Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:46 am BST

PDB ID	:	1YP4
Title	:	Crystal structure of potato tuber ADP-glucose pyrophosphorylase in complex with ADP-glucose
Authors	:	Jin, X.; Ballicora, M.A.; Preiss, J.; Geiger, J.H.
Deposited on	:	2005-01-29
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

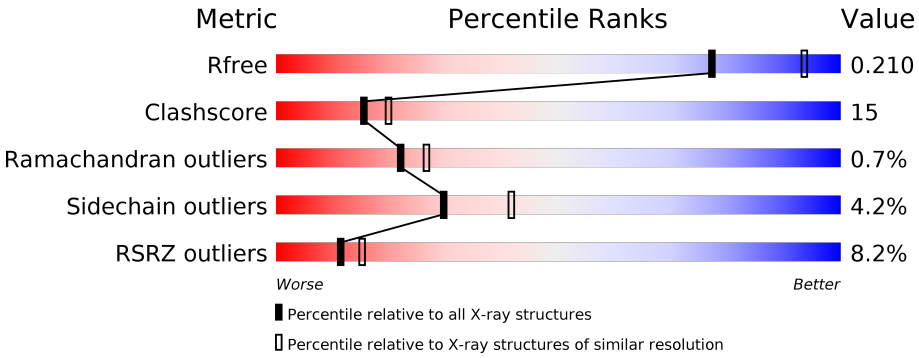
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	6% 70% 24%
1	B	451	9% 64% 31%
1	C	451	4% 68% 26%
1	D	451	12% 64% 29% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	1021	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14021 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.

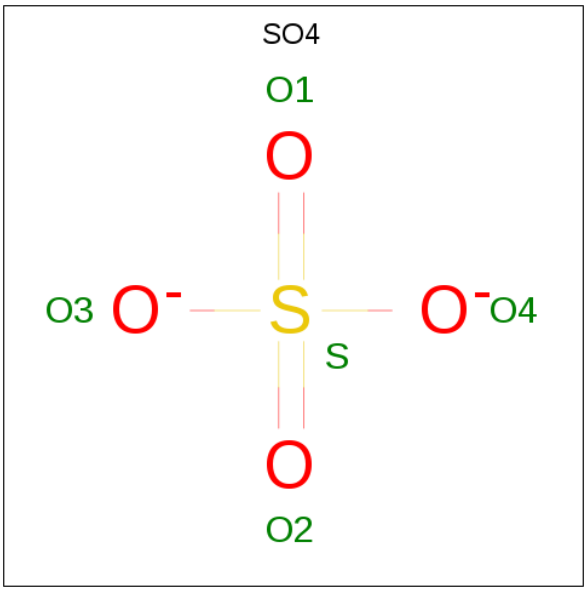
- Molecule 1 is a protein called Glucose-1-phosphate adenylyltransferase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3356	2136	568	636	16			
1	B	433	Total	C	N	O	S	0	0	0
			3350	2125	570	639	16			
1	C	434	Total	C	N	O	S	0	0	0
			3371	2144	570	641	16			
1	D	426	Total	C	N	O	S	0	0	0
			3301	2099	560	626	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: O_4S).



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

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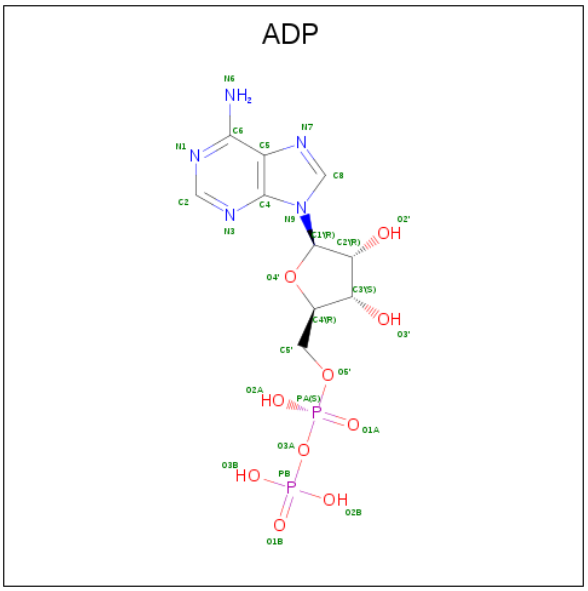
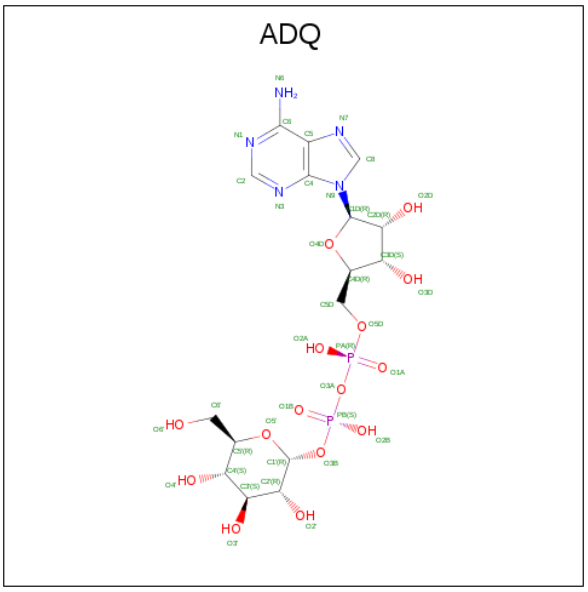
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0
3	C	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: ADQ) (formula: $C_{16}H_{25}N_5O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			38	16	5	15	2		

- Molecule 5 is water.

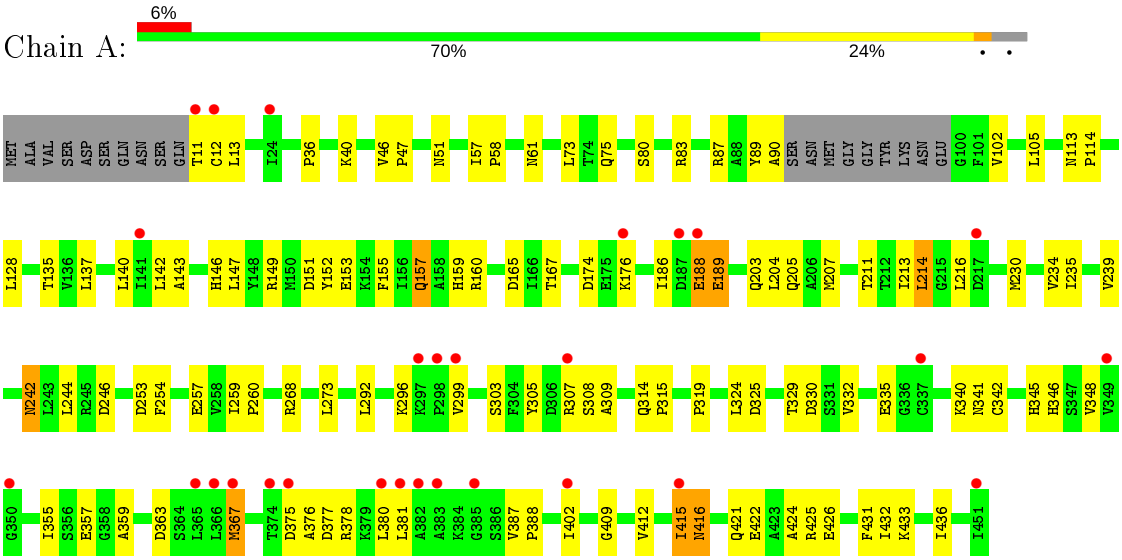
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total	O	0	0
			130	130		
5	B	106	Total	O	0	0
			106	106		
5	C	142	Total	O	0	0
			142	142		
5	D	93	Total	O	0	0
			93	93		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

