Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 10:54 PM EST

PDB ID	:	3VB0
Title	:	Crystal structure of 2,2',3-trihydroxybiphenyl 1,2-dioxygenase from dibenzofuran-degrading Sphingomonas wittichii strain RW1
Authors	:	Koksal, M.; Kumar, P.; Bolin, J.T.
Deposited on	:	2011-12-30
Resolution	:	2.10 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:

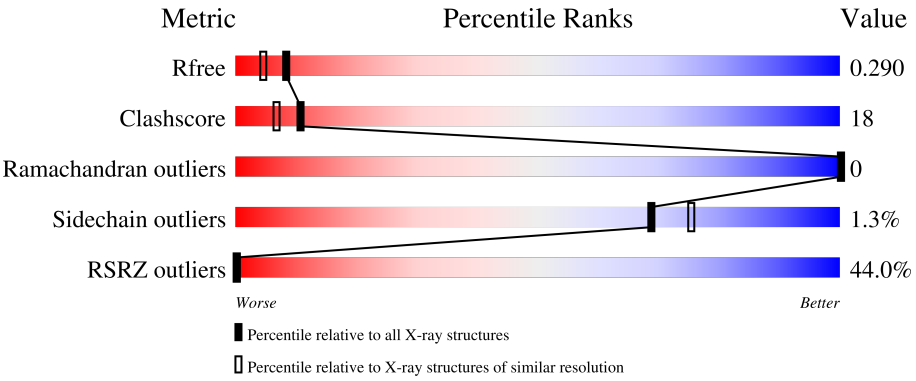
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	294	12% 90% 8% ·
1	B	294	15% 88% 10% ·
1	C	294	68% 58% 39% ··
1	D	294	79% 61% 36% ··

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	P6G	B	302	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9162 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.

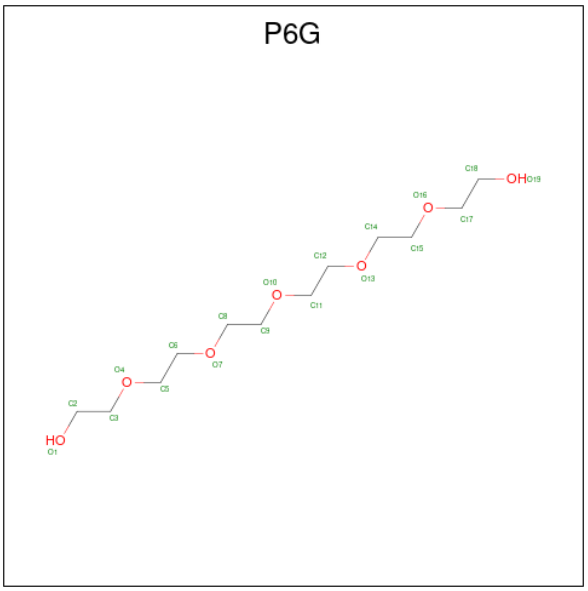
- Molecule 1 is a protein called Glyoxalase/bleomycin resistance protein/dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2238	1429	384	415	10			
1	B	289	Total	C	N	O	S	0	0	0
			2238	1429	384	415	10			
1	C	289	Total	C	N	O	S	0	0	0
			2238	1429	384	415	10			
1	D	289	Total	C	N	O	S	0	0	0
			2238	1429	384	415	10			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

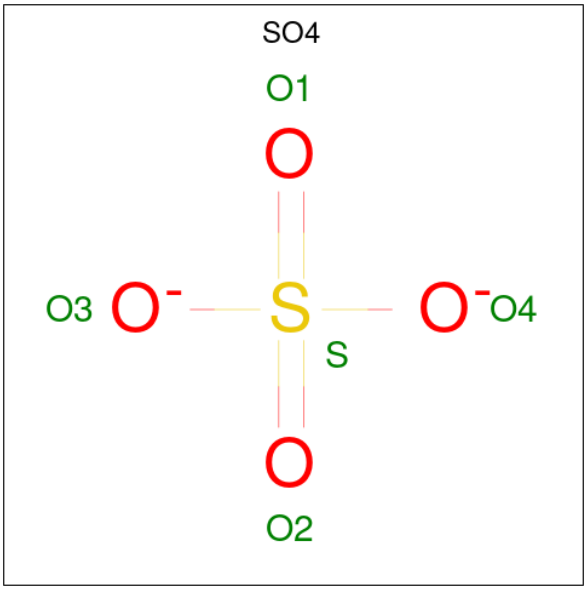
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 19 12 7	0	0
3	B	1	Total C O 19 12 7	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

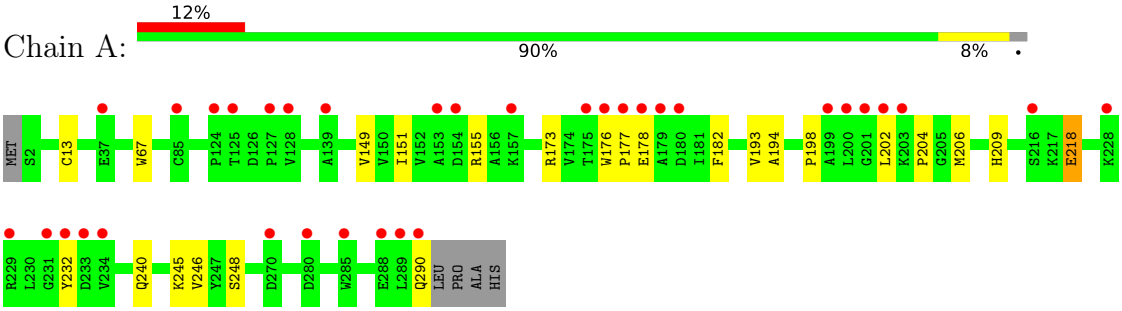
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	77	Total O 77 77	0	0
5	B	80	Total O 80 80	0	0
5	C	1	Total O 1 1	0	0

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.

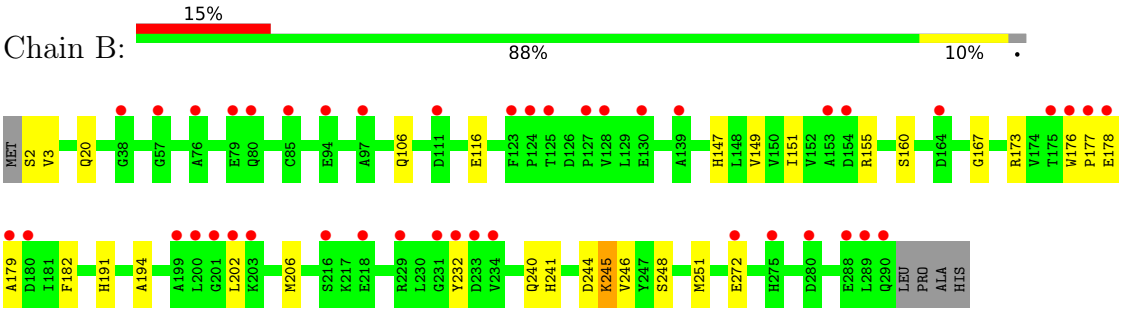
• Molecule 1: Glyoxalase/bleomycin resistance protein/dioxygenase

Chain A:



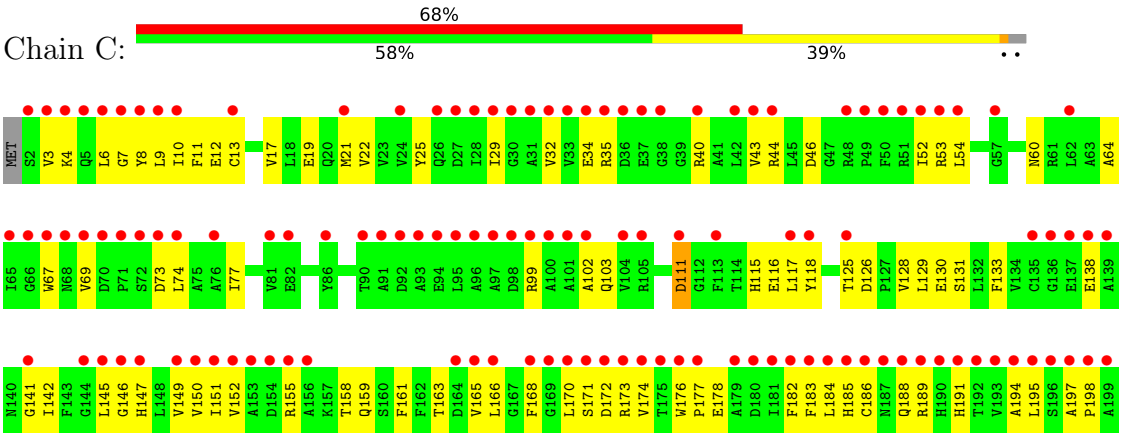
• Molecule 1: Glyoxalase/bleomycin resistance protein/dioxygenase

