



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2024 – 01:04 AM EDT

PDB ID : 1YP2
Title : Crystal structure of potato tuber ADP-glucose pyrophosphorylase
Authors : Jin, X.; Ballicora, M.A.; Preiss, J.; Geiger, J.H.
Deposited on : 2005-01-29
Resolution : 2.11 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

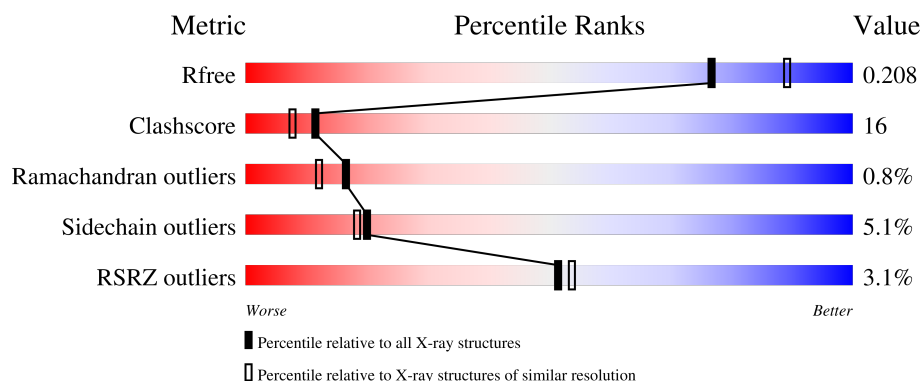
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	164625	7689 (2.14-2.10)
Clashscore	180529	8431 (2.14-2.10)
Ramachandran outliers	177936	8366 (2.14-2.10)
Sidechain outliers	177891	8367 (2.14-2.10)
RSRZ outliers	164620	7689 (2.14-2.10)

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 $\leq 5\%$. 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	451	<div> <div>0%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• 5%</div> </div> </div>
1	B	451	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>• 6%</div> </div> </div>
1	C	451	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>• •</div> </div> </div>
1	D	451	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>• 6%</div> </div> </div>

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
2	SO4	C	2010	-	-	X	-
3	PMB	A	3226	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14643 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 Glucose-1-phosphate adenylyltransferase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3346	2131	565	634	16			
1	B	426	Total	C	N	O	S	0	0	0
			3311	2105	561	629	16			
1	C	432	Total	C	N	O	S	0	0	0
			3367	2142	569	640	16			
1	D	423	Total	C	N	O	S	0	0	0
			3301	2102	558	625	16			

There are 4 discrepancies between the modelled and reference sequences:

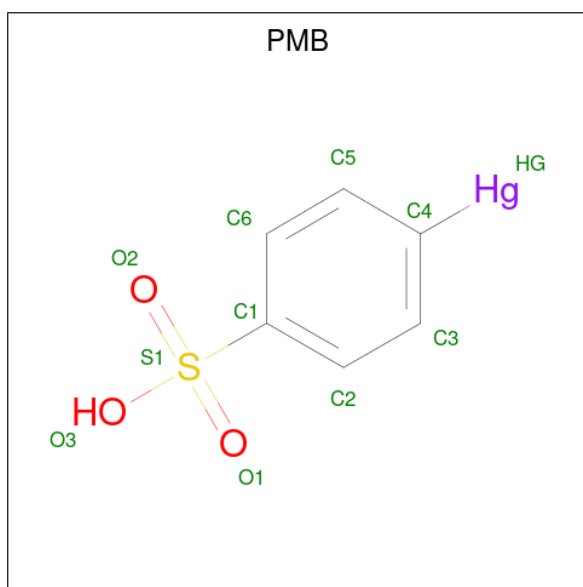
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P23509
B	1	MET	-	initiating methionine	UNP P23509
C	1	MET	-	initiating methionine	UNP P23509
D	1	MET	-	initiating methionine	UNP P23509

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is PARA-MERCURY-BENZENESULFONIC ACID (three-letter code: PMB) (formula: $C_6H_5HgO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Hg	O	S	0	0
			11	6	1	3	1		
3	B	1	Total	C	Hg	O	S	0	0
			11	6	1	3	1		
3	C	1	Total	C	Hg	O	S	0	0
			11	6	1	3	1		
3	D	1	Total	C	Hg	O	S	0	0
			11	6	1	3	1		

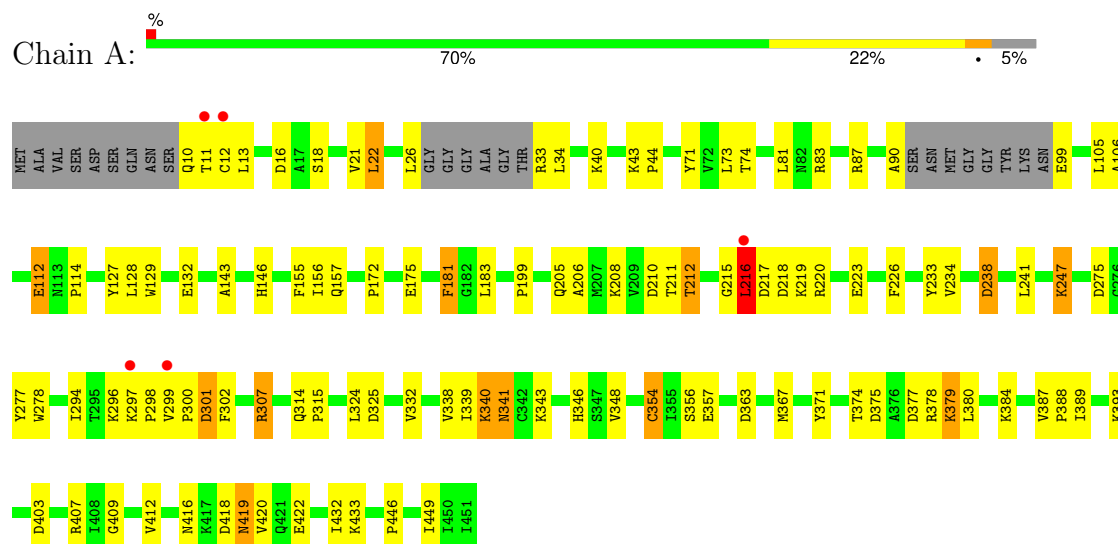
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	296	Total	O	0	0
			296	296		
4	B	286	Total	O	0	0
			286	286		
4	C	318	Total	O	0	0
			318	318		
4	D	314	Total	O	0	0
			314	314		

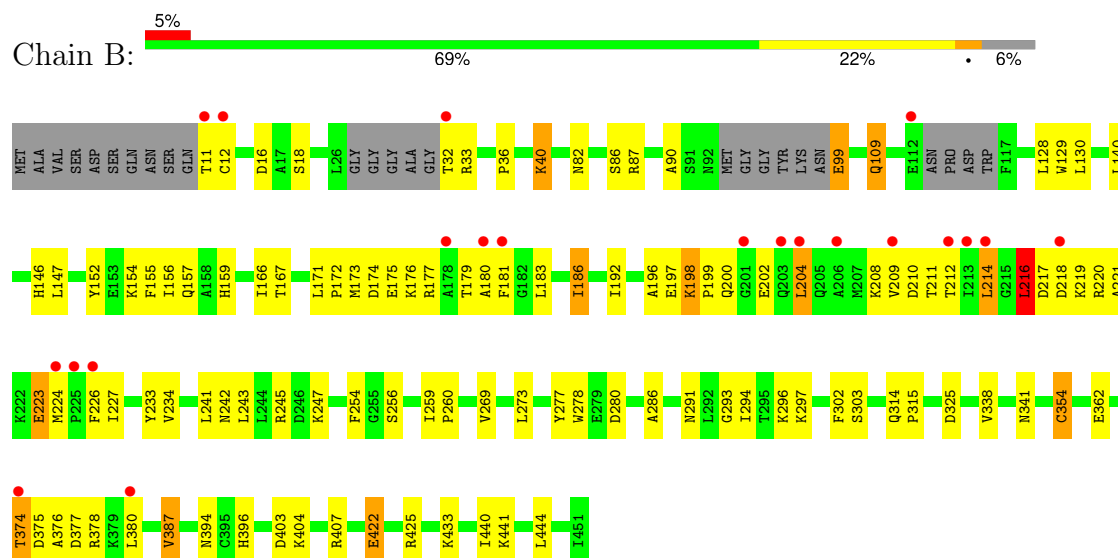
3 Residue-property plots

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: Glucose-1-phosphate adenylyltransferase small subunit

