



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:14 am BST

PDB ID : 1C7O  
Title : CRYSTAL STRUCTURE OF CYSTALYSIN FROM TREPONEMA DENTICOLOA CONTAINS A PYRIDOXAL 5'-PHOSPHATE-L-AMINOETHOXYVINYLGLYCINE COMPLEX  
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Deposited on : 2000-03-16  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

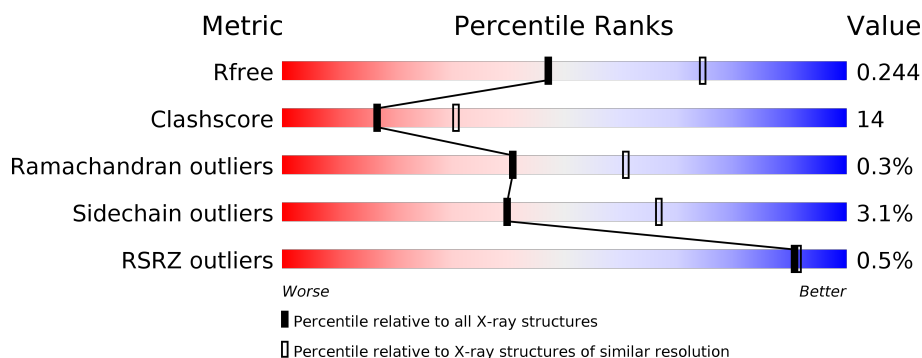
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	399	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>28%</div> <div>..</div> </div> </div>
1	B	399	<div> <div></div> <div>73%</div> <div>25%</div> <div>..</div> </div>
1	C	399	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>
1	D	399	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>..</div> </div> </div>
1	E	399	<div> <div></div> <div>67%</div> <div>30%</div> <div>..</div> </div>
1	F	399	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	399	<div><div>%</div><div><div></div></div><div>64%33%..</div></div>
1	H	399	<div><div></div><div>67%30%..</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27138 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 CRYSTALYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	B	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	C	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	D	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	E	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	F	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	G	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	H	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			

There are 24 discrepancies between the modelled and reference sequences:

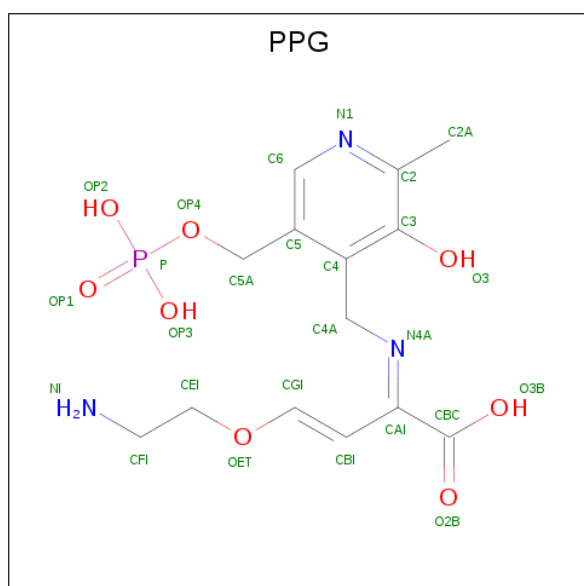
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLN	GLU	CONFLICT	UNP Q56257
A	154	GLN	GLU	CONFLICT	UNP Q56257
A	267	ALA	ILE	CONFLICT	UNP Q56257
B	88	GLN	GLU	CONFLICT	UNP Q56257
B	154	GLN	GLU	CONFLICT	UNP Q56257
B	267	ALA	ILE	CONFLICT	UNP Q56257
C	88	GLN	GLU	CONFLICT	UNP Q56257
C	154	GLN	GLU	CONFLICT	UNP Q56257
C	267	ALA	ILE	CONFLICT	UNP Q56257
D	88	GLN	GLU	CONFLICT	UNP Q56257
D	154	GLN	GLU	CONFLICT	UNP Q56257
D	267	ALA	ILE	CONFLICT	UNP Q56257
E	88	GLN	GLU	CONFLICT	UNP Q56257

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Chain	Residue	Modelled	Actual	Comment	Reference
E	154	GLN	GLU	CONFLICT	UNP Q56257
E	267	ALA	ILE	CONFLICT	UNP Q56257
F	88	GLN	GLU	CONFLICT	UNP Q56257
F	154	GLN	GLU	CONFLICT	UNP Q56257
F	267	ALA	ILE	CONFLICT	UNP Q56257
G	88	GLN	GLU	CONFLICT	UNP Q56257
G	154	GLN	GLU	CONFLICT	UNP Q56257
G	267	ALA	ILE	CONFLICT	UNP Q56257
H	88	GLN	GLU	CONFLICT	UNP Q56257
H	154	GLN	GLU	CONFLICT	UNP Q56257
H	267	ALA	ILE	CONFLICT	UNP Q56257

- Molecule 2 is (2E,3E)-4-(2-aminoethoxy)-2-[(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methyl]imino]but-3-enoic acid (three-letter code: PPG) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>3</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	B	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	C	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	D	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	E	1	Total	C	N	O	P	0	0
			26	14	3	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	G	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	H	1	Total	C	N	O	P	0	0
			26	14	3	8	1		

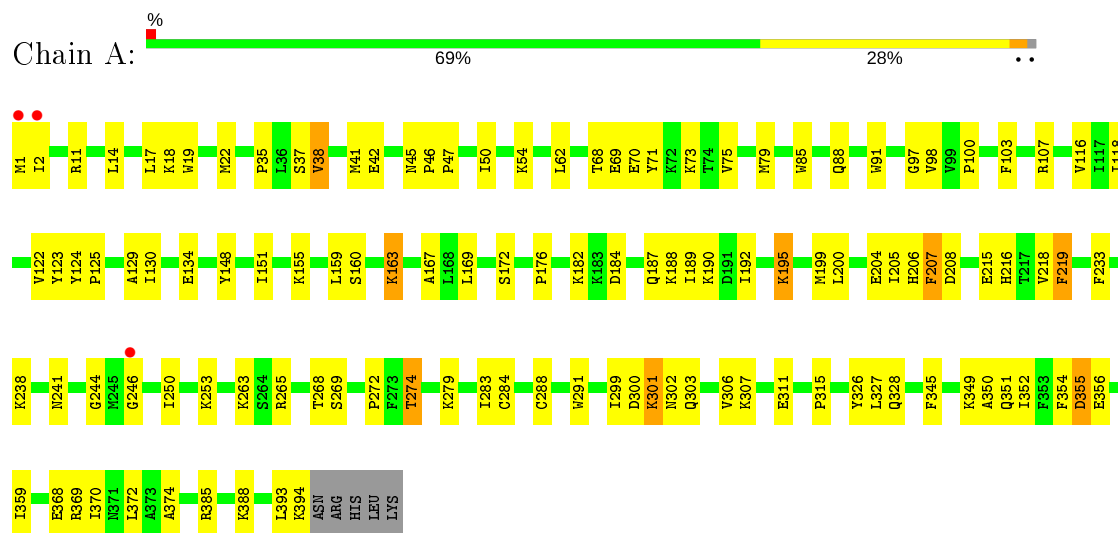
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	175	Total	O	0	0
			175	175		
3	B	181	Total	O	0	0
			181	181		
3	C	167	Total	O	0	0
			167	167		
3	D	139	Total	O	0	0
			139	139		
3	E	142	Total	O	0	0
			142	142		
3	F	180	Total	O	0	0
			180	180		
3	G	161	Total	O	0	0
			161	161		
3	H	129	Total	O	0	0
			129	129		

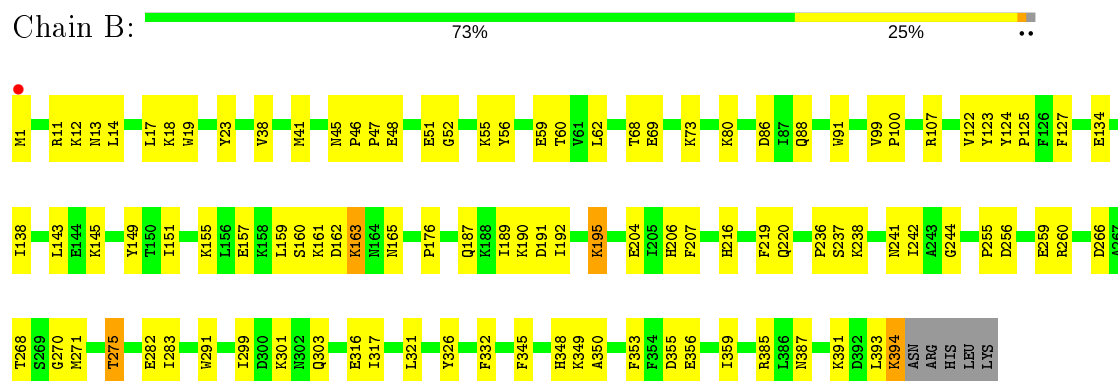
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

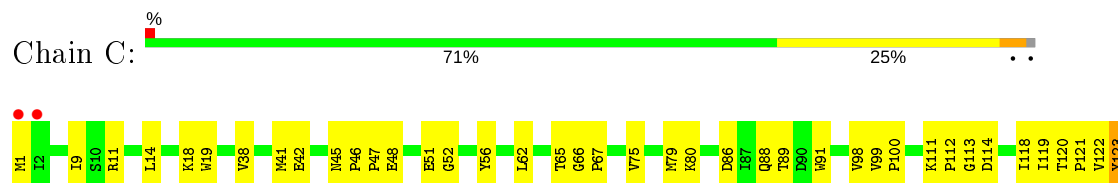
#### • Molecule 1: CYSTALYSIN



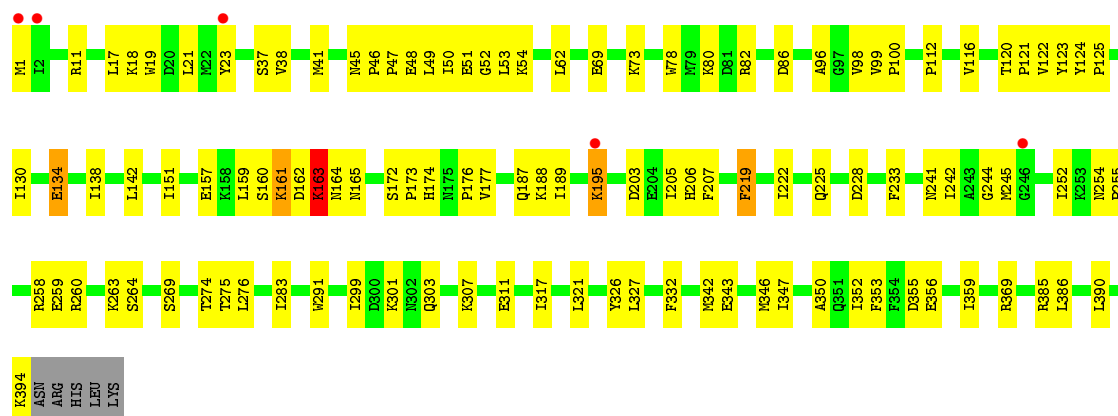
#### • Molecule 1: CYSTALYSIN



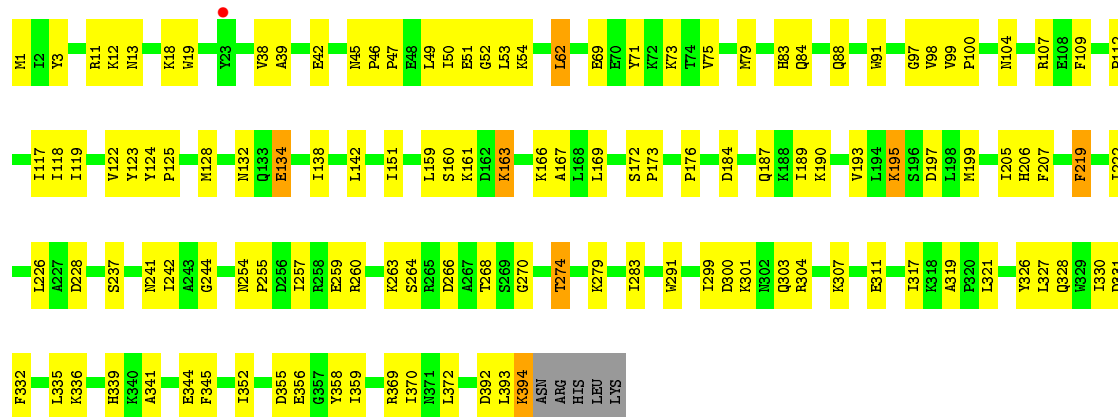
#### • Molecule 1: CYSTALYSIN



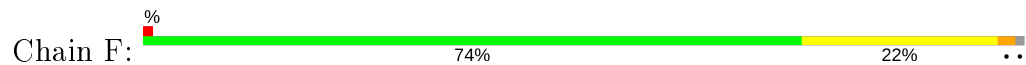
- Molecule 1: CYSTALYSIN



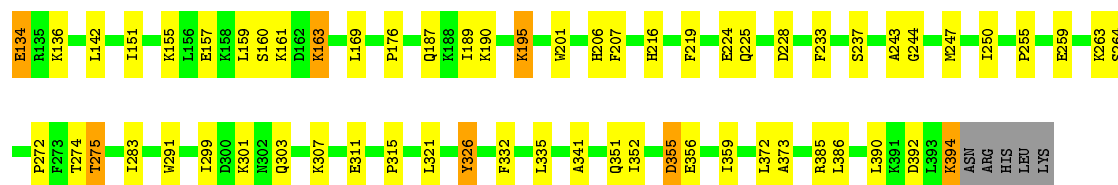
- Molecule 1: CYSTALYSIN



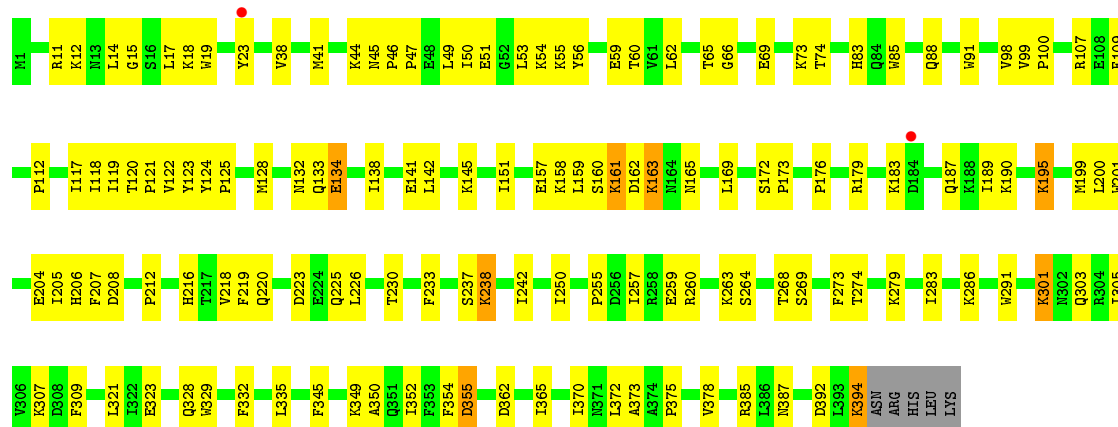
- Molecule 1: CYSTALYSIN



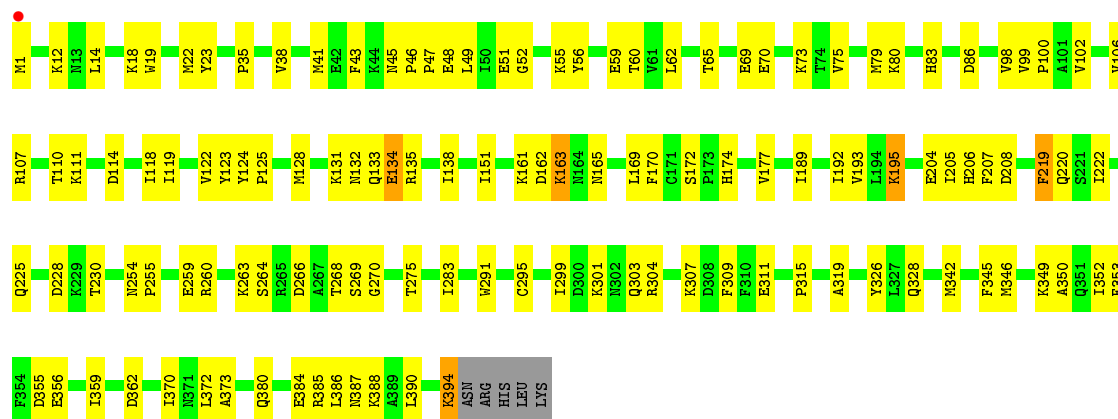




• Molecule 1: CYSTALYSIN



• Molecule 1: CYSTALYSIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.37Å 107.93Å 176.16Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.00-2.50) 91.9 (19.95-2.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.50Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.193 , 0.260 0.184 , 0.244	Depositor DCC
$R_{free}$ test set	5379 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 21.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.104 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	27138	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PPG

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	0.36	0/3283	0.62	0/4429
1	B	0.37	0/3283	0.63	0/4429
1	C	0.35	0/3283	0.62	1/4429 (0.0%)
1	D	0.34	0/3283	0.61	0/4429
1	E	0.35	0/3283	0.61	0/4429
1	F	0.37	0/3283	0.63	1/4429 (0.0%)
1	G	0.36	0/3283	0.61	1/4429 (0.0%)
1	H	0.35	0/3283	0.62	0/4429
All	All	0.36	0/26264	0.62	3/35432 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	355	ASP	N-CA-C	-6.22	94.20	111.00
1	C	355	ASP	N-CA-C	-5.80	95.34	111.00
1	G	355	ASP	N-CA-C	-5.20	96.96	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3207	0	3223	104	0
1	B	3207	0	3223	86	0
1	C	3207	0	3223	91	0
1	D	3207	0	3223	88	0
1	E	3207	0	3223	102	0
1	F	3207	0	3223	74	0
1	G	3207	0	3223	109	0
1	H	3207	0	3223	102	0
2	A	26	0	17	7	0
2	B	26	0	16	4	0
2	C	26	0	16	4	0
2	D	26	0	16	4	0
2	E	26	0	17	3	0
2	F	26	0	16	3	0
2	G	26	0	16	4	0
2	H	26	0	16	3	0
3	A	175	0	0	11	0
3	B	181	0	0	10	0
3	C	167	0	0	5	0
3	D	139	0	0	3	0
3	E	142	0	0	6	0
3	F	180	0	0	8	0
3	G	161	0	0	5	0
3	H	129	0	0	9	0
All	All	27138	0	25914	730	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 14.

