Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 10:56 AM EDT

PDB ID	:	1YP2 / pdb_00001yp2
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 (i) 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 (i)) were used in the production of this report:

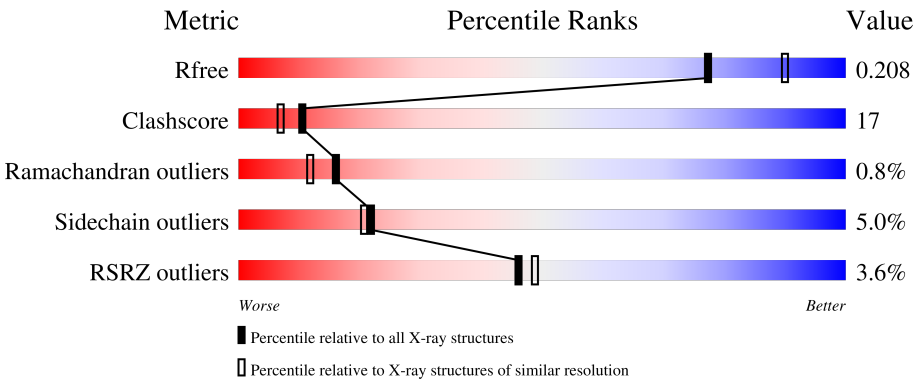
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.11 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 <=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	% 67% 24% • 5%
1	B	451	6% 67% 23% • 6%
1	C	451	4% 66% 25% • •
1	D	451	3% 66% 24% • • 6%

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 (i)

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.

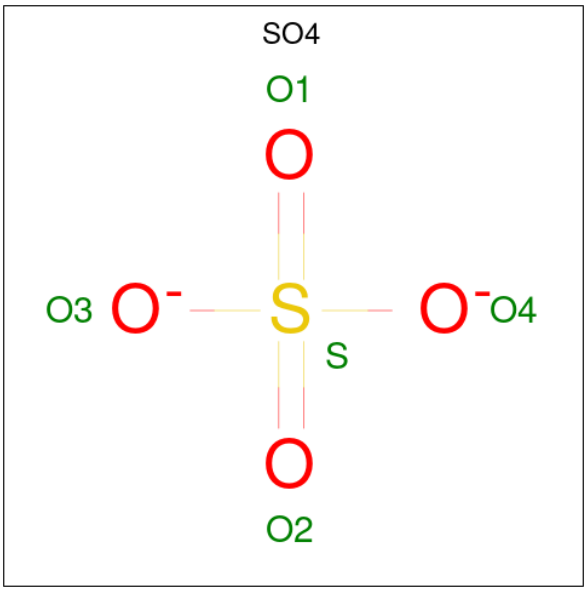
- Molecule 1 is a protein called Glucose-1-phosphate adenylyltransferase small subunit.

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

There are 4 discrepancies between the modelled and reference sequences:

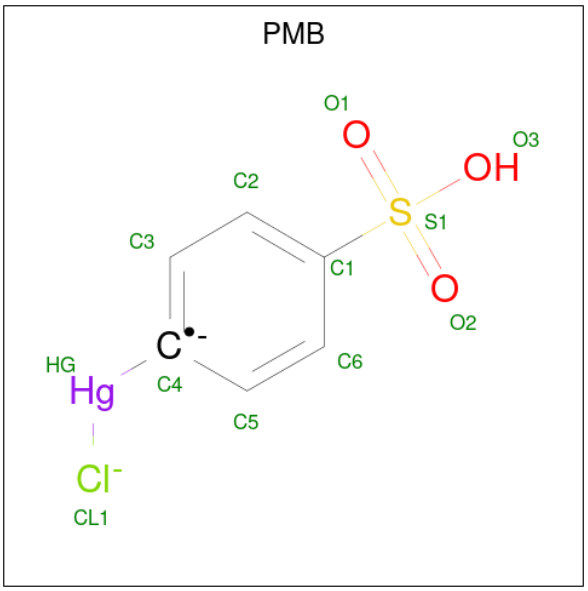
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P23509
B	1	MET	-	initiating methionine	UNP P23509
C	1	MET	-	initiating methionine	UNP P23509
D	1	MET	-	initiating methionine	UNP P23509

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 3 is PARA-MERCURY-BENZENESULFONIC ACID (CCD ID: PMB) (formula: $C_6H_5ClHgO_3S$).



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

- Molecule 4 is water.

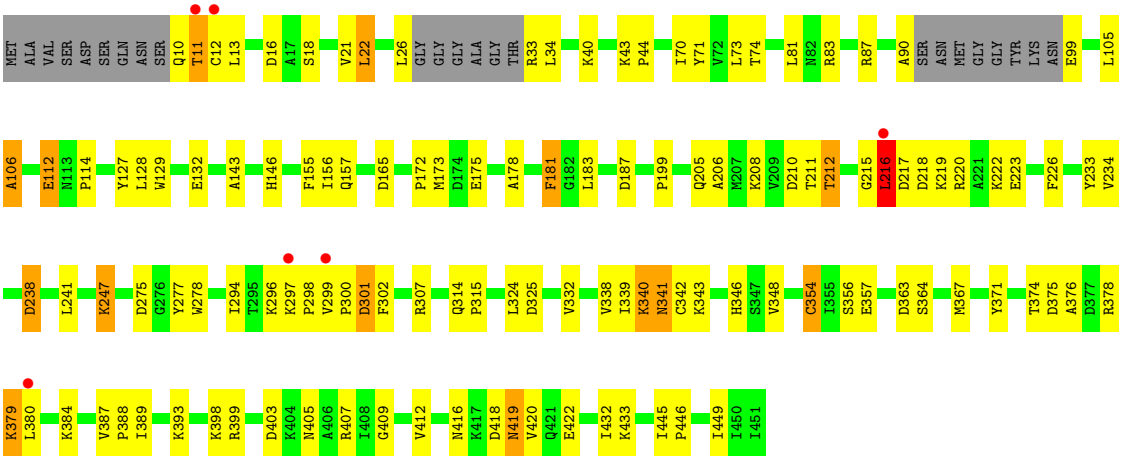
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	296	296	296	0	0
4	B	286	286	286	0	0
4	C	318	318	318	0	0
4	D	314	314	314	0	0

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.

