499:GLU:HG2	1:D:740:ASP:OD1	2.01	0.60
1:D:557:ILE:HD11	1:D:571:LEU:HB2	1.83	0.60
1:A:600:TRP:HE1	1:C:562:GLU:CD	2.09	0.60
1:D:666:GLN:NE2	3:D:3415:HOH:O	2.33	0.60
1:A:615:GLU:HB2	1:A:620:LYS:HG3	1.83	0.59
1:D:626:PRO:HB3	1:D:631:LYS:HB3	1.83	0.59
1:B:547:ARG:HB3	1:B:547:ARG:CZ	2.32	0.59
1:B:629:GLU:O	1:B:631:LYS:N	2.35	0.59
1:C:509:GLN:HE21	1:C:509:GLN:HA	1.67	0.59
1:D:628:LYS:HG2	1:D:631:LYS:HD2	1.85	0.59
1:D:544:ASN:OD1	1:D:566:TYR:OH	2.17	0.59
1:D:507:PHE:HD2	1:D:771:TYR:CD2	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:LEU:H	1:B:498:LEU:CD1	2.06	0.59
1:C:502:GLU:HG3	1:C:503:MET:N	2.17	0.59
1:B:752:GLU:HB2	3:B:3420:HOH:O	2.03	0.59
1:C:630:GLU:C	1:C:632:GLU:H	2.10	0.59
1:C:503:MET:O	1:C:507:PHE:N	2.27	0.58
1:C:629:GLU:OE1	1:C:646:SER:HA	2.03	0.58
1:A:685:PRO:HD2	1:A:769:PHE:CE2	2.36	0.58
1:D:499:GLU:O	1:D:502:GLU:HB3	2.03	0.58
1:C:538:PRO:HD3	3:C:3265:HOH:O	2.03	0.58
1:D:507:PHE:HD2	1:D:771:TYR:HD2	1.50	0.58
1:D:751:LEU:HD12	3:D:3234:HOH:O	2.03	0.58
1:B:498:LEU:C	1:B:500:PHE:H	2.11	0.58
1:B:707:GLU:OE2	1:C:708:HIS:NE2	2.36	0.58
1:B:499:GLU:HG2	1:B:502:GLU:OE2	2.04	0.57
1:C:670:GLU:HG3	3:C:3293:HOH:O	2.04	0.57
1:B:498:LEU:HD12	1:B:498:LEU:N	2.11	0.57
1:A:746:ILE:HB	1:A:771:TYR:CZ	2.40	0.57
1:B:562:GLU:N	3:B:3365:HOH:O	2.38	0.57
1:C:628:LYS:HB2	1:C:628:LYS:HZ3	1.68	0.57
1:A:628:LYS:O	1:A:629:GLU:HB2	2.04	0.57
1:B:679:TRP:CE2	1:B:721:ARG:HG2	2.39	0.57
1:D:498:LEU:C	1:D:500:PHE:H	2.10	0.57
1:B:533:ARG:HG3	1:B:533:ARG:NH1	2.19	0.57
1:A:618:SER:HB3	2:A:802:BGD:H15	1.87	0.56
1:A:690:SER:HB2	3:A:3009:HOH:O	2.05	0.56
1:C:657:GLN:NE2	1:C:670:GLU:OE2	2.39	0.56
1:A:561:GLN:NE2	3:A:3511:HOH:O	2.38	0.56
1:D:542:ASN:HD22	1:D:542:ASN:H	1.53	0.56
1:A:573:LYS:NZ	3:A:3424:HOH:O	2.37	0.56
1:B:547:ARG:CZ	1:B:547:ARG:CB	2.83	0.56
1:D:500:PHE:O	1:D:504:GLU:HG3	2.06	0.56
1:A:533:ARG:HG3	1:A:533:ARG:NH1	2.20	0.56
1:D:629:GLU:HG2	1:D:630:GLU:N	2.20	0.55
1:D:752:GLU:HB2	3:D:3249:HOH:O	2.06	0.55
1:A:633:MET:HE3	1:A:635:PHE:CZ	2.41	0.55
1:D:628:LYS:O	1:D:631:LYS:HB2	2.06	0.55
1:B:615:GLU:HB2	1:B:620:LYS:HG3	1.88	0.55
1:A:688:PRO:HG3	1:A:769:PHE:CE1	2.41	0.55
1:D:685:PRO:HD2	1:D:769:PHE:CZ	2.41	0.55
1:B:546:TYR:CD2	2:B:803:BGD:H382	2.41	0.55
1:A:736:ASP:OD2	1:D:697:LYS:NZ	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:603:LYS:HB3	1:C:605:ARG:HH12	1.70	0.55
1:D:661:GLU:HB2	1:D:668:THR:HG22	1.88	0.55
1:A:576:GLU:HG2	1:A:734:LEU:CD2	2.37	0.55
1:D:500:PHE:C	1:D:502:GLU:N	2.62	0.55
1:A:576:GLU:HG2	1:A:734:LEU:HD21	1.89	0.55
1:D:545:ARG:NH2	1:D:620:LYS:C	2.65	0.54
1:D:565:ASP:CG	1:D:565:ASP:O	2.50	0.54
1:D:497:LYS:HB2	1:D:499:GLU:OE1	2.07	0.54
1:D:498:LEU:C	1:D:500:PHE:N	2.63	0.54
1:D:647:GLU:HG3	1:D:656:ARG:HG2	1.89	0.54
1:B:708:HIS:HE2	1:C:707:GLU:CD	2.14	0.54
1:D:576:GLU:HG2	1:D:734:LEU:HD21	1.89	0.54
1:A:497:LYS:HD2	1:A:498:LEU:H	1.73	0.54
1:B:546:TYR:CZ	2:B:803:BGD:H42	2.43	0.54
1:C:503:MET:O	1:C:504:GLU:C	2.50	0.54
1:D:735:MET:HE2	1:D:741:PRO:O	2.08	0.53
1:A:720:GLY:HA3	3:A:3068:HOH:O	2.06	0.53
1:C:549:VAL:HG21	1:C:717:ALA:HB1	1.90	0.53
1:D:545:ARG:NE	1:D:620:LYS:O	2.40	0.53
1:B:628:LYS:O	1:B:631:LYS:HB3	2.09	0.53
1:C:548:ASP:OD1	2:C:804:BGD:H381	2.08	0.53
1:C:603:LYS:O	1:C:605:ARG:NH1	2.41	0.53
1:D:576:GLU:HG2	1:D:734:LEU:CD2	2.38	0.53
1:C:545:ARG:HG3	1:C:545:ARG:NH1	2.23	0.53
1:C:630:GLU:C	1:C:632:GLU:N	2.65	0.53
1:B:591:THR:O	1:B:591:THR:CG2	2.56	0.53
1:A:497:LYS:HB3	1:A:499:GLU:OE1	2.09	0.53
1:D:542:ASN:HD22	1:D:542:ASN:N	2.04	0.53
1:B:705:SER:OG	1:B:707:GLU:HG2	2.08	0.53
1:D:645:ILE:HG22	1:D:646:SER:N	2.23	0.52
1:C:573:LYS:HD3	3:C:3027:HOH:O	2.09	0.52
1:A:547:ARG:HG2	1:A:547:ARG:HH11	1.73	0.52
1:A:521:GLN:NE2	1:A:524:ARG:HD3	2.24	0.52
1:C:519:ILE:HA	1:C:522:ASP:OD2	2.10	0.52
1:A:594:HIS:HD2	3:A:3511:HOH:O	1.85	0.52
1:A:619:LEU:HD22	3:A:3063:HOH:O	2.09	0.52
1:B:500:PHE:CE1	1:B:775:ILE:O	2.62	0.52
1:C:630:GLU:H	1:C:644:LEU:HB3	1.74	0.52
1:A:547:ARG:HG2	1:A:547:ARG:NH1	2.25	0.52
1:D:575:GLU:O	1:D:578:GLN:N	2.42	0.52
1:A:584:THR:O	1:A:714:HIS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ARG:HG3	2:A:802:BGD:O2	2.10	0.51
1:C:618:SER:OG	2:C:804:BGD:H15	2.11	0.51
1:D:560:HIS:HB2	1:D:601:GLU:OE2	2.10	0.51
1:B:731:CYS:O	1:B:735:MET:HG3	2.09	0.51
1:C:684:VAL:HG23	3:C:3191:HOH:O	2.10	0.51
1:C:746:ILE:HB	1:C:771:TYR:CZ	2.46	0.51
1:A:619:LEU:O	2:A:802:BGD:H13	2.11	0.51
1:A:633:MET:O	1:A:634:ILE:HG13	2.11	0.51
1:B:500:PHE:HE1	1:B:775:ILE:O	1.93	0.51
1:C:548:ASP:OD2	2:C:804:BGD:H19	2.11	0.51
1:A:783:GLY:HA2	1:D:693:ASN:CG	2.35	0.50
1:D:545:ARG:HD3	1:D:546:TYR:HE1	1.74	0.50
1:C:611:ASN:HD21	1:C:621:CYS:HB2	1.75	0.50
1:C:628:LYS:NZ	1:C:628:LYS:CB	2.63	0.50
1:B:557:ILE:HD11	1:B:571:LEU:HB2	1.93	0.50
1:B:588:LEU:HB2	1:B:591:THR:HB	1.94	0.50
1:B:781:ILE:C	1:B:783:GLY:H	2.19	0.50
1:A:547:ARG:HD2	2:A:802:BGD:H41A	1.94	0.50
1:A:520:TYR:O	1:A:524:ARG:HG3	2.10	0.50
1:B:630:GLU:OE2	1:B:630:GLU:HA	2.12	0.50
1:C:715:CYS:SG	1:C:718:GLY:HA2	2.52	0.50
1:C:704:LEU:HB2	3:C:3173:HOH:O	2.11	0.50
1:C:503:MET:C	1:C:505:LYS:N	2.62	0.50
1:B:735:MET:HE2	1:B:741:PRO:O	2.11	0.50
1:D:542:ASN:H	1:D:542:ASN:ND2	2.09	0.50