All (730) 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:F:163:LYS:H	1:F:163:LYS:HD3	1.03	1.17
1:H:163:LYS:H	1:H:163:LYS:HD3	1.06	1.14
1:G:163:LYS:HD3	1:G:163:LYS:H	1.00	1.13
1:C:163:LYS:HD3	1:C:163:LYS:H	1.01	1.12
1:D:163:LYS:HD3	1:D:163:LYS:H	1.11	1.10
1:E:163:LYS:HD3	1:E:163:LYS:H	1.10	1.08
1:A:163:LYS:HD3	1:A:163:LYS:H	1.18	1.08
1:B:163:LYS:HD3	1:B:163:LYS:H	1.20	1.04
1:H:151:ILE:HD13	1:H:189:ILE:HD11	1.41	1.01
1:A:45:ASN:HD21	1:B:62:LEU:H	1.11	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:LYS:HD3	1:D:163:LYS:N	1.81	0.94
1:C:163:LYS:HD3	1:C:163:LYS:N	1.86	0.91
1:F:163:LYS:N	1:F:163:LYS:HD3	1.88	0.89
1:G:163:LYS:HD3	1:G:163:LYS:N	1.86	0.89
1:G:62:LEU:H	1:H:45:ASN:HD21	1.21	0.89
1:C:45:ASN:HD21	1:D:62:LEU:H	1.24	0.85
1:G:11:ARG:HA	1:G:14:LEU:HD12	1.58	0.85
1:G:163:LYS:CD	1:G:163:LYS:H	1.86	0.84
1:H:163:LYS:HD3	1:H:163:LYS:N	1.90	0.84
1:E:45:ASN:HD21	1:F:62:LEU:H	1.25	0.84
1:A:62:LEU:H	1:B:45:ASN:HD21	1.23	0.84
1:C:151:ILE:HD13	1:C:189:ILE:HD11	1.60	0.83
1:F:151:ILE:HD13	1:F:189:ILE:HD11	1.57	0.83
1:E:47:PRO:O	1:E:51:GLU:HG2	1.76	0.83
1:F:11:ARG:HA	1:F:14:LEU:HD12	1.61	0.82
1:C:163:LYS:H	1:C:163:LYS:CD	1.86	0.81
1:F:163:LYS:CD	1:F:163:LYS:H	1.84	0.80
1:E:163:LYS:HD3	1:E:163:LYS:N	1.94	0.80
1:D:18:LYS:HD3	1:D:38:VAL:HB	1.64	0.79
1:A:163:LYS:CD	1:A:163:LYS:H	1.93	0.79
1:E:163:LYS:CD	1:E:163:LYS:H	1.95	0.78
1:H:163:LYS:H	1:H:163:LYS:CD	1.90	0.77
1:D:299:ILE:HD13	1:D:326:TYR:HB3	1.66	0.77
1:B:151:ILE:CD1	1:B:189:ILE:HD11	2.15	0.76
1:E:51:GLU:HG3	3:E:5503:HOH:O	1.85	0.76
1:G:45:ASN:HD21	1:H:62:LEU:H	1.33	0.76
1:H:299:ILE:HD13	1:H:326:TYR:HB3	1.67	0.75
1:D:99:VAL:HB	1:D:100:PRO:HD3	1.69	0.74
1:A:107:ARG:HD2	3:B:2539:HOH:O	1.86	0.74
1:D:356:GLU:O	1:D:359:ILE:HG12	1.88	0.74
1:C:299:ILE:HD13	1:C:326:TYR:HB3	1.69	0.73
1:E:62:LEU:H	1:F:45:ASN:HD21	1.37	0.73
1:C:62:LEU:H	1:D:45:ASN:HD21	1.36	0.73
1:C:269:SER:HB3	1:D:269:SER:HB3	1.71	0.72
1:G:260:ARG:O	1:G:263:LYS:HG2	1.90	0.72
1:H:133:GLN:O	1:H:134:GLU:HB2	1.89	0.72
1:A:38:VAL:HG13	2:A:1500:PPG:HGI	1.72	0.72
1:F:255:PRO:O	1:F:259:GLU:HG3	1.90	0.72
1:B:255:PRO:O	1:B:259:GLU:HG3	1.89	0.71
1:G:190:LYS:HG3	1:G:226:LEU:HD22	1.72	0.71
1:A:2:ILE:HA	3:A:1592:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:GLN:HE22	1:E:190:LYS:NZ	1.89	0.70
1:E:255:PRO:O	1:E:259:GLU:HG3	1.92	0.70
1:F:41:MET:HG2	1:F:373:ALA:HB1	1.74	0.69
1:G:151:ILE:HD12	1:G:189:ILE:HD11	1.72	0.69
1:G:118:ILE:HG22	1:G:169:LEU:HB3	1.73	0.69
1:C:151:ILE:CD1	1:C:189:ILE:HD11	2.23	0.69
1:E:128:MET:O	1:E:132:ASN:HB2	1.92	0.69
1:C:98:VAL:HG21	1:C:205:ILE:HD12	1.75	0.69
1:B:163:LYS:H	1:B:163:LYS:CD	2.02	0.69
1:B:17:LEU:HD23	2:B:2500:PPG:HNI2	1.59	0.68
1:B:350:ALA:O	1:B:385:ARG:HD2	1.93	0.68
1:F:224:GLU:HG2	3:F:6566:HOH:O	1.94	0.67
1:G:255:PRO:O	1:G:259:GLU:HG3	1.94	0.67
1:D:255:PRO:O	1:D:259:GLU:HG3	1.94	0.67
1:A:107:ARG:NE	1:A:268:THR:HG21	2.10	0.67
1:B:162:ASP:HB3	1:B:165:ASN:ND2	2.09	0.67
1:G:123:TYR:CZ	1:G:125:PRO:HG2	2.29	0.67
1:E:197:ASP:HA	3:E:5617:HOH:O	1.94	0.66
1:H:356:GLU:O	1:H:359:ILE:HG12	1.94	0.66
1:H:163:LYS:HB3	3:H:8518:HOH:O	1.96	0.66
1:D:124:TYR:CD1	1:D:125:PRO:HD3	2.30	0.66
1:G:47:PRO:O	1:G:51:GLU:HG2	1.95	0.66
1:E:119:ILE:HG22	1:E:142:LEU:HG	1.77	0.66
1:H:255:PRO:O	1:H:259:GLU:HG3	1.96	0.66
1:H:122:VAL:HG22	1:H:123:TYR:N	2.11	0.65
1:B:11:ARG:HA	1:B:14:LEU:HD12	1.78	0.65
1:C:124:TYR:CG	1:C:125:PRO:HD3	2.31	0.65
1:C:88:GLN:HB2	1:C:91:TRP:CD1	2.32	0.65
1:C:255:PRO:O	1:C:259:GLU:HG3	1.97	0.65
1:E:151:ILE:HD13	1:E:189:ILE:HD11	1.79	0.65
1:G:124:TYR:CD1	1:G:125:PRO:HD3	2.31	0.65
1:A:122:VAL:HG22	1:A:123:TYR:N	2.12	0.64
1:H:162:ASP:HB3	1:H:165:ASN:ND2	2.12	0.64
1:A:62:LEU:H	1:B:45:ASN:ND2	1.95	0.64
1:A:184:ASP:HB3	3:A:1508:HOH:O	1.98	0.64
1:B:299:ILE:HD13	1:B:326:TYR:HB3	1.79	0.64
1:D:138:ILE:HG13	1:D:165:ASN:OD1	1.98	0.64
1:G:46:PRO:HG3	1:G:291:TRP:CD2	2.33	0.64
1:A:103:PHE:CE2	1:A:129:ALA:HA	2.34	0.63
1:D:123:TYR:CZ	1:D:125:PRO:HG2	2.34	0.63
1:G:62:LEU:H	1:H:45:ASN:ND2	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:HD3	1:A:163:LYS:N	2.02	0.63
1:B:124:TYR:CG	1:B:125:PRO:HD3	2.34	0.63
1:A:151:ILE:CD1	1:A:189:ILE:HD11	2.28	0.63
1:B:163:LYS:HD3	1:B:163:LYS:N	2.03	0.63
1:A:123:TYR:CZ	1:A:125:PRO:HG2	2.34	0.62
1:A:17:LEU:HD22	2:A:1500:PPG:HNI2	1.65	0.62
1:F:46:PRO:HG3	1:F:291:TRP:CD2	2.33	0.62
1:G:151:ILE:CD1	1:G:189:ILE:HD11	2.28	0.62
1:C:99:VAL:HB	1:C:100:PRO:HD3	1.81	0.62
1:F:56:TYR:O	1:F:60:THR:HG22	1.99	0.62
1:D:50:ILE:O	1:D:54:LYS:HG3	2.00	0.62
1:E:122:VAL:HG22	1:E:123:TYR:H	1.64	0.62
1:B:195:LYS:C	1:B:195:LYS:HD2	2.20	0.62
1:E:99:VAL:HB	1:E:100:PRO:HD3	1.81	0.62
1:F:11:ARG:HG3	1:F:19:TRP:NE1	2.15	0.62
1:C:172:SER:O	1:C:204:GLU:HG2	2.00	0.62
1:C:80:LYS:HD3	1:C:86:ASP:OD1	2.00	0.62
1:A:274:THR:HA	1:B:244:GLY:O	1.99	0.61
1:D:122:VAL:HG22	1:D:123:TYR:N	2.15	0.61
1:B:56:TYR:CE1	1:B:60:THR:HG21	2.35	0.61
1:D:195:LYS:HG2	1:G:88:GLN:CD	2.20	0.61
1:B:206:HIS:HE1	2:B:2500:PPG:O3	1.82	0.61
1:G:17:LEU:HD22	2:G:7500:PPG:HNI2	1.66	0.61
1:A:300:ASP:O	1:A:303:GLN:HG2	1.99	0.61
1:E:219:PHE:O	1:E:222:ILE:HG12	2.01	0.61
1:H:56:TYR:CE1	1:H:60:THR:HG21	2.36	0.61
1:A:215:GLU:HB2	3:A:1556:HOH:O	2.01	0.61
1:E:107:ARG:HE	1:E:268:THR:HG21	1.65	0.61
1:F:206:HIS:HE1	2:F:6500:PPG:O3	1.83	0.61
1:C:47:PRO:O	1:C:51:GLU:HG2	2.01	0.61
1:G:375:PRO:HB2	1:G:378:VAL:HG23	1.82	0.61
1:B:122:VAL:HG22	1:B:123:TYR:N	2.17	0.60
1:G:183:LYS:O	1:G:187:GLN:HG2	2.02	0.60
1:H:41:MET:HG2	1:H:373:ALA:HB1	1.83	0.60
1:G:237:SER:HA	1:G:242:ILE:HG13	1.83	0.60
1:B:88:GLN:HB2	1:B:91:TRP:CD1	2.36	0.60
1:C:118:ILE:HG22	1:C:169:LEU:HB3	1.84	0.60
1:A:75:VAL:O	1:A:79:MET:HG2	2.01	0.60
1:C:162:ASP:HB3	1:C:165:ASN:ND2	2.17	0.60
1:H:1:MET:SD	1:H:47:PRO:HB2	2.41	0.60
1:B:11:ARG:HB2	1:B:19:TRP:CD1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:PRO:O	1:H:51:GLU:HG2	2.02	0.60
1:H:18:LYS:HB2	1:H:38:VAL:HB	1.82	0.60
1:C:187:GLN:HE22	1:C:190:LYS:NZ	1.99	0.60
1:C:112:PRO:HB3	1:C:134:GLU:HB3	1.84	0.59
1:D:124:TYR:CG	1:D:125:PRO:HD3	2.37	0.59
1:D:151:ILE:CD1	1:D:189:ILE:HD11	2.32	0.59
1:E:206:HIS:HE1	2:E:5500:PPG:O3	1.86	0.59
1:E:190:LYS:HG3	1:E:226:LEU:HD22	1.84	0.59
1:H:206:HIS:HE1	2:H:8500:PPG:O3	1.85	0.59
1:C:11:ARG:HB2	1:C:19:TRP:CD1	2.38	0.59
1:D:187:GLN:HA	1:D:187:GLN:HE21	1.66	0.59
1:H:384:GLU:HG3	1:H:388:LYS:NZ	2.18	0.59
1:C:46:PRO:HG3	1:C:291:TRP:CD2	2.38	0.59
1:A:307:LYS:O	1:A:311:GLU:HG3	2.03	0.59
1:B:11:ARG:HG3	1:B:19:TRP:NE1	2.18	0.59
1:A:124:TYR:CG	1:A:125:PRO:HD3	2.38	0.59
1:E:123:TYR:CZ	1:E:125:PRO:HG2	2.37	0.59
1:A:122:VAL:HG22	1:A:123:TYR:H	1.67	0.58
1:C:52:GLY:HA3	1:C:283:ILE:HD13	1.85	0.58
1:B:160:SER:OG	1:B:195:LYS:NZ	2.36	0.58
1:D:46:PRO:HG3	1:D:291:TRP:CD2	2.38	0.58
1:H:99:VAL:HB	1:H:100:PRO:HD3	1.84	0.58
1:A:118:ILE:HG22	1:A:169:LEU:HB3	1.85	0.58
1:H:52:GLY:HA3	1:H:283:ILE:HD13	1.86	0.58
1:C:206:HIS:HE1	2:C:3500:PPG:O3	1.86	0.58
1:C:394:LYS:HB2	1:C:394:LYS:HZ2	1.68	0.58
1:H:195:LYS:HD2	1:H:195:LYS:O	2.03	0.58
1:C:138:ILE:HG13	1:C:165:ASN:OD1	2.02	0.58
1:G:220:GLN:HB3	1:G:230:THR:HG21	1.85	0.58
1:G:162:ASP:HB3	1:G:165:ASN:ND2	2.18	0.57
1:G:172:SER:O	1:G:204:GLU:HG2	2.03	0.57
1:A:107:ARG:HE	1:A:268:THR:HG21	1.69	0.57
1:B:123:TYR:CZ	1:B:125:PRO:HG2	2.38	0.57
1:B:151:ILE:HD13	1:B:189:ILE:HD11	1.86	0.57
1:C:238:LYS:HE2	2:C:3500:PPG:H4A2	1.86	0.57
1:D:163:LYS:CD	1:D:163:LYS:H	2.00	0.57
1:F:124:TYR:CD1	1:F:125:PRO:HD3	2.39	0.57
1:G:124:TYR:CG	1:G:125:PRO:HD3	2.39	0.57
1:A:388:LYS:HB3	3:A:1529:HOH:O	2.03	0.57
1:E:321:LEU:HD12	3:E:5620:HOH:O	2.03	0.57
1:F:111:LYS:HG2	1:F:114:ASP:OD1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:GLU:O	1:F:73:LYS:HG3	2.04	0.57
1:G:50:ILE:O	1:G:54:LYS:HG3	2.04	0.57
1:A:187:GLN:HE22	1:A:190:LYS:NZ	2.03	0.57
1:E:39:ALA:HB2	2:E:5500:PPG:O2B	2.04	0.57
1:E:118:ILE:HG22	1:E:169:LEU:HB3	1.86	0.57
1:G:206:HIS:HE1	2:G:7500:PPG:O3	1.88	0.57
1:F:41:MET:HG2	1:F:373:ALA:CB	2.34	0.57
1:H:118:ILE:HG22	1:H:169:LEU:HB3	1.86	0.57
1:A:11:ARG:HB2	1:A:19:TRP:CD1	2.40	0.56
1:B:107:ARG:HD2	3:B:2510:HOH:O	2.04	0.56
1:A:91:TRP:CZ2	1:A:253:LYS:HG3	2.40	0.56
1:G:112:PRO:HB3	1:G:134:GLU:HB3	1.86	0.56
1:H:311:GLU:O	1:H:315:PRO:HG3	2.05	0.56
1:H:69:GLU:O	1:H:73:LYS:HG3	2.05	0.56
1:H:394:LYS:HD3	3:H:8521:HOH:O	2.03	0.56
1:C:122:VAL:HG22	1:C:123:TYR:N	2.20	0.56
1:H:111:LYS:HG2	1:H:114:ASP:OD1	2.04	0.56
1:A:167:ALA:HB2	1:A:199:MET:HB2	1.87	0.56
1:C:394:LYS:HB2	1:C:394:LYS:NZ	2.19	0.56
1:E:187:GLN:HE22	1:E:190:LYS:HZ1	1.54	0.56
1:A:350:ALA:O	1:A:385:ARG:HD2	2.05	0.56
1:E:319:ALA:HB2	1:E:330:ILE:HG23	1.87	0.56
1:F:52:GLY:HA3	1:F:283:ILE:HD13	1.86	0.56
1:G:392:ASP:O	1:G:394:LYS:HE3	2.05	0.56
1:C:269:SER:CB	1:D:269:SER:HB3	2.34	0.56
1:D:1:MET:CE	1:D:48:GLU:HG3	2.36	0.56
1:B:99:VAL:HB	1:B:100:PRO:HD3	1.87	0.56
1:D:187:GLN:HA	1:D:187:GLN:NE2	2.21	0.56
1:E:69:GLU:O	1:E:73:LYS:HG3	2.06	0.56
1:E:98:VAL:HG21	1:E:205:ILE:HD12	1.88	0.56
1:A:205:ILE:HA	3:A:1526:HOH:O	2.05	0.55
1:B:123:TYR:CE1	2:B:2500:PPG:N4A	2.74	0.55
1:C:124:TYR:HB3	1:C:359:ILE:O	2.06	0.55
1:G:18:LYS:HD3	1:G:38:VAL:HB	1.89	0.55
1:A:123:TYR:CG	1:A:125:PRO:HD2	2.41	0.55
1:B:107:ARG:NE	1:B:268:THR:HG21	2.21	0.55
1:B:23:TYR:HE2	3:B:2660:HOH:O	1.90	0.55
1:C:98:VAL:HG13	1:C:233:PHE:HB3	1.87	0.55
1:G:69:GLU:O	1:G:73:LYS:HG3	2.06	0.55
1:B:145:LYS:HB2	3:B:2594:HOH:O	2.06	0.55
1:B:151:ILE:HD12	1:B:189:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ILE:HG22	1:C:142:LEU:HG	1.88	0.55
1:G:238:LYS:NZ	2:G:7500:PPG:H4A1	2.22	0.55
1:H:174:HIS:HD2	1:H:177:VAL:HG22	1.70	0.55
1:H:46:PRO:HG3	1:H:291:TRP:CD2	2.41	0.55
1:F:80:LYS:HD3	1:F:86:ASP:OD1	2.07	0.55
1:E:107:ARG:NE	1:E:268:THR:HG21	2.22	0.54
1:A:50:ILE:O	1:A:54:LYS:HG3	2.08	0.54
1:F:99:VAL:HB	1:F:100:PRO:HD3	1.88	0.54
1:B:238:LYS:HZ1	2:B:2500:PPG:H5A1	1.71	0.54
1:F:118:ILE:HG22	1:F:169:LEU:HB3	1.90	0.54
1:G:200:LEU:HB3	1:G:230:THR:OG1	2.07	0.54
1:F:272:PRO:HG3	3:F:6538:HOH:O	2.07	0.54
1:B:192:ILE:O	1:B:195:LYS:HE3	2.08	0.54
1:E:122:VAL:HG22	1:E:123:TYR:N	2.23	0.54
1:F:195:LYS:HD2	1:F:195:LYS:O	2.08	0.54
1:A:155:LYS:O	1:A:159:LEU:HG	2.07	0.54
1:B:204:GLU:OE1	1:B:216:HIS:HE1	1.90	0.54
1:D:52:GLY:HA3	1:D:283:ILE:HD13	1.90	0.54
1:G:99:VAL:HB	1:G:100:PRO:HD3	1.89	0.54
1:G:56:TYR:O	1:G:60:THR:HG22	2.08	0.54
1:C:9:ILE:HD11	1:C:42:GLU:HA	1.90	0.54
1:E:299:ILE:HD13	1:E:326:TYR:HB3	1.90	0.53
1:H:124:TYR:CG	1:H:125:PRO:HD3	2.43	0.53
1:C:275:THR:HG22	1:D:244:GLY:O	2.09	0.53
1:E:46:PRO:HG3	1:E:291:TRP:CD2	2.42	0.53
1:E:50:ILE:O	1:E:54:LYS:HG3	2.09	0.53
1:G:199:MET:CE	1:G:257:ILE:HD13	2.39	0.53
1:G:11:ARG:HB2	1:G:19:TRP:CD1	2.43	0.53
1:B:18:LYS:HB2	1:B:38:VAL:HB	1.91	0.53
1:D:275:THR:HG23	1:D:276:LEU:N	2.23	0.53
1:F:11:ARG:HG3	1:F:19:TRP:CE2	2.42	0.53
1:H:345:PHE:O	1:H:349:LYS:HB2	2.09	0.53
1:H:380:GLN:HG3	3:H:8519:HOH:O	2.08	0.53
1:H:350:ALA:O	1:H:385:ARG:HD2	2.09	0.53
1:E:51:GLU:HG3	3:E:5526:HOH:O	2.08	0.53
1:G:107:ARG:HB2	1:G:133:GLN:OE1	2.08	0.53
1:G:98:VAL:HG21	1:G:205:ILE:HD12	1.91	0.53
1:G:301:LYS:O	1:G:305:ILE:HG13	2.09	0.53
1:A:2:ILE:HG23	3:A:1592:HOH:O	2.09	0.53
1:E:317:ILE:HG23	1:E:331:ASP:O	2.08	0.53
1:H:65:THR:OG1	1:H:275:THR:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LYS:O	1:A:283:ILE:HG13	2.08	0.53
1:A:311:GLU:O	1:A:315:PRO:HG3	2.09	0.53
1:B:1:MET:CE	1:B:48:GLU:HG3	2.39	0.53
1:D:352:ILE:HG23	1:D:352:ILE:O	2.08	0.53
1:E:124:TYR:CG	1:E:125:PRO:HD3	2.44	0.53
1:E:11:ARG:HB2	1:E:19:TRP:CD1	2.43	0.53
1:G:138:ILE:HG22	1:G:159:LEU:HD13	1.90	0.53
1:G:350:ALA:O	1:G:385:ARG:HD2	2.09	0.53
1:C:356:GLU:O	1:C:359:ILE:HG12	2.09	0.53
1:G:354:PHE:HE1	1:G:370:ILE:HD12	1.73	0.53
1:H:123:TYR:CZ	1:H:125:PRO:HG2	2.44	0.53
1:B:236:PRO:HG2	1:B:242:ILE:HD11	1.91	0.52
1:C:1:MET:HE3	1:C:48:GLU:HG3	1.91	0.52
1:C:297:LYS:HG2	3:C:3613:HOH:O	2.08	0.52
1:G:88:GLN:HB2	1:G:91:TRP:CD1	2.44	0.52
1:H:263:LYS:HG3	1:H:264:SER:N	2.24	0.52
1:A:195:LYS:C	1:A:195:LYS:HD2	2.29	0.52
1:A:45:ASN:ND2	1:B:62:LEU:H	1.94	0.52
1:D:47:PRO:O	1:D:51:GLU:HG2	2.09	0.52
1:F:160:SER:OG	1:F:195:LYS:NZ	2.43	0.52
1:F:55:LYS:O	1:F:59:GLU:HG3	2.10	0.52
1:H:124:TYR:CD1	1:H:125:PRO:HD3	2.45	0.52
1:H:80:LYS:HD3	1:H:86:ASP:OD1	2.09	0.52
1:D:116:VAL:HB	1:D:130:ILE:HD13	1.91	0.52
1:G:55:LYS:O	1:G:59:GLU:HG3	2.08	0.52
1:A:200:LEU:HD21	1:A:219:PHE:CD1	2.45	0.52
1:C:119:ILE:HD12	1:C:170:PHE:HE1	1.75	0.52
1:H:192:ILE:O	1:H:195:LYS:HE3	2.10	0.52
1:H:43:PHE:HA	3:H:8531:HOH:O	2.09	0.52
1:A:160:SER:OG	1:A:195:LYS:NZ	2.42	0.52
1:B:348:HIS:HD2	3:B:2678:HOH:O	1.93	0.52
1:C:123:TYR:CG	1:C:125:PRO:HD2	2.45	0.52
1:G:123:TYR:CG	1:G:125:PRO:HD2	2.44	0.52
1:G:107:ARG:HE	1:G:268:THR:HG21	1.74	0.52
1:H:384:GLU:HG2	3:H:8601:HOH:O	2.10	0.52
1:C:392:ASP:C	1:C:394:LYS:N	2.62	0.52
1:E:160:SER:OG	1:E:195:LYS:NZ	2.43	0.52
1:B:317:ILE:HD13	1:B:332:PHE:CE2	2.45	0.51
1:A:238:LYS:NZ	2:A:1500:PPG:H4A1	2.25	0.51
1:C:88:GLN:HB2	1:C:91:TRP:NE1	2.26	0.51
1:F:119:ILE:HG22	1:F:142:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:ILE:CD1	1:E:189:ILE:HD11	2.39	0.51
1:H:98:VAL:O	1:H:102:VAL:HG23	2.10	0.51
1:A:1:MET:SD	1:A:47:PRO:HB2	2.50	0.51
1:D:350:ALA:O	1:D:385:ARG:HD2	2.11	0.51
1:A:46:PRO:HG3	1:A:291:TRP:CD2	2.45	0.51
1:D:317:ILE:HD13	1:D:332:PHE:CE2	2.45	0.51
1:E:332:PHE:O	1:E:335:LEU:HB2	2.10	0.51
1:E:189:ILE:O	1:E:193:VAL:HG23	2.11	0.51
1:G:117:ILE:HA	1:G:138:ILE:HB	1.92	0.51
1:H:123:TYR:CG	1:H:125:PRO:HD2	2.46	0.51
1:A:98:VAL:HG13	1:A:233:PHE:HB3	1.92	0.51
1:F:263:LYS:HG3	1:F:264:SER:N	2.26	0.51
1:H:56:TYR:O	1:H:60:THR:HG22	2.11	0.51
1:A:18:LYS:HE3	1:A:42:GLU:OE2	2.10	0.50
1:H:174:HIS:CD2	1:H:177:VAL:HG22	2.46	0.50
1:H:151:ILE:CD1	1:H:189:ILE:HD11	2.26	0.50
1:B:88:GLN:O	1:B:91:TRP:HB2	2.10	0.50
1:G:123:TYR:CD2	1:G:125:PRO:HD2	2.46	0.50
1:A:88:GLN:HB2	1:A:91:TRP:CD1	2.45	0.50
1:C:124:TYR:CD1	1:C:125:PRO:HD3	2.46	0.50
1:D:49:LEU:HA	1:D:283:ILE:HG21	1.94	0.50
1:G:44:LYS:HG3	3:G:7507:HOH:O	2.11	0.50
1:A:163:LYS:N	1:A:163:LYS:CD	2.69	0.50
1:A:18:LYS:HB2	1:A:38:VAL:HB	1.94	0.50
1:F:12:LYS:O	1:F:14:LEU:HG	2.10	0.50
1:F:392:ASP:C	1:F:394:LYS:N	2.63	0.50
1:H:122:VAL:HG22	1:H:123:TYR:H	1.73	0.50
1:H:228:ASP:O	1:H:254:ASN:HB2	2.11	0.50
1:G:328:GLN:HB3	1:G:370:ILE:CG2	2.41	0.50
1:H:352:ILE:HG23	1:H:352:ILE:O	2.11	0.50
1:E:11:ARG:NH1	1:E:42:GLU:OE2	2.45	0.50
1:E:317:ILE:HD11	1:E:335:LEU:HD13	1.94	0.50
1:E:244:GLY:HA3	1:F:275:THR:HG22	1.93	0.50
1:B:124:TYR:CD1	1:B:125:PRO:HD3	2.47	0.50
1:G:199:MET:HE3	1:G:257:ILE:HD13	1.92	0.50
1:A:148:TYR:OH	1:A:182:LYS:NZ	2.45	0.50
1:C:56:TYR:CD1	1:C:279:LYS:HG2	2.47	0.50
1:C:301:LYS:O	1:C:305:ILE:HG13	2.12	0.49
1:E:345:PHE:CE1	1:E:393:LEU:HD22	2.47	0.49
1:F:155:LYS:O	1:F:159:LEU:HG	2.12	0.49
1:B:123:TYR:CG	1:B:125:PRO:HD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:VAL:CG2	1:C:205:ILE:HD12	2.41	0.49
1:C:301:LYS:HD3	1:C:305:ILE:HD11	1.94	0.49
1:C:75:VAL:O	1:C:79:MET:HG2	2.11	0.49
1:H:303:GLN:HB3	1:H:372:LEU:HD13	1.94	0.49
1:A:215:GLU:HG3	3:A:1645:HOH:O	2.12	0.49
1:C:288:CYS:HA	3:C:3585:HOH:O	2.11	0.49
1:D:353:PHE:CD1	1:D:353:PHE:N	2.79	0.49
1:G:279:LYS:O	1:G:283:ILE:HG13	2.12	0.49
1:F:351:GLN:O	1:F:385:ARG:NH1	2.45	0.49
1:B:237:SER:HA	1:B:242:ILE:HG13	1.94	0.49
1:H:80:LYS:HE2	1:H:86:ASP:OD1	2.13	0.49
1:C:195:LYS:C	1:C:195:LYS:HD2	2.33	0.49
1:C:45:ASN:ND2	1:D:62:LEU:H	2.03	0.49
1:D:123:TYR:CD1	1:D:125:PRO:HD2	2.47	0.49
1:F:122:VAL:HG22	1:F:123:TYR:N	2.28	0.49
1:G:332:PHE:HD2	1:G:335:LEU:HD22	1.78	0.49
1:H:55:LYS:O	1:H:59:GLU:HG3	2.13	0.49
1:B:256:ASP:O	1:B:260:ARG:HG3	2.13	0.49
1:B:124:TYR:HB3	1:B:359:ILE:O	2.13	0.49
1:B:46:PRO:HG3	1:B:291:TRP:CD2	2.48	0.49
1:G:200:LEU:HD12	1:G:201:TRP:N	2.28	0.49
1:H:220:GLN:HB3	1:H:230:THR:HG21	1.95	0.48
1:H:309:PHE:CZ	1:H:387:ASN:HB2	2.47	0.48
1:H:22:MET:SD	1:H:35:PRO:HD3	2.53	0.48
1:C:392:ASP:C	1:C:394:LYS:H	2.15	0.48
1:E:303:GLN:HB3	1:E:372:LEU:HD13	1.95	0.48
1:H:195:LYS:HD2	1:H:195:LYS:C	2.33	0.48
1:G:128:MET:O	1:G:132:ASN:HB2	2.13	0.48
1:A:97:GLY:C	1:A:100:PRO:HD2	2.33	0.48
1:F:123:TYR:CD2	1:F:125:PRO:HD2	2.49	0.48
1:G:345:PHE:O	1:G:349:LYS:HB2	2.14	0.48
1:G:375:PRO:HD2	1:G:378:VAL:HG21	1.96	0.48
1:E:195:LYS:HD2	1:E:195:LYS:C	2.34	0.48
1:G:122:VAL:HG22	1:G:123:TYR:N	2.28	0.48