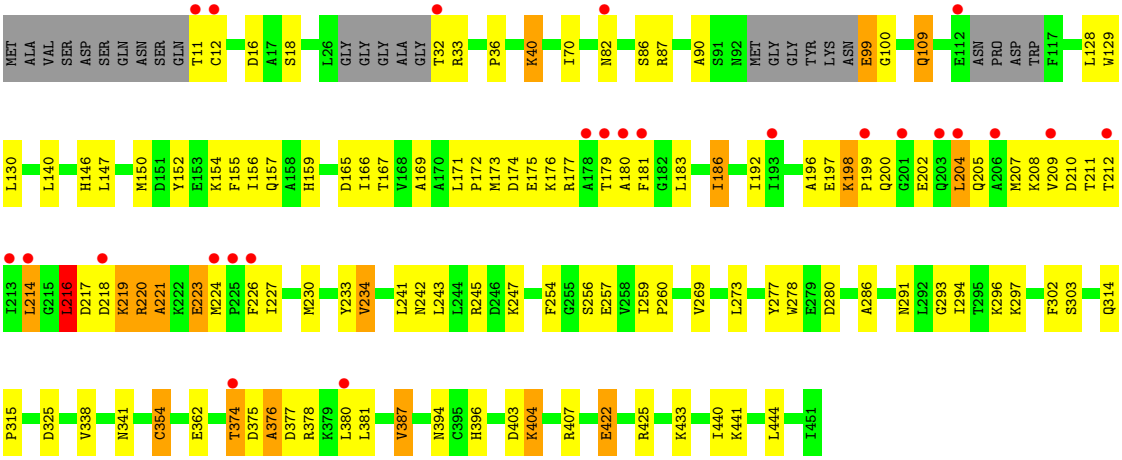
• Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit

Chain A:



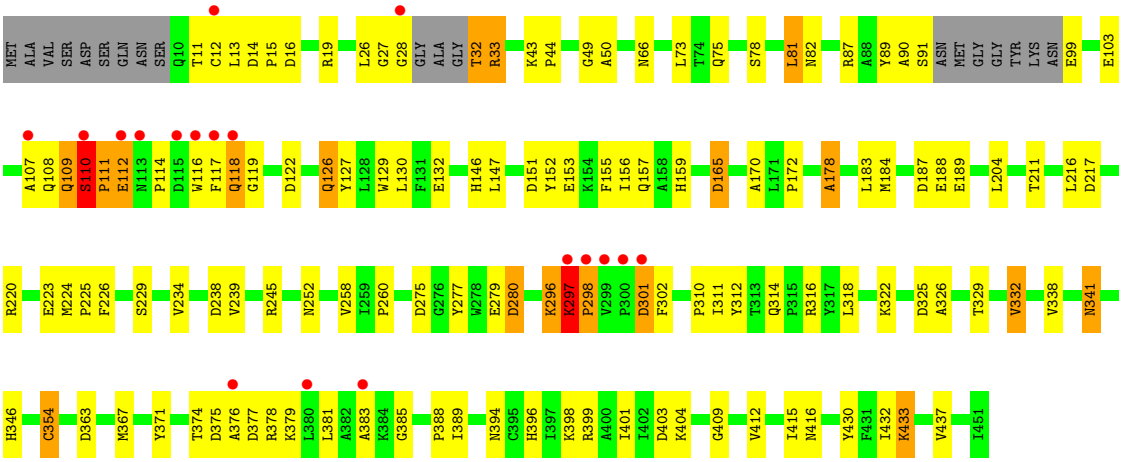
• Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit

Chain B:



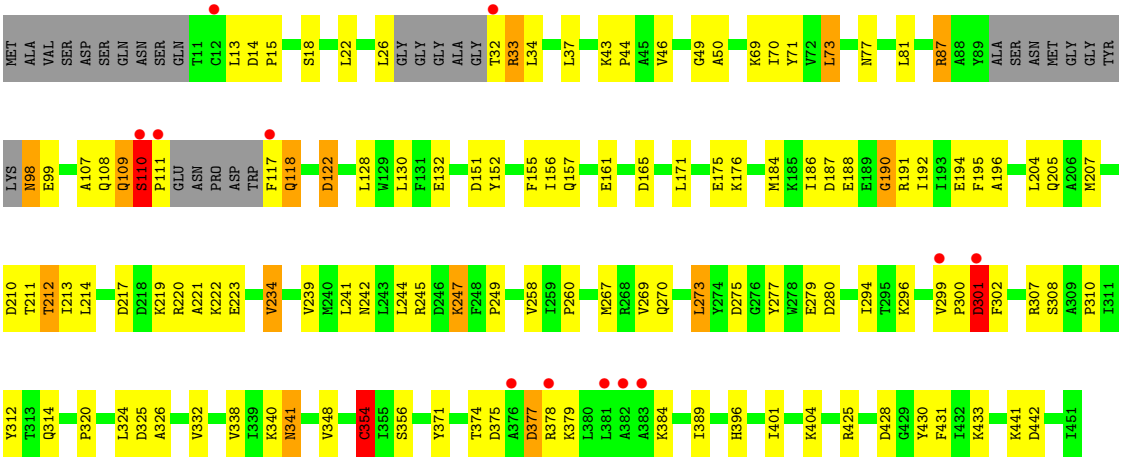
• Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	5215 reflections (4.91%)	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]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[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 (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	0.66	2/3409 (0.1%)	1.03	9/4613 (0.2%)
1	B	0.64	1/3369 (0.0%)	1.06	10/4556 (0.2%)
1	C	0.66	1/3430 (0.0%)	1.10	18/4641 (0.4%)
1	D	0.65	2/3360 (0.1%)	1.09	19/4543 (0.4%)
All	All	0.65	6/13568 (0.0%)	1.07	56/18353 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	CYS	N-CA	7.52	1.55	1.46
1	D	354	CYS	N-CA	7.45	1.55	1.46
1	D	354	CYS	C-O	7.05	1.32	1.24
1	A	354	CYS	CA-CB	6.71	1.63	1.53
1	A	354	CYS	CB-SG	6.14	2.01	1.81
1	C	354	CYS	C-O	5.85	1.31	1.24