1:C:502:GLU:HG3	1:C:503:MET:H	1.77	0.50
1:D:563:ASP:OD1	1:D:564:ASN:N	2.45	0.49
1:D:567:ILE:HA	3:D:3235:HOH:O	2.11	0.49
1:A:592:CYS:N	3:A:3070:HOH:O	2.45	0.49
1:B:509:GLN:HA	1:B:509:GLN:NE2	2.28	0.49
1:B:649:ILE:HG12	1:B:654:THR:OG1	2.12	0.49
1:C:738:ARG:NH1	1:C:744:VAL:HA	2.25	0.49
1:D:505:LYS:O	1:D:508:GLU:HB3	2.13	0.49
1:C:545:ARG:HD2	1:C:716:SER:O	2.12	0.49
1:D:533:ARG:HH11	1:D:533:ARG:CG	2.25	0.49
1:D:628:LYS:CG	1:D:631:LYS:HD2	2.42	0.49
1:D:502:GLU:O	1:D:505:LYS:N	2.46	0.49
1:D:575:GLU:O	1:D:576:GLU:C	2.55	0.49
1:C:509:GLN:HA	1:C:509:GLN:NE2	2.28	0.49
1:D:498:LEU:O	1:D:498:LEU:CD1	2.52	0.49
1:B:644:LEU:HA	1:B:658:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:SER:C	1:A:744:VAL:H	2.21	0.49
1:C:542:ASN:N	1:C:542:ASN:HD22	2.11	0.49
1:D:752:GLU:O	1:D:755:LYS:HB2	2.12	0.49
1:B:576:GLU:HG2	1:B:734:LEU:CD2	2.43	0.49
1:D:508:GLU:OE1	1:D:512:LYS:HG3	2.12	0.48
1:A:542:ASN:N	1:A:542:ASN:HD22	2.11	0.48
1:A:633:MET:HE2	1:A:642:LEU:HD23	1.94	0.48
1:A:741:PRO:O	1:A:744:VAL:HG23	2.12	0.48
1:C:584:THR:O	1:C:714:HIS:HB2	2.14	0.48
1:D:770:SER:O	1:D:771:TYR:C	2.55	0.48
1:A:547:ARG:HD3	2:A:802:BGD:O34	2.12	0.48
1:B:629:GLU:C	1:B:631:LYS:N	2.72	0.48
1:C:631:LYS:O	1:C:632:GLU:O	2.31	0.48
1:D:715:CYS:SG	1:D:718:GLY:HA2	2.53	0.48
1:A:635:PHE:HA	3:A:3046:HOH:O	2.12	0.48
3:B:3334:HOH:O	1:C:699:ARG:HG2	2.11	0.48
1:C:523:ILE:HD11	1:C:747:LYS:CD	2.43	0.48
1:A:633:MET:CE	1:A:642:LEU:HD23	2.44	0.48
1:B:542:ASN:N	1:B:542:ASN:HD22	2.11	0.48
1:D:612:ARG:HG2	3:D:3451:HOH:O	2.13	0.48
1:A:653:TYR:CD1	1:A:653:TYR:C	2.92	0.48
1:B:620:LYS:NZ	3:B:3316:HOH:O	2.43	0.48
1:C:513:SER:O	1:C:514:GLY:C	2.57	0.48
1:C:591:THR:O	1:C:591:THR:CG2	2.61	0.48
1:A:557:ILE:HD11	1:A:571:LEU:HB2	1.94	0.48
1:A:657:GLN:NE2	1:A:670:GLU:OE2	2.46	0.48
1:C:557:ILE:HD11	1:C:571:LEU:HB2	1.96	0.48
1:C:684:VAL:CG2	3:C:3191:HOH:O	2.62	0.48
1:D:691:PHE:O	1:D:694:PHE:HB3	2.14	0.48
1:C:533:ARG:HG3	1:C:533:ARG:NH1	2.21	0.47
1:D:652:TYR:CD2	1:D:690:SER:HB2	2.49	0.47
1:A:691:PHE:O	1:A:694:PHE:HB3	2.14	0.47
1:C:628:LYS:O	1:C:631:LYS:N	2.47	0.47
1:D:500:PHE:O	1:D:501:MET:C	2.57	0.47
1:C:530:PHE:HB3	1:C:531:PRO:HD2	1.96	0.47
1:A:509:GLN:HA	1:A:509:GLN:NE2	2.28	0.47
1:A:615:GLU:HB2	1:A:620:LYS:HG2	1.96	0.47
1:A:781:ILE:C	1:A:783:GLY:H	2.22	0.47
1:B:499:GLU:CB	1:B:502:GLU:OE2	2.62	0.47
1:C:533:ARG:HH11	1:C:533:ARG:CG	2.23	0.47
1:C:502:GLU:CD	1:C:742:SER:HB3	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:546:TYR:CD2	2:D:805:BGD:H382	2.50	0.47
1:B:519:ILE:HA	1:B:522:ASP:OD2	2.14	0.47
1:C:650:LYS:HE2	3:C:3472:HOH:O	2.13	0.47
1:C:666:GLN:NE2	3:C:3353:HOH:O	2.47	0.47
1:C:519:ILE:O	1:C:523:ILE:HD12	2.14	0.47
1:D:547:ARG:HA	3:D:3367:HOH:O	2.14	0.47
1:B:732:LEU:HD23	1:B:732:LEU:HA	1.80	0.46
1:A:775:ILE:O	1:A:778:ALA:HB3	2.16	0.46
1:B:707:GLU:CD	1:C:708:HIS:CE1	2.93	0.46
1:D:645:ILE:HD11	1:D:659:GLU:HB2	1.96	0.46
1:B:576:GLU:HG2	1:B:734:LEU:HD21	1.97	0.46
1:D:615:GLU:HB2	1:D:620:LYS:CG	2.43	0.46
1:D:760:LEU:O	1:D:761:ILE:HB	2.16	0.46
1:B:670:GLU:HG3	3:B:3141:HOH:O	2.15	0.46
1:D:550:SER:O	1:D:758:MET:HE3	2.15	0.46
1:C:546:TYR:CG	2:C:804:BGD:H382	2.51	0.46
1:C:702:GLY:O	1:C:705:SER:HB3	2.16	0.46
1:C:781:ILE:C	1:C:783:GLY:H	2.23	0.46
1:B:591:THR:O	1:B:591:THR:HG23	2.16	0.46
1:C:517:ALA:O	1:C:521:GLN:NE2	2.49	0.46
1:D:547:ARG:HD2	2:D:805:BGD:H27	1.98	0.46
1:B:508:GLU:OE1	1:B:508:GLU:HA	2.16	0.45
1:C:775:ILE:O	1:C:778:ALA:HB3	2.16	0.45
1:D:503:MET:O	1:D:775:ILE:HD11	2.16	0.45
1:A:497:LYS:N	1:A:782:MET:HE2	2.31	0.45
1:C:606:GLY:O	1:C:711:VAL:HG23	2.17	0.45
1:D:781:ILE:C	1:D:783:GLY:H	2.24	0.45
1:C:631:LYS:HD2	1:C:631:LYS:HA	1.52	0.45
1:B:735:MET:HG2	1:B:744:VAL:HG21	1.98	0.45
1:C:526:GLU:O	3:C:3470:HOH:O	2.21	0.45
1:B:665:THR:O	1:B:666:GLN:HB2	2.15	0.45
1:C:665:THR:C	3:C:3292:HOH:O	2.59	0.45
1:D:505:LYS:HG3	3:D:3271:HOH:O	2.17	0.45
1:D:628:LYS:HG3	1:D:631:LYS:HB2	1.99	0.45
1:C:539:LYS:HE3	3:C:3294:HOH:O	2.17	0.45
1:C:735:MET:HE2	1:C:741:PRO:O	2.17	0.45
1:D:520:TYR:CE2	1:D:524:ARG:HD3	2.52	0.45
1:C:547:ARG:HE	1:C:547:ARG:HB3	1.58	0.45
1:C:647:GLU:HB3	3:C:3207:HOH:O	2.17	0.45
1:C:760:LEU:O	1:C:761:ILE:HB	2.17	0.45
1:D:657:GLN:NE2	1:D:670:GLU:OE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:GLU:HB2	1:A:668:THR:HG22	1.99	0.45
1:C:576:GLU:HG2	1:C:734:LEU:HD21	1.99	0.45
1:D:774:VAL:O	1:D:778:ALA:HB2	2.17	0.45
1:A:742:SER:C	1:A:744:VAL:N	2.75	0.44
1:B:499:GLU:CG	1:B:502:GLU:OE2	2.65	0.44
1:A:503:MET:HE1	1:A:741:PRO:HB2	2.00	0.44
1:C:685:PRO:HD2	1:C:769:PHE:CD2	2.52	0.44
1:D:661:GLU:HB2	1:D:668:THR:CG2	2.48	0.44
1:C:526:GLU:C	3:C:3160:HOH:O	2.59	0.44
1:D:746:ILE:HG13	1:D:771:TYR:CD1	2.52	0.44
1:A:616:LYS:C	1:A:618:SER:H	2.26	0.44
1:C:591:THR:O	1:C:591:THR:HG23	2.17	0.44
1:A:633:MET:HE3	1:A:635:PHE:HZ	1.82	0.44
1:B:685:PRO:HD2	1:B:769:PHE:CE1	2.52	0.44
1:C:661:GLU:HG3	1:C:668:THR:HG23	1.99	0.44
1:C:746:ILE:HG13	1:C:771:TYR:CE2	2.53	0.44
1:B:579:ARG:CZ	1:B:733:LEU:HD11	2.48	0.44
1:D:613:VAL:HG12	1:D:621:CYS:C	2.42	0.44
1:B:774:VAL:O	1:B:778:ALA:HB2	2.18	0.43
1:D:692:LEU:O	1:D:693:ASN:C	2.61	0.43
1:D:544:ASN:OD1	1:D:568:ASN:ND2	2.45	0.43
1:A:648:ASP:OD2	1:A:650:LYS:NZ	2.49	0.43