1:G:172:SER:O	1:G:204:GLU:HA	2.13	0.48
1:A:187:GLN:HE22	1:A:190:LYS:HZ3	1.61	0.48
1:D:78:TRP:O	1:D:82:ARG:HB2	2.13	0.48
1:F:303:GLN:HB3	1:F:372:LEU:HD13	1.95	0.48
1:H:128:MET:O	1:H:132:ASN:HB2	2.13	0.48
1:C:111:LYS:HG2	1:C:114:ASP:OD1	2.14	0.48
1:D:49:LEU:O	1:D:53:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:GLN:HE22	1:E:190:LYS:HZ3	1.60	0.48
1:F:187:GLN:HE22	1:F:190:LYS:NZ	2.11	0.48
1:G:158:LYS:O	1:G:161:LYS:HB2	2.13	0.48
1:G:85:TRP:CE2	1:G:218:VAL:HG11	2.49	0.48
1:H:386:LEU:O	1:H:390:LEU:HG	2.13	0.48
1:D:138:ILE:HG22	1:D:159:LEU:HD13	1.96	0.48
1:A:301:LYS:HG3	3:A:1621:HOH:O	2.13	0.47
1:E:300:ASP:O	1:E:303:GLN:HG2	2.14	0.47
1:B:41:MET:HB2	1:B:241:ASN:ND2	2.29	0.47
1:C:128:MET:O	1:C:132:ASN:HB2	2.14	0.47
1:D:160:SER:OG	1:D:195:LYS:NZ	2.47	0.47
1:C:244:GLY:O	1:D:274:THR:HA	2.13	0.47
1:H:328:GLN:HB3	1:H:370:ILE:CG2	2.44	0.47
1:C:119:ILE:HD12	1:C:170:PHE:CE1	2.50	0.47
1:C:350:ALA:O	1:C:385:ARG:HD2	2.14	0.47
1:E:109:PHE:CZ	1:E:257:ILE:HG23	2.49	0.47
1:E:328:GLN:HB3	1:E:370:ILE:CG2	2.44	0.47
1:E:97:GLY:O	1:E:100:PRO:HD2	2.14	0.47
1:G:157:GLU:O	1:G:161:LYS:HD3	2.14	0.47
1:A:151:ILE:HD12	1:A:189:ILE:HD11	1.95	0.47
1:A:207:PHE:CD2	1:A:207:PHE:C	2.88	0.47
1:B:187:GLN:HE22	1:B:190:LYS:NZ	2.12	0.47
1:D:1:MET:HE3	1:D:48:GLU:HG3	1.96	0.47
1:A:37:SER:HB2	1:A:355:ASP:OD1	2.13	0.47
1:D:11:ARG:HG3	1:D:19:TRP:NE1	2.29	0.47
1:D:174:HIS:HD2	1:D:177:VAL:HG22	1.78	0.47
1:H:138:ILE:HG13	1:H:165:ASN:OD1	2.14	0.47
1:E:98:VAL:CG2	1:E:205:ILE:HD12	2.45	0.47
1:F:299:ILE:HD13	1:F:326:TYR:HB3	1.97	0.47
1:B:163:LYS:HE2	3:B:2574:HOH:O	2.15	0.47
1:D:123:TYR:CG	1:D:125:PRO:HD2	2.49	0.47
1:D:69:GLU:O	1:D:73:LYS:HG3	2.14	0.47
1:E:97:GLY:C	1:E:100:PRO:HD2	2.34	0.47
1:G:17:LEU:HD22	2:G:7500:PPG:NI	2.28	0.47
1:H:260:ARG:O	1:H:263:LYS:HG2	2.14	0.47
1:H:384:GLU:HG3	1:H:388:LYS:HZ2	1.80	0.47
1:D:206:HIS:HE1	2:D:4500:PPG:O3	1.97	0.47
1:D:228:ASP:O	1:D:254:ASN:HB2	2.14	0.47
1:G:11:ARG:CA	1:G:14:LEU:HD12	2.38	0.47
1:C:123:TYR:CZ	1:C:125:PRO:HG2	2.50	0.47
1:E:187:GLN:NE2	1:E:190:LYS:NZ	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:THR:O	1:F:274:THR:HG23	2.15	0.47
1:F:307:LYS:HD2	1:F:321:LEU:HG	1.96	0.47
1:A:351:GLN:O	1:A:385:ARG:NH1	2.48	0.47
1:D:327:LEU:HD13	1:D:369:ARG:NH1	2.29	0.47
1:E:187:GLN:NE2	1:E:190:LYS:HZ1	2.13	0.47
1:E:263:LYS:HG3	1:E:264:SER:N	2.29	0.47
1:F:247:MET:HB3	3:F:6625:HOH:O	2.14	0.47
1:A:216:HIS:HD2	3:A:1550:HOH:O	1.98	0.47
1:B:191:ASP:HB2	3:B:2607:HOH:O	2.15	0.47
1:F:225:GLN:O	1:F:228:ASP:HB2	2.15	0.47
1:H:1:MET:HE1	1:H:48:GLU:HA	1.96	0.47
1:A:22:MET:SD	1:A:35:PRO:HD3	2.55	0.46
1:D:19:TRP:O	1:D:23:TYR:HD1	1.98	0.46
1:E:260:ARG:HA	1:E:263:LYS:HG2	1.97	0.46
1:H:225:GLN:O	1:H:228:ASP:HB2	2.15	0.46
1:A:233:PHE:HD2	1:A:250:ILE:HD12	1.80	0.46
1:A:356:GLU:O	1:A:359:ILE:HG12	2.15	0.46
1:B:62:LEU:HD23	1:B:275:THR:HG21	1.98	0.46
1:B:387:ASN:OD1	1:B:391:LYS:HE3	2.15	0.46
1:B:47:PRO:O	1:B:51:GLU:HG2	2.15	0.46
1:B:80:LYS:HD3	1:B:86:ASP:OD1	2.15	0.46
1:G:83:HIS:HE1	1:G:208:ASP:OD1	1.98	0.46
1:B:1:MET:HE3	1:B:48:GLU:HG3	1.97	0.46
1:C:11:ARG:HA	1:C:14:LEU:HD12	1.96	0.46
1:C:160:SER:OG	1:C:195:LYS:NZ	2.47	0.46
1:C:352:ILE:O	1:C:352:ILE:HG23	2.16	0.46
1:H:266:ASP:HA	1:H:270:GLY:HA2	1.97	0.46
1:D:120:THR:HB	1:D:121:PRO:HA	1.97	0.46
1:D:1:MET:HE1	1:D:48:GLU:HG3	1.97	0.46
1:E:138:ILE:CG2	1:E:159:LEU:HD22	2.46	0.46
1:E:339:HIS:HB2	1:E:358:TYR:HD2	1.80	0.46
1:E:356:GLU:O	1:E:359:ILE:HG12	2.15	0.46
1:D:219:PHE:O	1:D:222:ILE:HG12	2.16	0.46
1:H:189:ILE:O	1:H:193:VAL:HG23	2.16	0.46
1:H:219:PHE:O	1:H:222:ILE:HG12	2.15	0.46
1:A:123:TYR:CD2	1:A:125:PRO:HD2	2.51	0.46
1:C:11:ARG:HG3	1:C:19:TRP:NE1	2.30	0.46
1:G:212:PRO:HB2	3:G:7532:HOH:O	2.16	0.46
1:H:75:VAL:O	1:H:79:MET:HG2	2.16	0.46
1:C:172:SER:HA	1:C:173:PRO:C	2.35	0.46
1:D:122:VAL:HG22	1:D:123:TYR:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:LYS:HD3	1:D:86:ASP:OD1	2.16	0.46
1:F:163:LYS:CD	1:F:163:LYS:N	2.64	0.46
1:C:113:GLY:HA2	1:C:136:LYS:NZ	2.30	0.46
1:D:17:LEU:HD23	2:D:4500:PPG:HNI2	1.81	0.46
1:E:123:TYR:CE1	2:E:5500:PPG:N4A	2.84	0.46
1:H:328:GLN:HB2	1:H:372:LEU:HD11	1.98	0.46
1:A:122:VAL:CG2	1:A:123:TYR:N	2.79	0.45
1:A:85:TRP:CD2	1:A:218:VAL:HG11	2.51	0.45
1:C:172:SER:O	1:C:204:GLU:HA	2.17	0.45
1:D:142:LEU:HA	3:D:4571:HOH:O	2.16	0.45
1:F:124:TYR:CG	1:F:125:PRO:HD3	2.51	0.45
1:F:84:GLN:HB3	3:F:6669:HOH:O	2.15	0.45
1:E:83:HIS:HB3	3:E:5566:HOH:O	2.16	0.45
1:G:56:TYR:CE1	1:G:60:THR:HG21	2.51	0.45
1:H:122:VAL:CG2	1:H:123:TYR:N	2.77	0.45
1:H:295:CYS:O	1:H:299:ILE:HG13	2.17	0.45
1:E:279:LYS:O	1:E:283:ILE:HG13	2.17	0.45
1:G:263:LYS:HG3	1:G:264:SER:N	2.32	0.45
1:G:65:THR:O	1:G:273:PHE:HA	2.16	0.45
1:F:195:LYS:HB3	1:F:195:LYS:HE3	1.73	0.45
1:F:237:SER:HB2	1:F:243:ALA:HA	1.98	0.45
1:G:260:ARG:HA	1:G:263:LYS:HG2	1.97	0.45
1:A:122:VAL:CG2	1:A:123:TYR:H	2.30	0.45
1:A:244:GLY:O	1:B:275:THR:HG22	2.17	0.45
1:A:107:ARG:CZ	1:A:268:THR:HG21	2.46	0.45
1:E:392:ASP:C	1:E:394:LYS:N	2.70	0.45
1:F:233:PHE:HD2	1:F:250:ILE:HD12	1.82	0.45
1:G:12:LYS:O	1:G:14:LEU:HG	2.17	0.45
1:D:275:THR:HG23	1:D:276:LEU:H	1.80	0.45
1:A:238:LYS:HZ1	2:A:1500:PPG:H5A1	1.82	0.45
1:A:272:PRO:HG3	3:A:1528:HOH:O	2.16	0.45
1:D:41:MET:HB2	1:D:241:ASN:ND2	2.32	0.45
1:E:117:ILE:HA	1:E:138:ILE:HB	1.98	0.45
1:E:266:ASP:HA	1:E:270:GLY:HA2	1.98	0.45
1:G:352:ILE:HD13	1:G:354:PHE:CZ	2.52	0.45
1:D:195:LYS:HG3	1:G:88:GLN:HG3	1.99	0.45
1:B:107:ARG:HE	1:B:268:THR:HG21	1.82	0.45
1:D:116:VAL:HB	1:D:130:ILE:CD1	2.46	0.45
1:D:386:LEU:O	1:D:390:LEU:HG	2.17	0.45
1:F:38:VAL:HG13	2:F:6500:PPG:HBI	1.98	0.45
1:A:328:GLN:HB2	1:A:372:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLY:HA3	1:B:283:ILE:HD13	1.98	0.45
1:A:85:TRP:CE2	1:A:218:VAL:HG11	2.52	0.44
1:B:122:VAL:HG22	1:B:123:TYR:H	1.81	0.44
1:D:37:SER:OG	1:D:38:VAL:N	2.50	0.44
1:E:71:TYR:O	1:E:75:VAL:HG23	2.17	0.44
1:G:46:PRO:HG3	1:G:291:TRP:CE3	2.52	0.44
1:D:205:ILE:HA	3:D:4566:HOH:O	2.17	0.44
1:E:123:TYR:CG	1:E:125:PRO:HD2	2.51	0.44
1:E:303:GLN:HG3	1:E:304:ARG:N	2.32	0.44
1:G:85:TRP:CD2	1:G:218:VAL:HG11	2.52	0.44
1:C:176:PRO:HB3	1:C:369:ARG:HD3	1.99	0.44
1:G:160:SER:OG	1:G:195:LYS:NZ	2.49	0.44
1:G:233:PHE:HD2	1:G:250:ILE:HD12	1.82	0.44
1:H:19:TRP:O	1:H:23:TYR:HD1	2.00	0.44
1:H:41:MET:HG2	1:H:373:ALA:CB	2.46	0.44
1:C:123:TYR:CD1	1:C:125:PRO:HD2	2.52	0.44
1:E:317:ILE:HD13	1:E:332:PHE:CE2	2.52	0.44
1:E:339:HIS:HB2	1:E:358:TYR:CD2	2.53	0.44
1:H:342:MET:O	1:H:346:MET:HG2	2.18	0.44
1:H:362:ASP:HB2	3:H:8553:HOH:O	2.15	0.44
1:D:260:ARG:O	1:D:263:LYS:HG2	2.18	0.44
1:E:3:TYR:CD2	1:E:291:TRP:HD1	2.36	0.44
1:E:392:ASP:C	1:E:394:LYS:H	2.20	0.44
1:H:131:LYS:HB2	1:H:131:LYS:HE3	1.82	0.44
1:A:263:LYS:NZ	1:F:341:ALA:HB2	2.32	0.44
1:C:133:GLN:O	1:C:134:GLU:HB2	2.18	0.44
1:C:300:ASP:O	1:C:303:GLN:HG2	2.18	0.44
1:D:21:LEU:HD12	1:D:21:LEU:O	2.17	0.44
1:F:195:LYS:C	1:F:195:LYS:HD2	2.37	0.44
1:G:19:TRP:O	1:G:23:TYR:HD1	2.00	0.44
1:G:98:VAL:CG2	1:G:205:ILE:HD12	2.48	0.44
1:A:11:ARG:HB2	1:A:19:TRP:CG	2.52	0.44
1:A:284:CYS:HA	1:A:288:CYS:SG	2.58	0.44
1:B:124:TYR:HA	1:B:127:PHE:HD1	1.82	0.44
1:B:162:ASP:HB3	1:B:165:ASN:HD22	1.80	0.44
1:C:317:ILE:HD13	1:C:332:PHE:CE2	2.53	0.44
1:F:216:HIS:HD2	3:F:6515:HOH:O	2.00	0.44
1:G:179:ARG:NE	1:G:323:GLU:OE1	2.43	0.44
1:C:187:GLN:HE22	1:C:190:LYS:HZ1	1.66	0.44
1:A:116:VAL:HB	1:A:130:ILE:HD13	2.00	0.43
1:E:328:GLN:HB3	1:E:370:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:303:GLN:HG3	1:H:304:ARG:N	2.33	0.43
1:B:55:LYS:O	1:B:59:GLU:HG3	2.17	0.43
1:C:41:MET:HB2	1:C:241:ASN:CG	2.39	0.43
1:E:112:PRO:HA	1:E:134:GLU:O	2.18	0.43
1:H:353:PHE:N	1:H:353:PHE:CD1	2.86	0.43
1:B:316:GLU:OE2	1:B:316:GLU:N	2.43	0.43
1:E:166:LYS:O	1:E:167:ALA:HB2	2.17	0.43
1:E:228:ASP:O	1:E:254:ASN:HB2	2.17	0.43
1:H:12:LYS:O	1:H:14:LEU:HG	2.18	0.43
1:A:184:ASP:O	1:A:188:LYS:HG3	2.18	0.43
1:D:151:ILE:HD13	1:D:189:ILE:HD11	1.98	0.43
1:F:68:THR:O	1:F:71:TYR:HB3	2.18	0.43
1:H:70:GLU:HB3	3:H:8552:HOH:O	2.17	0.43
1:A:17:LEU:HD21	1:B:271:MET:CE	2.48	0.43
1:A:299:ILE:HD13	1:A:326:TYR:HB3	2.01	0.43
1:B:356:GLU:O	1:B:359:ILE:HG12	2.18	0.43
1:D:157:GLU:O	1:D:161:LYS:HD3	2.19	0.43
1:E:254:ASN:HA	1:E:255:PRO:HD3	1.89	0.43
1:G:352:ILE:HA	3:G:7598:HOH:O	2.17	0.43
1:A:374:ALA:HB2	3:A:1524:HOH:O	2.19	0.43
1:D:225:GLN:CD	1:D:225:GLN:H	2.21	0.43
1:E:18:LYS:HD3	1:E:38:VAL:HB	2.00	0.43
1:G:195:LYS:C	1:G:195:LYS:HD2	2.39	0.43
1:D:162:ASP:O	1:D:164:ASN:N	2.52	0.43
1:D:98:VAL:HG13	1:D:233:PHE:HB3	2.00	0.43
1:F:311:GLU:O	1:F:315:PRO:HG3	2.17	0.43
1:G:145:LYS:HB3	1:G:145:LYS:HE3	1.90	0.43
1:A:302:ASN:O	1:A:306:VAL:HG23	2.19	0.43
1:B:303:GLN:HG3	1:B:321:LEU:HD22	2.01	0.43
1:E:352:ILE:O	1:E:352:ILE:HG23	2.18	0.43
1:F:352:ILE:HA	3:F:6580:HOH:O	2.18	0.43
1:F:392:ASP:C	1:F:394:LYS:H	2.22	0.43
1:A:328:GLN:HB3	1:A:370:ILE:CG2	2.49	0.43
1:A:352:ILE:CG2	1:A:352:ILE:O	2.67	0.43
1:A:41:MET:HB2	1:A:241:ASN:CG	2.39	0.43
1:C:120:THR:HB	1:C:121:PRO:HA	2.01	0.43
1:E:260:ARG:O	1:E:263:LYS:HG2	2.19	0.43
1:A:192:ILE:O	1:A:195:LYS:HE3	2.18	0.43
1:A:300:ASP:OD1	1:A:303:GLN:NE2	2.49	0.43
1:C:119:ILE:CG2	1:C:142:LEU:HG	2.49	0.43
1:E:241:ASN:ND2	1:F:61:VAL:HG13	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:MET:HG2	1:G:373:ALA:HB1	2.00	0.43
1:B:282:GLU:HG2	3:B:2603:HOH:O	2.18	0.42
1:B:353:PHE:N	1:B:353:PHE:CD1	2.87	0.42
1:F:356:GLU:O	1:F:359:ILE:HG12	2.19	0.42
1:F:80:LYS:HA	1:F:80:LYS:HD2	1.91	0.42
2:H:8500:PPG:HEI2	3:H:8556:HOH:O	2.19	0.42
1:C:203:ASP:OD1	2:C:3500:PPG:N1	2.52	0.42
1:D:172:SER:HA	1:D:173:PRO:C	2.39	0.42
1:E:12:LYS:HG2	1:E:13:ASN:ND2	2.34	0.42
1:G:216:HIS:CD2	3:G:7516:HOH:O	2.72	0.42
1:G:107:ARG:NE	1:G:268:THR:HG21	2.34	0.42
1:G:362:ASP:HA	1:G:365:ILE:HG13	2.01	0.42
1:B:12:LYS:HG2	1:B:13:ASN:ND2	2.34	0.42
1:B:266:ASP:HA	1:B:270:GLY:HA2	2.02	0.42
1:E:237:SER:HA	1:E:242:ILE:HG13	2.01	0.42
1:E:307:LYS:O	1:E:311:GLU:HG3	2.19	0.42
1:F:332:PHE:O	1:F:335:LEU:HB2	2.20	0.42
1:G:303:GLN:HB3	1:G:372:LEU:HD13	2.01	0.42
1:A:11:ARG:HA	1:A:14:LEU:HD12	2.01	0.42
1:A:98:VAL:HG21	1:A:205:ILE:HD12	2.01	0.42
1:E:104:ASN:HB2	3:E:5536:HOH:O	2.18	0.42
1:E:327:LEU:HB3	1:E:369:ARG:HD2	2.02	0.42
1:E:274:THR:HA	1:F:244:GLY:O	2.19	0.42
1:F:352:ILE:HG23	1:F:352:ILE:O	2.19	0.42
1:F:386:LEU:O	1:F:390:LEU:HG	2.19	0.42
1:A:238:LYS:HZ1	2:A:1500:PPG:H4A1	1.85	0.42
1:G:352:ILE:HG23	1:G:352:ILE:O	2.19	0.42
1:H:309:PHE:HZ	1:H:387:ASN:HB2	1.83	0.42
1:B:62:LEU:CD2	1:B:275:THR:HG21	2.49	0.42
1:B:69:GLU:O	1:B:73:LYS:HG3	2.20	0.42
1:F:123:TYR:CZ	1:F:125:PRO:HG2	2.55	0.42
1:G:332:PHE:O	1:G:335:LEU:HB2	2.19	0.42
1:G:49:LEU:O	1:G:53:LEU:HG	2.19	0.42
1:H:124:TYR:HB3	1:H:359:ILE:O	2.20	0.42
1:D:122:VAL:CG2	1:D:123:TYR:N	2.81	0.42
1:D:252:ILE:O	1:D:258:ARG:NH1	2.44	0.42
1:D:303:GLN:HG3	1:D:321:LEU:HD22	2.02	0.42
1:E:119:ILE:CG2	1:E:142:LEU:HG	2.47	0.42
1:A:172:SER:O	1:A:204:GLU:HA	2.20	0.42
1:A:206:HIS:HE1	2:A:1500:PPG:O3	2.02	0.42
1:B:238:LYS:HA	1:B:238:LYS:HD2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LYS:HB2	1:C:38:VAL:HB	2.01	0.42
1:D:17:LEU:CD2	2:D:4500:PPG:HNI2	2.32	0.42
1:D:347:ILE:HG23	1:D:353:PHE:CE2	2.54	0.42
1:D:203:ASP:OD1	2:D:4500:PPG:N1	2.53	0.42
1:H:122:VAL:CG2	1:H:123:TYR:H	2.33	0.42
1:H:263:LYS:CG	1:H:264:SER:N	2.82	0.42
1:H:307:LYS:HB2	1:H:319:ALA:O	2.19	0.42
1:H:307:LYS:O	1:H:311:GLU:HG3	2.19	0.42
1:A:354:PHE:CD2	1:A:368:GLU:HB3	2.55	0.42
1:A:69:GLU:O	1:A:73:LYS:HG3	2.20	0.42
1:B:345:PHE:O	1:B:349:LYS:HB2	2.19	0.42
1:G:307:LYS:HD2	1:G:321:LEU:HG	2.02	0.42
1:G:328:GLN:HB3	1:G:370:ILE:HG22	2.02	0.42
1:B:220:GLN:HG3	3:B:2526:HOH:O	2.20	0.41
1:B:68:THR:HB	3:B:2584:HOH:O	2.19	0.41
1:C:41:MET:HB2	1:C:241:ASN:ND2	2.35	0.41
1:D:18:LYS:CD	1:D:38:VAL:HB	2.42	0.41
1:E:123:TYR:CD2	1:E:125:PRO:HD2	2.55	0.41
1:G:120:THR:HB	1:G:121:PRO:HA	2.02	0.41
1:A:207:PHE:HE2	1:A:208:ASP:OD2	2.03	0.41
1:D:342:MET:O	1:D:346:MET:HG2	2.20	0.41
1:F:157:GLU:O	1:F:161:LYS:HD3	2.20	0.41
1:H:111:LYS:HA	1:H:135:ARG:NH2	2.35	0.41
1:H:123:TYR:CD1	1:H:125:PRO:HD2	2.56	0.41
1:G:269:SER:HB3	1:H:269:SER:HB3	2.02	0.41
1:A:123:TYR:CE1	2:A:1500:PPG:N4A	2.89	0.41
1:G:223:ASP:OD1	1:G:225:GLN:N	2.54	0.41
1:B:11:ARG:HB2	1:B:19:TRP:CG	2.55	0.41
1:C:263:LYS:HG3	1:C:264:SER:N	2.35	0.41
2:C:3500:PPG:H4A1	2:C:3500:PPG:H5A1	1.84	0.41
1:C:89:THR:HG23	3:C:3535:HOH:O	2.18	0.41
1:D:263:LYS:CG	1:D:264:SER:N	2.83	0.41
1:E:52:GLY:HA3	1:E:283:ILE:HD13	2.01	0.41
1:E:45:ASN:ND2	1:F:62:LEU:HG	2.35	0.41
1:H:119:ILE:HD12	1:H:170:PHE:CE1	2.55	0.41
1:A:123:TYR:CD1	1:A:125:PRO:HD2	2.55	0.41
1:B:122:VAL:CG2	1:B:123:TYR:N	2.82	0.41
1:B:1:MET:HE1	1:B:48:GLU:HG3	2.02	0.41
1:E:172:SER:HA	1:E:173:PRO:C	2.40	0.41
1:F:216:HIS:CD2	3:F:6515:HOH:O	2.72	0.41
1:H:123:TYR:CD2	1:H:125:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:THR:HG22	1:C:66:GLY:N	2.36	0.41
1:E:336:LYS:HD3	1:E:336:LYS:HA	1.81	0.41
1:G:11:ARG:HG3	1:G:19:TRP:NE1	2.35	0.41
1:G:109:PHE:CZ	1:G:257:ILE:HG23	2.55	0.41
1:H:49:LEU:HA	1:H:283:ILE:HG21	2.03	0.41
1:C:220:GLN:HB3	1:C:230:THR:HG21	2.02	0.41
1:F:17:LEU:HD23	2:F:6500:PPG:NI	2.36	0.41
1:A:68:THR:O	1:A:71:TYR:HB3	2.21	0.41
1:D:112:PRO:HB3	1:D:134:GLU:HB3	2.03	0.41
3:C:3631:HOH:O	1:D:96:ALA:HB3	2.20	0.41
1:G:119:ILE:HG22	1:G:142:LEU:HG	2.02	0.41
1:H:205:ILE:HA	3:H:8605:HOH:O	2.21	0.41
1:A:345:PHE:O	1:A:349:LYS:HB2	2.20	0.41
1:B:143:LEU:O	1:B:149:TYR:HA	2.21	0.41
1:B:157:GLU:O	1:B:161:LYS:HD3	2.21	0.41
1:C:18:LYS:HD3	1:C:38:VAL:HB	2.03	0.41
1:H:107:ARG:HE	1:H:268:THR:HG21	1.85	0.41
1:H:46:PRO:HA	1:H:47:PRO:HD3	1.93	0.41
1:A:265:ARG:HG2	1:A:265:ARG:O	2.20	0.41
1:C:136:LYS:N	1:C:136:LYS:HD2	2.36	0.41
1:D:343:GLU:OE2	1:D:356:GLU:HG3	2.20	0.41
1:F:133:GLN:O	1:F:134:GLU:HB2	2.21	0.41
1:F:201:TRP:HB3	1:F:233:PHE:HE1	1.86	0.41
1:F:9:ILE:HG12	3:F:6522:HOH:O	2.20	0.41
1:G:172:SER:HA	1:G:173:PRO:C	2.41	0.41
1:H:123:TYR:CE1	2:H:8500:PPG:N4A	2.89	0.41
1:C:207:PHE:CD2	1:C:207:PHE:C	2.92	0.41
1:G:15:GLY:O	1:H:65:THR:HA	2.21	0.41
1:G:309:PHE:CZ	1:G:387:ASN:HB2	2.55	0.41
1:H:172:SER:O	1:H:204:GLU:HA	2.21	0.41
1:A:345:PHE:CE1	1:A:393:LEU:HD22	2.56	0.40
1:E:124:TYR:CD1	1:E:125:PRO:HD3	2.56	0.40
1:F:123:TYR:CG	1:F:125:PRO:HD2	2.56	0.40
1:G:394:LYS:NZ	3:G:7573:HOH:O	2.53	0.40
1:G:74:THR:OG1	1:G:286:LYS:HE3	2.21	0.40
1:A:268:THR:OG1	1:A:269:SER:N	2.53	0.40
1:A:70:GLU:OE2	1:A:70:GLU:HA	2.22	0.40
1:B:155:LYS:O	1:B:159:LEU:HG	2.21	0.40
1:C:122:VAL:CG2	1:C:123:TYR:N	2.84	0.40
1:D:188:LYS:HE2	1:D:188:LYS:HB3	1.90	0.40
1:D:353:PHE:HA	3:D:4636:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:PRO:HB3	1:E:134:GLU:HB3	2.03	0.40
1:E:163:LYS:CD	1:E:163:LYS:N	2.69	0.40
1:G:65:THR:HG22	1:G:66:GLY:N	2.36	0.40
1:B:393:LEU:O	1:B:394:LYS:CB	2.69	0.40
1:D:242:ILE:HB	1:D:245:MET:HG2	2.03	0.40
1:A:327:LEU:HB3	1:A:369:ARG:HD2	2.02	0.40
1:B:138:ILE:HG13	1:B:165:ASN:OD1	2.21	0.40
1:C:303:GLN:HG3	1:C:321:LEU:HD22	2.03	0.40
1:C:67:PRO:HD3	1:C:278:TYR:CE2	2.56	0.40
1:E:341:ALA:O	1:E:344:GLU:HB3	2.21	0.40
1:E:45:ASN:HB2	1:E:50:ILE:HD11	2.03	0.40
1:E:49:LEU:O	1:E:53:LEU:HG	2.21	0.40
1:E:75:VAL:O	1:E:79:MET:HG2	2.22	0.40
1:E:88:GLN:HB2	1:E:91:TRP:CD1	2.57	0.40
1:F:136:LYS:N	1:F:136:LYS:HD2	2.36	0.40
1:G:233:PHE:CD2	1:G:250:ILE:HD12	2.56	0.40
1:C:163:LYS:HG2	3:C:3612:HOH:O	2.21	0.40
1:C:198:LEU:O	1:C:229:LYS:HD2	2.22	0.40
1:C:266:ASP:HA	1:C:270:GLY:HA2	2.02	0.40
1:D:307:LYS:O	1:D:311:GLU:HG3	2.22	0.40
1:G:11:ARG:HB2	1:G:19:TRP:CG	2.56	0.40
1:H:106:VAL:O	1:H:110:THR:OG1	2.28	0.40
1:H:83:HIS:HE1	1:H:208:ASP:OD1	2.03	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	392/399 (98%)	368 (94%)	21 (5%)	3 (1%)	19	35
1	B	392/399 (98%)	371 (95%)	21 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	392/399 (98%)	372 (95%)	19 (5%)	1 (0%)	41	61
1	D	392/399 (98%)	375 (96%)	16 (4%)	1 (0%)	41	61
1	E	392/399 (98%)	374 (95%)	16 (4%)	2 (0%)	29	48
1	F	392/399 (98%)	377 (96%)	15 (4%)	0	100	100
1	G	392/399 (98%)	369 (94%)	22 (6%)	1 (0%)	41	61
1	H	392/399 (98%)	371 (95%)	21 (5%)	0	100	100
All	All	3136/3192 (98%)	2977 (95%)	151 (5%)	8 (0%)	41	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	LYS
1	A	274	THR
1	E	62	LEU
1	G	141	GLU
1	C	123	TYR
1	E	274	THR
1	A	38	VAL
1	A	246	GLY