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	110	SER	CA-C-N	10.08	132.44	119.84
1	C	110	SER	C-N-CA	10.08	132.44	119.84
1	D	33	ARG	N-CA-C	-8.94	102.36	113.18
1	C	376	ALA	N-CA-C	-8.48	102.00	111.07
1	C	165	ASP	N-CA-C	-8.19	103.42	113.41
1	C	430	TYR	N-CA-C	8.17	120.02	108.74
1	B	221	ALA	N-CA-C	-7.73	103.11	112.54
1	C	297	LYS	N-CA-C	7.27	123.37	113.77
1	C	296	LYS	N-CA-C	7.11	120.80	110.42
1	B	376	ALA	N-CA-C	-7.06	102.79	111.33
1	C	119	GLY	N-CA-C	7.05	119.20	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	258	VAL	N-CA-C	6.83	116.98	110.42
1	D	301	ASP	N-CA-C	-6.81	103.86	111.28
1	C	404	LYS	N-CA-C	6.68	119.65	110.24
1	C	258	VAL	N-CA-C	6.67	117.42	110.62
1	D	70	ILE	N-CA-C	6.53	117.52	108.12
1	B	234	VAL	N-CA-C	-6.46	99.12	108.17
1	D	165	ASP	N-CA-C	-6.45	105.54	113.41
1	C	401	ILE	N-CA-C	-6.43	98.37	107.75
1	D	260	PRO	N-CA-C	-6.33	105.27	113.57
1	A	354	CYS	N-CA-CB	6.31	120.72	110.43
1	A	445	ILE	CA-C-N	6.21	127.61	119.84
1	A	445	ILE	C-N-CA	6.21	127.61	119.84
1	D	247	LYS	N-CA-C	5.81	117.42	111.14
1	D	356	SER	N-CA-C	5.79	117.54	110.41
1	B	381	LEU	N-CA-C	-5.71	105.05	111.28
1	A	165	ASP	N-CA-C	-5.71	104.51	112.45
1	C	229	SER	N-CA-C	-5.71	102.03	110.48
1	A	106	ALA	N-CA-C	5.70	118.98	110.14
1	D	194	GLU	N-CA-C	5.61	116.93	108.46
1	D	109	GLN	N-CA-C	-5.54	106.47	113.18
1	A	178	ALA	N-CA-C	5.46	117.93	111.33
1	B	165	ASP	N-CA-C	-5.45	104.87	112.45
1	A	70	ILE	N-CA-C	5.45	115.97	108.12
1	C	260	PRO	N-CA-C	-5.42	106.47	113.57
1	D	326	ALA	N-CA-C	5.39	117.69	108.90
1	A	364	SER	N-CA-C	5.37	117.83	109.52
1	D	87	ARG	N-CA-C	5.35	117.12	111.28
1	C	178	ALA	N-CA-C	5.34	117.79	111.33
1	B	100	GLY	N-CA-C	5.29	120.34	112.41
1	D	401	ILE	N-CA-C	-5.26	100.06	107.75
1	D	404	LYS	N-CA-C	5.25	117.64	110.24
1	B	354	CYS	N-CA-C	-5.25	100.62	109.07
1	A	405	ASN	N-CA-C	5.12	118.66	111.90
1	B	169	ALA	N-CA-C	-5.11	102.71	110.28
1	C	326	ALA	N-CA-C	5.11	116.85	108.52
1	B	404	LYS	N-CA-C	5.10	117.43	110.24
1	C	301	ASP	N-CA-C	-5.09	105.73	111.28
1	D	234	VAL	N-CA-C	-5.08	101.00	108.11
1	C	311	ILE	N-CA-C	-5.07	101.28	108.58
1	D	46	VAL	CA-C-N	5.06	124.97	119.76
1	D	46	VAL	C-N-CA	5.06	124.97	119.76
1	B	70	ILE	N-CA-C	5.04	115.38	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	280	ASP	N-CA-C	-5.02	102.27	110.20
1	D	308	SER	N-CA-C	5.01	119.42	112.45
1	D	190	GLY	N-CA-C	-5.00	108.37	115.43

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	110	0
1	B	3311	0	3331	128	0
1	C	3367	0	3378	111	0
1	D	3301	0	3324	115	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	453	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 17.