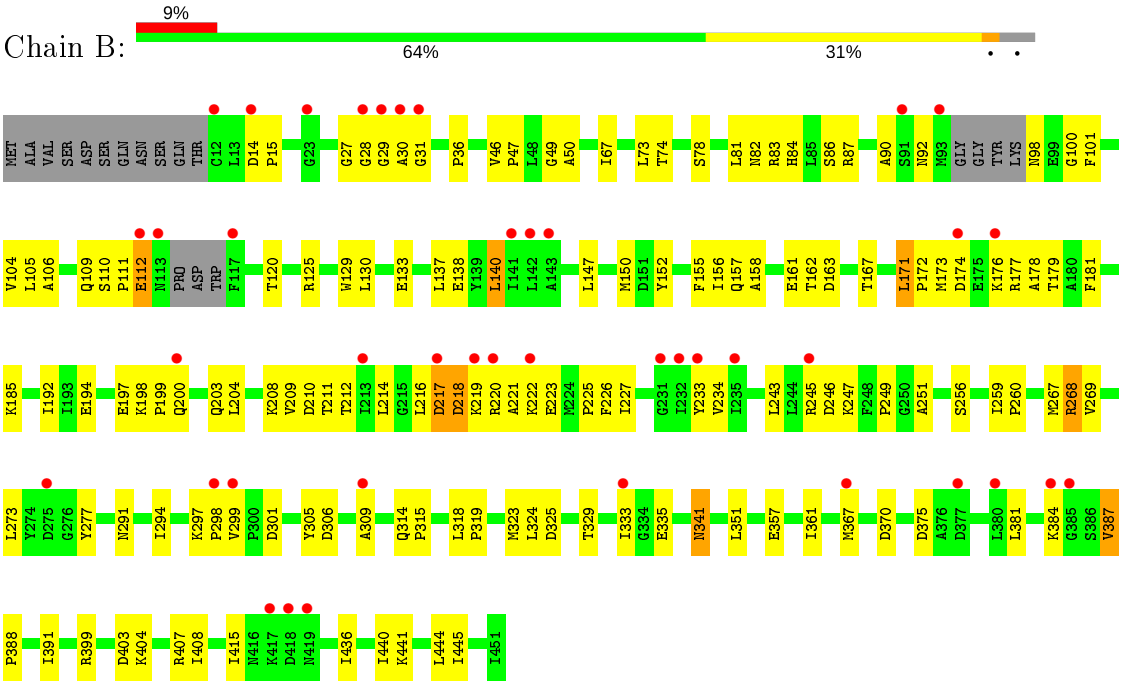
- Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit

Chain A:



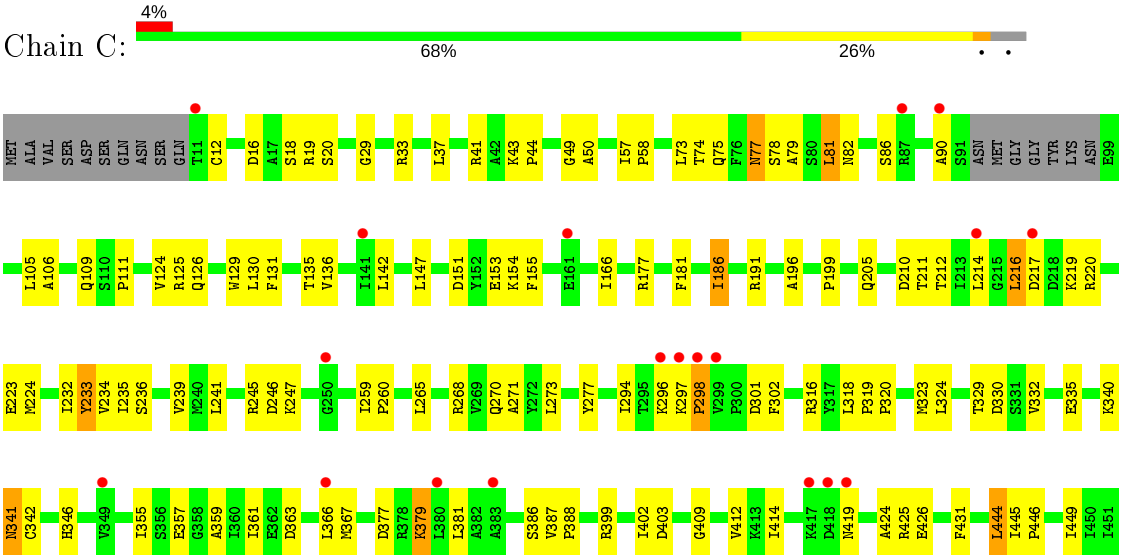
- Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit

Chain B:



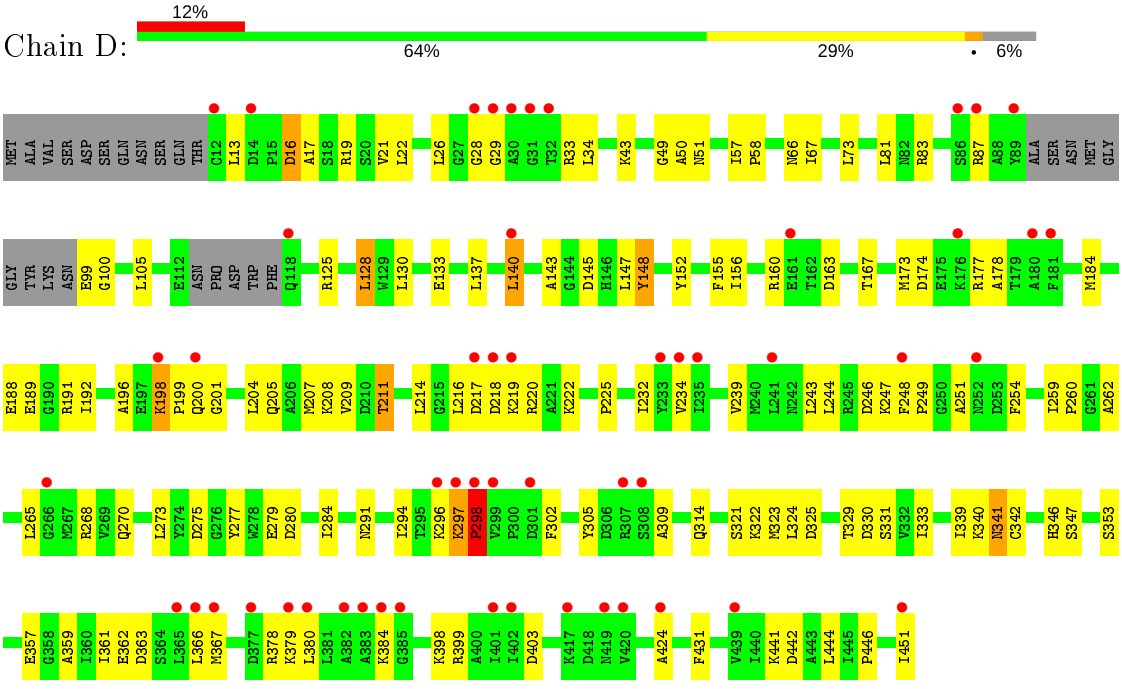
• Molecule 1: Glucose-1-phosphate adenylyltransferase small subunit