### 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	353/358 (99%)	344 (98%)	9 (2%)	47	73
1	B	353/358 (99%)	343 (97%)	10 (3%)	43	70
1	C	353/358 (99%)	343 (97%)	10 (3%)	43	70
1	D	353/358 (99%)	343 (97%)	10 (3%)	43	70
1	E	353/358 (99%)	339 (96%)	14 (4%)	31	56
1	F	353/358 (99%)	341 (97%)	12 (3%)	37	63
1	G	353/358 (99%)	340 (96%)	13 (4%)	34	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	353/358 (99%)	344 (98%)	9 (2%)	47 73
All	All	2824/2864 (99%)	2737 (97%)	87 (3%)	40 67

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	GLU
1	A	163	LYS
1	A	176	PRO
1	A	195	LYS
1	A	207	PHE
1	A	219	PHE
1	A	301	LYS
1	A	355	ASP
1	A	394	LYS
1	B	134	GLU
1	B	163	LYS
1	B	176	PRO
1	B	195	LYS
1	B	207	PHE
1	B	219	PHE
1	B	275	THR
1	B	301	LYS
1	B	355	ASP
1	B	394	LYS
1	C	134	GLU
1	C	163	LYS
1	C	176	PRO
1	C	195	LYS
1	C	207	PHE
1	C	219	PHE
1	C	275	THR
1	C	301	LYS
1	C	355	ASP
1	C	394	LYS
1	D	134	GLU
1	D	161	LYS
1	D	163	LYS
1	D	176	PRO
1	D	195	LYS
1	D	207	PHE
1	D	219	PHE