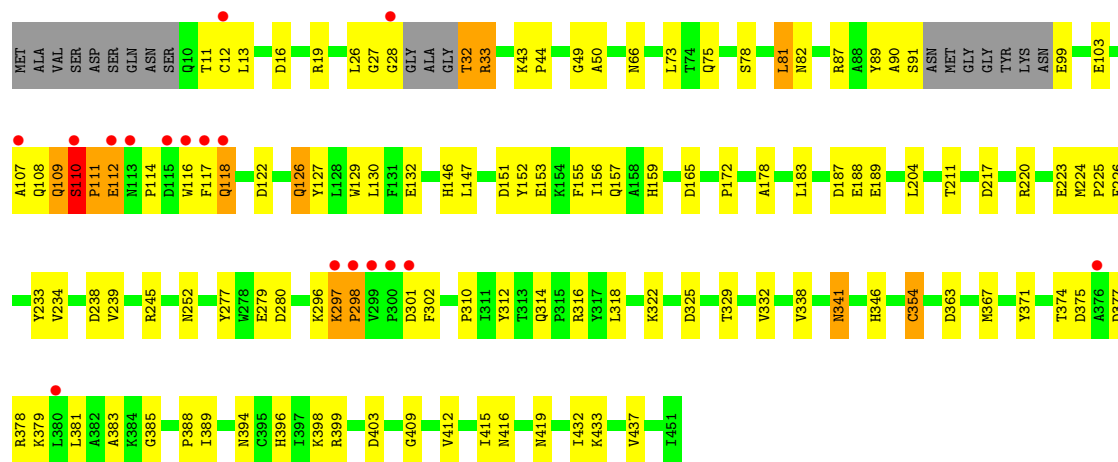


- Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit

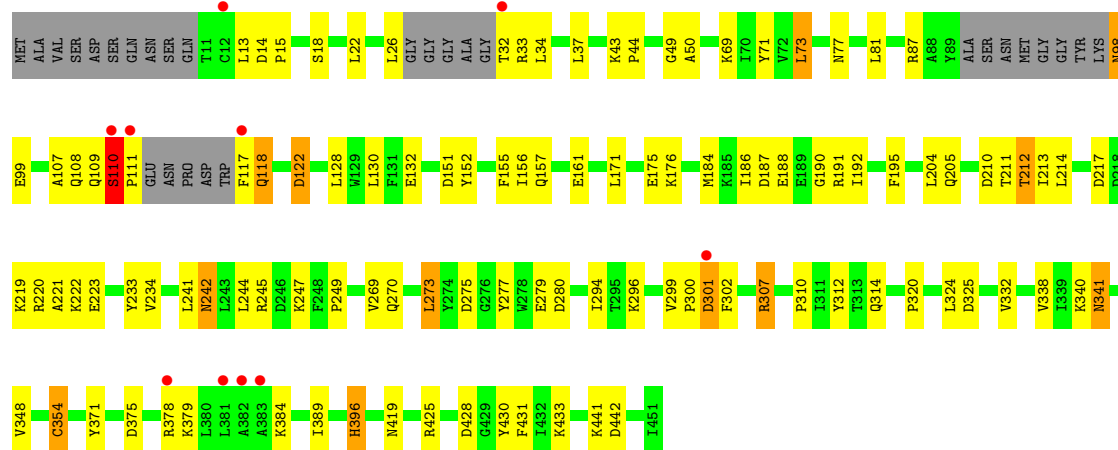


- Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit





• Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.47Å 137.55Å 91.62Å 90.00° 112.53° 90.00°	Depositor
Resolution (Å)	19.94 – 2.11 19.94 – 2.11	Depositor EDS
% Data completeness (in resolution range)	80.1 (19.94-2.11) 98.9 (19.94-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.172 , 0.229 0.208 , 0.208	Depositor DCC
R_{free} test set	5152 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14643	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PMB, 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	1/3409 (0.0%)	0.73	1/4613 (0.0%)
1	B	0.53	1/3369 (0.0%)	0.75	0/4556
1	C	0.53	0/3430	0.77	1/4641 (0.0%)
1	D	0.52	0/3360	0.75	0/4543
All	All	0.53	2/13568 (0.0%)	0.75	2/18353 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	CYS	CB-SG	11.34	2.01	1.82
1	B	354	CYS	CB-SG	-5.54	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	110	SER	C-N-CD	-6.75	105.76	120.60
1	A	354	CYS	N-CA-CB	5.62	120.72	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3346	0	3360	103	0
1	B	3311	0	3331	117	0
1	C	3367	0	3378	108	0
1	D	3301	0	3324	108	0
2	A	15	0	0	1	0
2	B	15	0	0	1	0
2	C	15	0	0	2	0
2	D	15	0	0	1	0
3	A	11	0	5	4	0
3	B	11	0	5	1	0
3	C	11	0	5	1	0
3	D	11	0	5	2	0
4	A	296	0	0	19	0
4	B	286	0	0	6	0
4	C	318	0	0	23	0
4	D	314	0	0	19	0
All	All	14643	0	13413	425	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 16.