1:C:730:THR:O	1:C:733:LEU:HB2	2.18	0.43
1:D:502:GLU:O	1:D:505:LYS:HB3	2.17	0.43
1:D:646:SER:H	1:D:657:GLN:HB3	1.82	0.43
1:D:681:ASP:HA	1:D:721:ARG:CZ	2.48	0.43
1:D:685:PRO:HD2	1:D:769:PHE:CE2	2.54	0.43
1:C:775:ILE:HG22	1:C:776:GLU:N	2.33	0.43
1:D:731:CYS:O	1:D:735:MET:HG3	2.18	0.43
1:A:648:ASP:OD2	1:A:650:LYS:HE2	2.18	0.43
1:A:681:ASP:O	1:A:682:PHE:HB2	2.18	0.43
1:B:697:LYS:HE2	3:B:3386:HOH:O	2.18	0.43
1:B:528:SER:HB3	1:B:530:PHE:CE1	2.53	0.43
1:B:650:LYS:HD2	1:B:653:TYR:CE1	2.54	0.43
1:C:738:ARG:HH11	1:C:744:VAL:HA	1.84	0.43
1:A:742:SER:O	1:A:744:VAL:N	2.52	0.43
1:B:499:GLU:CD	1:B:741:PRO:HD2	2.44	0.43
1:B:549:VAL:HG21	1:B:717:ALA:HB1	2.01	0.43
1:A:523:ILE:HG13	1:A:747:LYS:HD2	2.01	0.43
1:A:614:MET:HE3	1:A:614:MET:HB3	1.97	0.43
1:C:502:GLU:CG	1:C:503:MET:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:MET:HE2	1:A:742:SER:CA	2.49	0.43
1:B:499:GLU:OE1	1:B:740:ASP:OD1	2.37	0.43
1:C:507:PHE:CE2	1:C:516:TRP:HZ2	2.36	0.43
1:D:611:ASN:HD21	1:D:621:CYS:HB2	1.84	0.43
1:A:647:GLU:HG2	1:A:649:ILE:HD11	2.01	0.42
1:B:584:THR:O	1:B:714:HIS:HB2	2.19	0.42
1:B:691:PHE:O	1:B:694:PHE:HB3	2.19	0.42
1:A:575:GLU:H	1:A:575:GLU:CD	2.23	0.42
1:B:657:GLN:NE2	1:B:670:GLU:OE2	2.52	0.42
1:C:542:ASN:HD22	1:C:542:ASN:H	1.66	0.42
1:D:699:ARG:HA	1:D:704:LEU:HD12	2.01	0.42
1:A:547:ARG:HD2	2:A:802:BGD:C4	2.48	0.42
1:A:626:PRO:HB3	1:A:631:LYS:HB3	2.01	0.42
1:A:696:PHE:N	1:A:696:PHE:CD1	2.87	0.42
1:B:611:ASN:HD21	1:B:621:CYS:HB2	1.85	0.42
1:C:576:GLU:HG2	1:C:734:LEU:CD2	2.49	0.42
1:A:783:GLY:HA2	1:D:693:ASN:OD1	2.19	0.42
1:B:543:ARG:HD3	3:B:3096:HOH:O	2.19	0.42
1:C:508:GLU:OE1	1:C:508:GLU:HA	2.15	0.42
1:C:603:LYS:C	1:C:605:ARG:NH1	2.77	0.42
1:C:720:GLY:N	2:C:804:BGD:O50	2.40	0.42
1:D:574:MET:HE2	1:D:753:MET:HE3	2.01	0.42
1:D:752:GLU:HA	1:D:755:LYS:CE	2.46	0.42
1:A:627:GLN:H	1:A:631:LYS:CD	2.23	0.42
1:B:536:LYS:HA	1:B:536:LYS:HD3	1.84	0.42
1:B:760:LEU:O	1:B:761:ILE:HB	2.19	0.42
1:D:628:LYS:NZ	1:D:631:LYS:HD2	2.34	0.42
1:A:592:CYS:HB2	3:A:3070:HOH:O	2.18	0.42
1:B:676:TYR:CD2	1:B:679:TRP:HB2	2.55	0.42
1:C:533:ARG:NH1	1:C:533:ARG:CG	2.81	0.42
1:C:615:GLU:HB2	1:C:620:LYS:CG	2.44	0.42
1:C:740:ASP:HA	1:C:741:PRO:HD2	1.87	0.42
1:D:533:ARG:HG3	1:D:533:ARG:NH1	2.27	0.42
1:A:730:THR:O	1:A:733:LEU:HB2	2.20	0.42
1:B:498:LEU:C	1:B:500:PHE:N	2.75	0.42
1:A:533:ARG:NH1	1:A:533:ARG:CG	2.80	0.42
1:A:575:GLU:O	1:A:576:GLU:C	2.62	0.42
1:C:499:GLU:C	1:C:501:MET:N	2.76	0.42
1:C:539:LYS:H	1:C:539:LYS:HG2	1.64	0.42
1:C:499:GLU:C	1:C:501:MET:H	2.28	0.42
1:D:500:PHE:O	1:D:502:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:775:ILE:HG22	1:D:776:GLU:N	2.34	0.42
1:A:760:LEU:O	1:A:761:ILE:HB	2.19	0.41
1:B:614:MET:HE2	1:B:617:GLY:O	2.20	0.41
1:B:649:ILE:HG12	1:B:654:THR:CG2	2.49	0.41
1:D:502:GLU:C	1:D:504:GLU:H	2.26	0.41
1:D:778:ALA:O	1:D:782:MET:HG2	2.20	0.41
1:A:542:ASN:C	1:A:542:ASN:ND2	2.78	0.41
1:A:652:TYR:HA	1:A:678:THR:HG23	2.01	0.41
1:B:781:ILE:C	1:B:783:GLY:N	2.78	0.41
1:C:661:GLU:HB2	1:C:668:THR:HG22	2.01	0.41
1:A:629:GLU:HA	1:A:644:LEU:HD23	2.02	0.41
1:A:661:GLU:HG3	1:A:668:THR:HG23	2.01	0.41
1:D:609:MET:HG3	1:D:714:HIS:CE1	2.54	0.41
1:B:513:SER:O	1:B:514:GLY:C	2.63	0.41
1:C:609:MET:HG3	1:C:714:HIS:CE1	2.56	0.41
1:A:626:PRO:HA	1:A:631:LYS:HD3	2.02	0.41
1:C:536:LYS:HA	1:C:536:LYS:HD3	1.84	0.41
1:D:545:ARG:NH1	1:D:545:ARG:HG3	2.34	0.41
1:A:513:SER:O	1:A:514:GLY:C	2.64	0.41
1:A:542:ASN:HD22	1:A:542:ASN:H	1.67	0.41
1:A:692:LEU:O	1:A:696:PHE:CD1	2.73	0.41
1:A:530:PHE:HB3	1:A:531:PRO:HD2	2.01	0.41
1:A:647:GLU:HG2	1:A:649:ILE:CD1	2.51	0.41
1:D:661:GLU:HG3	1:D:668:THR:HG23	2.03	0.41
1:D:775:ILE:O	1:D:778:ALA:HB3	2.20	0.41
1:A:633:MET:CE	1:A:635:PHE:HZ	2.34	0.41
1:B:542:ASN:C	1:B:542:ASN:ND2	2.79	0.41
1:C:515:SER:O	1:C:519:ILE:HG13	2.20	0.41
1:D:533:ARG:CG	1:D:533:ARG:NH1	2.82	0.41
1:D:547:ARG:HH21	2:D:805:BGD:C5	2.34	0.41
1:A:515:SER:O	1:A:519:ILE:HG13	2.21	0.41
1:A:528:SER:HB3	1:A:530:PHE:CE1	2.56	0.41
1:C:574:MET:HE2	1:C:753:MET:CE	2.44	0.41
1:C:679:TRP:NE1	1:C:721:ARG:HG2	2.35	0.41
1:D:530:PHE:HB3	1:D:531:PRO:HD2	2.02	0.41
1:D:628:LYS:O	1:D:628:LYS:HG3	2.21	0.41
1:D:628:LYS:CD	1:D:631:LYS:HD2	2.51	0.41
1:B:626:PRO:HB2	1:B:644:LEU:HB2	2.03	0.40
1:A:536:LYS:HA	1:A:536:LYS:HD3	1.85	0.40
1:A:679:TRP:NE1	1:A:721:ARG:HG2	2.37	0.40
1:B:619:LEU:HD12	1:B:619:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:PHE:C	1:C:502:GLU:H	2.27	0.40
1:D:646:SER:OG	1:D:657:GLN:HB2	2.22	0.40
1:A:575:GLU:O	1:A:578:GLN:N	2.54	0.40
1:A:652:TYR:HA	1:A:678:THR:CG2	2.51	0.40
1:A:685:PRO:HD2	1:A:769:PHE:CD2	2.56	0.40
1:B:542:ASN:HD22	1:B:542:ASN:H	1.69	0.40
1:B:715:CYS:SG	1:B:718:GLY:HA2	2.60	0.40
1:B:719:ILE:HG13	1:B:720:GLY:N	2.37	0.40
1:C:537:LEU:N	1:C:537:LEU:CD1	2.85	0.40
1:C:735:MET:HG2	1:C:744:VAL:HG21	2.03	0.40
1:A:715:CYS:SG	1:A:718:GLY:HA2	2.61	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	285/295 (97%)	255 (90%)	27 (10%)	3 (1%)	11	22
1	B	285/295 (97%)	262 (92%)	18 (6%)	5 (2%)	6	12
1	C	285/295 (97%)	260 (91%)	21 (7%)	4 (1%)	9	17
1	D	285/295 (97%)	252 (88%)	28 (10%)	5 (2%)	6	12
All	All	1140/1180 (97%)	1029 (90%)	94 (8%)	17 (2%)	8	16