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Mol	Chain	Res	Type
1	D	301	LYS
1	D	355	ASP
1	D	394	LYS
1	E	1	MET
1	E	84	GLN
1	E	134	GLU
1	E	161	LYS
1	E	163	LYS
1	E	176	PRO
1	E	184	ASP
1	E	195	LYS
1	E	199	MET
1	E	207	PHE
1	E	219	PHE
1	E	301	LYS
1	E	355	ASP
1	E	394	LYS
1	F	11	ARG
1	F	134	GLU
1	F	163	LYS
1	F	176	PRO
1	F	195	LYS
1	F	207	PHE
1	F	219	PHE
1	F	275	THR
1	F	301	LYS
1	F	326	TYR
1	F	355	ASP
1	F	394	LYS
1	G	134	GLU
1	G	161	LYS
1	G	163	LYS
1	G	176	PRO
1	G	195	LYS
1	G	207	PHE
1	G	219	PHE
1	G	238	LYS
1	G	274	THR
1	G	301	LYS
1	G	329	TRP
1	G	355	ASP
1	G	394	LYS

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Mol	Chain	Res	Type
1	H	134	GLU
1	H	161	LYS
1	H	163	LYS
1	H	195	LYS
1	H	207	PHE
1	H	219	PHE
1	H	301	LYS
1	H	355	ASP
1	H	394	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	45	ASN
1	A	154	GLN
1	A	187	GLN
1	A	206	HIS
1	A	216	HIS
1	A	225	GLN
1	A	387	ASN
1	B	13	ASN
1	B	25	GLN
1	B	45	ASN
1	B	83	HIS
1	B	154	GLN
1	B	187	GLN
1	B	206	HIS
1	B	216	HIS
1	C	25	GLN
1	C	45	ASN
1	C	94	ASN
1	C	154	GLN
1	C	187	GLN
1	C	206	HIS
1	C	216	HIS
1	C	249	ASN
1	D	25	GLN
1	D	45	ASN
1	D	83	HIS
1	D	154	GLN
1	D	187	GLN

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Mol	Chain	Res	Type
1	D	206	HIS
1	D	216	HIS
1	D	225	GLN
1	E	25	GLN
1	E	45	ASN
1	E	154	GLN
1	E	187	GLN
1	E	206	HIS
1	E	216	HIS
1	E	313	ASN
1	F	25	GLN
1	F	45	ASN
1	F	154	GLN
1	F	187	GLN
1	F	206	HIS
1	F	216	HIS
1	G	25	GLN
1	G	45	ASN
1	G	83	HIS
1	G	187	GLN
1	G	206	HIS
1	G	216	HIS
1	G	225	GLN
1	G	339	HIS
1	G	387	ASN
1	H	13	ASN
1	H	25	GLN
1	H	45	ASN
1	H	154	GLN
1	H	187	GLN
1	H	206	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PPG	E	5500	-	24,26,26	3.94	9 (37%)	22,35,35	2.38	9 (40%)
2	PPG	H	8500	-	24,26,26	3.05	8 (33%)	22,35,35	2.64	8 (36%)
2	PPG	B	2500	-	24,26,26	3.83	7 (29%)	22,35,35	2.61	10 (45%)
2	PPG	G	7500	-	24,26,26	2.91	8 (33%)	22,35,35	2.09	8 (36%)
2	PPG	C	3500	-	24,26,26	2.89	8 (33%)	22,35,35	2.57	9 (40%)
2	PPG	F	6500	-	24,26,26	3.28	5 (20%)	22,35,35	2.48	9 (40%)
2	PPG	A	1500	-	24,26,26	3.40	8 (33%)	22,35,35	1.98	7 (31%)
2	PPG	D	4500	-	24,26,26	2.96	6 (25%)	22,35,35	2.41	9 (40%)