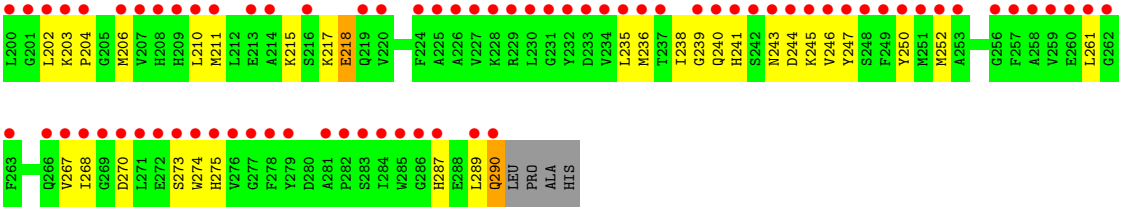
Chain B:



• Molecule 1: Glyoxalase/bleomycin resistance protein/dioxygenase

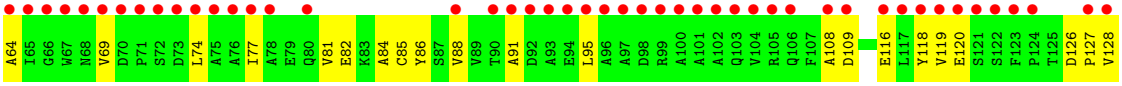
Chain C:

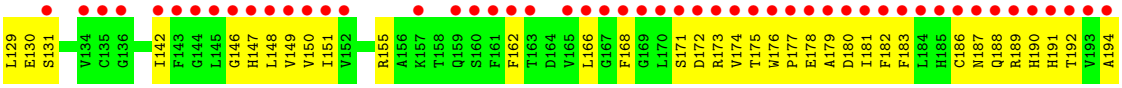


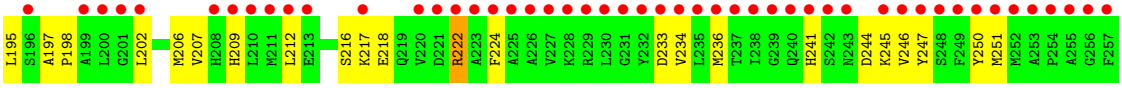


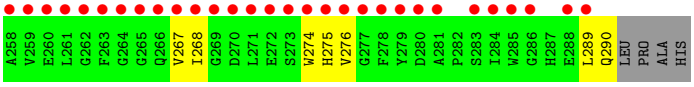
• Molecule 1: Glyoxalase/bleomycin resistance protein/dioxygenase

Chain D:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	131.59Å 131.59Å 103.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.85 – 2.10 34.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (92.85-2.10) 97.9 (34.54-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.289 0.254 , 0.290	Depositor DCC
R_{free} test set	2647 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	22.0	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.11 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9162	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9012e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P6G, FE2, SO4

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	0.55	1/2291 (0.0%)	0.61	0/3111
1	B	0.56	0/2291	0.61	0/3111
1	C	0.33	0/2291	0.47	0/3111
1	D	0.33	0/2291	0.48	0/3111
All	All	0.46	1/9164 (0.0%)	0.55	0/12444

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	CYS	CB-SG	-5.64	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2238	0	2173	26	0
1	B	2238	0	2173	33	0
1	C	2238	0	2173	135	0
1	D	2238	0	2173	140	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	19	0	26	2	0
3	B	19	0	26	9	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	77	0	0	0	0
5	B	80	0	0	0	0
5	C	1	0	0	0	0
All	All	9162	0	8744	325	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 18.