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	79.86Å 137.96Å 90.83Å 90.00° 112.91° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 25.83 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.99-2.30) 98.6 (25.83-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.244 0.205 , 0.210	Depositor DCC
R_{free} test set	3934 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14021	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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

5.1 Standard geometry

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

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	0.38	0/3420	0.64	0/4629
1	B	0.37	0/3409	0.63	0/4610
1	C	0.38	0/3435	0.65	0/4649
1	D	0.35	0/3360	0.62	0/4543
All	All	0.37	0/13624	0.63	0/18431

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3356	0	3372	85	0
1	B	3350	0	3360	120	0
1	C	3371	0	3383	113	0
1	D	3301	0	3324	99	0
2	A	20	0	0	0	0
2	B	20	0	0	3	0
2	C	20	0	0	1	0
2	D	20	0	0	2	0
3	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	27	0	12	0	0
4	B	38	0	22	4	0
5	A	130	0	0	6	0
5	B	106	0	0	6	1
5	C	142	0	0	12	1
5	D	93	0	0	5	0
All	All	14021	0	13485	399	1

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 15.

All (399) 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:D:297:LYS:HB3	1:D:298:PRO:HD2	1.27	1.11
1:B:268:ARG:HH11	1:B:268:ARG:HB3	1.06	1.10
1:D:125:ARG:HA	1:D:128:LEU:HD23	1.47	0.97
1:B:268:ARG:HB3	1:B:268:ARG:NH1	1.83	0.91
1:A:12:CYS:HB2	1:C:12:CYS:SG	2.10	0.91
1:B:367:MET:HG3	1:B:403:ASP:HA	1.53	0.90
1:C:367:MET:HG3	1:C:403:ASP:HA	1.52	0.90
1:C:426:GLU:HG2	1:C:431:PHE:CE1	2.08	0.89
1:B:219:LYS:H	1:B:219:LYS:HD2	1.35	0.88
1:A:378:ARG:HA	1:A:381:LEU:HD12	1.57	0.86
1:D:297:LYS:CB	1:D:298:PRO:HD2	2.06	0.86
1:A:426:GLU:HG2	1:A:431:PHE:HE1	1.41	0.86
1:B:387:VAL:HG22	1:B:407:ARG:HB3	1.59	0.83
1:A:40:LYS:H	1:A:113:ASN:HD21	1.27	0.83
1:A:75:GLN:HG2	1:A:114:PRO:HG2	1.60	0.82
1:D:297:LYS:HB3	1:D:298:PRO:CD	2.08	0.82
1:B:208:LYS:HE3	1:B:225:PRO:HG3	1.60	0.81
1:C:426:GLU:HG2	1:C:431:PHE:HE1	1.46	0.80
1:B:173:MET:HA	1:B:173:MET:HE3	1.66	0.76
1:B:384:LYS:NZ	1:B:384:LYS:HB3	1.99	0.76
1:C:155:PHE:CE2	1:C:234:VAL:HG23	2.20	0.76
1:A:259:ILE:HB	1:A:260:PRO:HD3	1.69	0.75
1:A:149:ARG:NH1	1:A:303:SER:O	2.21	0.73
1:C:125:ARG:HD2	5:C:1114:HOH:O	1.89	0.73
1:C:341:ASN:OD1	1:C:357:GLU:HG3	1.88	0.73
1:C:233:TYR:CD2	5:C:1153:HOH:O	2.41	0.72
1:C:332:VAL:HG12	1:D:322:LYS:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:LEU:HD12	1:D:143:ALA:HB2	1.73	0.71
1:D:341:ASN:HD22	1:D:341:ASN:H	1.38	0.70
1:D:218:ASP:O	1:D:222:LYS:HG2	1.91	0.70
1:D:87:ARG:HD2	1:D:314:GLN:OE1	1.93	0.69
1:A:214:LEU:HB3	1:A:273:LEU:HB2	1.75	0.69
1:A:325:ASP:O	1:A:341:ASN:HA	1.94	0.68
1:C:379:LYS:HE3	1:C:379:LYS:N	2.08	0.68
1:D:259:ILE:HB	1:D:260:PRO:HD3	1.75	0.68
1:A:155:PHE:CE2	1:A:234:VAL:HG23	2.27	0.68
1:C:377:ASP:O	1:C:381:LEU:HD23	1.94	0.68
1:C:86:SER:O	1:C:90:ALA:HB3	1.94	0.68
1:D:99:GLU:HG3	1:D:100:GLY:N	2.08	0.68
1:A:157:GLN:HG3	5:A:1100:HOH:O	1.94	0.68
1:B:109:GLN:HG2	1:C:126:GLN:NE2	2.09	0.67
1:B:384:LYS:HB3	1:B:384:LYS:HZ3	1.59	0.67
1:D:99:GLU:HG3	1:D:100:GLY:H	1.58	0.67
1:A:357:GLU:CD	1:A:357:GLU:H	1.97	0.67
1:C:296:LYS:HZ1	1:C:301:ASP:H	1.39	0.67
1:C:318:LEU:HD12	1:C:335:GLU:HG3	1.75	0.67
1:A:426:GLU:CG	1:A:431:PHE:HE1	2.06	0.67
1:A:40:LYS:H	1:A:113:ASN:ND2	1.92	0.67
1:D:291:ASN:O	1:D:294:ILE:HG12	1.95	0.66
1:C:323:MET:HE3	1:D:333:ILE:HD13	1.77	0.66
1:B:211:THR:O	1:B:216:LEU:HB2	1.96	0.66
1:A:149:ARG:NH2	1:A:309:ALA:O	2.29	0.65
1:D:277:TYR:CE2	1:D:302:PHE:HB2	2.32	0.65
1:B:367:MET:CG	1:B:403:ASP:HA	2.27	0.65
1:A:305:TYR:HB2	1:B:319:PRO:HD3	1.79	0.64
1:C:151:ASP:OD1	1:C:153:GLU:HB2	1.97	0.64