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	629	GLU
1	B	629	GLU
1	C	632	GLU
1	C	651	SER

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Mol	Chain	Res	Type
1	D	575	GLU
1	A	743	SER
1	B	498	LEU
1	B	630	GLU
1	B	575	GLU
1	C	761	ILE
1	D	563	ASP
1	D	647	GLU
1	D	761	ILE
1	A	761	ILE
1	B	761	ILE
1	C	630	GLU
1	D	503	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/268 (96%)	241 (94%)	16 (6%)	16	34
1	B	257/268 (96%)	239 (93%)	18 (7%)	14	29
1	C	254/268 (95%)	233 (92%)	21 (8%)	10	22
1	D	258/268 (96%)	244 (95%)	14 (5%)	20	41
All	All	1026/1072 (96%)	957 (93%)	69 (7%)	15	31

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	497	LYS
1	A	508	GLU
1	A	511	ASP
1	A	522	ASP
1	A	537	LEU
1	A	542	ASN
1	A	589	PRO
1	A	591	THR

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Mol	Chain	Res	Type
1	A	613	VAL
1	A	614	MET
1	A	619	LEU
1	A	636	GLU
1	A	668	THR
1	A	715	CYS
1	A	735	MET
1	A	775	ILE
1	B	508	GLU
1	B	511	ASP
1	B	521	GLN
1	B	537	LEU
1	B	542	ASN
1	B	547	ARG
1	B	591	THR
1	B	612	ARG
1	B	613	VAL
1	B	628	LYS
1	B	630	GLU
1	B	632	GLU
1	B	633	MET
1	B	636	GLU
1	B	668	THR
1	B	715	CYS
1	B	735	MET
1	B	775	ILE
1	C	502	GLU
1	C	503	MET
1	C	508	GLU
1	C	511	ASP
1	C	521	GLN
1	C	522	ASP
1	C	524	ARG
1	C	537	LEU
1	C	542	ASN
1	C	548	ASP
1	C	591	THR
1	C	628	LYS
1	C	630	GLU
1	C	636	GLU
1	C	651	SER
1	C	668	THR

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Mol	Chain	Res	Type
1	C	700	GLU
1	C	715	CYS
1	C	742	SER
1	C	772	LEU
1	C	775	ILE
1	D	511	ASP
1	D	523	ILE
1	D	537	LEU
1	D	542	ASN
1	D	561	GLN
1	D	591	THR
1	D	613	VAL
1	D	614	MET
1	D	619	LEU
1	D	631	LYS
1	D	636	GLU
1	D	668	THR
1	D	735	MET
1	D	775	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	GLN
1	A	521	GLN
1	A	542	ASN
1	A	561	GLN
1	A	578	GLN
1	A	594	HIS
1	A	693	ASN
1	B	509	GLN
1	B	542	ASN
1	B	560	HIS
1	B	611	ASN
1	B	627	GLN
1	B	657	GLN
1	B	666	GLN
1	B	693	ASN
1	B	762	GLN
1	C	509	GLN
1	C	542	ASN
1	C	560	HIS

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Mol	Chain	Res	Type
1	C	578	GLN
1	C	657	GLN
1	C	666	GLN
1	C	693	ASN
1	D	509	GLN
1	D	540	ASN
1	D	542	ASN
1	D	560	HIS
1	D	561	GLN
1	D	564	ASN
1	D	594	HIS
1	D	657	GLN
1	D	666	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGD	A	802	-	54,56,56	3.43	30 (55%)	73,83,83	1.22	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGD	D	805	-	54,56,56	3.29	27 (50%)	73,83,83	1.37	11 (15%)
2	BGD	C	804	-	54,56,56	3.27	30 (55%)	73,83,83	1.13	5 (6%)
2	BGD	B	803	-	54,56,56	3.29	28 (51%)	73,83,83	1.48	15 (20%)

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
2	BGD	A	802	-	-	6/61/71/71	0/3/3/3
2	BGD	D	805	-	-	12/61/71/71	0/3/3/3
2	BGD	C	804	-	-	9/61/71/71	0/3/3/3
2	BGD	B	803	-	-	4/61/71/71	0/3/3/3