All (325) 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:C:168:PHE:CD1	1:C:186:CYS:HB3	1.20	1.63
1:C:217:LYS:NZ	1:C:247:TYR:CZ	1.76	1.53
1:C:168:PHE:HE1	1:C:186:CYS:SG	1.32	1.52
1:D:176:TRP:NE1	1:D:178:GLU:HG2	1.24	1.51
1:D:176:TRP:NE1	1:D:178:GLU:CG	1.81	1.42
1:D:176:TRP:HE1	1:D:178:GLU:CG	1.33	1.32
1:C:168:PHE:CE1	1:C:186:CYS:SG	2.20	1.32
1:D:217:LYS:NZ	1:D:247:TYR:CZ	1.98	1.30
1:C:168:PHE:CE1	1:C:186:CYS:HB3	1.66	1.29
1:C:168:PHE:CE1	1:C:186:CYS:CB	2.16	1.29
1:C:168:PHE:CD1	1:C:186:CYS:CB	2.14	1.27
1:C:9:LEU:CD1	1:C:210:LEU:HD11	1.68	1.24
1:D:176:TRP:CD1	1:D:178:GLU:HG2	1.72	1.23
1:D:176:TRP:HE1	1:D:178:GLU:CD	1.46	1.18
1:D:86:TYR:CE1	1:D:109:ASP:HA	1.80	1.16
1:C:13:CYS:HA	1:C:60:ASN:OD1	1.44	1.14
1:D:126:ASP:C	1:D:130:GLU:OE1	1.89	1.11
1:C:203:LYS:O	1:C:206:MET:HG3	1.49	1.11
1:C:176:TRP:NE1	1:C:178:GLU:HG2	1.69	1.08
1:D:202:LEU:HD22	1:D:206:MET:HE2	1.36	1.07
1:C:149:VAL:HG22	1:C:194:ALA:HB3	1.37	1.05
1:A:176:TRP:NE1	1:A:178:GLU:CG	2.19	1.05
1:C:29:ILE:HD12	1:C:261:LEU:HD13	1.32	1.04
1:C:236:MET:CE	1:C:287:HIS:HB3	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TRP:NE1	1:A:178:GLU:HG2	1.73	1.04
1:D:155:ARG:HD2	1:D:182:PHE:CD2	1.93	1.03
1:C:9:LEU:HD13	1:C:210:LEU:HD11	1.41	1.00
1:C:217:LYS:NZ	1:C:247:TYR:OH	1.93	1.00
1:D:202:LEU:HD22	1:D:206:MET:CE	1.93	0.97
1:C:236:MET:HE3	1:C:287:HIS:HB3	1.43	0.97
1:D:188:GLN:HG3	1:D:268:ILE:O	1.65	0.96
1:A:176:TRP:HE1	1:A:178:GLU:CD	1.70	0.95
1:A:176:TRP:CD1	1:A:178:GLU:HG2	2.01	0.94
1:D:45:LEU:HD11	1:D:212:LEU:HD22	1.47	0.94
1:D:217:LYS:NZ	1:D:247:TYR:CE1	2.26	0.94
1:C:19:GLU:OE1	1:C:35:ARG:NH2	2.02	0.93
1:D:155:ARG:CD	1:D:182:PHE:CD2	2.51	0.93
1:C:217:LYS:NZ	1:C:247:TYR:CE1	2.24	0.92
1:D:45:LEU:HD11	1:D:212:LEU:CD2	2.00	0.92
1:D:244:ASP:OD2	1:D:246:VAL:HG22	1.69	0.91
1:D:173:ARG:HD2	1:D:182:PHE:CE1	2.05	0.91
1:D:36:ASP:OD2	1:D:40:ARG:HD2	1.70	0.91
1:D:82:GLU:OE1	1:D:88:VAL:N	2.02	0.91
1:C:176:TRP:NE1	1:C:178:GLU:CG	2.35	0.89
1:D:244:ASP:CG	1:D:246:VAL:HG22	1.92	0.89
1:B:251:MET:HE3	3:B:302:P6G:H62	1.55	0.89
1:C:19:GLU:CD	1:C:35:ARG:HH22	1.74	0.88
1:C:176:TRP:CD1	1:C:178:GLU:HG2	2.08	0.88
1:D:244:ASP:OD2	1:D:246:VAL:CG2	2.23	0.87
1:C:176:TRP:HE1	1:C:178:GLU:CG	1.87	0.86
1:D:45:LEU:CD1	1:D:212:LEU:HD22	2.05	0.86
1:C:168:PHE:HD1	1:C:186:CYS:CB	1.70	0.86
1:C:170:LEU:HA	1:C:184:LEU:HD23	1.57	0.86
1:D:86:TYR:HE1	1:D:109:ASP:HA	1.39	0.86
1:C:203:LYS:N	1:C:206:MET:SD	2.48	0.85
1:D:126:ASP:O	1:D:130:GLU:OE1	1.97	0.83
1:C:244:ASP:CG	1:C:246:VAL:HG23	1.99	0.82
1:D:17:VAL:HA	1:D:20:GLN:OE1	1.80	0.81
1:D:218:GLU:O	1:D:222:ARG:HG2	1.81	0.81
1:D:3:VAL:HG21	1:D:168:PHE:CE2	2.17	0.80
1:C:236:MET:HE2	1:C:287:HIS:HB3	1.63	0.79
1:C:13:CYS:CA	1:C:60:ASN:OD1	2.28	0.79
1:A:176:TRP:HE1	1:A:178:GLU:CG	1.90	0.79
1:C:241:HIS:HB2	1:C:244:ASP:OD1	1.83	0.79
1:B:251:MET:HE3	3:B:302:P6G:C6	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ASP:OD2	1:C:246:VAL:CG2	2.32	0.77
1:D:149:VAL:HG21	1:D:209:HIS:CE1	2.21	0.76
1:C:168:PHE:HE1	1:C:186:CYS:CB	1.75	0.75
1:D:176:TRP:NE1	1:D:178:GLU:HG3	1.95	0.75
1:B:173:ARG:NH1	1:C:273:SER:OG	2.20	0.75
1:C:244:ASP:OD2	1:C:246:VAL:HG23	1.86	0.74
1:C:236:MET:CE	1:C:287:HIS:CB	2.66	0.74
1:D:149:VAL:HG22	1:D:194:ALA:HB3	1.69	0.73
1:D:173:ARG:HH11	1:D:182:PHE:HZ	1.30	0.72
1:B:173:ARG:HH12	1:C:270:ASP:CG	1.93	0.72
1:B:173:ARG:NH1	1:C:270:ASP:CB	2.52	0.72
1:D:218:GLU:O	1:D:222:ARG:CG	2.38	0.72
1:C:149:VAL:CG2	1:C:194:ALA:HB3	2.17	0.71
1:C:159:GLN:O	1:C:163:THR:OG1	2.04	0.71
1:D:176:TRP:CE2	1:D:178:GLU:CG	2.72	0.70
1:D:24:VAL:HG13	1:D:251:MET:HE1	1.73	0.70
1:B:173:ARG:NH1	1:C:270:ASP:HB3	2.07	0.70
1:D:217:LYS:NZ	1:D:247:TYR:OH	2.25	0.70
1:D:174:VAL:HG23	1:D:183:PHE:CE2	2.26	0.69
1:C:236:MET:HE2	1:C:287:HIS:CB	2.22	0.69
1:D:24:VAL:HG13	1:D:251:MET:CE	2.23	0.69
1:D:155:ARG:CD	1:D:182:PHE:CE2	2.76	0.68
1:C:9:LEU:HD13	1:C:210:LEU:CD1	2.22	0.68
1:C:126:ASP:O	1:C:130:GLU:HG3	1.94	0.68
1:C:29:ILE:HD13	1:C:261:LEU:HD22	1.74	0.68
1:C:32:VAL:HG23	1:C:129:LEU:HD13	1.74	0.68
1:A:232:TYR:CZ	3:A:302:P6G:H31	2.29	0.68
1:C:9:LEU:HD12	1:C:210:LEU:HD11	1.71	0.67
1:B:251:MET:CE	3:B:302:P6G:H62	2.23	0.67
1:C:102:ALA:O	1:C:103:GLN:HG3	1.95	0.67
1:D:173:ARG:NH1	1:D:182:PHE:CZ	2.59	0.66
1:D:11:PHE:CE1	1:D:62:LEU:HD13	2.30	0.66
1:D:176:TRP:NE1	1:D:178:GLU:CD	2.31	0.66
1:C:149:VAL:HG22	1:C:194:ALA:CB	2.20	0.65
1:D:36:ASP:OD2	1:D:40:ARG:CD	2.44	0.65
1:C:161:PHE:CD1	1:C:165:VAL:HG21	2.32	0.65
1:D:176:TRP:CZ2	1:D:179:ALA:HB3	2.33	0.64
1:D:128:VAL:O	1:D:131:SER:OG	2.13	0.64
1:C:176:TRP:HB2	1:C:177:PRO:HD2	1.80	0.64
1:C:151:ILE:HG13	1:C:202:LEU:HB3	1.80	0.64
1:D:176:TRP:CE2	1:D:178:GLU:HG3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:PHE:HD1	1:C:186:CYS:HB3	0.84	0.63
1:B:149:VAL:HG22	1:B:194:ALA:HB3	1.80	0.63
1:B:232:TYR:CZ	3:B:302:P6G:H31	2.33	0.63
1:D:173:ARG:HD2	1:D:182:PHE:CZ	2.33	0.63
1:D:197:ALA:HB1	1:D:198:PRO:HD2	1.80	0.63
1:D:241:HIS:HB2	1:D:244:ASP:OD1	1.99	0.62
1:C:172:ASP:OD2	1:C:243:ASN:HB2	1.99	0.62
1:D:3:VAL:HG11	1:D:166:LEU:HD22	1.81	0.62
1:C:133:PHE:O	1:C:215:LYS:HE3	2.00	0.61
1:C:173:ARG:HD2	1:C:182:PHE:CE1	2.35	0.61
1:C:176:TRP:HE1	1:C:178:GLU:CD	2.04	0.61
1:C:3:VAL:HG23	1:C:166:LEU:O	2.01	0.61
1:D:17:VAL:HG11	1:D:60:ASN:OD1	2.00	0.61
1:D:162:PHE:HD2	1:D:168:PHE:CD2	2.19	0.60
1:C:67:TRP:HB2	1:C:117:LEU:HD23	1.82	0.60
1:B:176:TRP:NE1	1:B:178:GLU:HG2	2.17	0.60
1:C:176:TRP:HB2	1:C:177:PRO:CD	2.32	0.60
1:D:202:LEU:HD22	1:D:206:MET:HE1	1.83	0.60
1:D:216:SER:HB2	1:D:218:GLU:OE1	2.01	0.60
1:D:48:ARG:HG2	1:D:49:PRO:HD2	1.84	0.59
1:D:176:TRP:CH2	1:D:179:ALA:HB3	2.37	0.59
1:D:176:TRP:HB2	1:D:177:PRO:HD2	1.85	0.59
1:A:202:LEU:HD22	1:A:206:MET:CE	2.32	0.59
1:D:86:TYR:CD1	1:D:108:ALA:O	2.56	0.58
1:D:175:THR:OG1	1:D:180:ASP:OD1	2.21	0.58
1:C:10:ILE:HD12	1:C:64:ALA:HB3	1.84	0.58
1:D:74:LEU:HD22	1:D:119:VAL:HG23	1.85	0.58
1:C:73:ASP:HB3	1:C:77:ILE:HD11	1.86	0.58
1:D:176:TRP:HB2	1:D:177:PRO:CD	2.34	0.58
1:A:202:LEU:HD22	1:A:206:MET:HE2	1.84	0.58
1:C:146:GLY:HA2	1:C:189:ARG:CZ	2.33	0.58
1:C:3:VAL:CG1	1:C:67:TRP:HB3	2.33	0.57
1:D:81:VAL:HG12	1:D:86:TYR:HB2	1.85	0.57
1:B:173:ARG:NH1	1:C:270:ASP:CG	2.57	0.57
1:C:176:TRP:HE1	1:C:178:GLU:HG2	1.49	0.57
1:C:29:ILE:HD11	1:C:261:LEU:HB2	1.85	0.57
1:D:3:VAL:CG1	1:D:166:LEU:HD22	2.33	0.57
1:D:127:PRO:N	1:D:130:GLU:OE1	2.37	0.57
1:D:289:LEU:O	1:D:290:GLN:HB2	2.05	0.57
1:C:9:LEU:HD11	1:C:210:LEU:HD11	1.79	0.57
1:C:244:ASP:OD2	1:C:246:VAL:HG21	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:HD21	1:C:9:LEU:HD21	1.85	0.57
1:B:160:SER:HB2	1:C:275:HIS:HE1	1.68	0.57
1:D:202:LEU:CD2	1:D:206:MET:CE	2.77	0.56
1:D:244:ASP:OD2	1:D:246:VAL:HG21	2.03	0.56
1:A:149:VAL:HG22	1:A:194:ALA:HB3	1.86	0.56
1:D:3:VAL:HA	1:D:69:VAL:HG12	1.87	0.56
1:B:232:TYR:CG	3:B:302:P6G:H51	2.41	0.56
1:C:155:ARG:HD2	1:C:182:PHE:CD2	2.40	0.56
1:D:128:VAL:HG23	1:D:129:LEU:N	2.21	0.56
1:C:29:ILE:CD1	1:C:261:LEU:HB2	2.36	0.56
1:A:173:ARG:HH11	1:A:182:PHE:HZ	1.53	0.56
1:D:151:ILE:HD11	1:D:202:LEU:HD12	1.86	0.56
1:D:155:ARG:NE	1:D:182:PHE:CE2	2.75	0.55
1:C:197:ALA:HB1	1:C:198:PRO:HD2	1.88	0.55
1:D:10:ILE:HD12	1:D:64:ALA:HB3	1.88	0.55
1:D:13:CYS:HB2	1:D:18:LEU:HD12	1.88	0.55
1:C:268:ILE:HD12	1:C:274:TRP:CD2	2.42	0.55
1:D:22:VAL:HG21	1:D:35:ARG:HH21	1.73	0.54
1:B:202:LEU:HD22	1:B:206:MET:CE	2.38	0.54
1:D:84:ALA:O	1:D:85:CYS:HB2	2.07	0.54
1:D:173:ARG:NH1	1:D:182:PHE:HZ	1.97	0.54