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	PPG	E	5500	-	-	4/16/21/21	0/1/1/1
2	PPG	H	8500	-	-	6/16/21/21	0/1/1/1
2	PPG	B	2500	-	-	5/16/21/21	0/1/1/1
2	PPG	G	7500	-	-	3/16/21/21	0/1/1/1
2	PPG	C	3500	-	-	6/16/21/21	0/1/1/1
2	PPG	F	6500	-	-	4/16/21/21	0/1/1/1
2	PPG	A	1500	-	-	5/16/21/21	0/1/1/1
2	PPG	D	4500	-	-	5/16/21/21	0/1/1/1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5500	PPG	CAI-N4A	14.48	1.53	1.30
2	B	2500	PPG	CAI-N4A	11.70	1.48	1.30
2	A	1500	PPG	CAI-N4A	11.03	1.47	1.30
2	B	2500	PPG	C5-C4	10.57	1.55	1.40
2	F	6500	PPG	CAI-N4A	10.20	1.46	1.30
2	H	8500	PPG	CAI-N4A	9.84	1.45	1.30
2	F	6500	PPG	C5-C4	9.82	1.54	1.40
2	D	4500	PPG	CAI-N4A	9.56	1.45	1.30
2	A	1500	PPG	C5-C4	8.31	1.52	1.40
2	C	3500	PPG	CAI-N4A	7.95	1.42	1.30
2	D	4500	PPG	C5-C4	7.94	1.51	1.40
2	C	3500	PPG	C3-C2	7.74	1.48	1.40
2	E	5500	PPG	C5-C4	7.73	1.51	1.40
2	G	7500	PPG	CAI-N4A	7.61	1.42	1.30
2	G	7500	PPG	C5-C4	7.44	1.50	1.40
2	B	2500	PPG	C3-C2	7.32	1.48	1.40
2	H	8500	PPG	C5-C4	7.16	1.50	1.40
2	A	1500	PPG	C3-C2	6.42	1.47	1.40
2	C	3500	PPG	C5-C4	6.01	1.48	1.40
2	E	5500	PPG	C3-C2	5.43	1.46	1.40
2	H	8500	PPG	C3-C2	5.21	1.46	1.40
2	D	4500	PPG	C3-C2	4.51	1.45	1.40
2	G	7500	PPG	CBC-CAI	-4.27	1.45	1.52
2	E	5500	PPG	CBI-CAI	-4.22	1.38	1.46
2	F	6500	PPG	C3-C2	4.06	1.45	1.40
2	F	6500	PPG	C2-N1	3.98	1.41	1.33
2	G	7500	PPG	CBI-CAI	-3.97	1.39	1.46
2	G	7500	PPG	C2-N1	3.97	1.41	1.33
2	E	5500	PPG	C4A-N4A	-3.87	1.40	1.46
2	B	2500	PPG	C2-N1	3.61	1.40	1.33
2	E	5500	PPG	CBI-CGI	3.19	1.44	1.32
2	F	6500	PPG	CBI-CGI	3.16	1.44	1.32
2	E	5500	PPG	C2-N1	3.14	1.39	1.33
2	B	2500	PPG	CBI-CGI	3.12	1.44	1.32
2	D	4500	PPG	C2-N1	3.07	1.39	1.33
2	G	7500	PPG	C3-C2	2.93	1.43	1.40
2	A	1500	PPG	C2-N1	2.87	1.39	1.33
2	A	1500	PPG	C5A-C5	2.75	1.58	1.50
2	C	3500	PPG	C3-C4	2.74	1.44	1.40
2	H	8500	PPG	C2-N1	2.71	1.39	1.33
2	B	2500	PPG	C5A-C5	2.70	1.58	1.50
2	H	8500	PPG	C3-C4	2.70	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	PPG	CBI-CGI	2.67	1.42	1.32
2	G	7500	PPG	C4A-C4	2.65	1.58	1.52
2	D	4500	PPG	C4A-C4	2.64	1.58	1.52
2	H	8500	PPG	P-OP3	-2.64	1.44	1.54
2	C	3500	PPG	C4A-N4A	-2.61	1.42	1.46
2	H	8500	PPG	CBI-CGI	2.60	1.42	1.32
2	E	5500	PPG	C3-C4	2.59	1.44	1.40
2	C	3500	PPG	C2-N1	2.59	1.38	1.33
2	A	1500	PPG	OET-CGI	2.56	1.46	1.36
2	C	3500	PPG	CBI-CGI	2.47	1.41	1.32
2	G	7500	PPG	CBI-CGI	2.39	1.41	1.32
2	H	8500	PPG	C2A-C2	2.26	1.54	1.50
2	A	1500	PPG	OET-CEI	2.15	1.50	1.43
2	B	2500	PPG	CBI-CAI	2.14	1.49	1.46
2	C	3500	PPG	P-OP3	-2.11	1.46	1.54
2	D	4500	PPG	CBI-CGI	2.04	1.40	1.32
2	E	5500	PPG	P-OP3	-2.01	1.47	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8500	PPG	C2A-C2-C3	8.03	130.81	120.89
2	C	3500	PPG	C2A-C2-C3	7.82	130.55	120.89
2	B	2500	PPG	C2A-C2-C3	6.15	128.49	120.89
2	E	5500	PPG	C2A-C2-C3	6.14	128.47	120.89
2	D	4500	PPG	C2A-C2-C3	6.09	128.41	120.89
2	F	6500	PPG	C2A-C2-C3	5.28	127.41	120.89
2	A	1500	PPG	C2A-C2-C3	5.14	127.24	120.89
2	G	7500	PPG	C2A-C2-C3	4.97	127.02	120.89
2	F	6500	PPG	C4A-C4-C5	4.90	125.65	119.73
2	H	8500	PPG	C6-N1-C2	4.72	127.91	119.17
2	B	2500	PPG	OP2-P-OP4	-4.49	94.77	106.73
2	H	8500	PPG	C3-C2-N1	-4.40	115.08	120.77
2	D	4500	PPG	C4A-C4-C5	4.22	124.82	119.73
2	C	3500	PPG	C6-N1-C2	3.95	126.48	119.17
2	F	6500	PPG	C6-N1-C2	3.93	126.45	119.17
2	E	5500	PPG	C6-N1-C2	3.87	126.33	119.17
2	C	3500	PPG	C3-C2-N1	-3.82	115.83	120.77
2	B	2500	PPG	C6-N1-C2	3.77	126.15	119.17
2	B	2500	PPG	C4A-C4-C5	3.67	124.16	119.73
2	A	1500	PPG	C4A-C4-C5	3.65	124.13	119.73
2	D	4500	PPG	C6-N1-C2	3.65	125.92	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5500	PPG	C4A-C4-C5	3.64	124.12	119.73
2	C	3500	PPG	C6-C5-C4	3.54	120.62	118.12
2	G	7500	PPG	C6-N1-C2	3.50	125.66	119.17
2	F	6500	PPG	O3-C3-C4	3.50	128.39	118.13
2	E	5500	PPG	C6-C5-C4	3.39	120.51	118.12
2	D	4500	PPG	C3-C2-N1	-3.38	116.40	120.77
2	F	6500	PPG	C5-C6-N1	-3.37	118.20	123.82
2	G	7500	PPG	C3-C2-N1	-3.35	116.44	120.77
2	G	7500	PPG	C4A-C4-C5	3.34	123.76	119.73
2	E	5500	PPG	C3-C2-N1	-3.23	116.60	120.77
2	A	1500	PPG	C6-N1-C2	3.21	125.12	119.17
2	B	2500	PPG	O3-C3-C4	3.19	127.48	118.13
2	H	8500	PPG	O3-C3-C4	3.19	127.48	118.13
2	D	4500	PPG	OP2-P-OP4	-3.14	98.37	106.73
2	F	6500	PPG	O3-C3-C2	-3.10	110.73	117.49
2	F	6500	PPG	C6-C5-C4	3.07	120.29	118.12
2	G	7500	PPG	C5-C6-N1	-3.06	118.72	123.82
2	C	3500	PPG	O3-C3-C4	3.06	127.10	118.13
2	B	2500	PPG	C5-C6-N1	-3.03	118.78	123.82
2	E	5500	PPG	O3-C3-C4	2.95	126.80	118.13
2	D	4500	PPG	O3-C3-C4	2.95	126.79	118.13
2	B	2500	PPG	C6-C5-C4	2.93	120.19	118.12
2	A	1500	PPG	O3-C3-C4	2.91	126.67	118.13
2	B	2500	PPG	O3-C3-C2	-2.88	111.22	117.49
2	F	6500	PPG	C3-C2-N1	-2.80	117.15	120.77
2	B	2500	PPG	C3-C2-N1	-2.76	117.20	120.77
2	G	7500	PPG	C6-C5-C4	2.71	120.04	118.12
2	A	1500	PPG	C3-C2-N1	-2.70	117.27	120.77
2	H	8500	PPG	C5-C6-N1	-2.70	119.33	123.82
2	D	4500	PPG	C5-C6-N1	-2.55	119.57	123.82
2	G	7500	PPG	O3-C3-C4	2.53	125.54	118.13
2	E	5500	PPG	C5-C6-N1	-2.52	119.63	123.82
2	E	5500	PPG	C3-C4-C5	-2.48	116.34	118.72
2	D	4500	PPG	O3-C3-C2	-2.47	112.12	117.49
2	B	2500	PPG	C3-C4-C5	-2.43	116.39	118.72
2	C	3500	PPG	OP2-P-OP4	-2.39	100.38	106.73
2	C	3500	PPG	C5-C6-N1	-2.39	119.84	123.82
2	F	6500	PPG	OP2-P-OP4	-2.28	100.67	106.73
2	D	4500	PPG	C6-C5-C4	2.28	119.73	118.12
2	E	5500	PPG	O3-C3-C2	-2.26	112.57	117.49
2	A	1500	PPG	O3-C3-C2	-2.19	112.71	117.49
2	H	8500	PPG	OP4-C5A-C5	2.18	113.50	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8500	PPG	O3-C3-C2	-2.17	112.76	117.49
2	G	7500	PPG	OP2-P-OP4	-2.15	101.02	106.73
2	A	1500	PPG	C5-C6-N1	-2.13	120.27	123.82
2	H	8500	PPG	OP2-P-OP4	-2.12	101.09	106.73
2	C	3500	PPG	C2A-C2-N1	-2.08	113.61	117.67
2	C	3500	PPG	O3-C3-C2	-2.07	112.98	117.49

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5500	PPG	CBI-CAI-N4A-C4A
2	E	5500	PPG	N4A-CAI-CBI-CGI
2	E	5500	PPG	CBC-CAI-CBI-CGI
2	E	5500	PPG	CAI-CBI-CGI-OET
2	H	8500	PPG	CBI-CAI-N4A-C4A
2	H	8500	PPG	N4A-CAI-CBI-CGI
2	H	8500	PPG	CBC-CAI-CBI-CGI
2	B	2500	PPG	C5A-OP4-P-OP1
2	B	2500	PPG	CBI-CAI-N4A-C4A
2	B	2500	PPG	CAI-CBI-CGI-OET
2	G	7500	PPG	CBI-CAI-N4A-C4A
2	G	7500	PPG	CAI-CBI-CGI-OET
2	C	3500	PPG	CBI-CAI-N4A-C4A
2	C	3500	PPG	N4A-CAI-CBI-CGI
2	C	3500	PPG	CBC-CAI-CBI-CGI
2	C	3500	PPG	CAI-CBI-CGI-OET
2	F	6500	PPG	CBI-CAI-N4A-C4A
2	F	6500	PPG	CAI-CBI-CGI-OET
2	A	1500	PPG	CBI-CAI-N4A-C4A
2	A	1500	PPG	N4A-CAI-CBI-CGI
2	A	1500	PPG	CBC-CAI-CBI-CGI
2	A	1500	PPG	CAI-CBI-CGI-OET
2	D	4500	PPG	CBI-CAI-N4A-C4A
2	D	4500	PPG	CAI-CBI-CGI-OET
2	C	3500	PPG	C5-C4-C4A-N4A
2	C	3500	PPG	C3-C4-C4A-N4A
2	B	2500	PPG	N4A-CAI-CBI-CGI
2	F	6500	PPG	N4A-CAI-CBI-CGI
2	B	2500	PPG	CBC-CAI-CBI-CGI
2	F	6500	PPG	CBC-CAI-CBI-CGI
2	H	8500	PPG	C3-C4-C4A-N4A

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Mol	Chain	Res	Type	Atoms
2	H	8500	PPG	C5A-OP4-P-OP1
2	D	4500	PPG	C5A-OP4-P-OP1
2	H	8500	PPG	C5-C4-C4A-N4A
2	D	4500	PPG	N4A-CAI-CBI-CGI
2	G	7500	PPG	C6-C5-C5A-OP4
2	A	1500	PPG	CFI-CEI-OET-CGI
2	D	4500	PPG	CBC-CAI-CBI-CGI

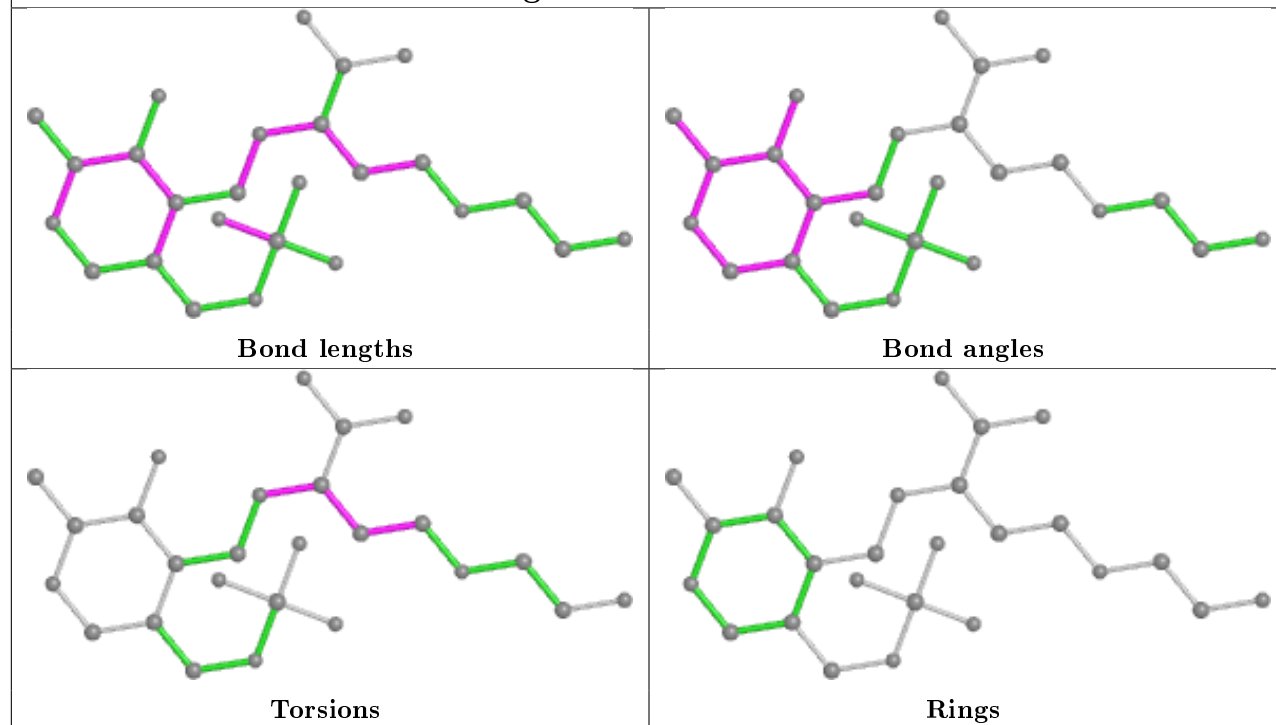
There are no ring outliers.

8 monomers are involved in 32 short contacts:

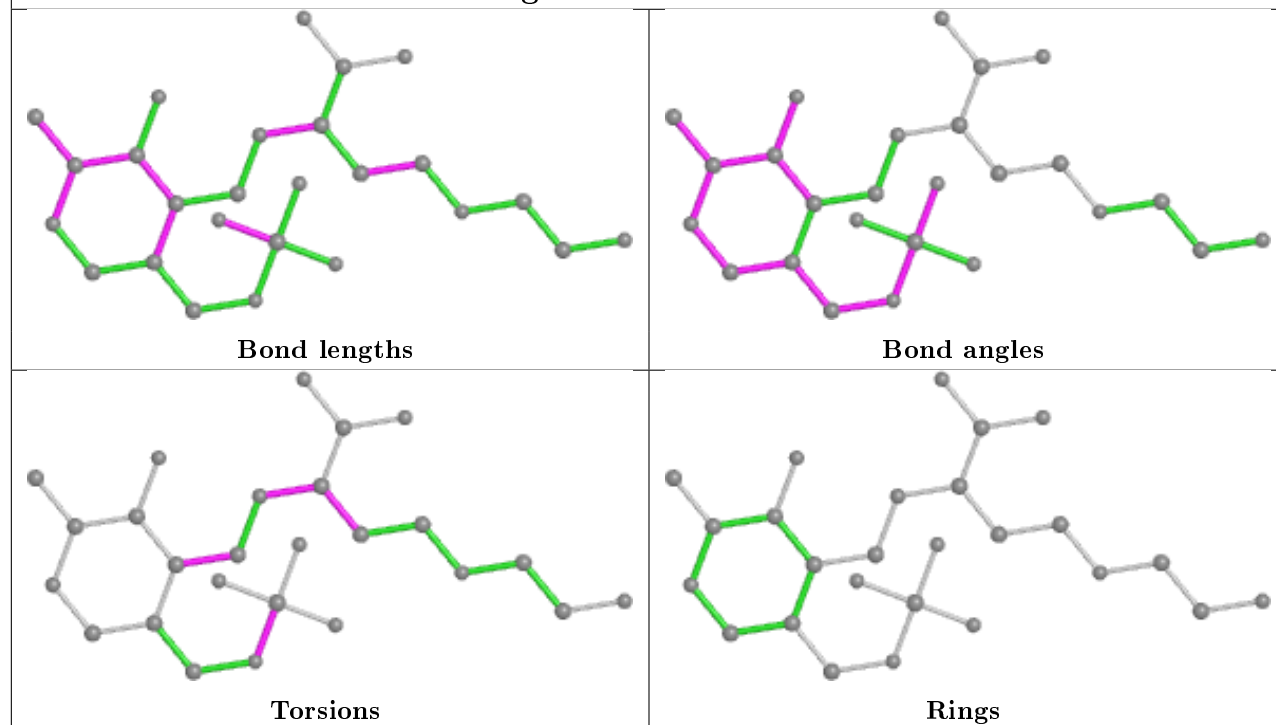
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	5500	PPG	3	0
2	H	8500	PPG	3	0
2	B	2500	PPG	4	0
2	G	7500	PPG	4	0
2	C	3500	PPG	4	0
2	F	6500	PPG	3	0
2	A	1500	PPG	7	0
2	D	4500	PPG	4	0

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.