All (425) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:CYS:CB	1:A:354:CYS:SG	2.01	1.49
1:B:11:THR:HA	1:B:157:GLN:HE22	1.09	1.13
1:A:33:ARG:HE	1:A:43:LYS:NZ	1.50	1.09
1:B:387:VAL:HG13	1:B:444:LEU:HD11	1.36	1.03
1:B:87:ARG:HD2	1:C:99:GLU:HG2	1.41	1.02
1:B:40:LYS:HE3	1:B:441:LYS:HB3	1.38	1.02
1:C:297:LYS:HG3	1:C:298:PRO:HD3	1.44	1.00
1:C:109:GLN:H	1:C:109:GLN:HE21	1.02	0.96
1:A:33:ARG:HE	1:A:43:LYS:HZ1	0.99	0.93
1:B:216:LEU:HD23	1:B:217:ASP:H	1.32	0.92
1:B:11:THR:HA	1:B:157:GLN:NE2	1.88	0.89
1:C:332:VAL:HG13	1:D:320:PRO:HB2	1.54	0.89
1:D:108:GLN:HG2	1:D:110:SER:H	1.38	0.88
1:D:110:SER:CB	1:D:111:PRO:HD2	2.03	0.86
3:D:3229:PMB:HG	3:D:3229:PMB:C4	1.83	0.86
1:D:217:ASP:OD1	1:D:220:ARG:HD3	1.76	0.85
1:D:108:GLN:HE21	1:D:110:SER:HA	1.42	0.85
3:C:3228:PMB:H5	4:C:3310:HOH:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ALA:HA	1:B:198:LYS:HE3	1.59	0.84
3:D:3229:PMB:HG	3:D:3229:PMB:HG	0.88	0.84
1:C:109:GLN:HE21	1:C:109:GLN:N	1.76	0.84
1:D:107:ALA:HB2	1:D:117:PHE:CE2	2.15	0.82
1:B:387:VAL:HG22	1:B:407:ARG:HB3	1.60	0.81
1:B:11:THR:HG21	1:B:154:LYS:HE3	1.62	0.81
1:D:110:SER:OG	1:D:111:PRO:HD2	1.80	0.81
1:B:175:GLU:HA	1:B:226:PHE:HE2	1.46	0.81
1:B:109:GLN:H	1:B:109:GLN:HE21	1.28	0.80
1:C:377:ASP:O	1:C:381:LEU:HD13	1.82	0.80
1:D:338:VAL:HG23	1:D:354:CYS:HA	1.65	0.79
1:C:33:ARG:HG3	1:C:33:ARG:HH11	1.48	0.79
1:C:375:ASP:O	1:C:379:LYS:HG3	1.82	0.78
1:B:11:THR:CA	1:B:157:GLN:HE22	1.93	0.78
1:D:108:GLN:NE2	1:D:110:SER:HA	1.98	0.78
1:B:214:LEU:HB2	1:B:273:LEU:HD22	1.65	0.78
1:B:214:LEU:HD13	1:B:214:LEU:H	1.50	0.77
1:B:208:LYS:HG2	1:B:226:PHE:CZ	2.19	0.77
1:D:77:ASN:HB2	4:D:3421:HOH:O	1.84	0.77
1:C:297:LYS:CG	1:C:298:PRO:HD3	2.15	0.76
1:A:10:GLN:O	1:C:11:THR:HG22	1.83	0.76
1:C:33:ARG:H	1:C:33:ARG:HD3	1.49	0.76
1:B:293:GLY:HA2	1:B:296:LYS:HE2	1.68	0.76
1:A:99:GLU:HA	4:D:3537:HOH:O	1.87	0.74
1:C:217:ASP:OD1	1:C:220:ARG:HD3	1.88	0.74
1:A:33:ARG:NE	1:A:43:LYS:NZ	2.33	0.74
1:D:108:GLN:HG2	1:D:110:SER:N	2.03	0.74
1:A:354:CYS:SG	3:A:3226:PMB:HG	2.06	0.73
1:A:384:LYS:HD3	4:A:3443:HOH:O	1.88	0.73
1:A:422:GLU:OE1	1:A:433:LYS:HE2	1.88	0.73
1:C:132:GLU:HG2	4:C:3515:HOH:O	1.90	0.72
1:C:33:ARG:HG3	1:C:33:ARG:NH1	2.03	0.72
1:B:354:CYS:SG	3:B:3227:PMB:HG	2.04	0.72
1:A:238:ASP:N	1:A:238:ASP:OD2	2.23	0.71
1:B:208:LYS:HG2	1:B:226:PHE:CE1	2.25	0.71
1:A:324:LEU:HD11	1:B:297:LYS:HD3	1.70	0.71
1:C:118:GLN:O	1:C:252:ASN:HB3	1.90	0.71
1:B:171:LEU:HD22	1:B:172:PRO:HD2	1.71	0.71
1:C:107:ALA:HB2	1:C:117:PHE:CE1	2.26	0.71
1:A:33:ARG:HB2	4:A:3475:HOH:O	1.90	0.70
1:B:375:ASP:HA	1:B:378:ARG:HD2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ARG:NH2	1:C:99:GLU:HA	2.07	0.70
1:D:375:ASP:O	1:D:379:LYS:HG2	1.92	0.69
3:A:3226:PMB:C4	4:A:3462:HOH:O	2.41	0.69
1:D:280:ASP:HB2	4:D:3346:HOH:O	1.91	0.69
1:A:297:LYS:HB3	1:A:298:PRO:HD3	1.75	0.69
1:C:109:GLN:H	1:C:109:GLN:NE2	1.85	0.69
1:A:33:ARG:NE	1:A:43:LYS:HZ1	1.83	0.69
1:D:242:ASN:HD21	1:D:247:LYS:NZ	1.91	0.69
1:B:293:GLY:O	1:B:296:LYS:HG2	1.93	0.68
1:D:277:TYR:CE2	1:D:302:PHE:HB2	2.28	0.68
1:B:179:THR:HG22	1:B:204:LEU:HG	1.74	0.68
1:B:362:GLU:OE1	1:B:396:HIS:HE1	1.76	0.68
1:D:242:ASN:HD21	1:D:247:LYS:HZ1	1.42	0.68
1:B:387:VAL:HG13	1:B:444:LEU:CD1	2.19	0.68
1:C:16:ASP:OD1	1:C:19:ARG:HG2	1.94	0.68
1:B:259:ILE:HB	1:B:260:PRO:HD3	1.76	0.67
1:D:219:LYS:HE3	1:D:223:GLU:OE1	1.94	0.67
1:A:83:ARG:HD2	4:A:3396:HOH:O	1.94	0.67
1:B:175:GLU:HA	1:B:226:PHE:CE2	2.27	0.67
1:A:354:CYS:SG	4:A:3415:HOH:O	2.53	0.66
1:B:209:VAL:HG21	4:B:3454:HOH:O	1.95	0.66
1:D:210:ASP:OD1	1:D:212:THR:HB	1.95	0.66
1:B:211:THR:HA	1:B:214:LEU:HD11	1.77	0.66
1:C:108:GLN:NE2	1:C:110:SER:O	2.29	0.65
1:B:40:LYS:HE2	1:B:440:ILE:CG2	2.26	0.65
1:B:216:LEU:HD23	1:B:217:ASP:N	2.09	0.65
1:C:110:SER:HB2	1:C:111:PRO:CD	2.28	0.64
1:A:87:ARG:NH2	1:A:87:ARG:HB3	2.12	0.64
1:B:211:THR:O	1:B:216:LEU:HB3	1.97	0.64
1:B:374:THR:HG22	1:B:374:THR:O	1.98	0.63
1:D:241:LEU:HD11	1:D:245:ARG:HD3	1.79	0.63
1:B:192:ILE:HD12	1:B:269:VAL:HG12	1.80	0.63
1:B:254:PHE:O	1:B:259:ILE:HG12	1.98	0.63
1:B:109:GLN:HE21	1:B:109:GLN:N	1.97	0.63
1:B:220:ARG:HG2	1:B:220:ARG:HH21	1.64	0.63
1:B:394:ASN:ND2	4:B:3345:HOH:O	2.31	0.63
1:B:422:GLU:OE1	1:B:433:LYS:HD2	1.99	0.63
1:C:277:TYR:CE2	1:C:302:PHE:HB2	2.34	0.63
1:A:26:LEU:HD23	1:A:73:LEU:HB2	1.82	0.62
1:A:220:ARG:HD2	4:A:3480:HOH:O	1.98	0.62
1:B:129:TRP:CE2	1:C:110:SER:HA	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:LEU:HD23	1:C:388:PRO:HA	1.81	0.62
1:D:109:GLN:HB3	4:D:3418:HOH:O	1.97	0.62
1:D:109:GLN:O	1:D:110:SER:HB2	1.99	0.62
1:D:294:ILE:HA	1:D:300:PRO:HB3	1.79	0.62
1:A:211:THR:HG21	1:A:216:LEU:HD12	1.80	0.62
1:B:196:ALA:O	1:B:199:PRO:HD3	1.99	0.62
1:C:152:TYR:O	1:C:156:ILE:HG12	1.99	0.62
1:A:357:GLU:OE2	1:A:393:LYS:HE3	1.99	0.62
1:D:33:ARG:HH21	1:D:33:ARG:HG3	1.65	0.62
1:D:378:ARG:NH1	4:D:3423:HOH:O	2.33	0.62
1:D:223:GLU:HB3	4:D:3489:HOH:O	2.00	0.61
1:B:177:ARG:HB3	1:B:181:PHE:HE1	1.66	0.61
1:A:26:LEU:HD21	1:A:73:LEU:HD12	1.83	0.60
1:A:132:GLU:HG3	4:A:3421:HOH:O	2.01	0.60
1:A:210:ASP:OD2	1:A:212:THR:HB	2.01	0.60
1:C:117:PHE:HE1	4:C:3449:HOH:O	1.84	0.60
1:C:325:ASP:O	1:C:341:ASN:HA	2.01	0.60
1:C:432:ILE:HG12	1:C:437:VAL:HG22	1.83	0.60
1:B:216:LEU:CD2	1:B:217:ASP:H	2.10	0.60
1:B:425:ARG:HD3	4:B:3445:HOH:O	2.01	0.60
1:D:296:LYS:HD3	1:D:301:ASP:OD2	2.01	0.59
1:C:394:ASN:HB3	4:C:3384:HOH:O	2.01	0.59
1:B:387:VAL:CG1	1:B:444:LEU:HD11	2.20	0.59
1:D:184:MET:HG2	1:D:195:PHE:CE2	2.38	0.59
1:A:277:TYR:CE1	1:A:301:ASP:HB3	2.37	0.59
1:C:32:THR:N	4:C:3408:HOH:O	2.35	0.59
1:D:33:ARG:HD3	4:D:3427:HOH:O	2.03	0.59
1:C:117:PHE:CD1	4:C:3397:HOH:O	2.52	0.59
1:A:219:LYS:HG2	1:A:223:GLU:OE2	2.02	0.59
1:B:374:THR:HB	1:B:377:ASP:OD2	2.03	0.58
1:B:374:THR:O	1:B:376:ALA:N	2.32	0.58
1:C:151:ASP:OD1	1:C:153:GLU:HB2	2.03	0.58
1:B:216:LEU:HD21	1:B:220:ARG:HB3	1.84	0.58
1:B:186:ILE:HD13	1:B:186:ILE:H	1.68	0.58
1:A:143:ALA:O	1:A:146:HIS:HE1	1.86	0.57
1:C:33:ARG:H	1:C:33:ARG:CD	2.13	0.57
1:B:173:MET:CE	1:B:177:ARG:HD3	2.34	0.57
1:B:200:GLN:HA	1:B:204:LEU:HB2	1.85	0.57
1:D:132:GLU:OE2	1:D:241:LEU:HD22	2.04	0.57
1:C:155:PHE:CE2	1:C:234:VAL:HG23	2.40	0.57
1:A:340:LYS:HG3	1:A:356:SER:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLN:HG3	1:C:110:SER:H	1.70	0.57
1:A:338:VAL:HG23	1:A:354:CYS:HA	1.87	0.56
1:C:338:VAL:HG23	1:C:338:VAL:O	2.05	0.56