1:B:176:TRP:HB2	1:B:177:PRO:CD	2.37	0.54
1:D:155:ARG:CZ	1:D:182:PHE:CZ	2.91	0.54
1:B:246:VAL:HG12	1:B:248:SER:HB3	1.89	0.54
1:D:148:LEU:HD11	1:D:207:VAL:HG13	1.90	0.54
1:C:17:VAL:HG21	1:C:60:ASN:ND2	2.22	0.53
1:D:155:ARG:CZ	1:D:182:PHE:CE2	2.92	0.53
1:B:151:ILE:HG13	1:B:202:LEU:HB3	1.90	0.53
1:C:4:LYS:HE2	1:C:142:ILE:HD12	1.91	0.53
1:C:69:VAL:HG21	1:C:74:LEU:HD13	1.90	0.53
1:B:202:LEU:HD22	1:B:206:MET:HE2	1.90	0.53
1:D:244:ASP:OD1	1:D:246:VAL:HG22	2.08	0.53
1:D:3:VAL:CG2	1:D:168:PHE:CE2	2.90	0.53
1:D:176:TRP:HH2	1:D:181:ILE:HD12	1.74	0.53
1:D:151:ILE:HG13	1:D:202:LEU:CD1	2.40	0.52
1:D:3:VAL:HG21	1:D:168:PHE:CZ	2.44	0.52
1:D:176:TRP:CH2	1:D:181:ILE:HD12	2.45	0.52
1:C:21:MET:HE2	1:C:25:TYR:HE2	1.75	0.52
1:D:173:ARG:CZ	1:D:180:ASP:OD1	2.57	0.52
1:C:17:VAL:HG21	1:C:60:ASN:HD21	1.74	0.52
1:D:174:VAL:HG23	1:D:183:PHE:HE2	1.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ARG:HD3	1:D:182:PHE:CE2	2.44	0.51
1:C:236:MET:CE	1:C:287:HIS:CG	2.93	0.51
1:D:174:VAL:CG2	1:D:183:PHE:CE2	2.94	0.51
1:D:241:HIS:CB	1:D:244:ASP:OD1	2.58	0.51
1:D:149:VAL:CG2	1:D:209:HIS:CE1	2.93	0.51
1:C:29:ILE:CD1	1:C:261:LEU:HD13	2.23	0.51
1:C:197:ALA:HB1	1:C:198:PRO:CD	2.40	0.51
1:D:45:LEU:HD11	1:D:212:LEU:HD21	1.88	0.51
1:D:202:LEU:CD2	1:D:206:MET:HE1	2.40	0.51
1:C:147:HIS:HB3	1:C:191:HIS:O	2.11	0.51
1:D:126:ASP:N	1:D:130:GLU:OE1	2.44	0.51
1:B:160:SER:HB2	1:C:275:HIS:CE1	2.45	0.50
1:A:149:VAL:HG21	1:A:209:HIS:CE1	2.46	0.50
1:D:45:LEU:CD1	1:D:212:LEU:CD2	2.75	0.50
1:C:155:ARG:CD	1:C:182:PHE:CD2	2.95	0.50
1:B:251:MET:CE	3:B:302:P6G:C6	2.85	0.50
1:D:32:VAL:HG23	1:D:129:LEU:CD1	2.42	0.50
1:D:126:ASP:H	1:D:130:GLU:CD	2.15	0.50
1:D:224:PHE:HE1	1:D:234:VAL:HG11	1.78	0.49
1:D:7:GLY:HA3	1:D:118:TYR:OH	2.13	0.49
1:A:176:TRP:NE1	1:A:178:GLU:HG3	2.23	0.49
1:C:111:ASP:OD1	1:C:152:VAL:HA	2.12	0.49
1:C:236:MET:HB2	1:C:250:TYR:HB2	1.95	0.49
1:C:7:GLY:HA3	1:C:118:TYR:OH	2.13	0.48
1:D:151:ILE:HG13	1:D:202:LEU:HD13	1.95	0.48
1:A:176:TRP:CE2	1:A:178:GLU:CG	2.94	0.48
1:D:45:LEU:HD13	1:D:212:LEU:HD22	1.91	0.48
1:D:147:HIS:HB3	1:D:191:HIS:O	2.13	0.48
1:C:73:ASP:O	1:C:77:ILE:HG13	2.13	0.48
1:C:217:LYS:HG3	1:C:247:TYR:CE2	2.48	0.48
1:D:218:GLU:O	1:D:222:ARG:HG3	2.12	0.48
1:D:148:LEU:CD1	1:D:207:VAL:HG13	2.43	0.48
1:C:12:GLU:O	1:C:60:ASN:HA	2.14	0.48
1:C:3:VAL:HG13	1:C:67:TRP:HB3	1.96	0.47
1:C:128:VAL:O	1:C:131:SER:OG	2.26	0.47
1:C:203:LYS:O	1:C:206:MET:CG	2.41	0.47
1:D:91:ALA:HB1	1:D:95:LEU:HB3	1.96	0.47
1:A:240:GLN:HA	1:A:246:VAL:O	2.14	0.47
1:A:176:TRP:CE2	1:A:178:GLU:HG3	2.49	0.47
1:C:29:ILE:HD12	1:C:261:LEU:CD1	2.24	0.47
1:C:241:HIS:CB	1:C:244:ASP:OD1	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:MET:HE1	3:B:302:P6G:H52	1.97	0.47
1:C:289:LEU:O	1:C:290:GLN:HB2	2.13	0.47
1:C:240:GLN:HA	1:C:246:VAL:O	2.15	0.47
1:B:106:GLN:HG3	1:B:116:GLU:HG2	1.97	0.47
1:D:44:ARG:NH2	1:D:126:ASP:OD2	2.45	0.47
1:D:162:PHE:CD2	1:D:168:PHE:CE2	3.03	0.47
1:B:155:ARG:HD3	1:B:182:PHE:CD2	2.51	0.46
1:C:203:LYS:HB3	1:C:204:PRO:HD2	1.97	0.46
1:C:29:ILE:CD1	1:C:261:LEU:HD22	2.44	0.46
1:D:48:ARG:CG	1:D:49:PRO:HD2	2.45	0.46
1:D:77:ILE:O	1:D:81:VAL:HG23	2.15	0.46
1:B:173:ARG:HH12	1:C:270:ASP:CB	2.26	0.46
1:C:11:PHE:HB2	1:C:54:LEU:HD23	1.97	0.46
1:B:232:TYR:CD2	3:B:302:P6G:H51	2.51	0.46
1:C:158:THR:HG22	1:C:195:LEU:HD11	1.97	0.46
1:C:171:SER:OG	1:C:185:HIS:ND1	2.30	0.46
1:A:155:ARG:HD3	1:A:182:PHE:CD2	2.51	0.46
1:D:22:VAL:HG13	1:D:33:VAL:HG11	1.96	0.46
1:D:168:PHE:CD1	1:D:186:CYS:HB3	2.50	0.46
1:D:86:TYR:CZ	1:D:109:ASP:HA	2.46	0.46
1:B:244:ASP:O	1:B:245:LYS:HB2	2.15	0.46
1:D:151:ILE:CD1	1:D:202:LEU:HD12	2.46	0.46
1:B:176:TRP:CH2	1:B:179:ALA:HB3	2.51	0.45
1:D:19:GLU:OE2	1:D:35:ARG:NH2	2.48	0.45
1:A:218:GLU:CD	1:A:218:GLU:H	2.18	0.45
1:C:239:GLY:C	1:C:287:HIS:CE1	2.89	0.45
1:C:3:VAL:HG11	1:C:67:TRP:HB3	1.98	0.45
1:C:10:ILE:HD11	1:C:99:ARG:CD	2.47	0.45
1:D:6:LEU:HB2	1:D:192:THR:CG2	2.47	0.45
1:B:20:GLN:HB3	3:B:302:P6G:H22	1.98	0.44
1:C:217:LYS:HG3	1:C:247:TYR:CD2	2.52	0.44
1:D:35:ARG:HD3	1:D:40:ARG:O	2.17	0.44
1:D:162:PHE:CD2	1:D:168:PHE:CD2	3.03	0.44
1:C:235:LEU:HD22	1:C:252:MET:HE2	1.99	0.44
1:D:11:PHE:CZ	1:D:62:LEU:HD13	2.52	0.44
1:D:19:GLU:CD	1:D:35:ARG:NH2	2.71	0.44
1:A:151:ILE:HG13	1:A:202:LEU:HB3	1.99	0.44
1:C:238:ILE:HG21	1:C:247:TYR:CZ	2.53	0.44
1:C:268:ILE:HD12	1:C:274:TRP:CE2	2.53	0.44
1:C:32:VAL:CG2	1:C:129:LEU:HD13	2.46	0.44
1:D:244:ASP:O	1:D:245:LYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LEU:HD23	1:C:211:MET:H	1.83	0.44
1:B:241:HIS:HB2	1:B:244:ASP:OD1	2.18	0.44
1:B:272:GLU:O	1:C:245:LYS:HE3	2.18	0.44
1:C:150:VAL:HG23	1:C:195:LEU:HD23	2.00	0.44
1:D:48:ARG:HE	1:D:120:GLU:CD	2.19	0.43
1:D:275:HIS:HD2	1:D:276:VAL:O	2.01	0.43
1:C:151:ILE:HD11	1:C:202:LEU:CD1	2.48	0.43
1:D:236:MET:HB2	1:D:250:TYR:HB2	2.00	0.43
1:A:176:TRP:HB2	1:A:177:PRO:CD	2.49	0.43
1:C:161:PHE:O	1:C:165:VAL:HB	2.18	0.43
1:D:146:GLY:HA2	1:D:189:ARG:CZ	2.49	0.43
1:C:141:GLY:HA3	1:C:188:GLN:HG2	2.01	0.43
1:D:32:VAL:HG23	1:D:129:LEU:HD11	2.01	0.43
1:B:2:SER:HB2	1:B:167:GLY:HA3	2.01	0.42
1:C:22:VAL:HG21	1:C:35:ARG:NH2	2.34	0.42
1:D:17:VAL:HG21	1:D:60:ASN:HD21	1.83	0.42
1:A:198:PRO:HG3	1:A:204:PRO:HD3	2.01	0.42
1:D:91:ALA:CB	1:D:95:LEU:HD23	2.48	0.42
1:B:147:HIS:HB3	1:B:191:HIS:O	2.18	0.42
1:B:240:GLN:HA	1:B:246:VAL:O	2.19	0.42
1:C:188:GLN:HB3	1:C:267:VAL:HG13	2.01	0.42
1:C:218:GLU:CD	1:C:218:GLU:H	2.23	0.42
1:D:168:PHE:CE1	1:D:186:CYS:HB3	2.55	0.42
1:A:176:TRP:HB2	1:A:177:PRO:HD2	2.00	0.42
1:D:188:GLN:HB3	1:D:267:VAL:HG13	2.00	0.42
1:C:40:ARG:NH2	1:C:53:ARG:NH2	2.68	0.42
1:D:162:PHE:HD2	1:D:168:PHE:CE2	2.38	0.42
1:D:142:ILE:HG22	1:D:187:ASN:HD22	1.85	0.42
1:C:168:PHE:HD1	1:C:186:CYS:CA	2.30	0.41
1:D:217:LYS:CE	1:D:247:TYR:CE1	3.01	0.41
1:C:67:TRP:NE1	1:C:115:HIS:ND1	2.52	0.41
1:C:8:TYR:OH	1:C:116:GLU:OE1	2.33	0.41
1:C:69:VAL:CG2	1:C:74:LEU:HD13	2.49	0.41
1:D:64:ALA:HB1	1:D:116:GLU:CD	2.40	0.41
1:A:232:TYR:CD2	3:A:302:P6G:H51	2.55	0.41
1:C:6:LEU:HG	1:C:145:LEU:CD2	2.51	0.41
1:C:21:MET:CE	1:C:25:TYR:CE2	3.03	0.41
1:C:174:VAL:HG23	1:C:183:PHE:CE2	2.55	0.41
1:D:172:ASP:OD2	1:D:190:HIS:NE2	2.46	0.41
1:C:138:GLU:OE2	1:C:215:LYS:NZ	2.47	0.41
1:A:67:TRP:HH2	1:A:193:VAL:CG2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TRP:NE1	1:A:178:GLU:CD	2.46	0.41
1:D:171:SER:HA	1:D:274:TRP:HE1	1.86	0.41
1:A:176:TRP:NE1	1:A:178:GLU:OE2	2.47	0.41
1:C:34:GLU:OE2	1:C:44:ARG:NH1	2.42	0.41
1:D:19:GLU:CD	1:D:35:ARG:HH22	2.24	0.41
1:A:246:VAL:CG1	1:A:248:SER:HB3	2.52	0.41
1:C:46:ASP:CA	1:C:129:LEU:HD23	2.51	0.41
1:D:142:ILE:HG22	1:D:187:ASN:ND2	2.36	0.40
1:D:150:VAL:HG22	1:D:195:LEU:HD23	2.03	0.40
1:D:128:VAL:CG2	1:D:129:LEU:N	2.84	0.40
1:D:155:ARG:NE	1:D:182:PHE:CD2	2.89	0.40
1:C:10:ILE:HD11	1:C:99:ARG:HD2	2.02	0.40
1:C:21:MET:CE	1:C:25:TYR:HE2	2.34	0.40
1:C:43:VAL:HB	1:C:52:ILE:HB	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	287/294 (98%)	283 (99%)	4 (1%)	0	100	100
1	B	287/294 (98%)	281 (98%)	6 (2%)	0	100	100
1	C	287/294 (98%)	282 (98%)	5 (2%)	0	100	100
1	D	287/294 (98%)	282 (98%)	5 (2%)	0	100	100
All	All	1148/1176 (98%)	1128 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/235 (98%)	228 (99%)	3 (1%)	69	75
1	B	231/235 (98%)	229 (99%)	2 (1%)	78	84
1	C	231/235 (98%)	227 (98%)	4 (2%)	60	67
1	D	231/235 (98%)	228 (99%)	3 (1%)	69	75
All	All	924/940 (98%)	912 (99%)	12 (1%)	69	75