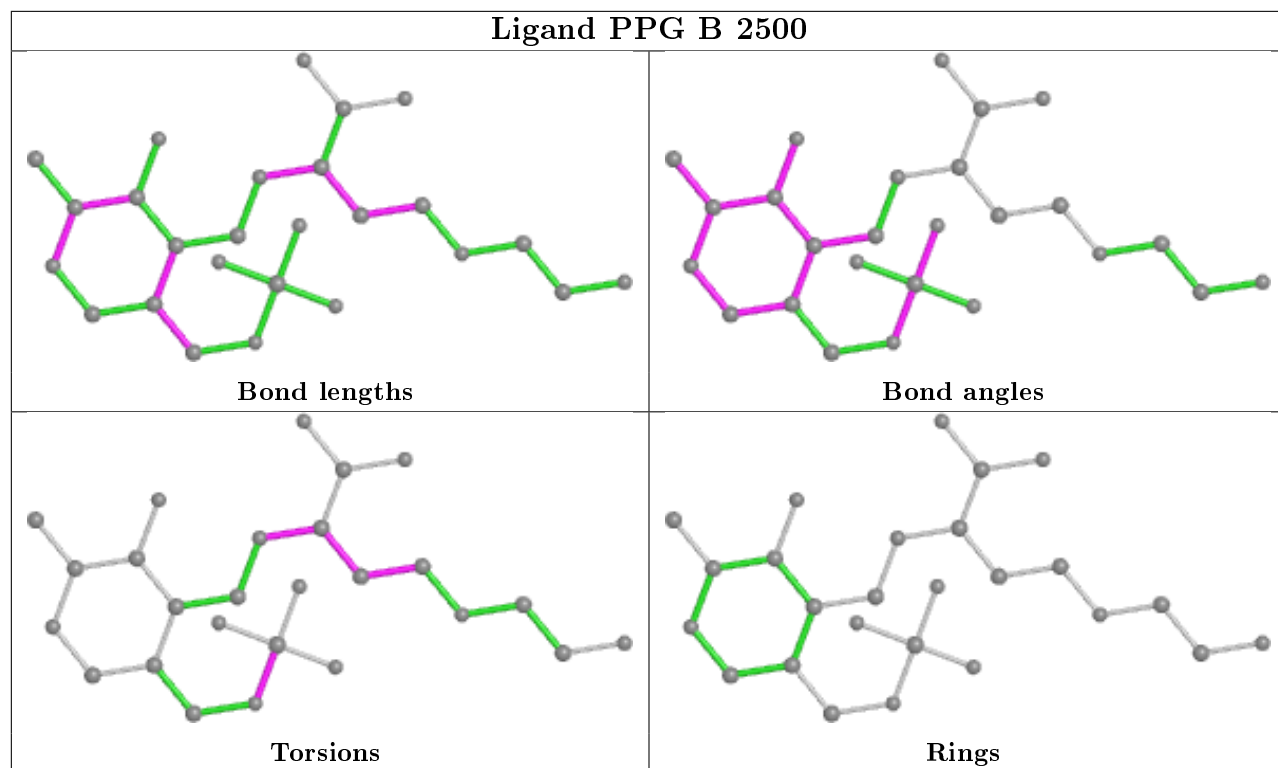
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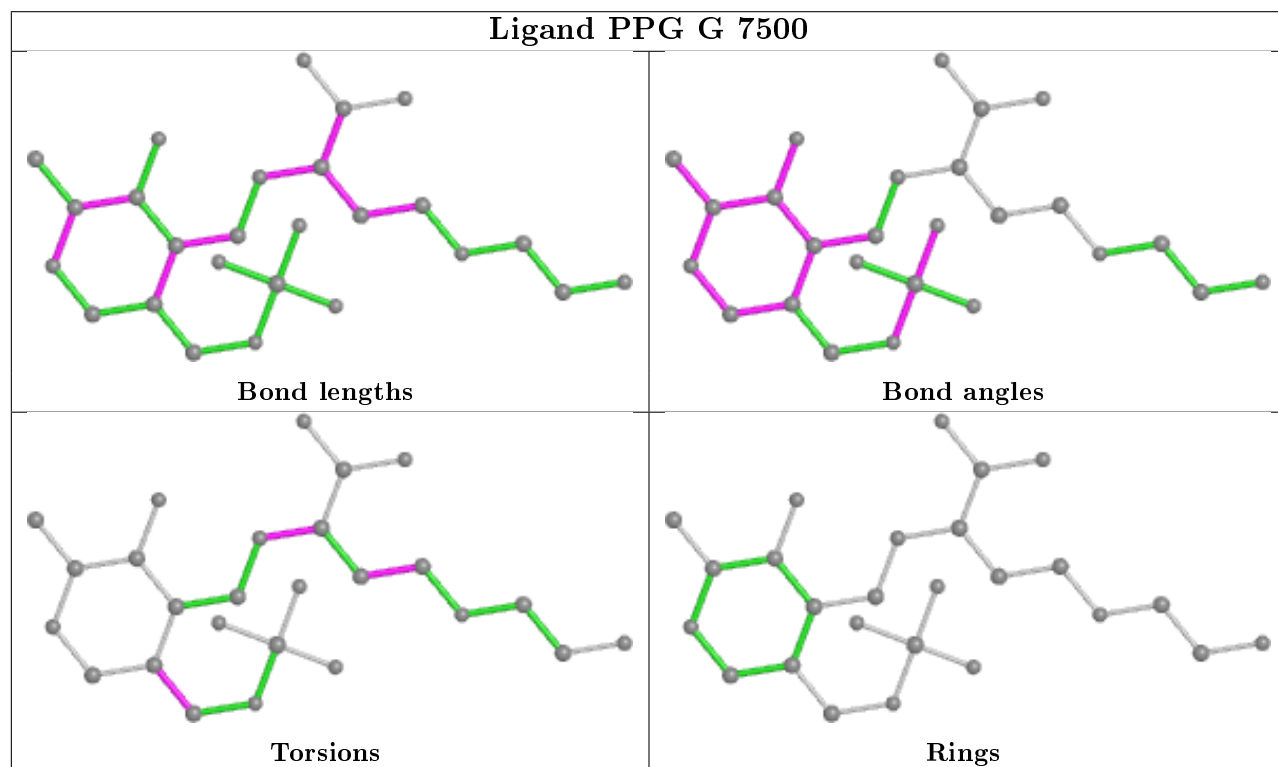
## Ligand PPG H 8500



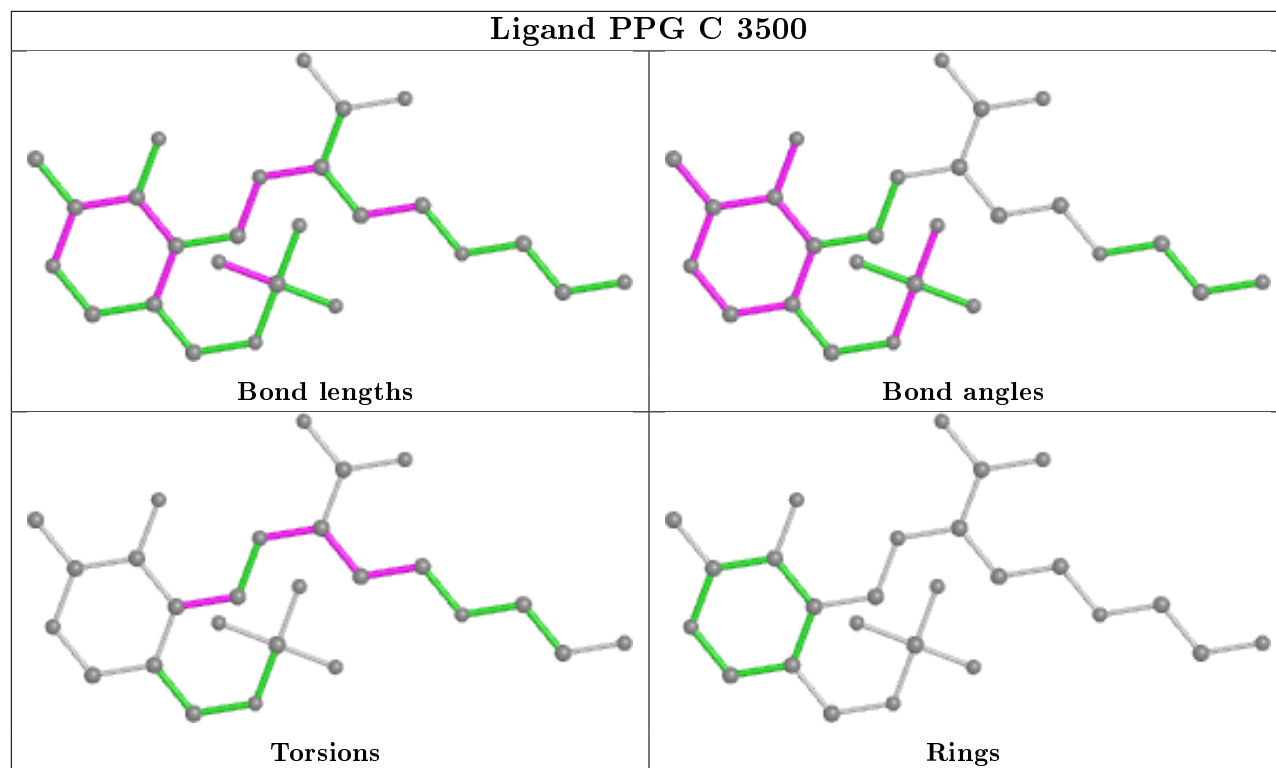
## Ligand PPG B 2500



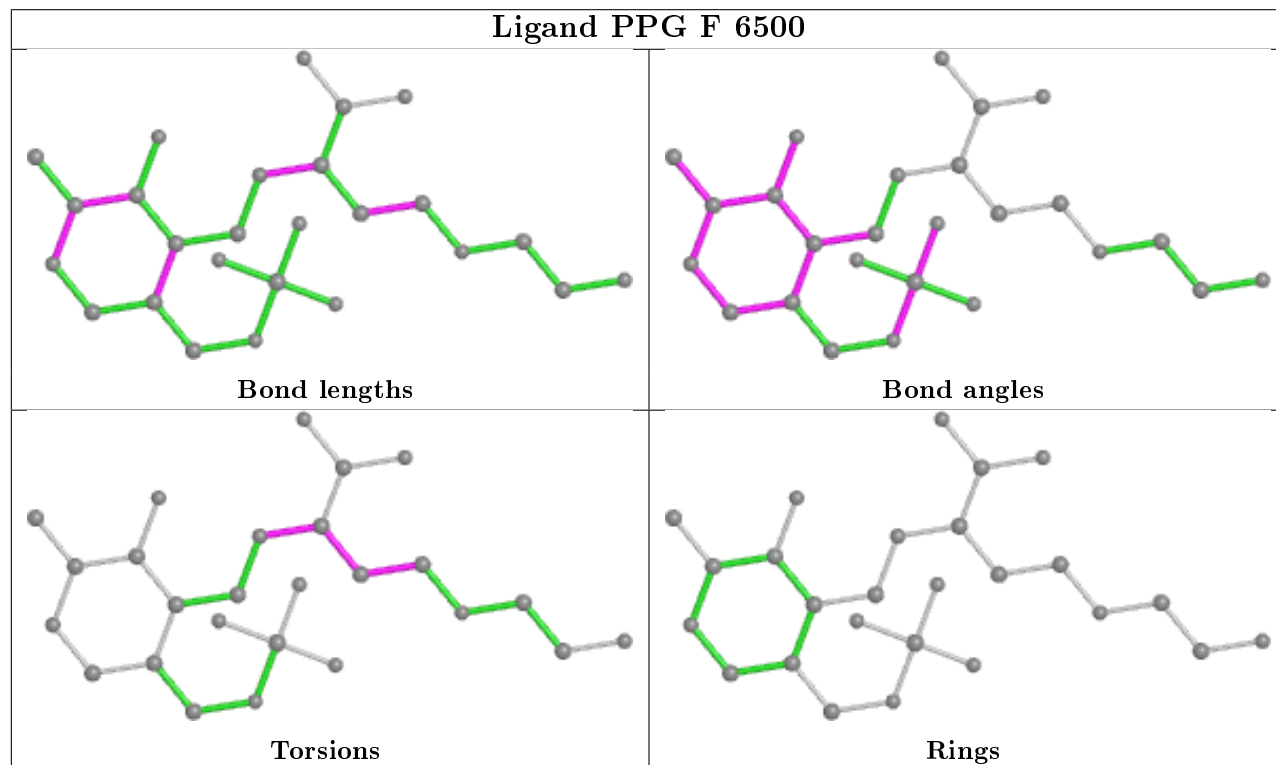
## Ligand PPG G 7500

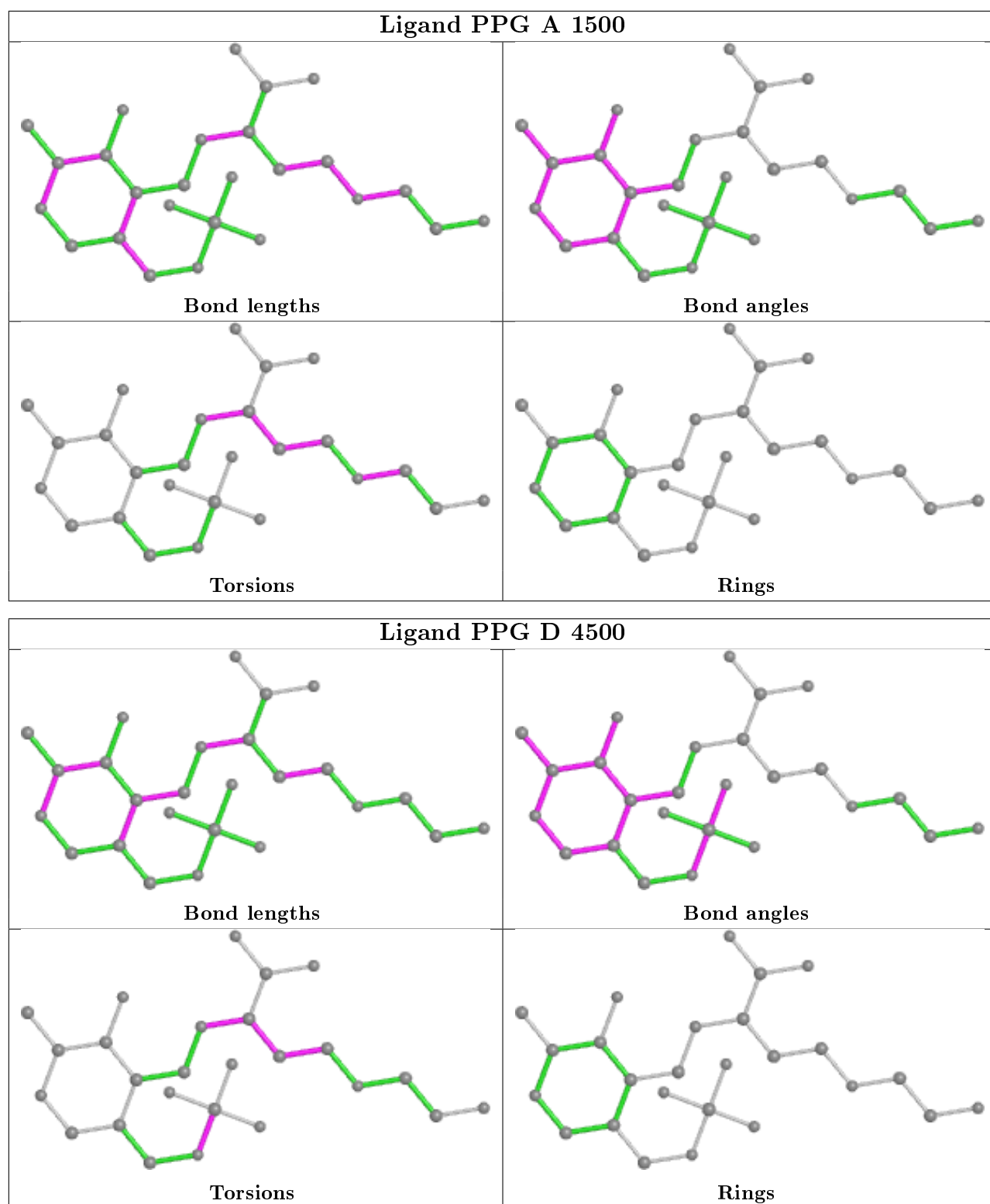


## Ligand PPG C 3500



## Ligand PPG F 6500





## 5.7 Other polymers ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	394/399 (98%)	-0.54	3 (0%) 86 87	19, 30, 44, 71	0
1	B	394/399 (98%)	-0.69	1 (0%) 94 94	12, 23, 36, 70	0
1	C	394/399 (98%)	-0.61	2 (0%) 91 91	17, 28, 42, 78	0
1	D	394/399 (98%)	-0.48	5 (1%) 77 79	19, 32, 48, 69	0
1	E	394/399 (98%)	-0.52	1 (0%) 94 94	18, 32, 48, 64	0
1	F	394/399 (98%)	-0.67	2 (0%) 91 91	12, 24, 38, 72	0
1	G	394/399 (98%)	-0.49	2 (0%) 91 91	19, 33, 46, 57	0
1	H	394/399 (98%)	-0.51	1 (0%) 94 94	16, 30, 47, 74	0
All	All	3152/3192 (98%)	-0.56	17 (0%) 91 91	12, 29, 45, 78	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	9.3
1	H	1	MET	5.4
1	F	1	MET	5.0
1	B	1	MET	4.7
1	A	2	ILE	4.3
1	D	1	MET	3.6
1	A	1	MET	3.0
1	D	2	ILE	2.9
1	D	246	GLY	2.8
1	G	23	TYR	2.6
1	D	195	LYS	2.5
1	F	2	ILE	2.5
1	G	184	ASP	2.4
1	D	23	TYR	2.2
1	C	2	ILE	2.1
1	A	246	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	23	TYR	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

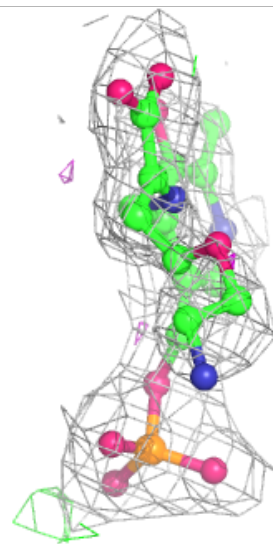
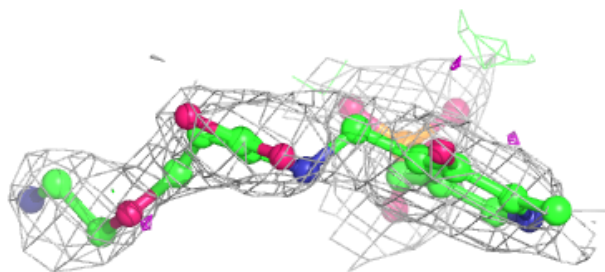
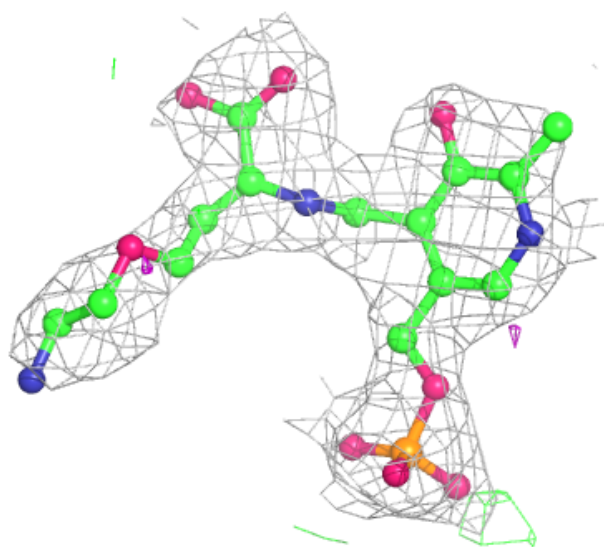
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PPG	G	7500	26/26	0.90	0.19	37,45,56,58	0
2	PPG	E	5500	26/26	0.94	0.15	28,39,52,53	0
2	PPG	D	4500	26/26	0.95	0.14	34,40,49,54	0
2	PPG	H	8500	26/26	0.96	0.14	30,35,55,55	0
2	PPG	C	3500	26/26	0.96	0.11	32,37,54,57	0
2	PPG	B	2500	26/26	0.96	0.13	27,32,47,51	0
2	PPG	A	1500	26/26	0.97	0.11	33,37,50,51	0
2	PPG	F	6500	26/26	0.97	0.12	17,26,44,45	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.