1:A:73:LEU:HD23	1:A:105:LEU:HB2	1.78	0.64
1:D:188:GLU:HG3	1:D:189:GLU:HG3	1.78	0.64
1:B:67:ILE:HD13	1:B:140:LEU:HD12	1.80	0.64
1:B:268:ARG:HH11	1:B:268:ARG:CB	1.96	0.64
1:B:87:ARG:HD2	1:B:314:GLN:OE1	1.98	0.63
1:D:155:PHE:CE2	1:D:234:VAL:HG23	2.34	0.63
1:C:355:ILE:HD13	1:C:361:ILE:HD12	1.81	0.63
1:C:73:LEU:HD23	1:C:105:LEU:HB2	1.81	0.62
1:C:268:ARG:HG3	1:C:268:ARG:HH21	1.65	0.62
1:A:268:ARG:HG2	5:A:1132:HOH:O	1.99	0.62
1:B:370:ASP:OD1	1:B:404:LYS:HE2	1.99	0.62
1:B:220:ARG:HA	1:B:220:ARG:NE	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:CG	5:A:1132:HOH:O	2.48	0.62
1:A:329:THR:CG2	1:A:345:HIS:HD2	2.13	0.61
1:C:214:LEU:HB3	1:C:273:LEU:HB2	1.81	0.61
1:C:33:ARG:HD3	5:C:1130:HOH:O	2.01	0.61
1:B:192:ILE:HD12	1:B:269:VAL:HG12	1.83	0.61
1:B:341:ASN:OD1	1:B:357:GLU:HG3	2.00	0.61
1:D:49:GLY:O	1:D:50:ALA:HB3	2.01	0.60
1:A:377:ASP:O	1:A:381:LEU:HG	2.00	0.60
1:C:216:LEU:HD22	1:C:217:ASP:H	1.66	0.60
1:B:384:LYS:O	1:B:384:LYS:HG2	2.02	0.60
1:B:73:LEU:HD23	1:B:105:LEU:HB2	1.83	0.60
1:C:446:PRO:HG2	1:C:449:ILE:HG13	1.83	0.60
1:B:110:SER:HA	1:C:129:TRP:CZ2	2.36	0.59
1:D:220:ARG:HG3	1:D:220:ARG:HH11	1.66	0.59
1:A:330:ASP:O	1:A:346:HIS:HA	2.03	0.59
1:A:87:ARG:HD2	1:A:314:GLN:OE1	2.02	0.59
1:D:268:ARG:HH11	1:D:268:ARG:HG3	1.68	0.59
1:A:165:ASP:HB3	1:A:239:VAL:HG21	1.85	0.59
1:B:217:ASP:CG	1:B:218:ASP:H	2.07	0.59
1:D:331:SER:HB3	1:D:347:SER:O	2.03	0.58
1:D:207:MET:O	1:D:209:VAL:HG13	2.04	0.58
1:C:277:TYR:CD2	1:C:302:PHE:HB2	2.38	0.58
1:D:147:LEU:O	1:D:148:TYR:HB3	2.03	0.58
1:A:235:ILE:CD1	1:A:254:PHE:HZ	2.17	0.58
1:B:351:LEU:N	1:B:351:LEU:HD23	2.19	0.57
1:D:33:ARG:HD3	5:D:1107:HOH:O	2.04	0.57
1:B:318:LEU:HD12	1:B:335:GLU:HG3	1.87	0.57
1:B:361:ILE:N	1:B:361:ILE:HD12	2.20	0.57
1:D:16:ASP:HB2	1:D:19:ARG:HD2	1.87	0.56
1:C:186:ILE:H	1:C:186:ILE:HD13	1.70	0.56
1:C:196:ALA:O	1:C:199:PRO:HD3	2.06	0.56
1:D:184:MET:SD	1:D:192:ILE:HD13	2.45	0.56
1:C:381:LEU:HD12	1:C:386:SER:HB3	1.87	0.56
1:D:246:ASP:O	1:D:249:PRO:HD3	2.06	0.56
1:A:415:ILE:HD13	1:A:415:ILE:H	1.71	0.56
1:C:320:PRO:HG3	1:D:51:ASN:ND2	2.20	0.56
1:B:173:MET:HE2	1:B:174:ASP:OD1	2.07	0.55
1:C:16:ASP:OD2	1:C:18:SER:HB2	2.05	0.55
1:D:214:LEU:HB3	1:D:273:LEU:HB2	1.88	0.55
1:D:66:ASN:HB2	5:D:1079:HOH:O	2.06	0.55
1:B:208:LYS:HE3	1:B:225:PRO:CG	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ASP:OD1	1:B:212:THR:HB	2.07	0.55
1:B:297:LYS:HB2	1:B:298:PRO:HA	1.89	0.55
1:C:294:ILE:HD11	1:C:332:VAL:HG21	1.88	0.55
1:D:208:LYS:HG3	1:D:225:PRO:HB2	1.88	0.55
1:D:346:HIS:HD2	1:D:363:ASP:OD1	1.90	0.55
1:A:421:GLN:NE2	5:A:1149:HOH:O	2.40	0.55
1:C:444:LEU:CD1	1:C:444:LEU:C	2.75	0.55
1:A:140:LEU:HD11	1:A:142:LEU:HD21	1.90	0.54
1:C:78:SER:HB3	5:C:1148:HOH:O	2.07	0.54
1:D:137:LEU:HD12	1:D:160:ARG:NH2	2.22	0.54
1:D:362:GLU:O	1:D:398:LYS:HA	2.08	0.54
1:A:211:THR:HG21	1:A:216:LEU:HD22	1.88	0.54
1:A:140:LEU:CD1	1:A:142:LEU:HG	2.38	0.54
1:B:259:ILE:HB	1:B:260:PRO:HD3	1.89	0.54
1:B:185:LYS:HB2	1:B:194:GLU:HB2	1.90	0.54
1:C:296:LYS:NZ	1:C:301:ASP:H	2.06	0.54
1:B:87:ARG:HG2	1:B:314:GLN:HG3	1.90	0.53
1:A:57:ILE:HB	1:A:58:PRO:CD	2.38	0.53
1:B:243:LEU:HD21	1:B:267:MET:SD	2.48	0.53
1:D:451:ILE:HG22	1:D:451:ILE:OXT	2.09	0.53
1:A:61:ASN:HB3	1:A:152:TYR:CE1	2.44	0.53
1:D:125:ARG:HA	1:D:128:LEU:CD2	2.31	0.53
1:D:34:LEU:HD12	1:D:43:LYS:HE3	1.90	0.53
1:B:67:ILE:CD1	1:B:140:LEU:HD12	2.39	0.53
1:B:197:GLU:HG2	1:B:256:SER:OG	2.09	0.53
1:B:220:ARG:HE	1:B:220:ARG:HA	1.73	0.53
1:C:324:LEU:HB3	1:C:340:LYS:HA	1.91	0.53
1:C:355:ILE:HD13	1:C:361:ILE:CD1	2.39	0.53
1:A:242:ASN:ND2	1:A:246:ASP:HB2	2.24	0.52
1:A:409:GLY:O	1:A:412:VAL:HG23	2.10	0.52
1:C:259:ILE:HG13	5:C:1153:HOH:O	2.09	0.52
1:D:239:VAL:HG12	1:D:243:LEU:HD12	1.92	0.52
1:A:11:THR:HG23	1:A:12:CYS:N	2.24	0.52