All (453) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:242:ASN:HD21	1:D:247:LYS:HZ1	1.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD2	1:A:238:ASP:N	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:374:THR:HG22	1:B:374:THR:O	1.98	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:220:ARG:HD3	1:B:224:MET:HE2	1.84	0.60
1:C:112:GLU:C	1:C:114:PRO:HD3	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:339:ILE:C	3:A:3226:PMB:H3	2.29	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:108:GLN:HE21	1:C:110:SER:C	2.13	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
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:B:150:MET:HE2	1:B:152:TYR:HD2	1.71	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:216:LEU:HD11	1:B:224:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:175:GLU:CD	1:D:205:GLN:HE22	2.15	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:C:383:ALA:C	1:C:385:GLY:H	2.16	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:A:112:GLU:C	1:A:114:PRO:HD3	2.34	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: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
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:B:230:MET:HE3	1:B:278:TRP:CD1	2.44	0.53
1:D:219:LYS:HD2	1:D:222:LYS:NZ	2.24	0.53
1:D:239:VAL:HG13	1:D:267:MET:HE1	1.91	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:C:187:ASP:OD1	1:C:187:ASP:C	2.52	0.52
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:14:ASP:HA	1:D:15:PRO:C	2.35	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:D:196:ALA:HB3	1:D:207:MET:HE2	1.93	0.51
1:C:49:GLY:O	1:C:50:ALA:HB3	2.10	0.51
1:D:190:GLY:C	1:D:270:GLN:NE2	2.68	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:C:170:ALA:HB2	1:C:184:MET:HE1	1.92	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
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: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:B:173:MET:HE2	1:B:177:ARG:HD3	1.94	0.49
1:C:354:CYS:SG	1:C:378:ARG:NH1	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:175:GLU:HB3	1:D:176:LYS:HZ2	1.77	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:C:225:PRO:HG2	1:C:226:PHE:CE1	2.48	0.48
1:C:415:ILE:O	1:C:416:ASN:C	2.56	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:A:296:LYS:HD3	1:A:299:VAL:O	2.13	0.48
1:B:196:ALA:CB	1:B:207:MET:HE2	2.44	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
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: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:C:383:ALA:C	1:C:385:GLY:N	2.70	0.47
1:B:374:THR:O	1:B:375:ASP:HB3	2.15	0.47
1:B:173:MET:HE1	1:B:177:ARG:HD3	1.97	0.47
1:A:215:GLY:O	1:A:216:LEU:C	2.58	0.46
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:338:VAL:HG23	1:A:338:VAL:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:173:MET:HB3	1:A:173:MET:HE2	1.68	0.46
1:A:217:ASP:O	1:A:218:ASP:C	2.59	0.46
1:D:214:LEU:HB3	1:D:273:LEU:HB2	1.96	0.46
1:B:150:MET:HE2	1:B:152:TYR:CD2	2.51	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:90:ALA:C	4:A:3408:HOH:O	2.60	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
1:B:109:GLN:H	1:B:109:GLN:NE2	2.07	0.45
1:C:117:PHE:HE2	1:C:126:GLN:CD	2.25	0.45
1:D:13:LEU:HD11	1:D:156:ILE:HB	1.99	0.45
1:D:196:ALA:CB	1:D:207:MET:HE2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:220:ARG:HH22	1:C:275:ASP:CG	2.24	0.45
1:D:371:TYR:OH	1:D:389:ILE:HD11	2.17	0.45
1:C:14:ASP:HA	1:C:15:PRO:C	2.42	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:D:187:ASP:CG	1:D:191:ARG:HB3	2.43	0.44
1:B:173:MET:HE2	1:B:177:ARG:HB2	2.00	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
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:D:374:THR:OG1	1:D:377:ASP:CG	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:374:THR:C	1:A:376:ALA:N	2.77	0.43
1:B:86:SER:HA	1:B:90:ALA:HB3	2.00	0.43
1:A:314:GLN:HA	1:A:315:PRO:HD3	1.90	0.43
1:B:171:LEU:HD13	1:B:171:LEU:C	2.43	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:B:197:GLU:O	1:B:198:LYS:C	2.62	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:207:MET:O	1:B:208:LYS:C	2.63	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:A:357:GLU:H	1:A:357:GLU:CD	2.17	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: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
1:B:280:ASP:O	1:B:286:ALA:HB1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:ARG:HH22	1:D:275:ASP:CG	2.23	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:A:342:CYS:C	1:A:343:LYS:HD2	2.44	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:B:374:THR:C	1:B:376:ALA:N	2.78	0.41
1:A:378:ARG:C	1:A:379:LYS:HE2	2.46	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:A:398:LYS:O	1:A:399:ARG:C	2.62	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: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:A:187:ASP:OD2	1:A:187:ASP:C	2.64	0.40
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:379:LYS:HE2	1:A:379:LYS:HA	2.02	0.40
1:B:257:GLU:C	1:B:260:PRO:HD2	2.46	0.40
1:A:146:HIS:CG	1:A:278:TRP:CH2	3.10	0.40
1:A:374:THR:C	1:A:376:ALA:H	2.30	0.40
1:A:380:LEU:HD22	4:A:3463:HOH:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	24 22
1	B	418/451 (93%)	387 (93%)	26 (6%)	5 (1%)	10 6
1	C	426/451 (94%)	402 (94%)	19 (4%)	5 (1%)	10 6
1	D	415/451 (92%)	398 (96%)	16 (4%)	1 (0%)	43 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%)	23	23
1	B	356/375 (95%)	337 (95%)	19 (5%)	20	18
1	C	362/375 (96%)	344 (95%)	18 (5%)	22	21
1	D	356/375 (95%)	338 (95%)	18 (5%)	21	20
All	All	1434/1500 (96%)	1362 (95%)	72 (5%)	22	21

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
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	222	LYS
1	A	233	TYR
1	A	238	ASP
1	A	247	LYS
1	A	301	ASP
1	A	340	LYS
1	A	341	ASN
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

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Mol	Chain	Res	Type
1	B	147	LEU
1	B	186	ILE
1	B	204	LEU
1	B	205	GLN
1	B	214	LEU
1	B	216	LEU
1	B	219	LYS
1	B	220	ARG
1	B	223	GLU
1	B	233	TYR
1	B	387	VAL
1	B	422	GLU
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	216	LEU
1	C	297	LYS
1	C	332	VAL
1	C	341	ASN
1	C	433	LYS
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

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Mol	Chain	Res	Type
1	D	244	LEU
1	D	273	LEU
1	D	301	ASP
1	D	341	ASN
1	D	354	CYS
1	D	377	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) 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	126	GLN
1	A	146	HIS
1	A	252	ASN
1	A	270	GLN
1	A	341	ASN
1	A	416	ASN
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	64	ASN
1	C	108	GLN
1	C	109	GLN
1	C	126	GLN
1	C	270	GLN
1	C	341	ASN
1	C	396	HIS
1	D	66	ASN
1	D	75	GLN