1:A:183:LEU:HD12	1:A:199:PRO:HG3	1.85	0.56
1:B:241:LEU:HD11	1:B:245:ARG:NH2	2.19	0.56
1:D:110:SER:HB3	1:D:111:PRO:HD2	1.84	0.56
1:B:179:THR:O	1:B:198:LYS:HB3	2.06	0.56
1:D:152:TYR:O	1:D:156:ILE:HG12	2.05	0.56
1:A:407:ARG:HD2	4:A:3465:HOH:O	2.05	0.56
1:B:216:LEU:HD21	1:B:220:ARG:CB	2.36	0.56
1:D:49:GLY:O	1:D:50:ALA:HB3	2.05	0.56
1:A:73:LEU:HD23	1:A:105:LEU:HB2	1.88	0.56
1:A:354:CYS:SG	1:A:354:CYS:CA	2.94	0.56
1:C:112:GLU:C	1:C:114:PRO:HD3	2.27	0.55
1:B:16:ASP:OD1	1:B:18:SER:HB3	2.05	0.55
1:A:325:ASP:O	1:A:341:ASN:HA	2.06	0.55
1:C:82:ASN:HB3	4:C:3407:HOH:O	2.07	0.55
1:A:99:GLU:OE2	1:A:99:GLU:N	2.39	0.55
1:C:109:GLN:HG3	4:C:3325:HOH:O	2.07	0.55
1:B:277:TYR:CE2	1:B:302:PHE:HB2	2.42	0.55
1:B:325:ASP:O	1:B:341:ASN:HA	2.06	0.55
1:D:22:LEU:HD21	1:D:71:TYR:HD1	1.71	0.55
1:B:217:ASP:OD2	1:B:219:LYS:HE3	2.06	0.55
1:B:314:GLN:NE2	2:B:2009:SO4:O2	2.40	0.54
1:C:153:GLU:HB3	4:C:3455:HOH:O	2.06	0.54
1:C:332:VAL:CG1	1:D:320:PRO:HB2	2.32	0.54
1:B:32:THR:HA	4:B:3420:HOH:O	2.07	0.54
1:C:316:ARG:HD3	2:C:2010:SO4:O3	2.07	0.54
1:D:26:LEU:HD12	1:D:26:LEU:N	2.22	0.54
1:B:220:ARG:HG2	1:B:220:ARG:NH2	2.22	0.54
1:D:155:PHE:CZ	1:D:234:VAL:HG23	2.42	0.54
1:D:300:PRO:HB2	1:D:302:PHE:O	2.07	0.54
1:D:314:GLN:NE2	2:D:2011:SO4:O1	2.41	0.54
1:B:33:ARG:HH21	1:B:33:ARG:HG3	1.73	0.54
1:D:87:ARG:NE	1:D:314:GLN:OE1	2.41	0.54
1:A:172:PRO:HA	1:A:226:PHE:O	2.08	0.53
1:B:197:GLU:HG3	1:B:256:SER:HA	1.89	0.53
1:A:277:TYR:CE2	1:A:302:PHE:HB2	2.43	0.53
1:A:339:ILE:C	3:A:3226:PMB:H3	2.29	0.53
1:D:186:ILE:HD12	1:D:190:GLY:HA2	1.90	0.53
1:D:279:GLU:HG3	4:D:3323:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ARG:NH1	4:D:3240:HOH:O	2.40	0.53
1:B:12:CYS:H	1:B:157:GLN:NE2	2.07	0.53
1:D:219:LYS:HD2	1:D:222:LYS:NZ	2.24	0.53
1:D:425:ARG:HG3	1:D:430:TYR:CZ	2.44	0.53
1:D:310:PRO:HG2	1:D:312:TYR:CE2	2.44	0.53
1:D:107:ALA:HB2	1:D:117:PHE:CZ	2.43	0.53
1:A:181:PHE:CD1	1:A:181:PHE:N	2.77	0.52
1:B:152:TYR:O	1:B:156:ILE:HG12	2.10	0.52
1:C:108:GLN:HE21	1:C:110:SER:C	2.13	0.52
1:B:217:ASP:O	1:B:221:ALA:N	2.42	0.52
1:D:108:GLN:HG2	1:D:110:SER:HA	1.92	0.52
1:A:380:LEU:HB2	4:A:3463:HOH:O	2.09	0.52
1:B:362:GLU:OE1	1:B:396:HIS:CE1	2.61	0.52
1:C:66:ASN:HB2	4:C:3330:HOH:O	2.09	0.52
1:D:341:ASN:HD22	1:D:341:ASN:H	1.58	0.52
1:A:157:GLN:HG3	4:A:3518:HOH:O	2.09	0.52
1:C:341:ASN:ND2	1:C:341:ASN:H	2.08	0.52
1:B:214:LEU:HD13	1:B:214:LEU:N	2.23	0.52
1:C:89:TYR:O	1:C:91:SER:N	2.43	0.51
1:C:13:LEU:HD11	1:C:156:ILE:HB	1.92	0.51
1:B:241:LEU:HD11	1:B:245:ARG:CZ	2.40	0.51
1:C:371:TYR:OH	1:C:389:ILE:HD11	2.10	0.51
1:A:21:VAL:HG21	1:A:156:ILE:HD13	1.91	0.51
1:A:371:TYR:OH	1:A:389:ILE:HD11	2.11	0.51
1:D:219:LYS:HD2	1:D:222:LYS:HZ3	1.76	0.51
1:D:296:LYS:HG3	4:D:3493:HOH:O	2.10	0.51
1:C:87:ARG:NH2	4:C:3511:HOH:O	2.44	0.51
1:C:409:GLY:O	1:C:412:VAL:HG23	2.11	0.51
1:C:49:GLY:O	1:C:50:ALA:HB3	2.10	0.51
1:B:338:VAL:HG23	1:B:354:CYS:HA	1.92	0.50
1:D:325:ASP:O	1:D:341:ASN:HA	2.11	0.50
1:B:338:VAL:HG23	1:B:338:VAL:O	2.11	0.50
1:D:98:ASN:ND2	4:D:3420:HOH:O	2.44	0.50
1:C:383:ALA:HB2	4:C:3351:HOH:O	2.11	0.50
1:D:431:PHE:HE2	1:D:433:LYS:HE3	1.76	0.50
1:B:183:LEU:HD13	1:B:226:PHE:CD1	2.45	0.50
1:D:175:GLU:CD	1:D:205:GLN:HE22	2.15	0.50
1:C:396:HIS:HD2	4:C:3459:HOH:O	1.93	0.50
1:A:416:ASN:HD21	1:A:420:VAL:H	1.58	0.49
1:B:223:GLU:OE1	1:B:223:GLU:O	2.29	0.49
1:C:367:MET:HG3	1:C:403:ASP:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PHE:CE2	1:B:234:VAL:HG23	2.48	0.49
1:D:33:ARG:HG3	1:D:33:ARG:NH2	2.27	0.49
1:D:22:LEU:HD21	1:D:71:TYR:CD1	2.46	0.49
1:D:211:THR:OG1	1:D:221:ALA:HA	2.13	0.49
1:B:291:ASN:O	1:B:294:ILE:HG12	2.13	0.49
1:C:383:ALA:C	1:C:385:GLY:H	2.16	0.49
1:D:188:GLU:HA	1:D:213:ILE:HD13	1.93	0.49
1:C:117:PHE:CZ	1:C:126:GLN:NE2	2.81	0.49
1:C:314:GLN:NE2	2:C:2010:SO4:O1	2.46	0.49
1:D:155:PHE:CE2	1:D:234:VAL:HG23	2.48	0.49
1:C:220:ARG:O	1:C:223:GLU:HG2	2.12	0.49
1:C:354:CYS:SG	1:C:378:ARG:NH1	2.86	0.49
1:C:33:ARG:HH11	1:C:33:ARG:CG	2.21	0.48
1:C:277:TYR:CD2	1:C:302:PHE:HB2	2.48	0.48
1:D:219:LYS:HA	1:D:222:LYS:HZ3	1.77	0.48
1:A:325:ASP:HB3	1:A:341:ASN:HB3	1.96	0.48
1:A:409:GLY:O	1:A:412:VAL:HG23	2.11	0.48
1:C:117:PHE:CE1	4:C:3397:HOH:O	2.65	0.48
1:D:277:TYR:CE1	1:D:301:ASP:HB2	2.47	0.48
1:A:112:GLU:C	1:A:114:PRO:HD3	2.34	0.48
1:A:332:VAL:HG22	1:A:348:VAL:HG22	1.94	0.48
1:C:117:PHE:HD1	4:C:3397:HOH:O	1.92	0.48
1:A:128:LEU:HD21	1:A:241:LEU:HA	1.94	0.48
1:A:367:MET:HG3	1:A:403:ASP:HA	1.94	0.48
1:C:26:LEU:CD2	1:C:73:LEU:HD22	2.43	0.48
1:B:217:ASP:OD2	1:B:219:LYS:HG3	2.14	0.48
1:B:173:MET:HE1	1:B:177:ARG:HD3	1.95	0.48
1:C:225:PRO:HG2	1:C:226:PHE:CE1	2.48	0.48
1:A:129:TRP:CE2	1:D:110:SER:HB2	2.49	0.48
1:B:159:HIS:HD2	1:B:167:THR:OG1	1.97	0.48
1:C:187:ASP:OD1	1:C:187:ASP:C	2.52	0.48
1:A:296:LYS:HD3	1:A:299:VAL:O	2.13	0.48
1:A:87:ARG:NH2	1:A:314:GLN:HG3	2.30	0.47
1:C:433:LYS:HG3	4:C:3403:HOH:O	2.14	0.47
1:D:18:SER:O	1:D:69:LYS:HE2	2.14	0.47
1:D:110:SER:CB	1:D:111:PRO:CD	2.81	0.47
1:D:299:VAL:HG12	1:D:300:PRO:HD2	1.95	0.47
1:A:301:ASP:HB2	4:A:3434:HOH:O	2.13	0.47
1:B:200:GLN:CA	1:B:204:LEU:HB2	2.44	0.47
1:C:110:SER:CB	1:C:111:PRO:CD	2.87	0.47
1:D:157:GLN:O	1:D:161:GLU:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:VAL:HG23	1:A:338:VAL:O	2.14	0.47
1:A:374:THR:OG1	1:A:377:ASP:OD1	2.21	0.47
1:B:40:LYS:HE2	1:B:440:ILE:HG22	1.94	0.47
1:D:175:GLU:HB3	1:D:176:LYS:NZ	2.29	0.47
1:A:12:CYS:SG	1:C:12:CYS:N	2.87	0.47
1:B:173:MET:HE2	1:B:177:ARG:HD3	1.95	0.47
1:B:216:LEU:CD2	1:B:217:ASP:N	2.73	0.47
1:D:117:PHE:HD1	4:D:3417:HOH:O	1.98	0.47
1:B:374:THR:O	1:B:375:ASP:HB3	2.15	0.47
1:B:174:ASP:HA	1:B:224:MET:HA	1.98	0.46
1:D:108:GLN:HG2	1:D:110:SER:CA	2.45	0.46
1:A:446:PRO:O	1:A:449:ILE:HG12	2.15	0.46
1:B:396:HIS:HD2	4:B:3346:HOH:O	1.98	0.46
1:C:238:ASP:HB2	4:C:3421:HOH:O	2.16	0.46
1:D:384:LYS:O	1:D:384:LYS:HG2	2.15	0.46
1:A:16:ASP:OD2	1:A:18:SER:HB3	2.15	0.46
1:B:159:HIS:CD2	1:B:167:THR:OG1	2.69	0.46
1:D:341:ASN:H	1:D:341:ASN:ND2	2.13	0.46
1:B:186:ILE:HD12	1:B:227:ILE:CD1	2.46	0.46
1:C:245:ARG:NH1	4:C:3538:HOH:O	2.43	0.46
1:A:418:ASP:O	1:A:419:ASN:CB	2.63	0.46
1:D:14:ASP:HA	1:D:15:PRO:C	2.35	0.46
1:D:190:GLY:C	1:D:270:GLN:NE2	2.68	0.46
1:D:396:HIS:HD2	4:D:3401:HOH:O	1.98	0.46
1:C:155:PHE:CE2	1:C:234:VAL:CG2	2.99	0.46
1:D:214:LEU:HB3	1:D:273:LEU:HB2	1.96	0.46