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	GLU
1	A	245	LYS
1	A	290	GLN
1	B	3	VAL
1	B	245	LYS
1	C	111	ASP
1	C	125	THR
1	C	218	GLU
1	C	290	GLN
1	D	18	LEU
1	D	222	ARG
1	D	233	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	110	ASN
1	D	275	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	303	-	4,4,4	0.19	0	6,6,6	0.11	0
3	P6G	B	302	-	18,18,18	0.46	0	17,17,17	0.56	0
4	SO4	A	303	-	4,4,4	0.12	0	6,6,6	0.09	0
3	P6G	A	302	-	18,18,18	0.50	0	17,17,17	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P6G	B	302	-	-	5/16/16/16	-
3	P6G	A	302	-	-	4/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

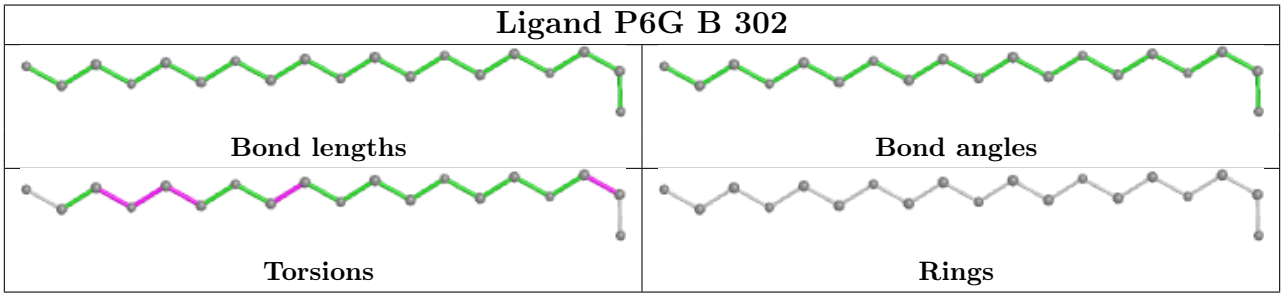
Mol	Chain	Res	Type	Atoms
3	A	302	P6G	O16-C17-C18-O19
3	A	302	P6G	O10-C11-C12-O13
3	B	302	P6G	C14-C15-O16-C17
3	B	302	P6G	C18-C17-O16-C15
3	B	302	P6G	O10-C11-C12-O13
3	B	302	P6G	O1-C2-C3-O4
3	A	302	P6G	C14-C15-O16-C17
3	B	302	P6G	O13-C14-C15-O16
3	A	302	P6G	O1-C2-C3-O4