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Mol	Chain	Res	Type
1	D	98	ASN
1	D	108	GLN
1	D	126	GLN
1	D	205	GLN
1	D	242	ASN
1	D	270	GLN
1	D	341	ASN
1	D	396	HIS
1	D	419	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	SO4	B	2006	-	4,4,4	0.40	0	6,6,6	0.12	0
2	SO4	D	2004	-	4,4,4	0.44	0	6,6,6	0.15	0
3	PMB	B	3227	4,1	7,11,12	3.02	3 (42%)	6,16,17	0.55	0
2	SO4	A	2007	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	D	2011	-	4,4,4	0.32	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	2001	-	4,4,4	0.39	0	6,6,6	0.21	0
2	SO4	A	2000	-	4,4,4	0.44	0	6,6,6	0.34	0
3	PMB	A	3226	1	7,11,12	1.51	2 (28%)	6,16,17	1.31	1 (16%)
2	SO4	C	2010	-	4,4,4	0.27	0	6,6,6	0.18	0
3	PMB	D	3229	4,1	7,11,12	2.76	3 (42%)	6,16,17	0.93	1 (16%)
2	SO4	C	2005	-	4,4,4	0.34	0	6,6,6	0.13	0
3	PMB	C	3228	4	7,11,12	5.67	4 (57%)	6,16,17	0.99	1 (16%)
2	SO4	A	2008	-	4,4,4	0.34	0	6,6,6	0.17	0
2	SO4	C	2002	-	4,4,4	0.41	0	6,6,6	0.28	0
2	SO4	B	2009	-	4,4,4	0.29	0	6,6,6	0.17	0
2	SO4	D	2003	-	4,4,4	0.33	0	6,6,6	0.22	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	A	3226	1	-	0/2/16/18	0/1/1/1
3	PMB	D	3229	4,1	-	2/2/16/18	0/1/1/1
3	PMB	B	3227	4,1	-	2/2/16/18	0/1/1/1
3	PMB	C	3228	4	-	0/2/16/18	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3228	PMB	C1-S1	12.55	1.97	1.74
3	B	3227	PMB	C1-S1	6.22	1.85	1.74
3	C	3228	PMB	C6-C5	6.01	1.49	1.35
3	D	3229	PMB	C1-S1	5.46	1.84	1.74
3	C	3228	PMB	C2-C1	4.86	1.45	1.36
3	B	3227	PMB	C6-C5	3.91	1.44	1.35
3	D	3229	PMB	C2-C1	3.44	1.42	1.36
3	D	3229	PMB	C6-C5	3.06	1.42	1.35
3	B	3227	PMB	C2-C1	2.98	1.41	1.36
3	A	3226	PMB	C6-C5	2.81	1.42	1.35
3	C	3228	PMB	C3-C2	2.45	1.48	1.41
3	A	3226	PMB	C2-C1	2.02	1.39	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3226	PMB	C2-C3-C4	-2.42	119.37	121.84
3	C	3228	PMB	C3-C4-C5	-2.24	115.41	118.60
3	D	3229	PMB	C2-C3-C4	-2.09	119.71	121.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

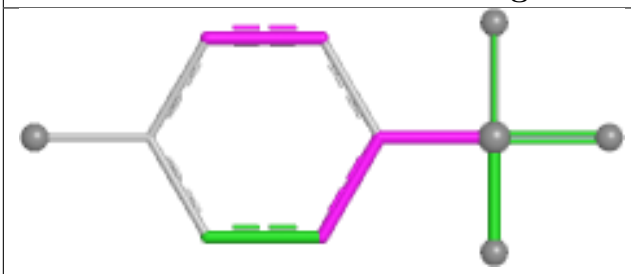
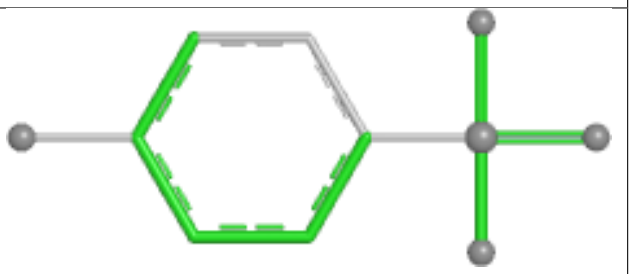
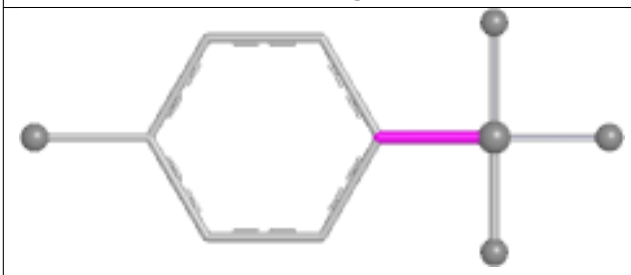
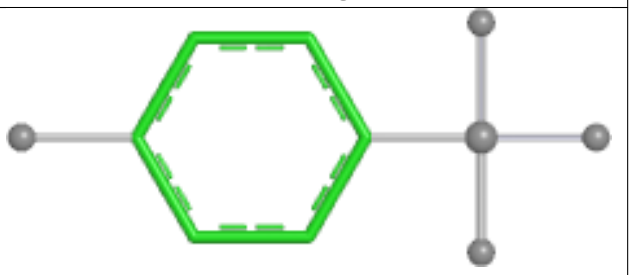
Mol	Chain	Res	Type	Atoms
3	B	3227	PMB	C2-C1-S1-O2
3	B	3227	PMB	C2-C1-S1-O1
3	D	3229	PMB	C2-C1-S1-O1
3	D	3229	PMB	C2-C1-S1-O2