1:C:129:TRP:N	4:C:3308:HOH:O	2.40	0.46
1:D:111:PRO:HD3	4:D:3446:HOH:O	2.16	0.45
1:A:211:THR:CG2	1:A:216:LEU:HD12	2.46	0.45
1:A:324:LEU:HD22	1:A:340:LYS:HE2	1.97	0.45
1:C:126:GLN:NE2	1:C:127:TYR:CE1	2.84	0.45
1:D:338:VAL:O	1:D:354:CYS:HA	2.15	0.45
1:A:87:ARG:NE	1:D:99:GLU:OE2	2.49	0.45
1:D:187:ASP:OD2	1:D:191:ARG:HB3	2.16	0.45
1:D:245:ARG:O	1:D:249:PRO:HB3	2.16	0.45
1:A:13:LEU:HD23	4:A:3518:HOH:O	2.15	0.45
1:A:341:ASN:H	1:A:341:ASN:ND2	2.13	0.45
1:A:346:HIS:O	1:A:363:ASP:HA	2.17	0.45
1:A:155:PHE:CE2	1:A:234:VAL:HG23	2.52	0.45
1:A:247:LYS:HA	1:A:247:LYS:HE3	1.98	0.45
1:A:379:LYS:CA	1:A:379:LYS:HE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLN:H	1:B:109:GLN:NE2	2.07	0.45
1:D:13:LEU:HD11	1:D:156:ILE:HB	1.99	0.45
1:B:314:GLN:HA	1:B:315:PRO:HD3	1.85	0.45
1:B:403:ASP:OD1	1:B:404:LYS:N	2.46	0.45
1:D:301:ASP:OD2	1:D:301:ASP:N	2.48	0.45
1:A:205:GLN:OE1	1:A:208:LYS:HE3	2.17	0.45
1:A:10:GLN:NE2	1:A:11:THR:HG23	2.31	0.45
1:B:146:HIS:CD2	1:B:278:TRP:CZ2	3.04	0.45
1:C:13:LEU:CD2	1:C:157:GLN:HG2	2.47	0.45
1:D:371:TYR:OH	1:D:389:ILE:HD11	2.17	0.45
1:C:383:ALA:C	1:C:385:GLY:N	2.70	0.44
1:D:87:ARG:HD3	1:D:314:GLN:OE1	2.17	0.44
1:A:74:THR:O	1:A:106:ALA:HA	2.18	0.44
1:D:441:LYS:O	1:D:442:ASP:HB2	2.17	0.44
1:A:26:LEU:CD2	1:A:73:LEU:HD12	2.47	0.44
1:A:129:TRP:CZ2	1:D:110:SER:HB2	2.52	0.44
1:A:378:ARG:CZ	1:A:378:ARG:HB2	2.46	0.44
1:D:118:GLN:HB2	1:D:122:ASP:OD2	2.17	0.44
1:A:206:ALA:HB1	4:A:3420:HOH:O	2.18	0.44
1:B:180:ALA:CA	1:B:198:LYS:HE3	2.37	0.44
1:D:192:ILE:HD12	1:D:269:VAL:HG12	2.00	0.44
1:B:186:ILE:HD12	1:B:227:ILE:HD13	1.98	0.44
1:C:28:GLY:HA3	1:C:75:GLN:H	1.81	0.44
1:D:220:ARG:NH2	1:D:275:ASP:OD2	2.40	0.44
1:A:87:ARG:HB3	1:A:87:ARG:HH21	1.80	0.44
1:B:209:VAL:HG22	1:B:210:ASP:N	2.33	0.44
1:C:378:ARG:NH1	4:C:3428:HOH:O	2.38	0.44
1:B:375:ASP:O	1:B:378:ARG:HB2	2.17	0.44
1:C:178:ALA:HB1	1:C:183:LEU:HD11	2.00	0.44
1:C:220:ARG:HA	1:C:223:GLU:HG2	2.00	0.44
1:C:277:TYR:CE1	1:C:301:ASP:HB3	2.53	0.44
1:C:338:VAL:HG23	1:C:354:CYS:HA	1.99	0.44
1:D:43:LYS:HB3	1:D:44:PRO:HD3	1.99	0.44
1:C:346:HIS:O	1:C:363:ASP:HA	2.17	0.44
1:A:294:ILE:HA	1:A:300:PRO:HB3	1.99	0.44
1:A:324:LEU:HD13	3:A:3226:PMB:O2	2.18	0.44
1:B:210:ASP:OD2	1:B:212:THR:OG1	2.36	0.43
1:C:110:SER:HB2	1:C:111:PRO:HD3	2.00	0.43
1:C:223:GLU:HG3	1:C:224:MET:HG3	2.00	0.43
1:A:294:ILE:HD11	1:A:332:VAL:HG21	2.00	0.43
1:C:146:HIS:HD2	1:C:280:ASP:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:GLU:OE2	1:C:189:GLU:HG3	2.17	0.43
1:B:171:LEU:HD13	1:B:172:PRO:O	2.17	0.43
1:D:332:VAL:HG22	1:D:348:VAL:HG22	2.00	0.43
1:A:40:LYS:HE2	4:A:3330:HOH:O	2.19	0.43
1:A:112:GLU:O	1:A:114:PRO:HD3	2.19	0.43
1:A:378:ARG:HH21	1:A:378:ARG:HG3	1.83	0.43
1:B:325:ASP:HB3	1:B:341:ASN:HB3	1.99	0.43
1:D:219:LYS:O	1:D:222:LYS:HG2	2.18	0.43
1:A:238:ASP:HA	4:A:3409:HOH:O	2.19	0.43
1:C:415:ILE:O	1:C:416:ASN:C	2.56	0.43
1:B:86:SER:HA	1:B:90:ALA:HB3	2.00	0.43
1:B:173:MET:HE2	1:B:177:ARG:HB2	2.01	0.43
1:A:314:GLN:HA	1:A:315:PRO:HD3	1.90	0.43
1:C:107:ALA:HA	1:C:117:PHE:CZ	2.54	0.43
1:A:146:HIS:HD2	4:A:3490:HOH:O	2.02	0.43
1:A:379:LYS:HE2	1:A:379:LYS:N	2.33	0.43
1:B:155:PHE:HE1	1:B:167:THR:HG22	1.84	0.43
1:B:171:LEU:HD22	1:B:172:PRO:CD	2.44	0.43
1:A:217:ASP:OD2	1:A:218:ASP:N	2.52	0.42
1:C:322:LYS:HB2	4:C:3377:HOH:O	2.18	0.42
1:D:324:LEU:HB2	1:D:340:LYS:HA	2.01	0.42
1:B:129:TRP:CZ2	1:C:110:SER:HA	2.54	0.42
1:D:32:THR:HG22	4:D:3452:HOH:O	2.18	0.42
1:D:98:ASN:N	4:D:3431:HOH:O	2.51	0.42
1:D:338:VAL:HG23	1:D:338:VAL:O	2.19	0.42
1:A:387:VAL:HA	1:A:388:PRO:HD3	1.86	0.42
1:C:153:GLU:O	1:C:157:GLN:HG3	2.19	0.42
1:C:78:SER:HB3	1:C:81:LEU:HB2	2.00	0.42
1:D:73:LEU:HD12	4:D:3458:HOH:O	2.19	0.42
1:B:219:LYS:HB2	1:B:219:LYS:NZ	2.34	0.42
1:D:217:ASP:OD1	1:D:220:ARG:CD	2.57	0.42
1:D:378:ARG:CZ	4:D:3474:HOH:O	2.67	0.42
1:B:197:GLU:O	1:B:199:PRO:N	2.53	0.42
1:A:275:ASP:CB	4:A:3491:HOH:O	2.67	0.42
1:B:11:THR:CG2	1:B:154:LYS:HE3	2.40	0.42
1:B:99:GLU:OE1	1:B:99:GLU:O	2.36	0.42
1:D:87:ARG:CD	1:D:314:GLN:OE1	2.67	0.42
1:A:215:GLY:O	1:A:216:LEU:C	2.58	0.42
1:B:166:ILE:HD11	1:B:243:LEU:CD1	2.50	0.42
1:B:242:ASN:HD21	1:B:247:LYS:HE2	1.85	0.42
1:D:108:GLN:CG	1:D:110:SER:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASP:O	1:B:286:ALA:HB1	2.20	0.42
1:A:22:LEU:HD21	1:A:71:TYR:CD1	2.54	0.41
1:A:43:LYS:HB3	1:A:44:PRO:HD3	2.01	0.41
1:C:43:LYS:N	1:C:44:PRO:CD	2.83	0.41
1:A:175:GLU:HA	1:A:226:PHE:CE1	2.55	0.41
1:C:172:PRO:HA	1:C:226:PHE:O	2.21	0.41
1:D:34:LEU:O	1:D:37:LEU:HB2	2.21	0.41
1:D:241:LEU:HD21	1:D:245:ARG:NH1	2.36	0.41
1:B:82:ASN:HB3	1:C:103:GLU:OE2	2.20	0.41
1:C:277:TYR:CZ	1:C:279:GLU:HG2	2.55	0.41
1:B:211:THR:OG1	1:B:221:ALA:HA	2.20	0.41
1:B:218:ASP:HA	1:B:221:ALA:HB3	2.03	0.41
1:C:27:GLY:HA2	4:C:3419:HOH:O	2.21	0.41
1:C:110:SER:CB	1:C:111:PRO:HD3	2.48	0.41
1:A:217:ASP:O	1:A:218:ASP:C	2.59	0.41
1:C:318:LEU:HD23	1:C:318:LEU:HA	1.83	0.41
1:A:127:TYR:OH	1:D:109:GLN:HG3	2.21	0.41
1:A:307:ARG:HA	1:A:307:ARG:HH11	1.85	0.41
1:A:314:GLN:NE2	2:A:2008:SO4:O4	2.54	0.41
1:B:212:THR:HG23	1:B:221:ALA:CB	2.51	0.41
1:B:303:SER:HA	4:B:3326:HOH:O	2.20	0.41
1:C:165:ASP:HB3	1:C:239:VAL:HG21	2.01	0.41
1:C:301:ASP:HA	4:C:3530:HOH:O	2.21	0.41
1:B:202:GLU:HA	1:B:202:GLU:OE2	2.21	0.41
1:C:398:LYS:HG3	1:C:399:ARG:N	2.36	0.41
1:C:156:ILE:O	1:C:159:HIS:HB3	2.22	0.40
1:D:132:GLU:HG3	4:D:3442:HOH:O	2.21	0.40
1:A:90:ALA:C	4:A:3408:HOH:O	2.60	0.40
1:A:379:LYS:HE2	1:A:379:LYS:HA	2.02	0.40
1:A:146:HIS:CG	1:A:278:TRP:CH2	3.10	0.40
1:A:380:LEU:HD22	4:A:3463:HOH:O	2.20	0.40
1:C:117:PHE:HE2	1:C:126:GLN:CD	2.25	0.40
1:C:296:LYS:HA	1:C:296:LYS:HD3	1.83	0.40
1:D:273:LEU:HD13	1:D:275:ASP:HB2	2.04	0.40
1:A:422:GLU:HA	1:A:432:ILE:O	2.21	0.40
1:C:310:PRO:HG2	1:C:312:TYR:CZ	2.56	0.40
1:D:425:ARG:NH1	1:D:428:ASP:OD2	2.54	0.40
1:C:329:THR:HG22	1:D:325:ASP:HA	2.04	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	422/451 (94%)	396 (94%)	24 (6%)	2 (0%)	25	22
1	B	418/451 (93%)	387 (93%)	26 (6%)	5 (1%)	11	6
1	C	426/451 (94%)	402 (94%)	19 (4%)	5 (1%)	11	6
1	D	415/451 (92%)	398 (96%)	16 (4%)	1 (0%)	44	44
All	All	1681/1804 (93%)	1583 (94%)	85 (5%)	13 (1%)	16	12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	LEU
1	A	419	ASN
1	B	176	LYS
1	B	374	THR
1	C	90	ALA
1	C	110	SER
1	C	111	PRO
1	D	110	SER
1	B	216	LEU
1	B	380	LEU
1	C	298	PRO
1	C	374	THR
1	B	198	LYS