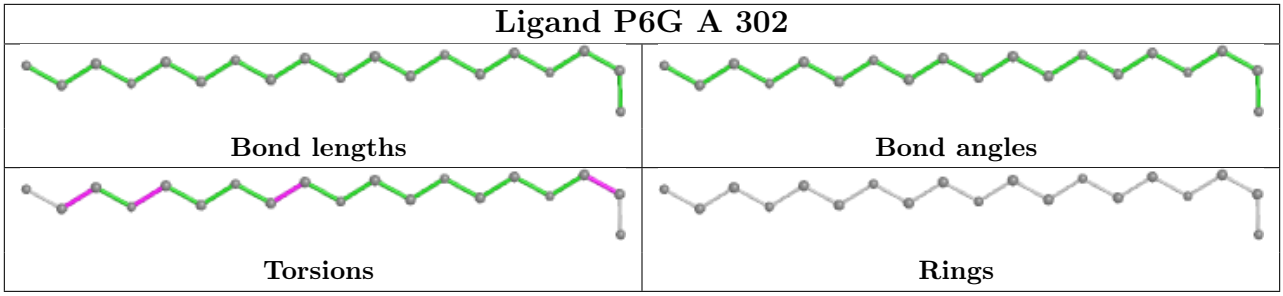
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	P6G	9	0
3	A	302	P6G	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	289/294 (98%)	0.72	34 (11%)	4 5	11, 23, 37, 46	289 (100%)
1	B	289/294 (98%)	0.72	43 (14%)	2 3	11, 23, 37, 45	289 (100%)
1	C	289/294 (98%)	5.50	200 (69%)	0 0	11, 23, 37, 44	289 (100%)
1	D	289/294 (98%)	5.39	232 (80%)	0 0	11, 22, 36, 44	289 (100%)
All	All	1156/1176 (98%)	3.08	509 (44%)	0 0	11, 23, 37, 46	1156 (100%)

All (509) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	232	TYR	29.1
1	C	227	VAL	22.7
1	C	28	ILE	22.2
1	D	123	PHE	20.6
1	C	152	VAL	20.0
1	D	62	LEU	18.4
1	C	230	LEU	18.4
1	C	71	PRO	18.1
1	C	91	ALA	17.9
1	C	259	VAL	17.2
1	C	229	ARG	16.8
1	C	258	ALA	16.8
1	D	60	ASN	16.6
1	D	163	THR	16.5
1	C	95	LEU	15.9
1	D	276	VAL	15.8
1	C	251	MET	15.8
1	D	122	SER	15.6
1	C	226	ALA	15.6
1	C	43	VAL	15.5
1	C	274	TRP	15.5

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Mol	Chain	Res	Type	RSRZ
1	C	252	MET	15.1
1	C	156	ALA	14.5
1	C	257	PHE	14.4
1	C	268	ILE	14.2
1	C	153	ALA	14.1
1	D	182	PHE	13.9
1	C	50	PHE	13.8
1	C	139	ALA	13.8
1	D	170	LEU	13.7
1	C	231	GLY	13.4
1	D	145	LEU	13.4
1	C	210	LEU	13.4
1	D	11	PHE	13.2
1	D	267	VAL	13.2
1	C	93	ALA	13.2
1	B	200	LEU	13.1
1	D	63	ALA	12.7
1	C	202	LEU	12.7
1	D	10	ILE	12.7
1	D	9	LEU	12.6
1	D	257	PHE	12.5
1	C	70	ASP	12.5
1	D	275	HIS	12.3
1	C	233	ASP	12.3
1	D	200	LEU	12.3
1	D	42	LEU	12.2
1	C	100	ALA	12.2
1	C	154	ASP	12.2
1	C	32	VAL	12.1
1	D	255	ALA	11.9
1	C	170	LEU	11.8
1	D	278	PHE	11.8
1	D	212	LEU	11.7
1	D	184	LEU	11.7
1	C	184	LEU	11.7
1	D	168	PHE	11.5
1	D	29	ILE	11.5
1	C	151	ILE	11.5
1	C	267	VAL	11.4
1	C	203	LYS	11.3
1	D	33	VAL	11.2
1	D	48	ARG	11.2

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Mol	Chain	Res	Type	RSRZ
1	D	64	ALA	11.1
1	C	99	ARG	11.0
1	C	92	ASP	11.0
1	D	54	LEU	10.9
1	C	155	ARG	10.9
1	C	147	HIS	10.9
1	D	261	LEU	10.7
1	D	274	TRP	10.6
1	B	85	CYS	10.6
1	D	77	ILE	10.6
1	D	231	GLY	10.5
1	C	42	LEU	10.3
1	C	27	ASP	10.2
1	D	61	ARG	10.2
1	D	50	PHE	10.2
1	D	22	VAL	10.2
1	C	169	GLY	10.2
1	C	118	TYR	10.1
1	D	6	LEU	10.1
1	C	81	VAL	10.1
1	C	235	LEU	10.1
1	C	196	SER	10.0
1	D	193	VAL	10.0
1	D	91	ALA	9.9
1	C	250	TYR	9.9
1	C	197	ALA	9.9
1	D	30	GLY	9.8
1	C	266	GLN	9.8
1	C	186	CYS	9.7
1	D	49	PRO	9.7
1	C	72	SER	9.7
1	D	273	SER	9.7
1	C	44	ARG	9.6
1	C	275	HIS	9.6
1	C	269	GLY	9.6
1	D	254	PRO	9.4
1	D	121	SER	9.4
1	D	186	CYS	9.3
1	C	189	ARG	9.2
1	D	100	ALA	9.2
1	C	234	VAL	9.2
1	C	185	HIS	9.2

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Mol	Chain	Res	Type	RSRZ
1	D	166	LEU	9.2
1	D	12	GLU	9.1
1	C	209	HIS	9.1
1	D	169	GLY	9.1
1	D	178	GLU	9.1
1	C	52	ILE	9.1
1	C	49	PRO	8.9
1	C	193	VAL	8.9
1	D	144	GLY	8.9
1	D	7	GLY	8.8
1	D	8	TYR	8.8
1	D	39	GLY	8.8
1	D	101	ALA	8.7
1	C	3	VAL	8.7
1	D	41	ALA	8.7
1	D	192	THR	8.6
1	C	253	ALA	8.6
1	D	256	GLY	8.6
1	C	7	GLY	8.6
1	D	271	LEU	8.6
1	D	38	GLY	8.5
1	A	200	LEU	8.5
1	D	268	ILE	8.5
1	C	246	VAL	8.5
1	C	273	SER	8.4
1	D	47	GLY	8.4
1	D	189	ARG	8.4
1	C	228	LYS	8.4
1	D	66	GLY	8.4
1	D	181	ILE	8.4
1	C	183	PHE	8.4
1	C	276	VAL	8.4
1	C	171	SER	8.4
1	C	244	ASP	8.3
1	C	277	GLY	8.3
1	C	8	TYR	8.3
1	C	284	ILE	8.3
1	D	247	TYR	8.2
1	C	214	ALA	8.2
1	C	195	LEU	8.1
1	D	265	GLY	8.0
1	D	246	VAL	8.0

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Mol	Chain	Res	Type	RSRZ
1	C	285	TRP	8.0
1	D	269	GLY	8.0
1	D	95	LEU	8.0
1	A	177	PRO	7.9
1	D	210	LEU	7.9
1	D	187	ASN	7.9
1	C	271	LEU	7.9
1	C	279	TYR	7.9
1	C	187	ASN	7.9
1	D	23	VAL	7.8
1	C	96	ALA	7.8
1	D	221	ASP	7.7
1	D	97	ALA	7.7
1	C	98	ASP	7.7
1	D	162	PHE	7.7
1	C	201	GLY	7.7
1	C	278	PHE	7.6
1	D	277	GLY	7.6
1	D	93	ALA	7.6
1	D	52	ILE	7.5
1	D	173	ARG	7.5
1	D	78	ALA	7.4
1	D	102	ALA	7.4
1	D	20	GLN	7.4
1	C	34	GLU	7.4
1	D	28	ILE	7.4
1	D	3	VAL	7.4
1	D	180	ASP	7.4
1	D	117	LEU	7.3
1	C	33	VAL	7.3
1	C	241	HIS	7.3
1	D	148	LEU	7.3
1	C	191	HIS	7.2
1	C	31	ALA	7.2
1	C	13	CYS	7.2
1	D	149	VAL	7.1
1	D	146	GLY	7.0
1	C	190	HIS	7.0
1	C	213	GLU	7.0
1	D	211	MET	7.0
1	B	178	GLU	6.9
1	C	62	LEU	6.9