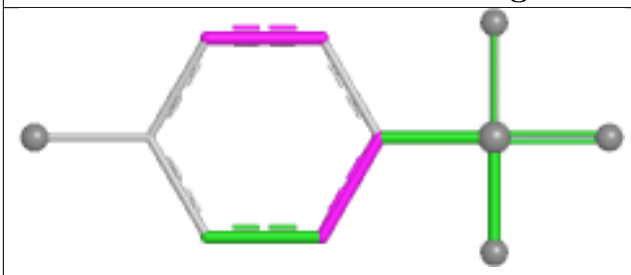
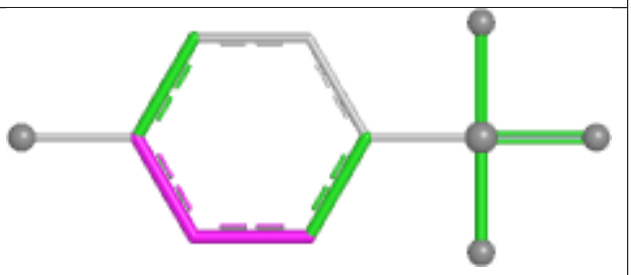
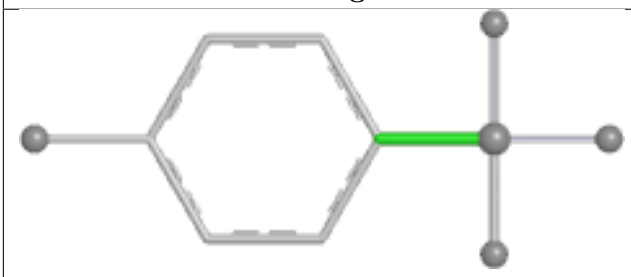
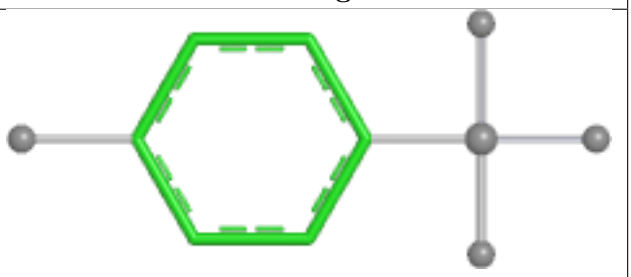
There are no ring outliers.

8 monomers are involved in 13 short contacts:

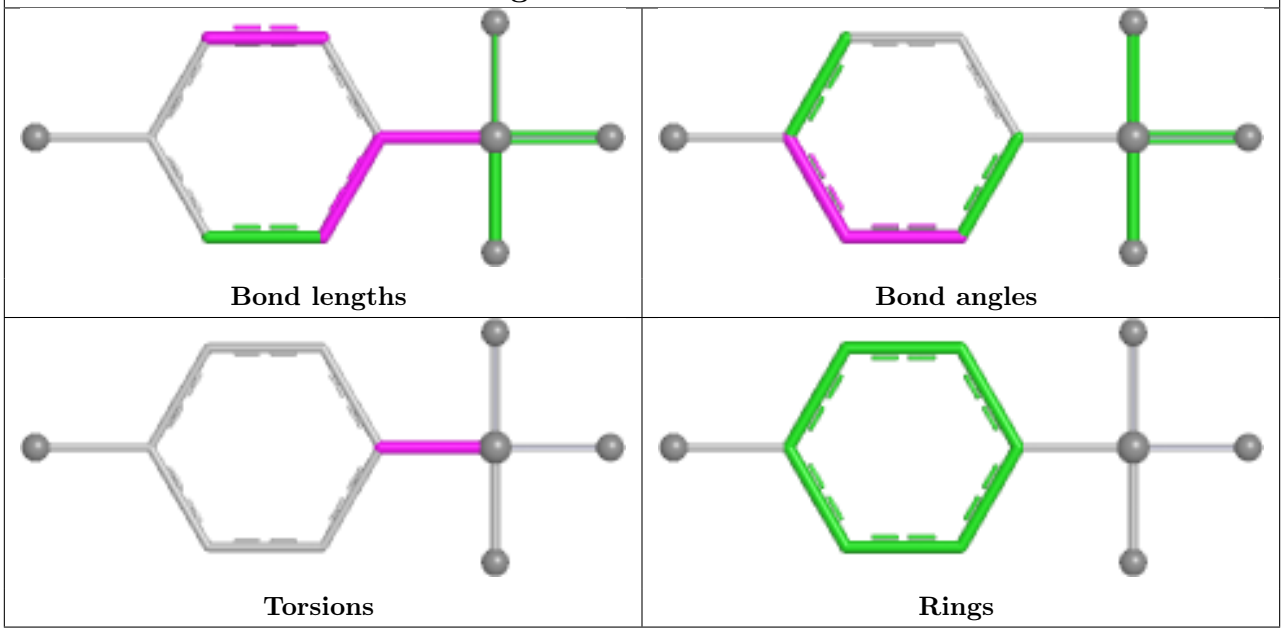
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3227	PMB	1	0
2	D	2011	SO4	1	0
3	A	3226	PMB	4	0
2	C	2010	SO4	2	0
3	D	3229	PMB	2	0
3	C	3228	PMB	1	0
2	A	2008	SO4	1	0
2	B	2009	SO4	1	0

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 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.