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	360/375 (96%)	343 (95%)	17 (5%)	22	21
1	B	356/375 (95%)	340 (96%)	16 (4%)	23	22
1	C	362/375 (96%)	344 (95%)	18 (5%)	20	19
1	D	356/375 (95%)	334 (94%)	22 (6%)	15	12
All	All	1434/1500 (96%)	1361 (95%)	73 (5%)	20	18

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	34	LEU
1	A	81	LEU
1	A	112	GLU
1	A	181	PHE
1	A	212	THR
1	A	216	LEU
1	A	233	TYR
1	A	238	ASP
1	A	247	LYS
1	A	301	ASP
1	A	307	ARG
1	A	340	LYS
1	A	341	ASN
1	A	343	LYS
1	A	375	ASP
1	A	379	LYS
1	B	36	PRO
1	B	40	LYS
1	B	99	GLU
1	B	109	GLN
1	B	128	LEU
1	B	130	LEU
1	B	140	LEU
1	B	147	LEU
1	B	186	ILE
1	B	204	LEU
1	B	214	LEU
1	B	216	LEU
1	B	223	GLU
1	B	233	TYR
1	B	387	VAL
1	B	422	GLU

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Mol	Chain	Res	Type
1	C	32	THR
1	C	33	ARG
1	C	81	LEU
1	C	109	GLN
1	C	112	GLU
1	C	116	TRP
1	C	118	GLN
1	C	122	ASP
1	C	126	GLN
1	C	130	LEU
1	C	147	LEU
1	C	204	LEU
1	C	211	THR
1	C	233	TYR
1	C	297	LYS
1	C	341	ASN
1	C	354	CYS
1	C	419	ASN
1	D	73	LEU
1	D	81	LEU
1	D	98	ASN
1	D	110	SER
1	D	118	GLN
1	D	122	ASP
1	D	128	LEU
1	D	130	LEU
1	D	151	ASP
1	D	171	LEU
1	D	204	LEU
1	D	212	THR
1	D	233	TYR
1	D	242	ASN
1	D	244	LEU
1	D	273	LEU
1	D	301	ASP
1	D	307	ARG
1	D	341	ASN
1	D	354	CYS
1	D	396	HIS
1	D	419	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	64	ASN
1	A	66	ASN
1	A	75	GLN
1	A	109	GLN
1	A	146	HIS
1	A	341	ASN
1	A	416	ASN
1	A	419	ASN
1	A	421	GLN
1	B	64	ASN
1	B	75	GLN
1	B	108	GLN
1	B	109	GLN
1	B	146	HIS
1	B	157	GLN
1	B	159	HIS
1	B	242	ASN
1	B	252	ASN
1	B	396	HIS
1	B	419	ASN
1	C	10	GLN
1	C	51	ASN
1	C	64	ASN
1	C	75	GLN
1	C	109	GLN
1	C	126	GLN
1	C	252	ASN
1	C	270	GLN
1	C	341	ASN
1	C	394	ASN
1	C	396	HIS
1	D	66	ASN
1	D	75	GLN
1	D	98	ASN
1	D	108	GLN
1	D	126	GLN
1	D	205	GLN
1	D	242	ASN
1	D	252	ASN
1	D	270	GLN
1	D	341	ASN
1	D	396	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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$
3	PMB	D	3229	1	8,11,11	2.33	5 (62%)	14,16,16	0.95	1 (7%)
2	SO4	A	2007	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	C	2002	-	4,4,4	0.41	0	6,6,6	0.28	0
2	SO4	D	2011	-	4,4,4	0.32	0	6,6,6	0.15	0
3	PMB	B	3227	-	8,11,11	2.48	4 (50%)	14,16,16	1.18	2 (14%)
2	SO4	A	2008	-	4,4,4	0.34	0	6,6,6	0.17	0
2	SO4	C	2010	-	4,4,4	0.27	0	6,6,6	0.18	0
3	PMB	A	3226	4,1	8,11,11	1.34	2 (25%)	14,16,16	1.42	3 (21%)
2	SO4	D	2003	-	4,4,4	0.33	0	6,6,6	0.22	0
2	SO4	A	2000	-	4,4,4	0.44	0	6,6,6	0.34	0
2	SO4	D	2004	-	4,4,4	0.44	0	6,6,6	0.15	0
2	SO4	C	2005	-	4,4,4	0.34	0	6,6,6	0.13	0
2	SO4	B	2001	-	4,4,4	0.39	0	6,6,6	0.21	0
2	SO4	B	2006	-	4,4,4	0.40	0	6,6,6	0.12	0
3	PMB	C	3228	-	8,11,11	5.07	5 (62%)	14,16,16	2.21	5 (35%)
2	SO4	B	2009	-	4,4,4	0.29	0	6,6,6	0.17	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	PMB	D	3229	1	-	0/6/6/6	0/1/1/1
3	PMB	B	3227	-	-	0/6/6/6	0/1/1/1
3	PMB	C	3228	-	-	0/6/6/6	0/1/1/1
3	PMB	A	3226	4,1	-	0/6/6/6	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3228	PMB	C1-S1	9.90	1.97	1.77
3	C	3228	PMB	C6-C5	6.50	1.49	1.38
3	C	3228	PMB	C3-C2	5.67	1.48	1.38
3	B	3227	PMB	C1-S1	4.23	1.85	1.77
3	C	3228	PMB	C2-C1	4.04	1.45	1.38
3	C	3228	PMB	C6-C1	3.92	1.45	1.38
3	D	3229	PMB	C1-S1	3.55	1.84	1.77
3	B	3227	PMB	C6-C5	3.55	1.44	1.38
3	D	3229	PMB	C3-C2	3.33	1.44	1.38
3	B	3227	PMB	C6-C1	2.93	1.43	1.38
3	D	3229	PMB	C6-C1	2.77	1.43	1.38
3	A	3226	PMB	C6-C1	2.56	1.42	1.38
3	B	3227	PMB	C3-C2	2.49	1.42	1.38
3	D	3229	PMB	C6-C5	2.36	1.42	1.38
3	D	3229	PMB	C2-C1	2.31	1.42	1.38
3	A	3226	PMB	C6-C5	2.01	1.42	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3228	PMB	C6-C1-C2	-5.09	113.83	120.47
3	C	3228	PMB	C3-C2-C1	4.49	123.81	119.44
3	B	3227	PMB	C3-C2-C1	2.86	122.22	119.44
3	A	3226	PMB	C2-C1-S1	-2.71	115.86	119.74
3	C	3228	PMB	C5-C6-C1	2.49	121.86	119.44
3	C	3228	PMB	C6-C1-S1	2.43	123.22	119.74
3	B	3227	PMB	C6-C1-C2	-2.36	117.39	120.47
3	C	3228	PMB	C2-C1-S1	2.23	122.94	119.74
3	A	3226	PMB	C3-C2-C1	2.21	121.59	119.44
3	A	3226	PMB	C6-C1-S1	2.21	122.90	119.74
3	D	3229	PMB	C3-C2-C1	2.09	121.47	119.44

There are no chirality outliers.

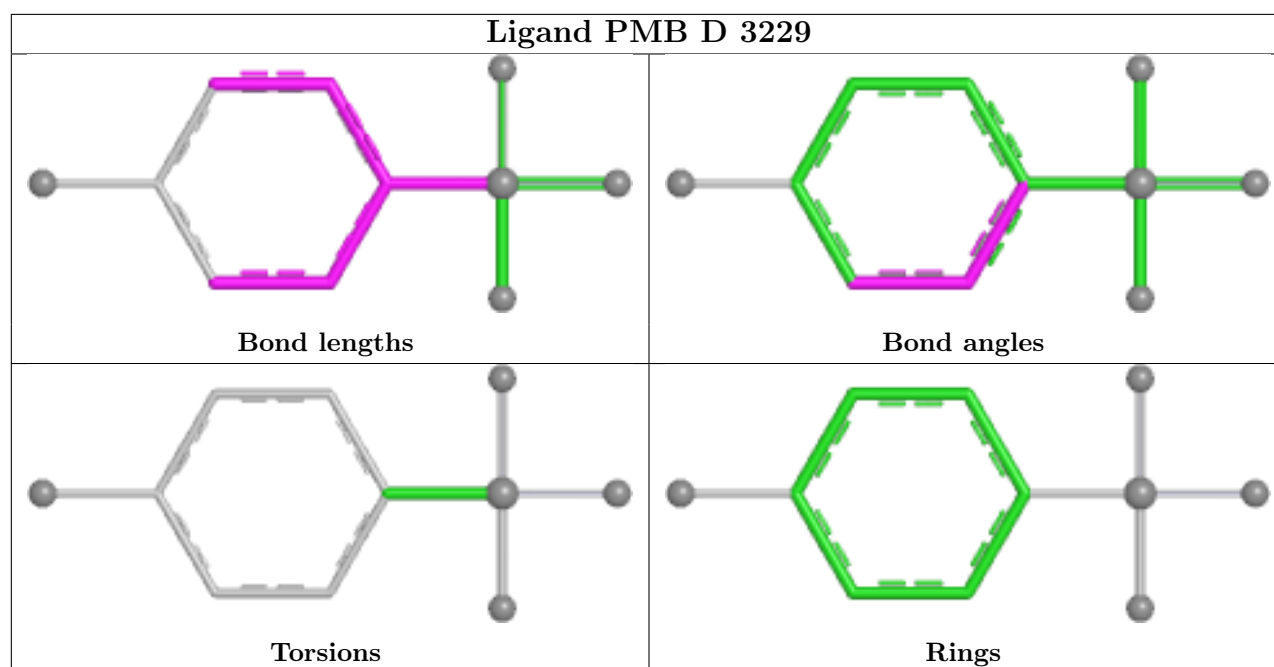
There are no torsion outliers.