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Mol	Chain	Res	Type	RSRZ
1	C	207	VAL	6.8
1	D	183	PHE	6.7
1	D	234	VAL	6.7
1	D	171	SER	6.6
1	C	38	GLY	6.6
1	C	101	ALA	6.6
1	C	104	VAL	6.6
1	D	208	HIS	6.6
1	A	176	TRP	6.6
1	C	24	VAL	6.6
1	D	238	ILE	6.6
1	C	182	PHE	6.5
1	C	5	GLN	6.5
1	D	188	GLN	6.5
1	D	279	TYR	6.5
1	B	177	PRO	6.5
1	C	260	GLU	6.5
1	D	31	ALA	6.5
1	C	242	SER	6.5
1	D	24	VAL	6.5
1	C	94	GLU	6.5
1	D	119	VAL	6.4
1	D	43	VAL	6.4
1	C	204	PRO	6.3
1	D	167	GLY	6.3
1	C	68	ASN	6.3
1	C	239	GLY	6.3
1	D	222	ARG	6.3
1	D	213	GLU	6.3
1	C	9	LEU	6.3
1	D	201	GLY	6.3
1	C	180	ASP	6.3
1	C	188	GLN	6.3
1	D	104	VAL	6.2
1	D	25	TYR	6.2
1	C	53	ARG	6.2
1	D	34	GLU	6.2
1	C	74	LEU	6.1
1	D	2	SER	6.1
1	D	270	ASP	6.1
1	B	199	ALA	6.0
1	D	53	ARG	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	258	ALA	6.0
1	D	69	VAL	6.0
1	C	135	CYS	6.0
1	A	179	ALA	6.0
1	C	146	GLY	6.0
1	C	208	HIS	6.0
1	C	150	VAL	6.0
1	D	103	GLN	6.0
1	C	4	LYS	5.9
1	C	2	SER	5.8
1	D	185	HIS	5.8
1	D	40	ARG	5.8
1	D	67	TRP	5.8
1	D	5	GLN	5.8
1	D	99	ARG	5.8
1	D	27	ASP	5.7
1	D	190	HIS	5.7
1	C	149	VAL	5.7
1	D	118	TYR	5.7
1	D	96	ALA	5.6
1	C	199	ALA	5.6
1	D	51	ARG	5.6
1	A	178	GLU	5.6
1	C	145	LEU	5.5
1	D	76	ALA	5.5
1	D	209	HIS	5.5
1	A	128	VAL	5.5
1	C	26	GLN	5.5
1	B	179	ALA	5.5
1	D	147	HIS	5.5
1	D	74	LEU	5.5
1	D	35	ARG	5.4
1	D	55	ASP	5.4
1	D	266	GLN	5.4
1	C	270	ASP	5.4
1	C	206	MET	5.4
1	C	36	ASP	5.4
1	A	199	ALA	5.4
1	C	243	ASN	5.3
1	B	231	GLY	5.3
1	D	259	VAL	5.3
1	D	120	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	236	MET	5.3
1	C	237	THR	5.2
1	D	21	MET	5.2
1	C	200	LEU	5.2
1	A	231	GLY	5.1
1	B	176	TRP	5.1
1	D	179	ALA	5.1
1	D	272	GLU	5.0
1	D	56	PRO	5.0
1	D	281	ALA	4.9
1	D	280	ASP	4.9
1	C	6	LEU	4.9
1	C	97	ALA	4.9
1	C	168	PHE	4.9
1	D	172	ASP	4.9
1	D	36	ASP	4.8
1	D	94	GLU	4.8
1	D	191	HIS	4.8
1	C	69	VAL	4.8
1	A	127	PRO	4.8
1	C	111	ASP	4.8
1	D	285	TRP	4.8
1	C	194	ALA	4.8
1	C	166	LEU	4.8
1	C	37	GLU	4.8
1	D	92	ASP	4.7
1	D	245	LYS	4.7
1	A	201	GLY	4.7
1	D	176	TRP	4.7
1	C	211	MET	4.7
1	D	98	ASP	4.7
1	D	159	GLN	4.6
1	D	175	THR	4.6
1	A	85	CYS	4.6
1	C	198	PRO	4.6
1	D	230	LEU	4.6
1	D	17	VAL	4.6
1	C	35	ARG	4.6
1	D	75	ALA	4.5
1	D	174	VAL	4.5
1	D	194	ALA	4.5
1	C	287	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	21	MET	4.4
1	D	4	LYS	4.4
1	D	68	ASN	4.4
1	D	227	VAL	4.4
1	B	201	GLY	4.4
1	D	65	ILE	4.4
1	D	232	TYR	4.4
1	A	233	ASP	4.4
1	B	290	GLN	4.4
1	A	289	LEU	4.4
1	C	181	ILE	4.4
1	A	154	ASP	4.4
1	C	73	ASP	4.3
1	D	109	ASP	4.3
1	C	192	THR	4.3
1	D	220	VAL	4.2
1	C	90	THR	4.2
1	C	172	ASP	4.2
1	D	239	GLY	4.2
1	D	252	MET	4.2
1	C	177	PRO	4.2
1	D	283	SER	4.2
1	D	80	GLN	4.0
1	D	284	ILE	4.0
1	C	256	GLY	4.0
1	D	131	SER	4.0
1	D	248	SER	4.0
1	B	202	LEU	3.9
1	D	236	MET	3.9
1	C	105	ARG	3.9
1	C	66	GLY	3.9
1	C	176	TRP	3.9
1	D	263	PHE	3.9
1	D	253	ALA	3.8
1	D	26	GLN	3.8
1	A	232	TYR	3.7
1	C	10	ILE	3.7
1	C	216	SER	3.7
1	D	228	LYS	3.7
1	C	102	ALA	3.7
1	C	290	GLN	3.7
1	C	175	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	275	HIS	3.6
1	A	285	TRP	3.6
1	D	142	ILE	3.6
1	D	32	VAL	3.6
1	C	125	THR	3.6
1	D	249	PHE	3.6
1	C	29	ILE	3.6
1	D	233	ASP	3.6
1	D	226	ALA	3.6
1	D	116	GLU	3.6
1	D	88	VAL	3.6
1	B	280	ASP	3.5
1	D	262	GLY	3.5
1	C	245	LYS	3.5
1	B	288	GLU	3.5
1	A	202	LEU	3.5
1	A	175	THR	3.5
1	B	154	ASP	3.5
1	B	164	ASP	3.5
1	D	235	LEU	3.5
1	D	37	GLU	3.5
1	D	223	ALA	3.5
1	B	272	GLU	3.4
1	D	70	ASP	3.4
1	D	143	PHE	3.4
1	D	150	VAL	3.4
1	A	125	THR	3.4
1	A	288	GLU	3.4
1	B	216	SER	3.4
1	C	283	SER	3.4
1	A	290	GLN	3.3
1	C	289	LEU	3.3
1	D	199	ALA	3.3
1	D	229	ARG	3.3
1	C	179	ALA	3.3
1	A	203	LYS	3.2
1	C	54	LEU	3.2
1	D	264	GLY	3.2
1	D	135	CYS	3.2
1	C	174	VAL	3.2
1	C	117	LEU	3.2
1	B	124	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	141	GLY	3.1
1	D	160	SER	3.1
1	B	94	GLU	3.1
1	D	45	LEU	3.1
1	D	157	LYS	3.1
1	D	240	GLN	3.1
1	B	180	ASP	3.1
1	C	48	ARG	3.1
1	D	289	LEU	3.1
1	D	124	PRO	3.1
1	D	134	VAL	3.1
1	D	13	CYS	3.0
1	C	165	VAL	3.0
1	B	130	GLU	3.0
1	D	90	THR	2.9
1	A	270	ASP	2.9
1	B	125	THR	2.9
1	B	79	GLU	2.9
1	C	82	GLU	2.9
1	C	173	ARG	2.9
1	C	136	GLY	2.9
1	D	108	ALA	2.9
1	D	241	HIS	2.9
1	A	157	LYS	2.9
1	C	272	GLU	2.9
1	C	67	TRP	2.9
1	C	240	GLN	2.9
1	C	40	ARG	2.8
1	B	128	VAL	2.8
1	D	237	THR	2.8
1	A	216	SER	2.8
1	A	229	ARG	2.8
1	C	57	GLY	2.8
1	C	248	SER	2.8
1	A	280	ASP	2.7
1	D	288	GLU	2.7
1	C	225	ALA	2.7
1	D	202	LEU	2.7
1	C	224	PHE	2.7
1	C	144	GLY	2.6
1	D	71	PRO	2.6
1	C	281	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	251	MET	2.6
1	B	233	ASP	2.6
1	D	128	VAL	2.6
1	B	289	LEU	2.6
1	D	165	VAL	2.6
1	D	224	PHE	2.6
1	D	250	TYR	2.6
1	C	282	PRO	2.6
1	D	44	ARG	2.5
1	C	86	TYR	2.5
1	A	37	GLU	2.5
1	B	175	THR	2.5
1	B	218	GLU	2.5
1	D	260	GLU	2.5
1	B	229	ARG	2.5
1	B	232	TYR	2.5
1	D	243	ASN	2.5
1	C	51	ARG	2.5
1	D	242	SER	2.5
1	B	38	GLY	2.5
1	C	262	GLY	2.5
1	B	76	ALA	2.5
1	C	76	ALA	2.5
1	A	234	VAL	2.5
1	D	225	ALA	2.5
1	C	219	GLN	2.4
1	C	220	VAL	2.4
1	B	97	ALA	2.4
1	B	139	ALA	2.4
1	B	203	LYS	2.4
1	D	151	ILE	2.4
1	C	247	TYR	2.4
1	D	286	GLY	2.4
1	B	127	PRO	2.4
1	D	105	ARG	2.4
1	D	106	GLN	2.3
1	D	196	SER	2.3
1	D	127	PRO	2.3
1	C	137	GLU	2.3
1	A	124	PRO	2.3
1	B	57	GLY	2.3
1	C	286	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	111	ASP	2.3
1	A	139	ALA	2.3
1	D	217	LYS	2.3
1	C	65	ILE	2.3
1	D	177	PRO	2.3
1	C	261	LEU	2.3
1	A	180	ASP	2.3
1	C	263	PHE	2.2
1	C	113	PHE	2.2
1	B	80	GLN	2.2
1	D	18	LEU	2.2
1	D	161	PHE	2.2
1	D	57	GLY	2.2
1	A	153	ALA	2.2
1	D	73	ASP	2.1
1	C	164	ASP	2.1
1	C	138	GLU	2.1
1	B	153	ALA	2.1
1	D	72	SER	2.1
1	B	123	PHE	2.1
1	C	30	GLY	2.1
1	A	228	LYS	2.0
1	B	234	VAL	2.0
1	C	249	PHE	2.0
1	D	136	GLY	2.0
1	D	152	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