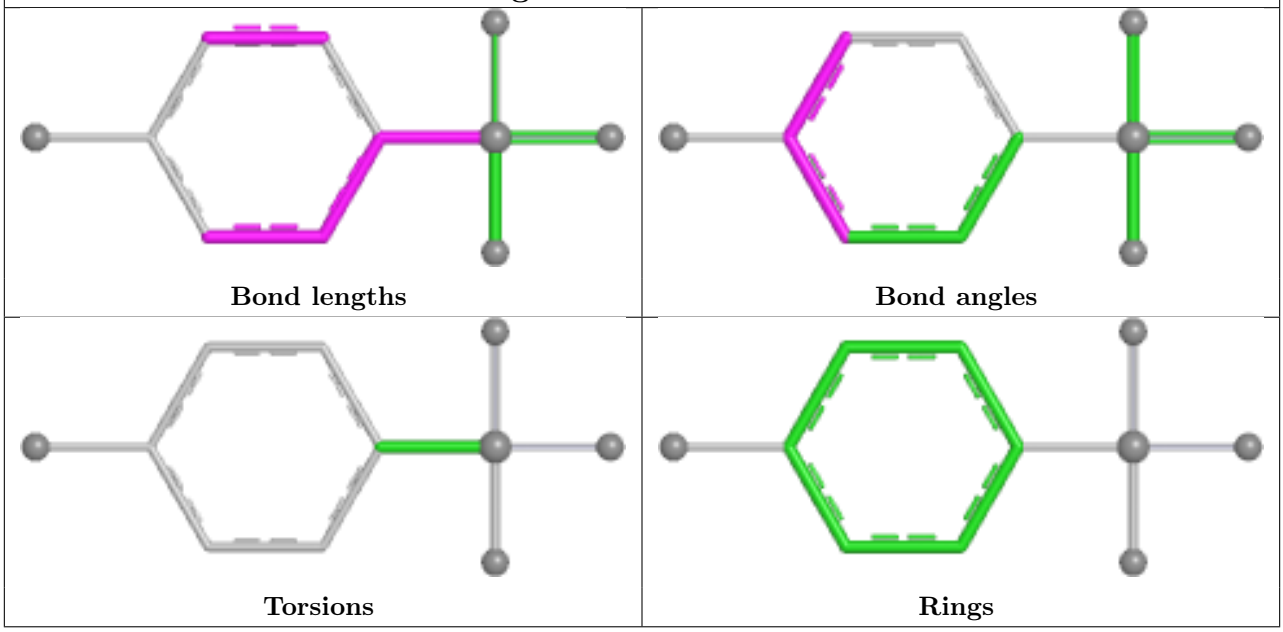
Ligand PMB B 3227	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PMB A 3226	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PMB D 3229



Ligand PMB C 3228



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.04	6 (1%)	73	76	14, 29, 63, 81	0
1	B	426/451 (94%)	0.15	25 (5%)	28	30	13, 31, 78, 81	0
1	C	432/451 (95%)	-0.02	18 (4%)	40	43	13, 27, 62, 81	0
1	D	423/451 (93%)	0.11	12 (2%)	55	58	15, 32, 68, 81	0
All	All	1709/1804 (94%)	0.05	61 (3%)	46	49	13, 30, 69, 81	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	111	PRO	4.0
1	C	113	ASN	3.9
1	D	117	PHE	3.7
1	C	300	PRO	3.5
1	C	115	ASP	3.5
1	C	28	GLY	3.4
1	C	112	GLU	3.2
1	C	117	PHE	3.2
1	D	383	ALA	3.2
1	C	380	LEU	3.1
1	D	382	ALA	3.1
1	B	214	LEU	3.1
1	B	224	MET	3.1
1	D	378	ARG	3.0
1	C	116	TRP	3.0
1	C	299	VAL	3.0
1	C	298	PRO	3.0
1	B	112	GLU	2.9
1	C	297	LYS	2.9
1	B	11	THR	2.9
1	B	12	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	118	GLN	2.8
1	B	178	ALA	2.8
1	B	206	ALA	2.8
1	B	213	ILE	2.8
1	B	209	VAL	2.7
1	C	110	SER	2.7
1	B	201	GLY	2.7
1	B	181	PHE	2.5
1	B	32	THR	2.5
1	C	107	ALA	2.5
1	B	204	LEU	2.5
1	A	12	CYS	2.5
1	B	374	THR	2.5
1	C	376	ALA	2.5
1	A	216	LEU	2.5
1	B	226	PHE	2.5
1	B	380	LEU	2.4
1	B	218	ASP	2.4
1	C	12	CYS	2.4
1	A	11	THR	2.4
1	B	180	ALA	2.3
1	D	12	CYS	2.3
1	C	301	ASP	2.3
1	D	110	SER	2.3
1	B	225	PRO	2.3
1	D	381	LEU	2.3
1	B	203	GLN	2.2
1	A	299	VAL	2.2
1	D	32	THR	2.2
1	D	301	ASP	2.2
1	B	212	THR	2.2
1	A	297	LYS	2.2
1	C	383	ALA	2.1
1	D	376	ALA	2.1
1	A	380	LEU	2.0
1	B	82	ASN	2.0
1	B	193	ILE	2.0
1	D	299	VAL	2.0
1	B	179	THR	2.0
1	B	199	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

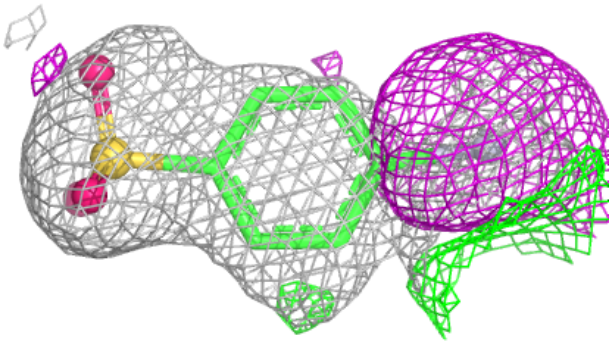
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