1:B:86:SER:HA	1:B:90:ALA:HB3	1.92	0.52
1:A:140:LEU:HD13	1:A:142:LEU:HG	1.92	0.52
1:C:166:ILE:HG12	1:C:235:ILE:HG12	1.92	0.52
1:C:324:LEU:O	1:D:329:THR:HA	2.10	0.52
1:A:305:TYR:CB	1:B:319:PRO:HD3	2.40	0.52
1:B:273:LEU:N	1:B:273:LEU:HD22	2.24	0.52
1:A:325:ASP:HB3	1:A:341:ASN:HB3	1.91	0.52
1:C:329:THR:HG22	1:D:325:ASP:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:THR:HG21	4:B:506:ADQ:H5'1	1.92	0.51
1:B:158:ALA:O	1:B:162:THR:HG23	2.10	0.51
1:D:155:PHE:HE1	1:D:167:THR:HG22	1.74	0.51
1:B:217:ASP:OD2	1:B:218:ASP:N	2.42	0.51
1:B:27:GLY:O	1:B:29:GLY:N	2.44	0.51
1:C:361:ILE:HD13	1:C:366:LEU:HD21	1.92	0.51
1:C:78:SER:CB	5:C:1148:HOH:O	2.57	0.51
1:C:424:ALA:C	1:C:425:ARG:HG2	2.30	0.51
1:A:342:CYS:HB2	1:A:359:ALA:O	2.11	0.51
1:B:83:ARG:HD2	5:C:1094:HOH:O	2.09	0.51
1:A:159:HIS:CD2	1:A:167:THR:OG1	2.64	0.51
1:D:384:LYS:O	1:D:384:LYS:HG2	2.11	0.51
1:B:31:GLY:HA3	2:B:1021:SO4:S	2.51	0.51
1:B:173:MET:HE3	1:B:174:ASP:H	1.74	0.51
1:D:441:LYS:O	1:D:442:ASP:HB2	2.11	0.51
1:D:341:ASN:ND2	1:D:357:GLU:HG3	2.26	0.50
1:A:332:VAL:CG2	1:A:348:VAL:HG13	2.41	0.50
1:B:100:GLY:O	1:B:101:PHE:HB3	2.10	0.50
1:D:330:ASP:O	1:D:346:HIS:HA	2.11	0.50
1:D:243:LEU:HD21	1:D:262:ALA:HB2	1.92	0.50
1:A:424:ALA:O	1:A:425:ARG:HD3	2.11	0.50
1:C:124:VAL:HG13	1:C:131:PHE:HE1	1.77	0.50
1:B:222:LYS:CA	1:B:222:LYS:HE2	2.41	0.50
1:D:353:SER:HB2	5:D:1087:HOH:O	2.10	0.50
1:D:378:ARG:C	1:D:380:LEU:H	2.15	0.50
1:A:186:ILE:HD13	1:A:214:LEU:HD21	1.92	0.50
1:B:150:MET:CE	1:B:155:PHE:HB2	2.42	0.50
1:B:29:GLY:O	1:B:30:ALA:HB3	2.12	0.50
1:D:201:GLY:O	1:D:205:GLN:HG2	2.12	0.50
1:A:159:HIS:HD2	1:A:167:THR:OG1	1.95	0.50
1:B:120:THR:CG2	4:B:506:ADQ:H5'1	2.42	0.49
1:D:198:LYS:N	1:D:198:LYS:HD2	2.27	0.49
1:C:216:LEU:CD2	1:C:217:ASP:H	2.25	0.49
1:D:220:ARG:NH1	1:D:220:ARG:HG3	2.26	0.49
1:B:173:MET:HE1	1:B:177:ARG:NH2	2.27	0.49
1:A:340:LYS:HG3	1:A:357:GLU:OE2	2.12	0.49
1:B:198:LYS:HE3	5:B:1124:HOH:O	2.12	0.49
1:A:253:ASP:O	1:A:257:GLU:HB2	2.12	0.49
1:B:440:ILE:HG22	1:B:441:LYS:N	2.27	0.49
1:D:268:ARG:HG3	1:D:268:ARG:NH1	2.28	0.49
1:B:82:ASN:ND2	1:B:104:VAL:HG21	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HD23	1:A:348:VAL:HG23	1.95	0.49
1:A:367:MET:HB2	1:A:402:ILE:O	2.13	0.49
1:C:86:SER:HA	1:C:90:ALA:HB2	1.94	0.49
1:D:83:ARG:HG3	1:D:83:ARG:HH21	1.78	0.49
1:B:222:LYS:HE2	1:B:222:LYS:HA	1.95	0.48
1:B:325:ASP:HB3	1:B:341:ASN:HA	1.95	0.48
1:C:77:ASN:ND2	1:C:78:SER:H	2.12	0.48
1:A:128:LEU:HD11	1:A:244:LEU:HB2	1.96	0.48
1:A:89:TYR:O	1:A:90:ALA:C	2.52	0.48
1:D:173:MET:HG2	1:D:177:ARG:HB2	1.96	0.48
1:B:155:PHE:CE2	1:B:234:VAL:HG23	2.48	0.48
1:A:11:THR:HG23	1:A:12:CYS:H	1.79	0.48
1:C:41:ARG:NH2	1:C:403:ASP:OD1	2.46	0.48
1:C:424:ALA:O	1:C:425:ARG:HG2	2.13	0.48
1:B:277:TYR:CD1	1:B:301:ASP:HB3	2.49	0.48
1:B:415:ILE:HG22	1:B:415:ILE:O	2.12	0.47
1:D:297:LYS:O	1:D:298:PRO:C	2.53	0.47
1:A:346:HIS:HD2	1:A:363:ASP:OD2	1.98	0.47
1:B:125:ARG:NH2	1:B:251:ALA:O	2.47	0.47
1:D:57:ILE:HB	1:D:58:PRO:HD3	1.95	0.47
1:A:324:LEU:O	1:B:329:THR:HA	2.15	0.47
1:C:245:ARG:HD3	1:C:246:ASP:OD1	2.15	0.47
1:D:211:THR:HB	1:D:216:LEU:HD12	1.96	0.47
1:A:296:LYS:HD3	1:A:299:VAL:O	2.14	0.47
1:A:415:ILE:HD13	1:A:415:ILE:N	2.29	0.47
1:B:177:ARG:HB3	1:B:181:PHE:HE1	1.80	0.47
1:B:220:ARG:CA	1:B:220:ARG:NE	2.78	0.47
1:C:216:LEU:HD22	1:C:217:ASP:N	2.30	0.47
1:C:377:ASP:O	1:C:381:LEU:CD2	2.63	0.47
1:D:57:ILE:HB	1:D:58:PRO:CD	2.44	0.47
1:B:314:GLN:HA	1:B:315:PRO:HD3	1.81	0.47
1:C:296:LYS:HZ1	1:C:301:ASP:N	2.08	0.47
1:D:196:ALA:O	1:D:199:PRO:HD3	2.14	0.47
1:A:80:SER:O	1:A:83:ARG:HG2	2.14	0.47
1:B:199:PRO:HB2	1:B:203:GLN:HG2	1.97	0.47
1:B:152:TYR:O	1:B:156:ILE:HD12	2.14	0.47
1:C:241:LEU:O	1:C:245:ARG:HB3	2.15	0.47