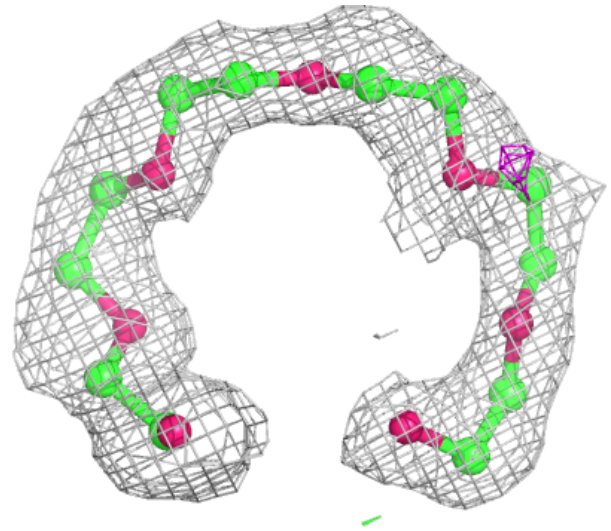
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

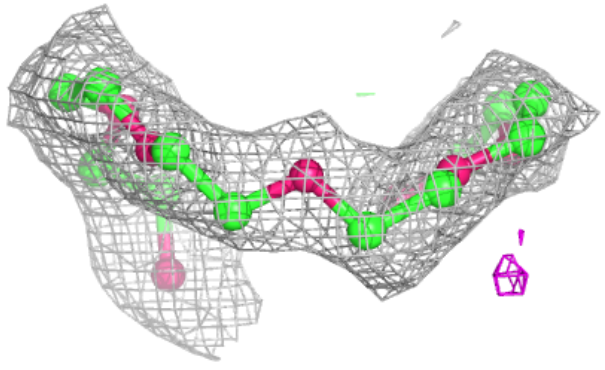
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	P6G	A	302	19/19	0.81	0.20	42,46,52,53	19
3	P6G	B	302	19/19	0.85	0.21	36,39,46,48	19
2	FE2	C	300	1/1	0.96	0.32	20,20,20,20	1
4	SO4	B	303	5/5	0.96	0.23	46,46,47,48	5
4	SO4	A	303	5/5	0.97	0.18	48,48,50,50	5
2	FE2	D	300	1/1	0.97	0.32	20,20,20,20	1
2	FE2	A	301	1/1	0.99	0.05	21,21,21,21	1
2	FE2	B	301	1/1	0.99	0.05	20,20,20,20	1

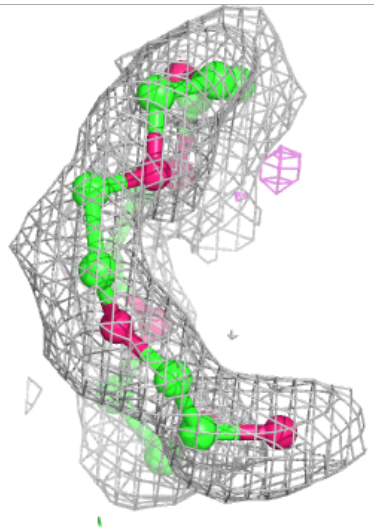
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G A 302:

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

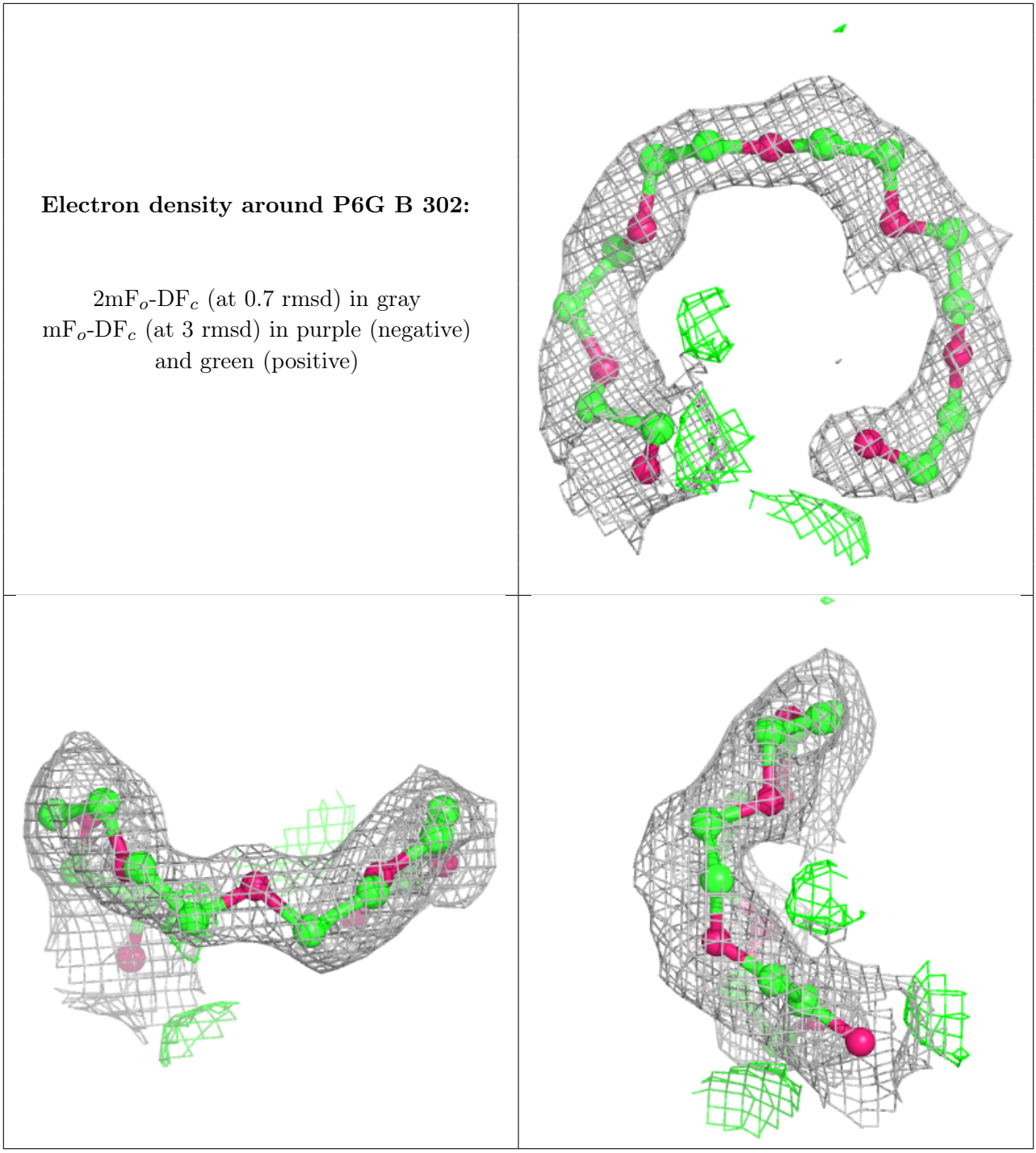






Electron density around P6G B 302:

$2mF_o$-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.