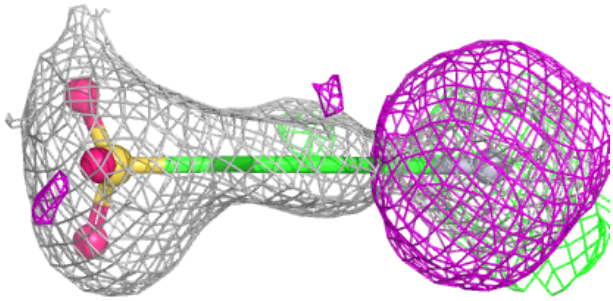
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PMB	A	3226	11/12	0.62	0.31	35,39,47,47	0
3	PMB	C	3228	11/12	0.88	0.22	20,46,50,51	0
2	SO4	D	2004	5/5	0.93	0.09	46,51,53,54	0
2	SO4	A	2008	5/5	0.94	0.08	44,46,47,49	0
2	SO4	B	2006	5/5	0.95	0.08	55,55,58,60	0
2	SO4	D	2011	5/5	0.96	0.07	35,40,42,43	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	11/12	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	11/12	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

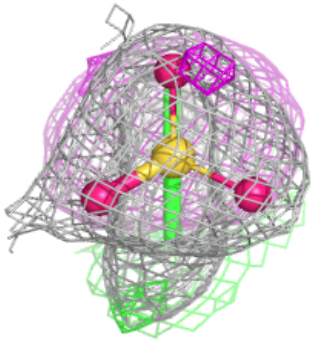
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

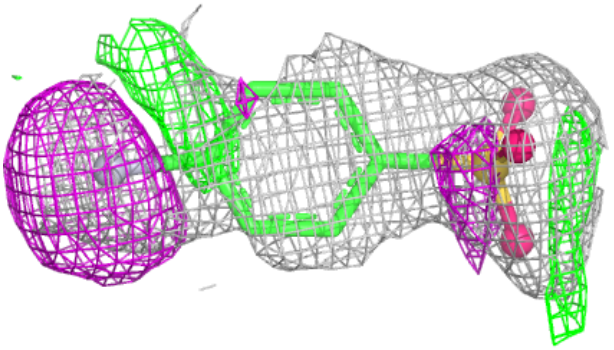


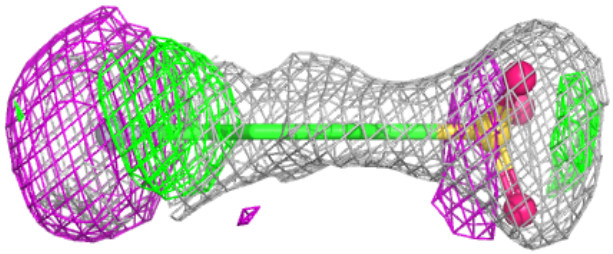


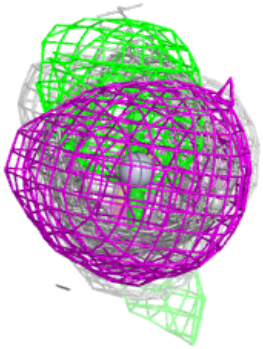


Electron density around PMB C 3228:

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

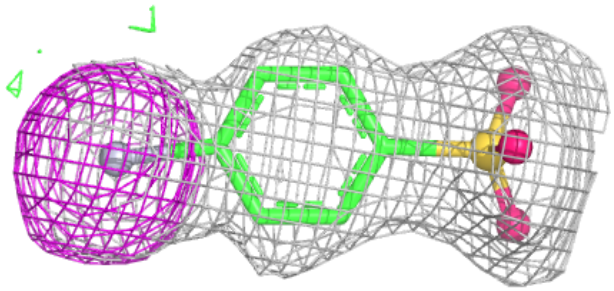


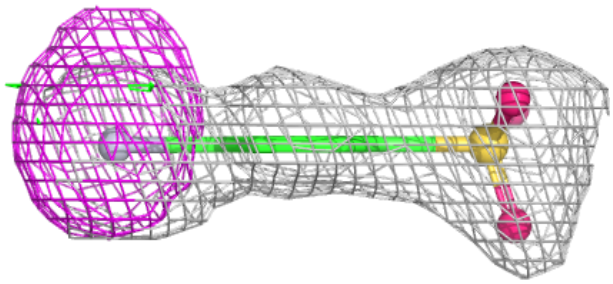


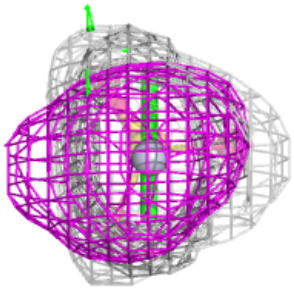


Electron density around PMB B 3227:

$2mF_o$-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:

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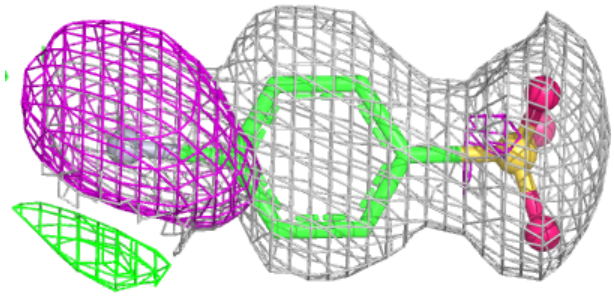
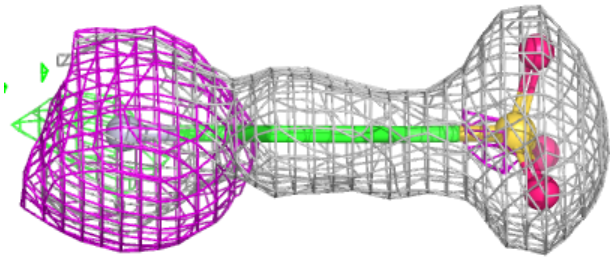
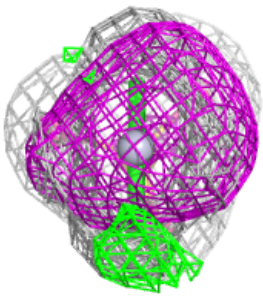
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.