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	803	BGD	C11-C10	7.04	1.50	1.39
2	A	802	BGD	C11-C10	6.95	1.50	1.39
2	B	803	BGD	C27-C28	6.76	1.50	1.39
2	D	805	BGD	C11-C10	6.55	1.49	1.39
2	A	802	BGD	C27-C28	6.46	1.50	1.39
2	D	805	BGD	C12-C10	6.16	1.48	1.39
2	A	802	BGD	C43-C42	6.11	1.48	1.38
2	D	805	BGD	C43-C42	6.05	1.48	1.38
2	A	802	BGD	C12-C10	6.01	1.48	1.39
2	C	804	BGD	C11-C10	5.98	1.48	1.39
2	A	802	BGD	C41-C44	5.94	1.49	1.39
2	C	804	BGD	C27-C28	5.91	1.49	1.39
2	C	804	BGD	C25-C28	5.91	1.49	1.39
2	B	803	BGD	C43-C44	5.86	1.49	1.39
2	B	803	BGD	C43-C42	5.79	1.48	1.38
2	C	804	BGD	C41-C44	5.72	1.48	1.39
2	D	805	BGD	C43-C44	5.70	1.48	1.39
2	A	802	BGD	C41-C40	5.69	1.48	1.38
2	D	805	BGD	C27-C28	5.62	1.48	1.39
2	B	803	BGD	C27-C26	5.59	1.47	1.38
2	C	804	BGD	C12-C10	5.55	1.47	1.39
2	A	802	BGD	C13-C11	5.49	1.48	1.38
2	D	805	BGD	P32-O33	5.44	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	805	BGD	C25-C28	5.43	1.48	1.39
2	A	802	BGD	C14-C12	5.43	1.48	1.38
2	D	805	BGD	C13-C11	5.28	1.47	1.38
2	C	804	BGD	P32-O33	5.27	1.59	1.50
2	A	802	BGD	P32-O33	5.22	1.58	1.50
2	A	802	BGD	C25-C28	5.20	1.48	1.39
2	B	803	BGD	C25-C28	5.19	1.48	1.39
2	C	804	BGD	C43-C44	5.16	1.47	1.39
2	C	804	BGD	C43-C42	5.10	1.47	1.38
2	B	803	BGD	P32-O33	5.04	1.58	1.50
2	D	805	BGD	C14-C12	5.03	1.47	1.38
2	B	803	BGD	C13-C11	4.94	1.47	1.38
2	B	803	BGD	C25-C24	4.85	1.46	1.38
2	A	802	BGD	C26-C23	4.85	1.48	1.38
2	B	803	BGD	C14-C12	4.78	1.47	1.38
2	B	803	BGD	C12-C10	4.70	1.46	1.39
2	D	805	BGD	C26-C23	4.68	1.48	1.38
2	C	804	BGD	C25-C24	4.64	1.46	1.38
2	C	804	BGD	C13-C11	4.63	1.46	1.38
2	B	803	BGD	C42-C39	4.61	1.48	1.38
2	A	802	BGD	C27-C26	4.61	1.46	1.38
2	C	804	BGD	C41-C40	4.60	1.46	1.38
2	C	804	BGD	C42-C39	4.58	1.48	1.38
2	B	803	BGD	C41-C44	4.58	1.47	1.39
2	D	805	BGD	C41-C44	4.52	1.46	1.39
2	D	805	BGD	C42-C39	4.51	1.47	1.38
2	C	804	BGD	C14-C12	4.51	1.46	1.38
2	C	804	BGD	C27-C26	4.51	1.46	1.38
2	D	805	BGD	C41-C40	4.49	1.46	1.38
2	B	803	BGD	C15-C14	4.42	1.48	1.38
2	C	804	BGD	C24-C23	4.41	1.47	1.38
2	A	802	BGD	C15-C14	4.32	1.47	1.38
2	D	805	BGD	C27-C26	4.32	1.45	1.38
2	D	805	BGD	C15-C14	4.25	1.47	1.38
2	A	802	BGD	C15-C13	4.24	1.47	1.38
2	A	802	BGD	F46-C45	4.21	1.43	1.37
2	D	805	BGD	F31-C29	4.21	1.43	1.37
2	D	805	BGD	C25-C24	4.20	1.45	1.38
2	B	803	BGD	C37-C52	4.18	1.60	1.52
2	B	803	BGD	F46-C45	4.18	1.43	1.37
2	C	804	BGD	C52-N54	-4.17	1.23	1.32
2	C	804	BGD	C26-C23	4.15	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	805	BGD	P48-O49	4.14	1.57	1.50
2	B	803	BGD	C26-C23	4.11	1.47	1.38
2	A	802	BGD	C52-N54	-4.08	1.23	1.32
2	D	805	BGD	C15-C13	4.03	1.47	1.38
2	A	802	BGD	C42-C39	4.03	1.46	1.38
2	B	803	BGD	C24-C23	3.97	1.46	1.38
2	A	802	BGD	C25-C24	3.94	1.45	1.38
2	A	802	BGD	C43-C44	3.94	1.45	1.39
2	B	803	BGD	C15-C13	3.93	1.46	1.38
2	C	804	BGD	C15-C13	3.89	1.46	1.38
2	C	804	BGD	C15-C14	3.88	1.46	1.38
2	A	802	BGD	C24-C23	3.82	1.46	1.38
2	A	802	BGD	F31-C29	3.79	1.42	1.37
2	C	804	BGD	F46-C45	3.76	1.42	1.37
2	C	804	BGD	F30-C29	3.64	1.42	1.37
2	A	802	BGD	C17-N16	3.61	1.53	1.45
2	A	802	BGD	F30-C29	3.58	1.42	1.37
2	D	805	BGD	C24-C23	3.48	1.45	1.38
2	C	804	BGD	C37-C52	3.43	1.59	1.52
2	B	803	BGD	F30-C29	3.22	1.41	1.37
2	B	803	BGD	C41-C40	3.21	1.44	1.38
2	D	805	BGD	F46-C45	3.21	1.41	1.37
2	D	805	BGD	C17-N16	3.20	1.52	1.45
2	B	803	BGD	F31-C29	3.16	1.41	1.37
2	C	804	BGD	P48-O49	3.14	1.55	1.50
2	A	802	BGD	C37-C52	3.14	1.58	1.52
2	D	805	BGD	C52-N54	-3.08	1.25	1.32
2	B	803	BGD	C29-C28	2.88	1.61	1.51
2	C	804	BGD	C29-C28	2.87	1.61	1.51
2	A	802	BGD	C45-C44	2.84	1.61	1.51
2	A	802	BGD	C29-C28	2.79	1.61	1.51
2	B	803	BGD	P48-O49	2.77	1.54	1.50
2	C	804	BGD	C45-C44	2.68	1.61	1.51
2	D	805	BGD	F30-C29	2.65	1.41	1.37
2	D	805	BGD	C29-C28	2.62	1.60	1.51
2	B	803	BGD	O53-C52	2.56	1.28	1.23
2	D	805	BGD	C37-C52	2.56	1.57	1.52
2	A	802	BGD	P48-O49	2.55	1.54	1.50
2	C	804	BGD	C17-N16	2.53	1.51	1.45
2	B	803	BGD	C52-N54	-2.48	1.27	1.32
2	C	804	BGD	F31-C29	2.29	1.40	1.37
2	A	802	BGD	C37-N36	2.27	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	805	BGD	C45-C44	2.24	1.59	1.51
2	B	803	BGD	C4-C5	2.20	1.55	1.50
2	A	802	BGD	C19-N18	2.19	1.50	1.45
2	C	804	BGD	O53-C52	2.17	1.27	1.23
2	B	803	BGD	C40-C39	2.15	1.43	1.38
2	C	804	BGD	C40-C39	2.15	1.43	1.38
2	A	802	BGD	C38-C37	2.15	1.59	1.54
2	C	804	BGD	C38-C37	2.12	1.59	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	805	BGD	P32-C29-C28	4.04	121.09	108.95
2	B	803	BGD	C10-C8-N16	3.60	123.71	117.04
2	C	804	BGD	P32-C29-C28	3.49	119.43	108.95
2	B	803	BGD	C43-C44-C45	3.38	123.78	120.03
2	C	804	BGD	P48-C45-C44	3.20	118.55	108.95
2	D	805	BGD	C43-C44-C45	3.18	123.56	120.03
2	A	802	BGD	C10-C8-N16	3.04	122.67	117.04
2	B	803	BGD	C27-C28-C29	3.02	123.38	120.03
2	B	803	BGD	C1-C17-N16	-3.00	103.00	111.11
2	B	803	BGD	P32-C29-C28	2.99	117.93	108.95
2	A	802	BGD	C27-C28-C29	2.85	123.20	120.03
2	D	805	BGD	C38-C37-N36	-2.82	104.99	110.83
2	B	803	BGD	O9-C8-N16	-2.73	117.27	122.47
2	D	805	BGD	C39-C38-C37	2.73	120.61	113.36
2	D	805	BGD	C20-C19-N18	-2.71	103.77	111.11
2	A	802	BGD	P32-C29-C28	2.66	116.94	108.95
2	B	803	BGD	O7-C5-C4	2.61	122.23	114.00
2	D	805	BGD	C10-C8-N16	2.56	121.78	117.04
2	D	805	BGD	O50-P48-O49	-2.51	106.81	112.96
2	D	805	BGD	O7-C5-C4	2.49	121.86	114.00
2	A	802	BGD	O34-P32-O33	-2.48	106.89	112.96
2	B	803	BGD	C38-C39-C40	-2.41	116.41	120.90
2	D	805	BGD	O34-P32-O33	-2.41	107.05	112.96
2	B	803	BGD	O51-P48-O49	-2.40	107.09	112.96
2	B	803	BGD	C17-N16-C8	-2.39	115.83	121.56
2	C	804	BGD	C20-C19-N18	-2.38	104.68	111.11
2	B	803	BGD	O50-P48-O49	-2.37	107.16	112.96
2	D	805	BGD	C19-N18-C1	2.33	126.66	121.65
2	B	803	BGD	P48-C45-C44	2.30	115.86	108.95
2	A	802	BGD	O51-P48-O49	-2.28	107.37	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	804	BGD	O7-C5-C4	2.26	121.12	114.00
2	A	802	BGD	O7-C5-C4	2.25	121.11	114.00
2	A	802	BGD	C19-C20-N36	2.20	121.32	116.63
2	B	803	BGD	C22-C19-C20	-2.20	104.68	110.30
2	C	804	BGD	O34-P32-O33	-2.13	107.75	112.96
2	B	803	BGD	O34-P32-O33	-2.12	107.77	112.96
2	D	805	BGD	C27-C28-C29	2.04	122.29	120.03
2	A	802	BGD	C3-C17-N16	-2.01	106.93	110.91
2	B	803	BGD	C3-C17-N16	2.00	114.87	110.91