1:D:155:PHE:CE2	1:D:232:ILE:HG22	2.50	0.47
1:A:13:LEU:CD2	1:A:157:GLN:HG2	2.44	0.47
1:B:157:GLN:O	1:B:161:GLU:HG3	2.15	0.47
5:B:1112:HOH:O	1:C:82:ASN:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASN:HD22	1:A:246:ASP:HB2	1.79	0.46
1:B:197:GLU:OE1	1:B:198:LYS:HE2	2.14	0.46
1:A:319:PRO:HD3	1:B:305:TYR:HB2	1.97	0.46
1:C:219:LYS:HD3	1:C:219:LYS:C	2.35	0.46
1:B:381:LEU:HD13	1:B:388:PRO:HA	1.96	0.46
1:C:57:ILE:HB	1:C:58:PRO:CD	2.44	0.46
1:D:200:GLN:HA	1:D:204:LEU:HB2	1.96	0.46
1:D:323:MET:HE2	1:D:339:ILE:HD12	1.98	0.46
1:B:137:LEU:O	1:B:138:GLU:HG3	2.15	0.46
1:B:200:GLN:HA	1:B:204:LEU:HB2	1.97	0.46
1:D:67:ILE:HD12	1:D:140:LEU:HD12	1.96	0.46
1:B:220:ARG:HE	1:B:220:ARG:CA	2.28	0.46
1:C:316:ARG:HD3	2:C:1010:SO4:O3	2.15	0.46
1:C:220:ARG:HA	1:C:223:GLU:HG2	1.98	0.46
1:A:137:LEU:HD12	1:A:160:ARG:NH2	2.31	0.46
1:D:191:ARG:N	1:D:270:GLN:NE2	2.64	0.46
1:C:79:ALA:HB3	5:C:1129:HOH:O	2.16	0.46
1:D:309:ALA:HB1	5:D:1029:HOH:O	2.16	0.45
1:A:307:ARG:HG3	1:A:308:SER:N	2.31	0.45
1:B:197:GLU:HG3	1:B:198:LYS:HD2	1.98	0.45
1:B:219:LYS:N	1:B:219:LYS:HD2	2.16	0.45
1:C:223:GLU:HG3	1:C:224:MET:HG3	1.97	0.45
1:B:298:PRO:HG2	1:B:299:VAL:HG22	1.98	0.45
1:B:86:SER:HA	1:B:90:ALA:CB	2.47	0.45
1:C:247:LYS:HE3	1:C:265:LEU:HD13	1.99	0.45
1:C:270:GLN:HG3	1:C:271:ALA:N	2.31	0.45
1:D:217:ASP:OD2	1:D:219:LYS:HB3	2.16	0.45
1:B:29:GLY:HA2	4:B:506:ADQ:C4	2.47	0.45
1:D:346:HIS:HE1	5:D:1074:HOH:O	1.99	0.45
1:B:133:GLU:HG2	1:C:79:ALA:HB1	1.97	0.45
1:D:324:LEU:HD12	1:D:340:LYS:HD2	1.99	0.45
1:B:444:LEU:HD23	1:B:445:ILE:N	2.32	0.45
1:B:129:TRP:CG	1:C:111:PRO:HD3	2.51	0.45
1:A:375:ASP:OD2	1:A:376:ALA:N	2.49	0.44
1:A:143:ALA:HB3	1:A:146:HIS:CE1	2.52	0.44
1:B:112:GLU:OE1	1:B:112:GLU:HA	2.16	0.44
1:B:351:LEU:H	1:B:351:LEU:CD2	2.30	0.44
1:B:46:VAL:HA	1:B:47:PRO:HD3	1.86	0.44
1:B:74:THR:O	1:B:106:ALA:HA	2.18	0.44
1:C:330:ASP:O	1:C:346:HIS:HA	2.17	0.44
1:C:74:THR:O	1:C:106:ALA:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:CYS:HB2	1:D:359:ALA:O	2.18	0.44
1:A:376:ALA:O	1:A:380:LEU:HD13	2.17	0.44
1:B:49:GLY:O	1:B:50:ALA:HB3	2.17	0.44
1:C:109:GLN:OE1	1:C:109:GLN:HA	2.16	0.44
1:B:399:ARG:CZ	1:B:436:ILE:HD11	2.48	0.44
1:D:220:ARG:NH2	1:D:275:ASP:OD1	2.51	0.44
1:B:246:ASP:O	1:B:249:PRO:HD3	2.18	0.44
1:B:444:LEU:C	1:B:444:LEU:HD23	2.38	0.44
1:A:90:ALA:HB2	1:A:102:VAL:H	1.81	0.44
1:B:399:ARG:CZ	1:B:436:ILE:CD1	2.96	0.44
1:C:154:LYS:HA	1:C:154:LYS:HD3	1.84	0.44
1:D:380:LEU:HD23	1:D:380:LEU:O	2.18	0.44
1:B:173:MET:O	1:B:226:PHE:HB2	2.18	0.43
1:B:98:ASN:ND2	5:B:1069:HOH:O	2.50	0.43
1:D:191:ARG:N	1:D:270:GLN:HE22	2.16	0.43
1:B:351:LEU:H	1:B:351:LEU:HD23	1.83	0.43
1:C:124:VAL:HG13	1:C:131:PHE:CE1	2.54	0.43
1:D:155:PHE:CE1	1:D:167:THR:HG22	2.53	0.43
1:A:426:GLU:HG2	1:A:431:PHE:CE1	2.33	0.43
1:B:325:ASP:O	1:B:341:ASN:HA	2.19	0.43
1:C:210:ASP:OD2	1:C:212:THR:OG1	2.37	0.43
1:C:332:VAL:HA	1:D:321:SER:O	2.19	0.43
1:B:221:ALA:C	1:B:222:LYS:HE2	2.38	0.43
1:C:414:ILE:O	1:C:414:ILE:HG22	2.19	0.43
1:B:323:MET:HE2	1:B:333:ILE:HD13	1.99	0.43
1:D:26:LEU:HD23	1:D:73:LEU:HD22	2.00	0.43
1:D:323:MET:HA	1:D:339:ILE:O	2.19	0.43
1:C:20:SER:O	1:C:136:VAL:HB	2.19	0.43
1:C:277:TYR:CE2	1:C:302:PHE:HB2	2.54	0.43
1:C:29:GLY:HA2	1:C:75:GLN:HB2	2.00	0.43
1:D:346:HIS:CD2	1:D:363:ASP:OD1	2.69	0.43
1:A:174:ASP:OD1	1:A:176:LYS:HG2	2.18	0.43
1:A:188:GLU:HA	1:A:213:ILE:HD13	2.01	0.43
1:C:135:THR:HG22	1:C:135:THR:O	2.17	0.43
1:C:297:LYS:N	1:C:298:PRO:HD2	2.33	0.43
1:C:357:GLU:H	1:C:357:GLU:CD	2.21	0.43
1:A:11:THR:OG1	1:A:12:CYS:N	2.51	0.43
1:A:421:GLN:HA	1:A:421:GLN:OE1	2.18	0.43
1:B:220:ARG:NH2	1:B:223:GLU:HB2	2.34	0.43
1:C:259:ILE:HB	1:C:260:PRO:HD3	2.00	0.43
1:A:324:LEU:HD11	1:B:297:LYS:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:GLY:O	1:C:412:VAL:HG23	2.19	0.43