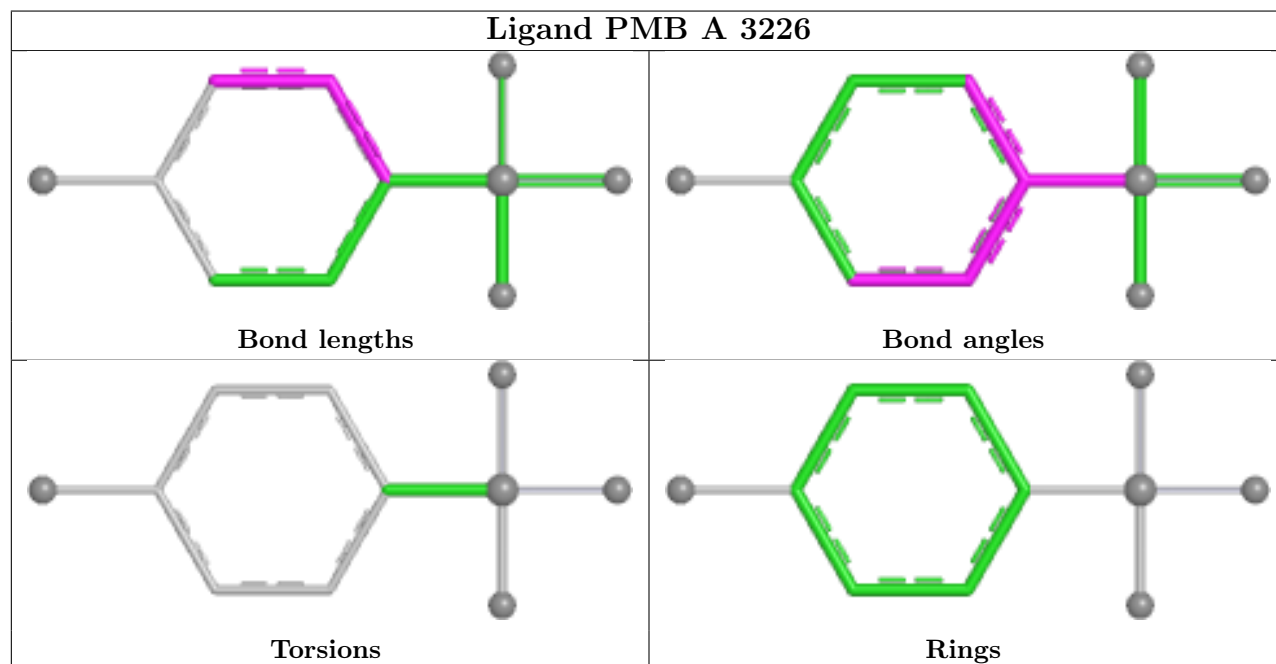
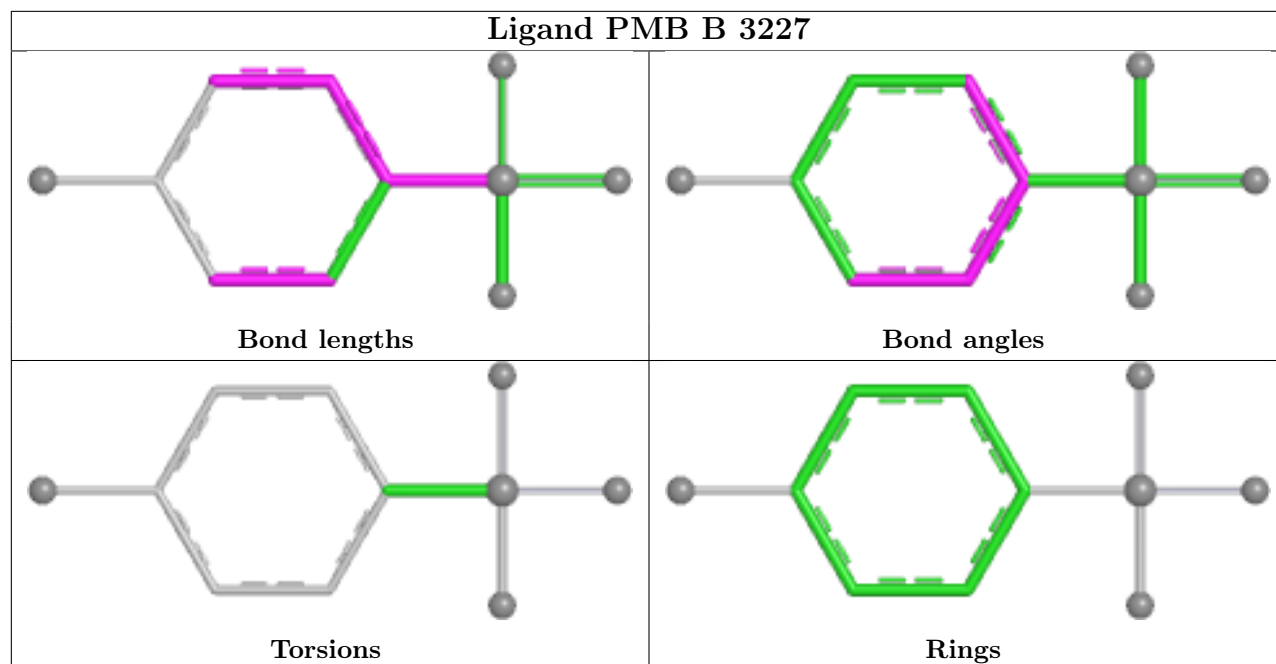
There are no ring outliers.

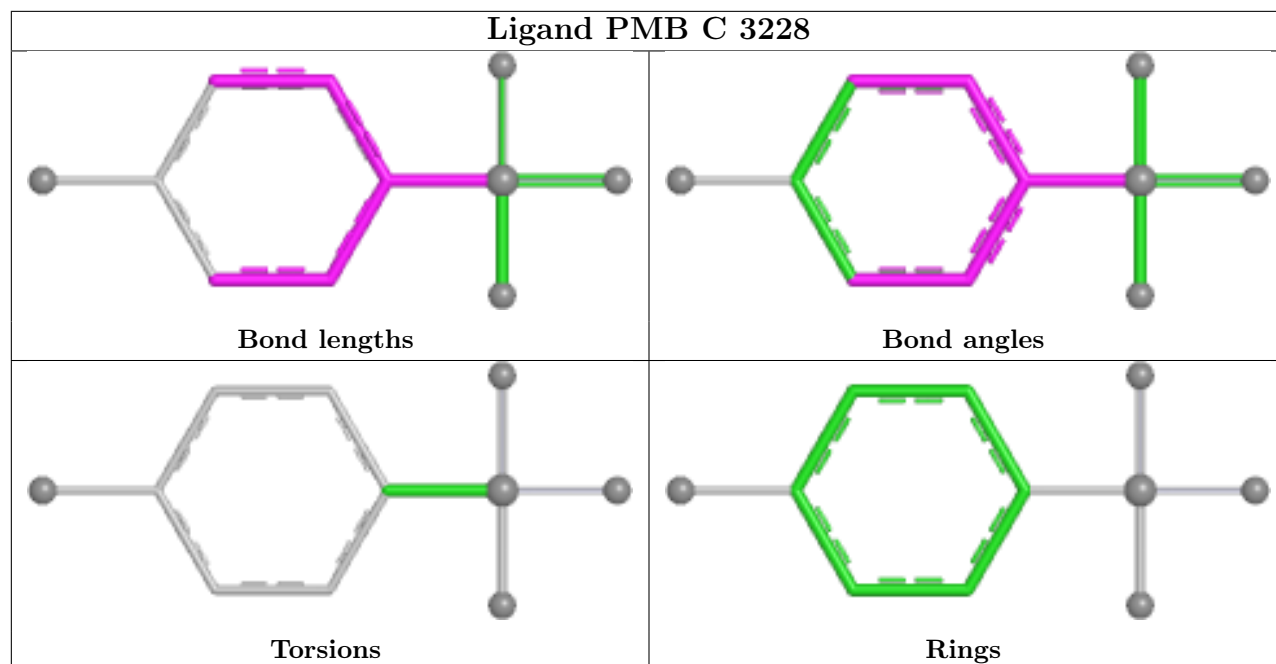
8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3229	PMB	2	0
2	D	2011	SO4	1	0
3	B	3227	PMB	1	0
2	A	2008	SO4	1	0
2	C	2010	SO4	2	0
3	A	3226	PMB	4	0
3	C	3228	PMB	1	0
2	B	2009	SO4	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	428/451 (94%)	-0.15	5 (1%) 76 77	14, 29, 63, 81	0
1	B	426/451 (94%)	0.04	21 (4%) 36 38	13, 31, 78, 81	0
1	C	432/451 (95%)	-0.12	17 (3%) 44 46	13, 27, 62, 81	0
1	D	423/451 (93%)	0.01	10 (2%) 59 62	15, 32, 68, 81	0
All	All	1709/1804 (94%)	-0.05	53 (3%) 51 54	13, 30, 69, 81	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	111	PRO	3.9
1	C	113	ASN	3.8
1	D	117	PHE	3.5
1	C	115	ASP	3.4
1	C	300	PRO	3.4
1	C	28	GLY	3.3
1	C	112	GLU	3.2
1	C	117	PHE	3.0
1	D	383	ALA	3.0
1	C	380	LEU	3.0
1	B	224	MET	3.0
1	B	214	LEU	3.0
1	D	378	ARG	3.0
1	D	382	ALA	3.0
1	B	112	GLU	2.9
1	C	297	LYS	2.9
1	C	299	VAL	2.8
1	C	298	PRO	2.8
1	C	116	TRP	2.8
1	B	11	THR	2.8
1	C	118	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	12	CYS	2.7
1	B	213	ILE	2.6
1	C	110	SER	2.6
1	B	178	ALA	2.6
1	B	206	ALA	2.6
1	B	209	VAL	2.6
1	B	201	GLY	2.5
1	B	181	PHE	2.4
1	B	32	THR	2.4
1	B	204	LEU	2.3
1	C	107	ALA	2.3
1	A	12	CYS	2.3
1	B	374	THR	2.3
1	B	218	ASP	2.3
1	A	216	LEU	2.3
1	C	376	ALA	2.3
1	B	226	PHE	2.3
1	B	380	LEU	2.3
1	C	12	CYS	2.2
1	A	11	THR	2.2
1	C	301	ASP	2.2
1	B	180	ALA	2.2
1	D	12	CYS	2.2
1	D	110	SER	2.2
1	B	203	GLN	2.2
1	D	301	ASP	2.1
1	B	225	PRO	2.1
1	D	381	LEU	2.1
1	D	32	THR	2.1
1	A	299	VAL	2.1
1	A	297	LYS	2.1
1	B	212	THR	2.1