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	804	BGD	C25-C28-C29-F31
2	C	804	BGD	C27-C28-C29-F31
2	D	805	BGD	C19-C22-C23-C26
2	D	805	BGD	C19-C22-C23-C24
2	C	804	BGD	N18-C19-C22-C23
2	D	805	BGD	O2-C1-C17-C3
2	A	802	BGD	F31-C29-P32-O33
2	D	805	BGD	N18-C1-C17-C3
2	D	805	BGD	C25-C28-C29-F30
2	D	805	BGD	C25-C28-C29-F31
2	D	805	BGD	C27-C28-C29-F30
2	D	805	BGD	C27-C28-C29-F31
2	D	805	BGD	O2-C1-C17-N16
2	A	802	BGD	N36-C37-C52-O53
2	A	802	BGD	N36-C37-C52-N54
2	C	804	BGD	N36-C37-C52-O53
2	C	804	BGD	N36-C37-C52-N54
2	C	804	BGD	C37-C38-C39-C42
2	C	804	BGD	C37-C38-C39-C40
2	A	802	BGD	C3-C4-C5-O7
2	B	803	BGD	C3-C4-C5-O7
2	A	802	BGD	C3-C4-C5-O6
2	B	803	BGD	C3-C4-C5-O6
2	D	805	BGD	C3-C4-C5-O6
2	D	805	BGD	C3-C4-C5-O7
2	C	804	BGD	C3-C4-C5-O7
2	D	805	BGD	N18-C1-C17-N16
2	B	803	BGD	O2-C1-C17-N16

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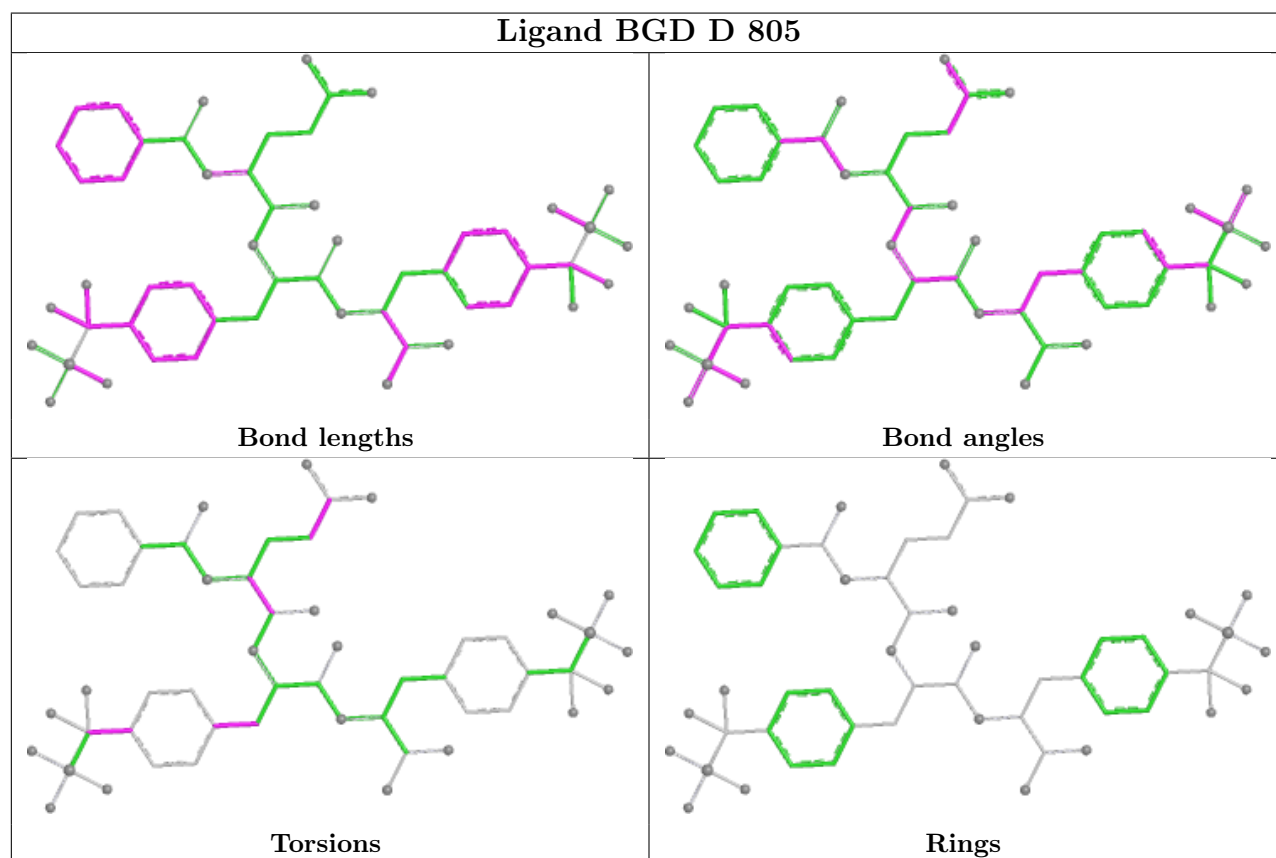
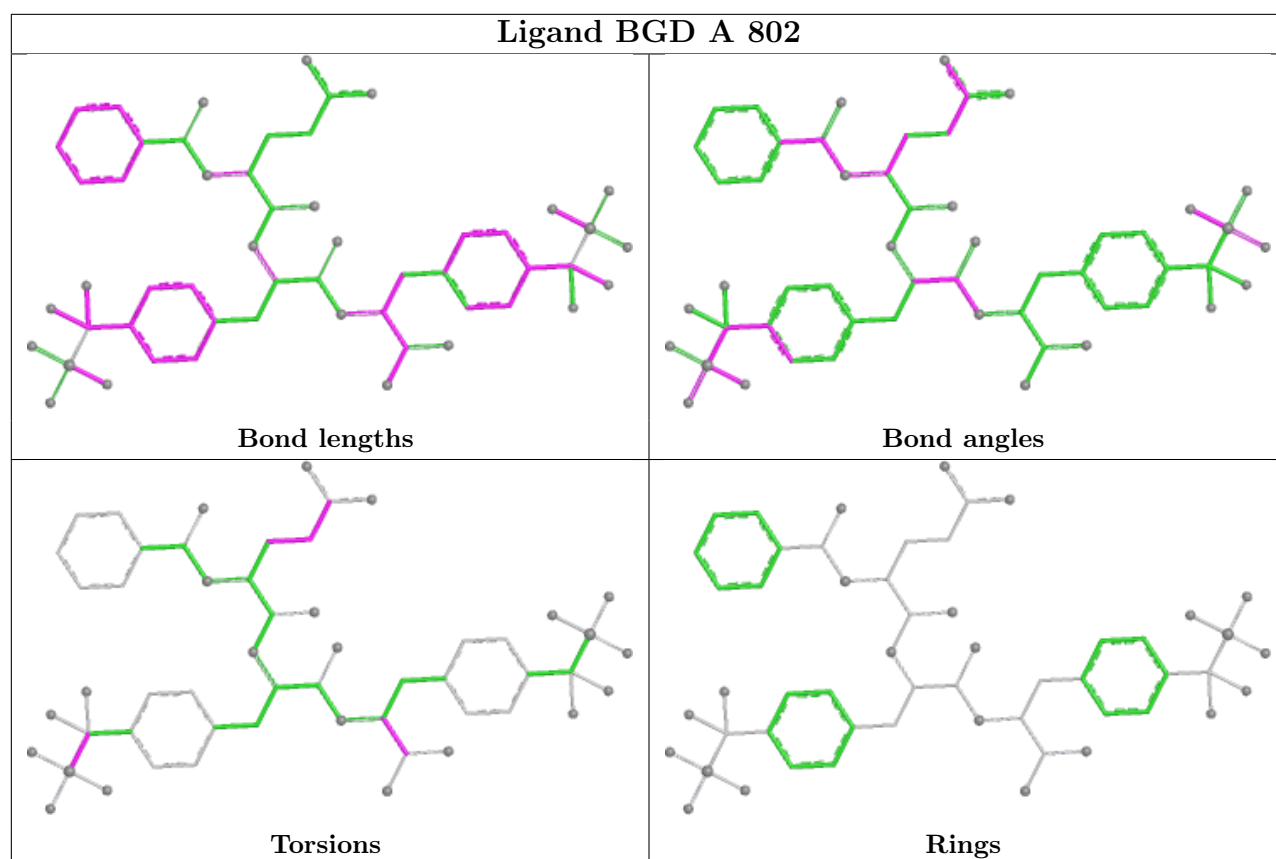
Mol	Chain	Res	Type	Atoms
2	C	804	BGD	C3-C4-C5-O6
2	B	803	BGD	O2-C1-C17-C3
2	A	802	BGD	C17-C3-C4-C5