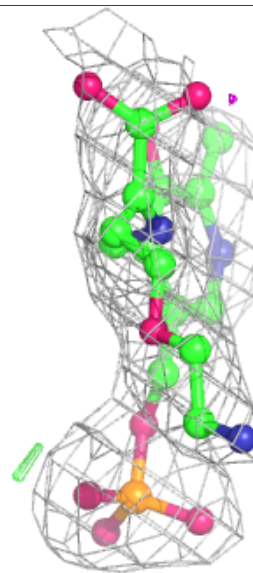
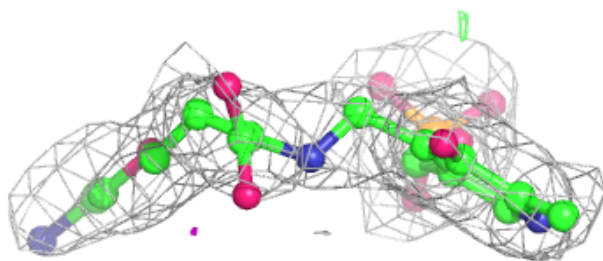
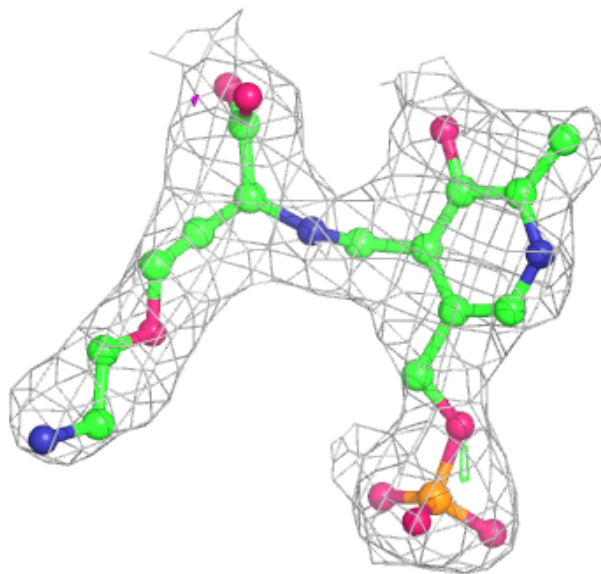
**Electron density around PPG G 7500:**

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



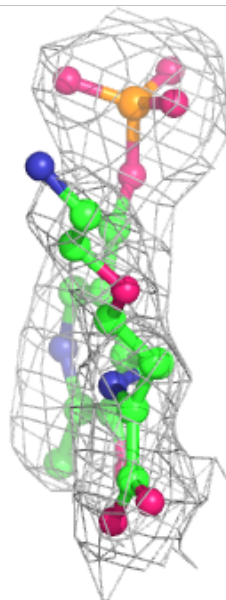
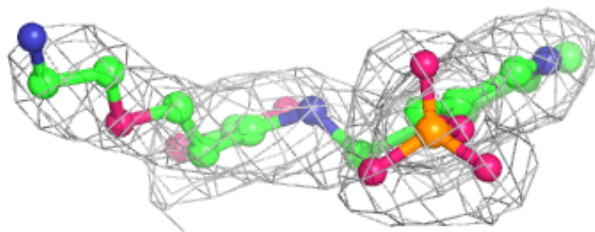
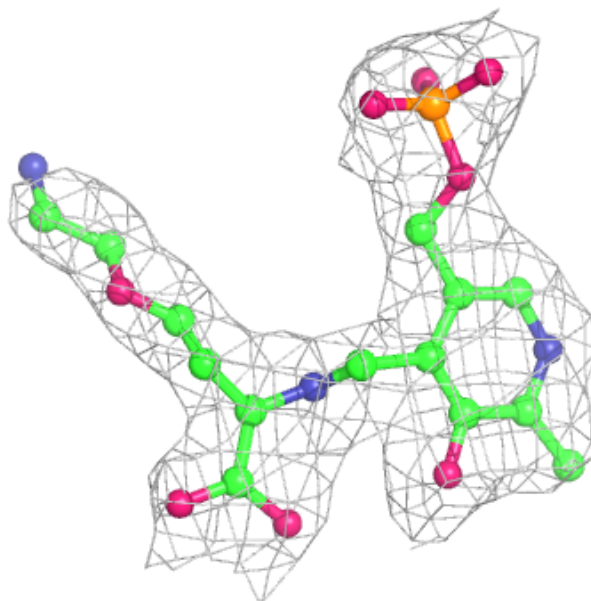
**Electron density around PPG E 5500:**

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



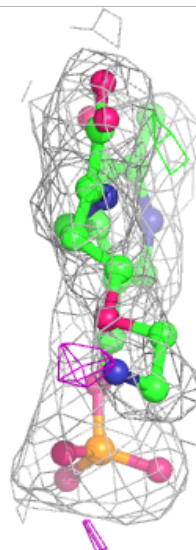
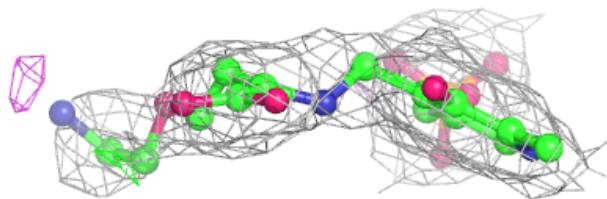
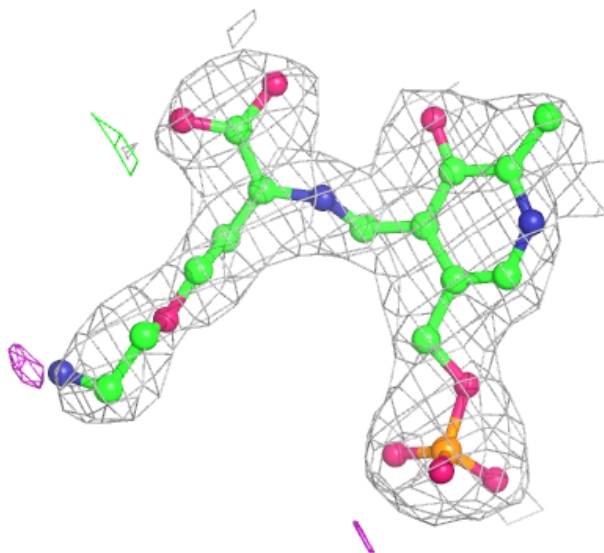
**Electron density around PPG D 4500:**

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



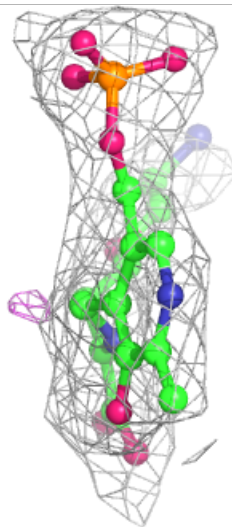
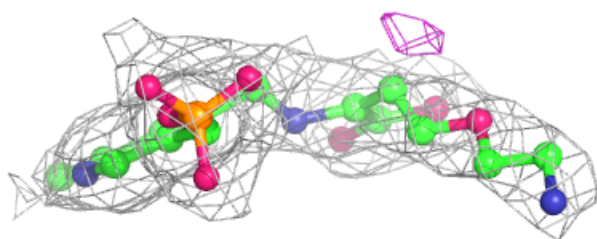
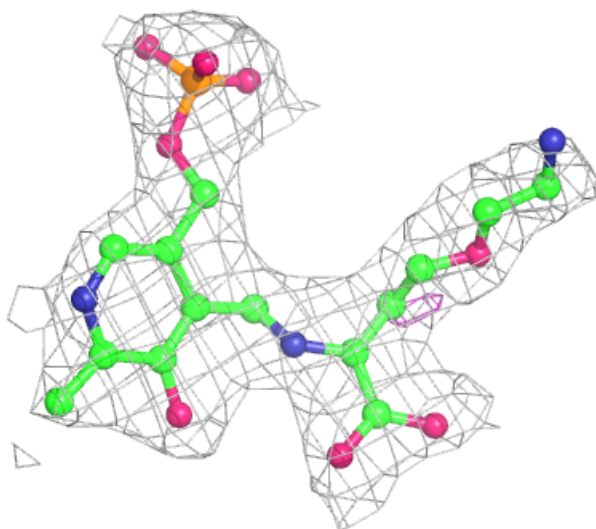
**Electron density around PPG H 8500:**

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



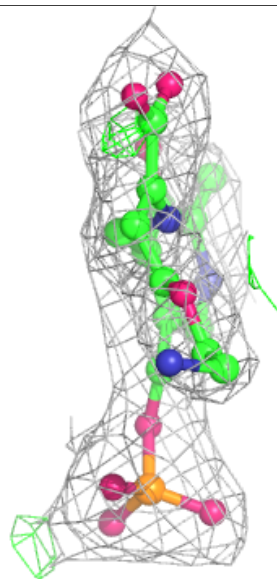
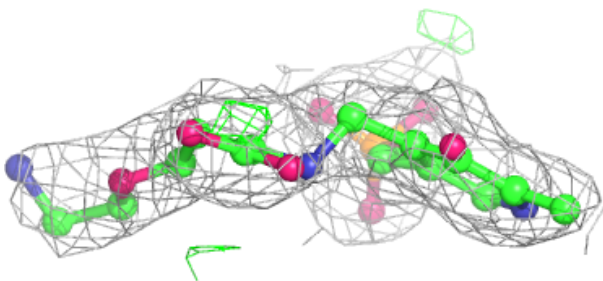
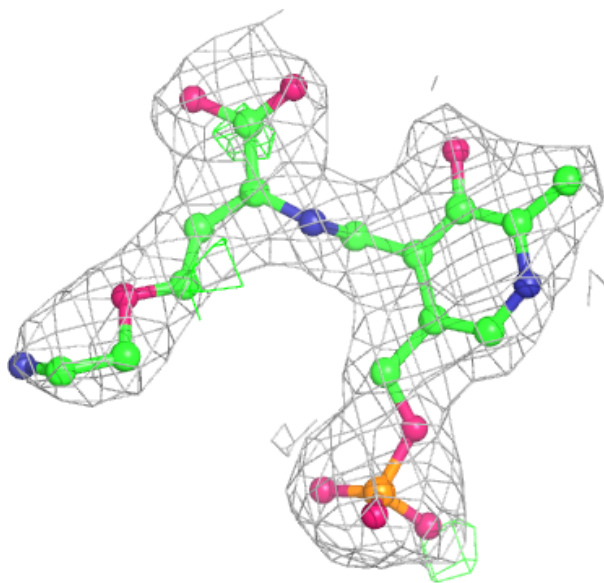
**Electron density around PPG C 3500:**

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



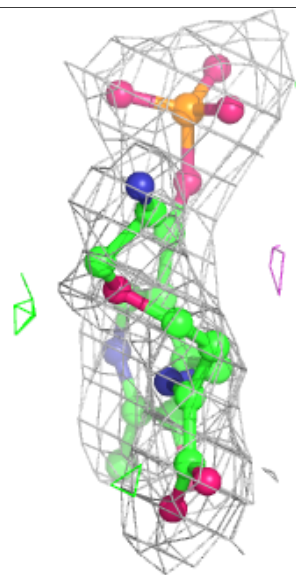
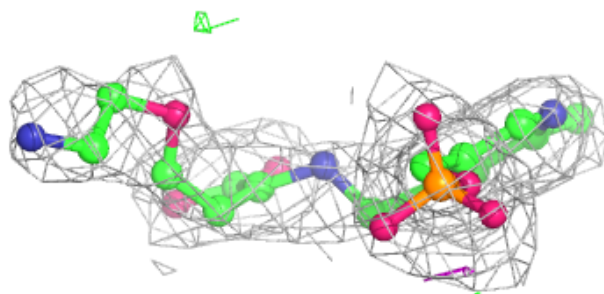
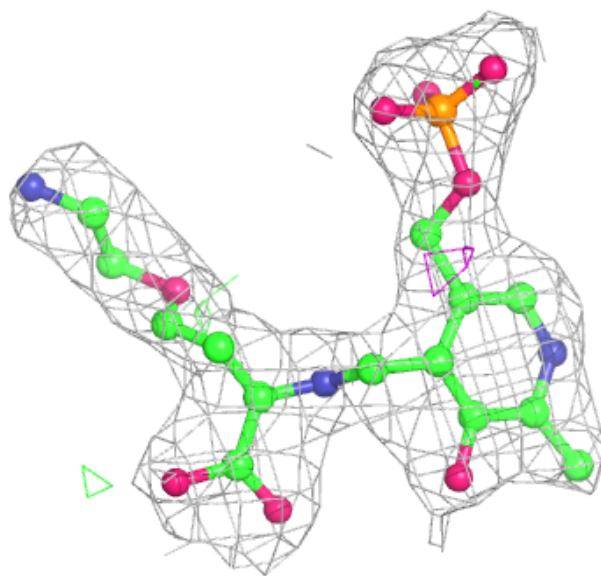
**Electron density around PPG B 2500:**

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



**Electron density around PPG A 1500:**

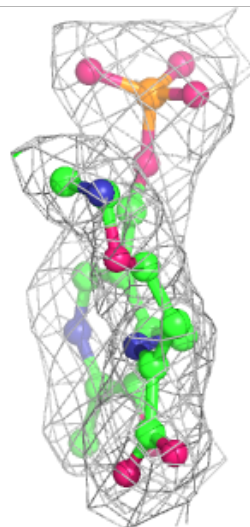
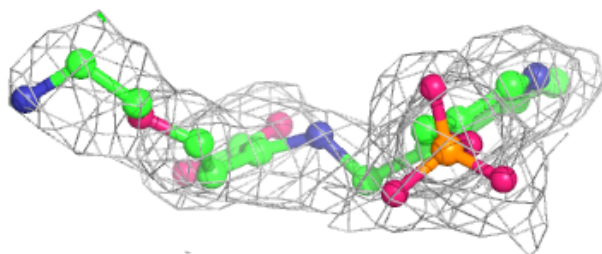
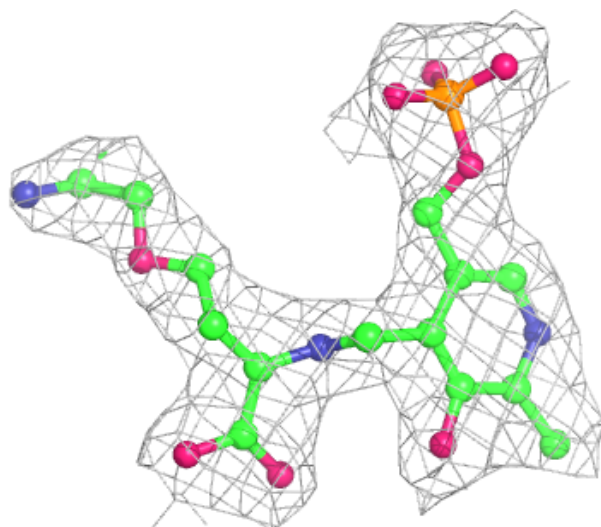
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PPG F 6500:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.