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

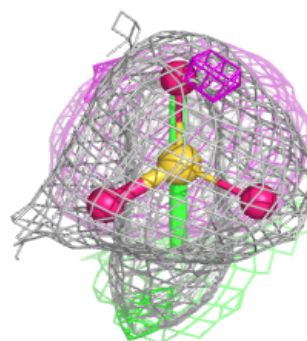
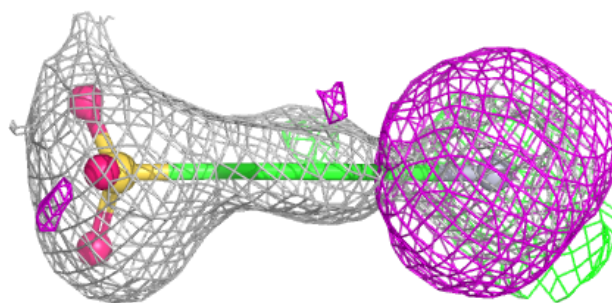
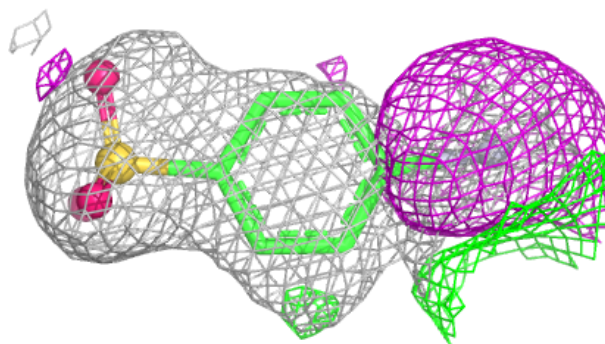
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PMB	A	3226	11/11	0.62	0.31	35,39,47,47	0
3	PMB	C	3228	11/11	0.88	0.22	20,46,50,51	0
2	SO4	D	2004	5/5	0.93	0.09	46,51,53,54	0
2	SO4	A	2008	5/5	0.94	0.08	44,46,47,49	0
2	SO4	B	2006	5/5	0.95	0.08	55,55,58,60	0
2	SO4	D	2011	5/5	0.96	0.07	35,40,42,43	0
2	SO4	C	2010	5/5	0.96	0.06	41,42,43,44	0
2	SO4	C	2005	5/5	0.96	0.09	47,48,50,51	0
3	PMB	B	3227	11/11	0.97	0.14	26,36,42,46	0
2	SO4	A	2007	5/5	0.97	0.07	48,48,49,52	0
3	PMB	D	3229	11/11	0.97	0.12	19,32,40,43	0
2	SO4	A	2000	5/5	0.98	0.05	28,29,30,31	0
2	SO4	D	2003	5/5	0.98	0.06	27,29,30,31	0
2	SO4	B	2009	5/5	0.98	0.07	36,39,41,41	0
2	SO4	B	2001	5/5	0.98	0.05	23,25,27,27	0
2	SO4	C	2002	5/5	0.99	0.04	23,24,26,28	0

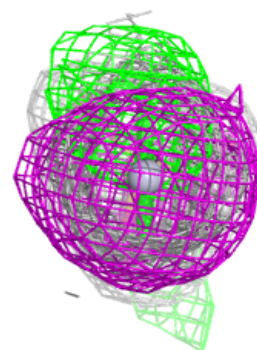
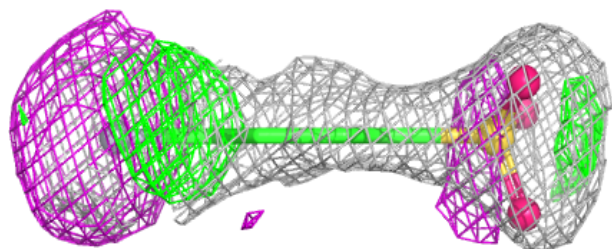
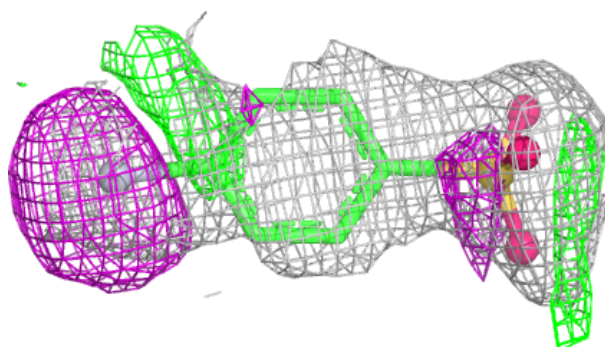
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PMB A 3226:

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

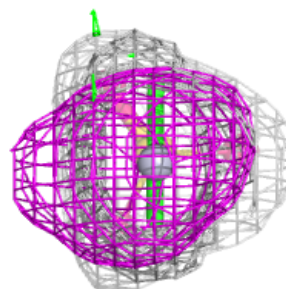
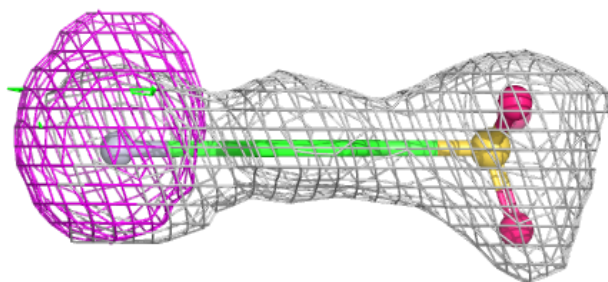
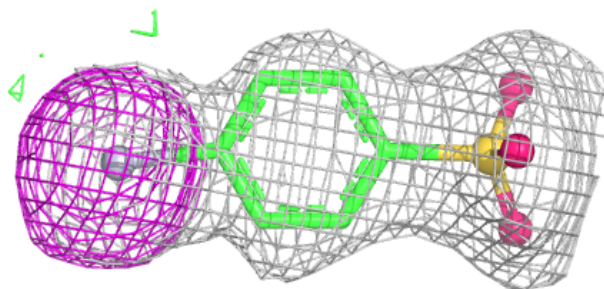
**Electron density around PMB C 3228:**

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

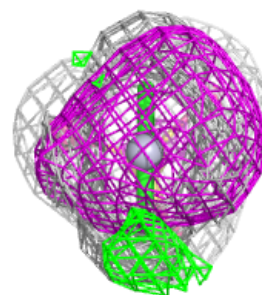
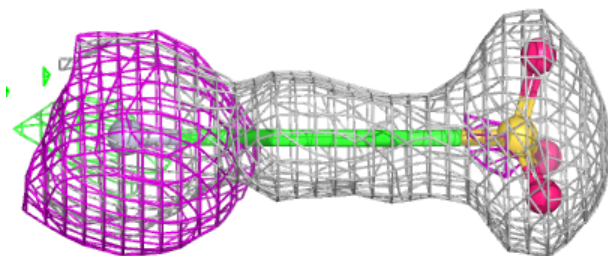
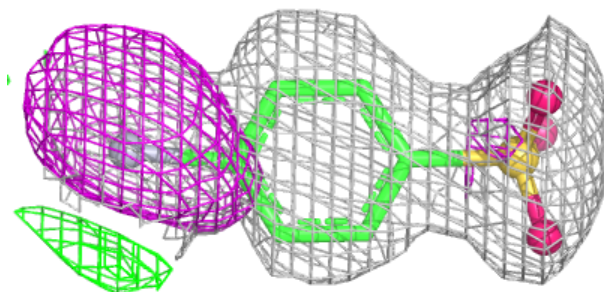


Electron density around PMB B 3227:

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

**Electron density around PMB D 3229:**

$2mF_o-DF_c$ (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.