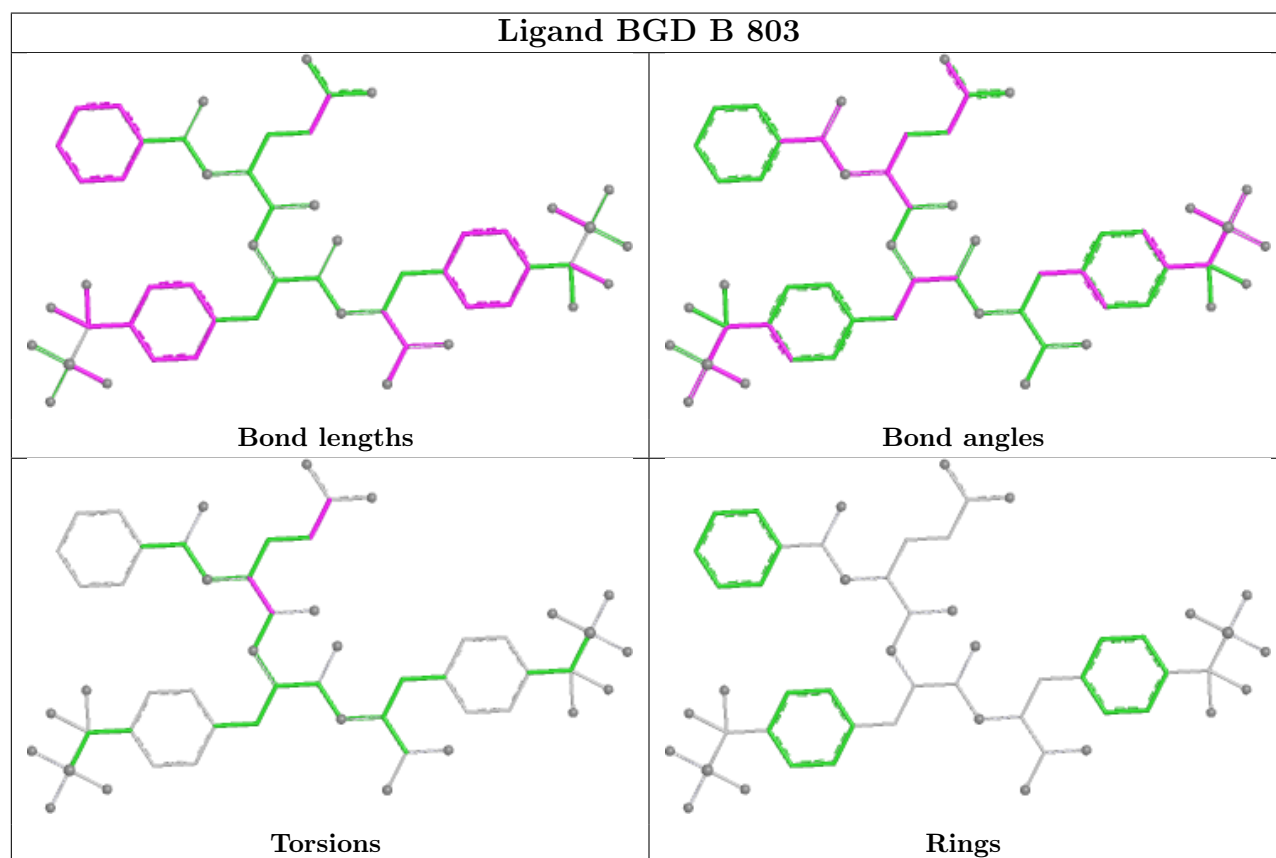
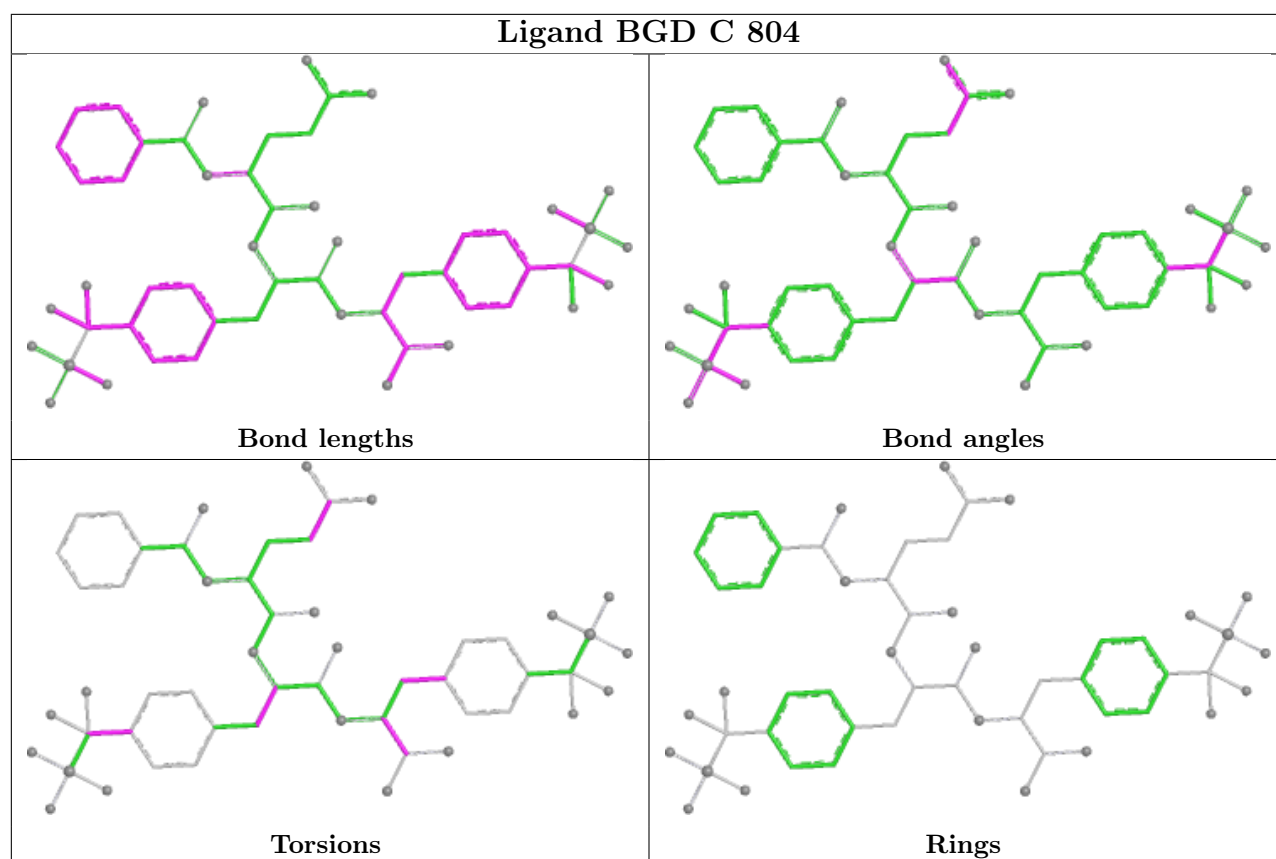
There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	BGD	6	0
2	D	805	BGD	3	0
2	C	804	BGD	5	0
2	B	803	BGD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	287/295 (97%)	0.31	15 (5%) 33 29	12, 37, 71, 100	0
1	B	287/295 (97%)	-0.02	5 (1%) 69 65	9, 27, 64, 92	0
1	C	287/295 (97%)	0.53	28 (9%) 13 11	13, 37, 84, 100	0
1	D	287/295 (97%)	1.07	60 (20%) 2 2	22, 54, 83, 100	0
All	All	1148/1180 (97%)	0.47	108 (9%) 14 12	9, 38, 80, 100	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	782	MET	5.4
1	A	781	ILE	4.6
1	D	622	ALA	4.6
1	D	780	PHE	4.5
1	B	781	ILE	4.5
1	D	535	ALA	4.3
1	B	780	PHE	4.0
1	C	500	PHE	4.0
1	A	783	GLY	4.0
1	C	497	LYS	4.0
1	A	736	ASP	4.0
1	A	782	MET	3.8
1	D	781	ILE	3.7
1	D	624	TYR	3.7
1	C	682	PHE	3.7
1	C	509	GLN	3.7
1	B	498	LEU	3.6
1	C	498	LEU	3.5
1	D	621	CYS	3.5
1	D	589	PRO	3.3
1	A	780	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	630	GLU	3.3
1	D	634	ILE	3.3
1	D	613	VAL	3.2
1	C	520	TYR	3.2
1	C	783	GLY	3.2
1	B	782	MET	3.1
1	D	537	LEU	3.1
1	D	659	GLU	3.1
1	C	684	VAL	3.1
1	D	591	THR	3.0
1	D	587	PRO	3.0
1	D	586	GLY	3.0
1	D	588	LEU	3.0
1	C	530	PHE	3.0
1	D	746	ILE	2.9
1	D	566	TYR	2.9
1	A	512	LYS	2.9
1	D	625	TRP	2.9
1	C	781	ILE	2.8
1	C	780	PHE	2.8
1	C	679	TRP	2.8
1	D	783	GLY	2.8
1	D	675	HIS	2.8
1	D	640	LEU	2.7
1	D	658	LEU	2.7
1	C	529	ASP	2.7
1	C	683	GLY	2.7
1	C	528	SER	2.7
1	D	563	ASP	2.7
1	D	614	MET	2.7
1	D	542	ASN	2.6
1	C	510	ILE	2.6
1	D	782	MET	2.6
1	D	629	GLU	2.6
1	C	507	PHE	2.6
1	D	630	GLU	2.6
1	D	592	CYS	2.6
1	D	541	LYS	2.5
1	D	663	LEU	2.5
1	D	534	VAL	2.5
1	D	540	ASN	2.5
1	C	563	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	498	LEU	2.4
1	D	638	THR	2.4
1	C	779	LYS	2.4
1	C	776	GLU	2.4
1	D	628	LYS	2.4
1	D	668	THR	2.3
1	D	619	LEU	2.3
1	D	655	VAL	2.3
1	D	660	LEU	2.3
1	D	635	PHE	2.3
1	A	561	GLN	2.3
1	A	614	MET	2.3
1	D	594	HIS	2.3
1	A	629	GLU	2.3
1	D	636	GLU	2.3
1	D	538	PRO	2.3
1	B	561	GLN	2.2
1	A	628	LYS	2.2
1	D	664	THR	2.2
1	C	501	MET	2.2
1	C	562	GLU	2.2
1	D	499	GLU	2.2
1	D	741	PRO	2.2
1	A	616	LYS	2.2
1	D	735	MET	2.2
1	D	498	LEU	2.2
1	D	557	ILE	2.2
1	A	686	GLU	2.2
1	D	595	PHE	2.2
1	C	680	PRO	2.1
1	D	696	PHE	2.1
1	D	648	ASP	2.1
1	A	501	MET	2.1
1	A	696	PHE	2.1
1	C	503	MET	2.1
1	D	623	GLN	2.1
1	D	611	ASN	2.1
1	D	616	LYS	2.0
1	D	677	THR	2.0
1	C	652	TYR	2.0
1	D	555	SER	2.0
1	D	533	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	536	LYS	2.0
1	C	523	ILE	2.0
1	D	665	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