1:C:78:SER:OG	1:C:81:LEU:HB2	2.19	0.43
1:B:247:LYS:HE2	5:B:1116:HOH:O	2.17	0.42
1:B:351:LEU:N	1:B:351:LEU:CD2	2.82	0.42
1:C:294:ILE:HD13	5:C:1096:HOH:O	2.18	0.42
1:C:41:ARG:HH22	1:C:403:ASP:CG	2.21	0.42
1:D:444:LEU:O	1:D:446:PRO:HD3	2.19	0.42
1:B:306:ASP:HB3	1:B:309:ALA:C	2.39	0.42
1:A:425:ARG:HH11	1:A:425:ARG:HG3	1.84	0.42
1:B:163:ASP:O	1:B:268:ARG:HD3	2.19	0.42
1:A:432:ILE:HA	1:A:436:ILE:O	2.20	0.42
1:B:133:GLU:HG2	1:C:79:ALA:CB	2.50	0.42
1:C:444:LEU:HD12	1:C:446:PRO:HD3	2.01	0.42
1:D:67:ILE:CD1	1:D:140:LEU:HD12	2.49	0.42
1:C:77:ASN:HD22	1:C:78:SER:H	1.66	0.42
1:B:181:PHE:CD2	4:B:506:ADQ:H6'2	2.54	0.42
1:C:186:ILE:HA	1:C:191:ARG:O	2.19	0.42
1:C:142:LEU:HD23	1:C:232:ILE:HG23	2.00	0.42
1:C:268:ARG:NH2	1:C:268:ARG:HG3	2.32	0.42
1:D:222:LYS:HE2	1:D:222:LYS:HA	2.02	0.42
1:A:46:VAL:HA	1:A:47:PRO:HD3	1.77	0.42
1:B:110:SER:HB2	1:B:111:PRO:HD2	2.02	0.42
1:B:155:PHE:HE1	1:B:167:THR:HG22	1.84	0.42
1:C:16:ASP:OD1	1:C:19:ARG:HG2	2.20	0.42
1:C:259:ILE:CD1	5:C:1153:HOH:O	2.67	0.42
1:D:174:ASP:O	1:D:178:ALA:HB2	2.20	0.42
1:A:40:LYS:N	1:A:113:ASN:HD21	2.07	0.41
1:A:387:VAL:HA	1:A:388:PRO:HD3	1.82	0.41
1:C:12:CYS:HB2	5:C:1127:HOH:O	2.20	0.41
1:D:155:PHE:CZ	1:D:234:VAL:HG23	2.54	0.41
1:D:341:ASN:H	1:D:341:ASN:ND2	2.10	0.41
1:D:424:ALA:HA	1:D:431:PHE:CD1	2.55	0.41
1:B:245:ARG:CZ	5:B:1098:HOH:O	2.67	0.41
1:B:384:LYS:NZ	1:B:384:LYS:CB	2.78	0.41
1:C:241:LEU:HD21	1:C:245:ARG:NH1	2.35	0.41
1:C:367:MET:HG2	1:C:402:ILE:O	2.20	0.41
1:B:291:ASN:O	1:B:294:ILE:HG12	2.21	0.41
1:B:391:ILE:HD13	1:B:408:ILE:HD12	2.01	0.41
1:C:177:ARG:HG2	1:C:181:PHE:HE1	1.86	0.41
1:C:236:SER:HB2	1:C:239:VAL:HG23	2.02	0.41
1:D:314:GLN:NE2	2:D:1011:SO4:O4	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LEU:HD11	1:B:227:ILE:HG12	2.03	0.41
1:C:37:LEU:HD22	1:C:367:MET:HE2	2.03	0.41
1:C:445:ILE:HA	1:C:446:PRO:HD2	1.88	0.41
1:A:433:LYS:C	1:A:433:LYS:HD3	2.40	0.41
1:B:222:LYS:N	1:B:222:LYS:HE2	2.35	0.41
1:C:346:HIS:HD2	1:C:363:ASP:OD1	2.03	0.41
1:C:446:PRO:HG2	1:C:449:ILE:CG1	2.48	0.41
1:A:151:ASP:OD1	1:A:153:GLU:HG3	2.21	0.41
1:A:51:ASN:ND2	1:A:335:GLU:HG2	2.36	0.41
1:B:14:ASP:HA	1:B:15:PRO:C	2.41	0.41
1:B:78:SER:HA	5:B:1071:HOH:O	2.19	0.41
1:C:205:GLN:HA	1:C:205:GLN:OE1	2.21	0.41
1:C:444:LEU:HD13	1:C:444:LEU:C	2.40	0.41
1:C:319:PRO:HD3	1:D:305:TYR:HB2	2.03	0.41
1:D:367:MET:HE3	1:D:403:ASP:OD1	2.21	0.41
1:A:205:GLN:C	1:A:207:MET:H	2.24	0.41
1:B:84:HIS:ND1	2:B:1009:SO4:O4	2.51	0.41
1:D:254:PHE:O	1:D:259:ILE:HG12	2.20	0.41
1:B:171:LEU:HB2	1:B:172:PRO:CD	2.51	0.41
1:C:77:ASN:O	1:C:111:PRO:HA	2.19	0.41
1:C:363:ASP:O	1:C:399:ARG:HA	2.20	0.41
1:D:33:ARG:HG3	2:D:1023:SO4:S	2.61	0.41
1:D:247:LYS:HD2	1:D:265:LEU:CD1	2.50	0.41
1:A:230:MET:N	5:A:1145:HOH:O	2.32	0.41
1:C:43:LYS:N	1:C:44:PRO:CD	2.83	0.41
1:D:277:TYR:CE1	1:D:279:GLU:HG2	2.56	0.41
1:B:31:GLY:HA3	2:B:1021:SO4:O2	2.21	0.41
1:C:379:LYS:HE3	1:C:379:LYS:CA	2.51	0.41
1:C:387:VAL:HG13	1:C:388:PRO:HD2	2.03	0.41
1:C:49:GLY:O	1:C:50:ALA:HB3	2.20	0.40
1:D:13:LEU:HD13	1:D:17:ALA:HB2	2.03	0.40
1:D:21:VAL:HG21	1:D:156:ILE:HD13	2.02	0.40
1:D:361:ILE:HD13	1:D:366:LEU:HD21	2.03	0.40
1:A:314:GLN:HA	1:A:315:PRO:HD3	1.89	0.40
1:C:181:PHE:HB3	5:C:1098:HOH:O	2.22	0.40
1:C:342:CYS:HB2	1:C:359:ALA:O	2.20	0.40
1:D:152:TYR:O	1:D:156:ILE:HG13	2.21	0.40
1:D:248:PHE:HB3	1:D:251:ALA:HB2	2.04	0.40
1:D:34:LEU:HA	1:D:284:ILE:HD12	2.03	0.40
1:D:49:GLY:O	1:D:50:ALA:CB	2.66	0.40
1:A:355:ILE:HG22	1:A:359:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:VAL:HG23	5:A:1046:HOH:O	2.22	0.40
1:A:189:GLU:N	1:A:189:GLU:OE1	2.55	0.40
1:D:296:LYS:O	1:D:297:LYS:O	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1123:HOH:O	5:C:1158:HOH:O[2_657]	2.19	0.01