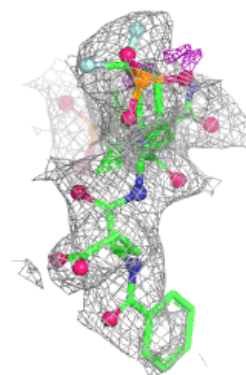
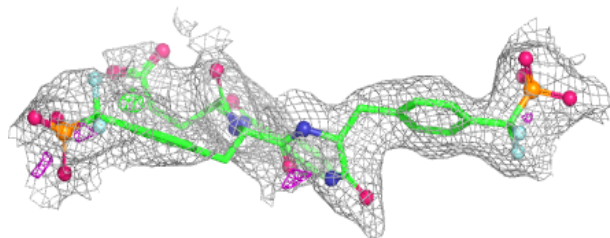
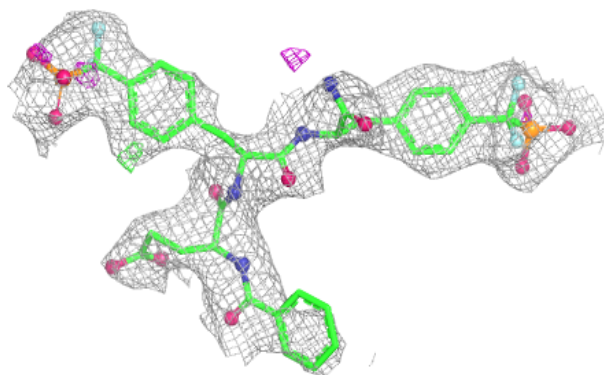
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGD	C	804	54/54	0.83	0.16	42,78,100,100	0
2	BGD	D	805	54/54	0.83	0.16	41,72,100,100	0
2	BGD	A	802	54/54	0.87	0.16	36,75,92,92	0
2	BGD	B	803	54/54	0.93	0.12	13,50,68,70	0

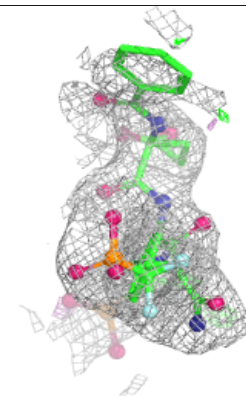
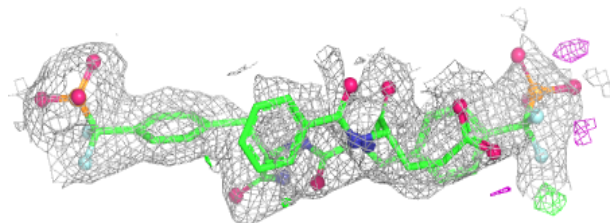
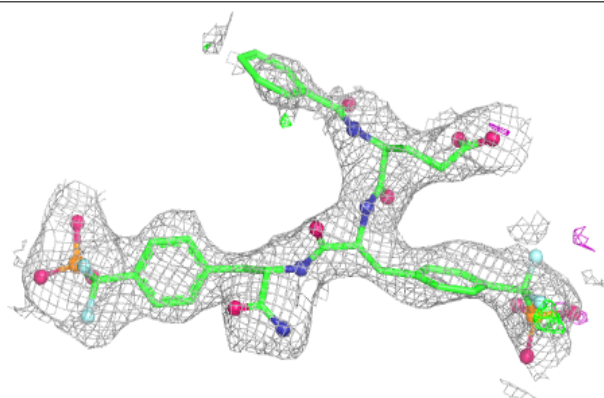
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BGD C 804:

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

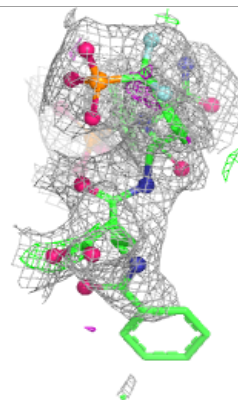
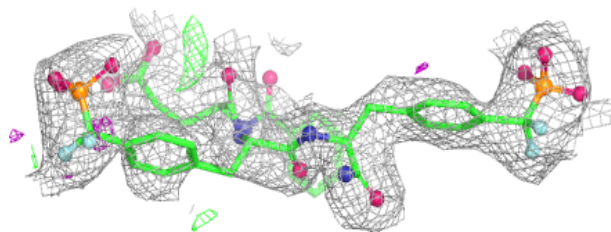
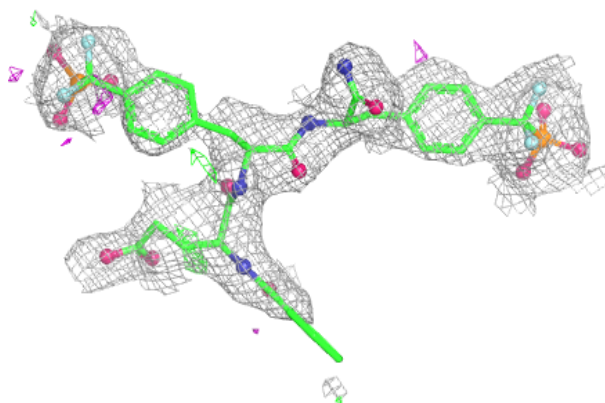
**Electron density around BGD D 805:**

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

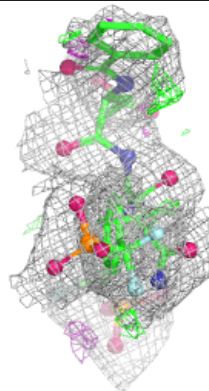
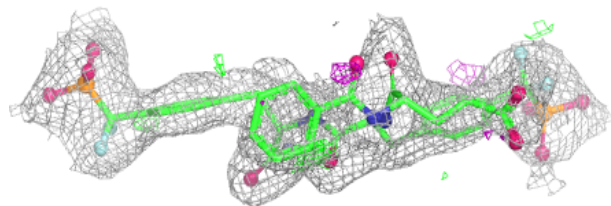
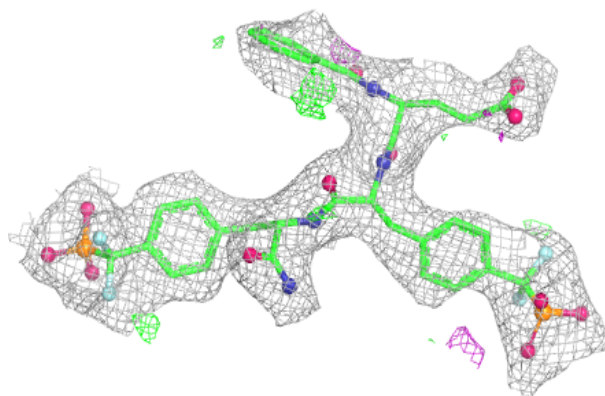


Electron density around BGD A 802:

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

**Electron density around BGD B 803:**

$2mF_o-DF_c$ (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.