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	428/451 (95%)	401 (94%)	26 (6%)	1 (0%)	47	58
1	B	427/451 (95%)	393 (92%)	30 (7%)	4 (1%)	17	20
1	C	430/451 (95%)	406 (94%)	23 (5%)	1 (0%)	47	58
1	D	420/451 (93%)	386 (92%)	28 (7%)	6 (1%)	11	11
All	All	1705/1804 (94%)	1586 (93%)	107 (6%)	12 (1%)	22	26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	217	ASP
1	D	297	LYS
1	D	298	PRO
1	B	28	GLY
1	B	218	ASP
1	C	298	PRO
1	D	29	GLY

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Mol	Chain	Res	Type
1	B	178	ALA
1	D	379	LYS
1	A	416	ASN
1	D	148	TYR
1	D	28	GLY

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	359/375 (96%)	345 (96%)	14 (4%)	32	46
1	B	358/375 (96%)	341 (95%)	17 (5%)	26	37
1	C	361/375 (96%)	349 (97%)	12 (3%)	38	53
1	D	353/375 (94%)	336 (95%)	17 (5%)	25	36
All	All	1431/1500 (95%)	1371 (96%)	60 (4%)	30	42

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	PRO
1	A	135	THR
1	A	147	LEU
1	A	157	GLN
1	A	188	GLU
1	A	189	GLU
1	A	203	GLN
1	A	204	LEU
1	A	214	LEU
1	A	242	ASN
1	A	367	MET
1	A	415	ILE
1	A	416	ASN
1	A	422	GLU
1	B	36	PRO
1	B	81	LEU

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Mol	Chain	Res	Type
1	B	92	ASN
1	B	112	GLU
1	B	130	LEU
1	B	140	LEU
1	B	147	LEU
1	B	171	LEU
1	B	176	LYS
1	B	179	THR
1	B	209	VAL
1	B	233	TYR
1	B	268	ARG
1	B	324	LEU
1	B	341	ASN
1	B	375	ASP
1	B	387	VAL
1	C	77	ASN
1	C	81	LEU
1	C	130	LEU
1	C	147	LEU
1	C	186	ILE
1	C	211	THR
1	C	216	LEU
1	C	233	TYR
1	C	341	ASN
1	C	379	LYS
1	C	419	ASN
1	C	444	LEU
1	D	16	ASP
1	D	22	LEU
1	D	81	LEU
1	D	105	LEU
1	D	128	LEU
1	D	130	LEU
1	D	133	GLU
1	D	140	LEU
1	D	145	ASP
1	D	163	ASP
1	D	198	LYS
1	D	211	THR
1	D	244	LEU
1	D	280	ASP
1	D	298	PRO

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Mol	Chain	Res	Type
1	D	341	ASN
1	D	399	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	64	ASN
1	A	66	ASN
1	A	113	ASN
1	A	146	HIS
1	A	157	GLN
1	A	159	HIS
1	A	203	GLN
1	A	252	ASN
1	A	270	GLN
1	A	314	GLN
1	A	345	HIS
1	A	346	HIS
1	A	416	ASN
1	A	419	ASN
1	B	64	ASN
1	B	75	GLN
1	B	82	ASN
1	B	113	ASN
1	B	146	HIS
1	B	205	GLN
1	B	242	ASN
1	B	314	GLN
1	B	421	GLN
1	C	64	ASN
1	C	66	ASN
1	C	77	ASN
1	C	82	ASN
1	C	126	GLN
1	C	146	HIS
1	C	203	GLN
1	C	242	ASN
1	C	252	ASN
1	C	270	GLN
1	C	346	HIS
1	C	396	HIS

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Mol	Chain	Res	Type
1	C	419	ASN
1	D	66	ASN
1	D	75	GLN
1	D	108	GLN
1	D	200	GLN
1	D	205	GLN
1	D	252	ASN
1	D	270	GLN
1	D	341	ASN
1	D	346	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

19 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	1009	-	4,4,4	0.22	0	6,6,6	0.08	0
3	ADP	C	558	-	24,29,29	0.95	1 (4%)	29,45,45	1.57	5 (17%)
3	ADP	A	557	-	24,29,29	1.04	1 (4%)	29,45,45	1.52	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	1006	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	A	1007	-	4,4,4	0.31	0	6,6,6	0.07	0
2	SO4	C	1022	-	4,4,4	0.20	0	6,6,6	0.18	0
2	SO4	C	1010	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	A	1000	-	4,4,4	0.14	0	6,6,6	0.21	0
2	SO4	B	1001	-	4,4,4	0.17	0	6,6,6	0.22	0
2	SO4	D	1023	-	4,4,4	0.29	0	6,6,6	0.07	0
2	SO4	C	1002	-	4,4,4	0.16	0	6,6,6	0.28	0
2	SO4	A	1008	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	C	1005	-	4,4,4	0.30	0	6,6,6	0.07	0
2	SO4	D	1004	-	4,4,4	0.29	0	6,6,6	0.05	0
4	ADQ	B	506	-	35,41,41	1.85	8 (22%)	45,63,63	3.49	10 (22%)
2	SO4	D	1003	-	4,4,4	0.34	0	6,6,6	0.27	0
2	SO4	A	1020	-	4,4,4	0.20	0	6,6,6	0.12	0
2	SO4	B	1021	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	D	1011	-	4,4,4	0.30	0	6,6,6	0.10	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	ADP	C	558	-	-	3/12/32/32	0/3/3/3
3	ADP	A	557	-	-	3/12/32/32	0/3/3/3
4	ADQ	B	506	-	-	7/19/59/59	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	506	ADQ	PB-O3B	-5.06	1.47	1.60
4	B	506	ADQ	C2-N3	3.99	1.38	1.32
4	B	506	ADQ	C4-N3	3.23	1.40	1.35
4	B	506	ADQ	C2-N1	3.09	1.39	1.33
3	A	557	ADP	C2-N1	3.04	1.39	1.33
4	B	506	ADQ	C3'-C2'	2.96	1.59	1.52
3	C	558	ADP	C2-N1	2.62	1.38	1.33
4	B	506	ADQ	O4D-C1D	2.45	1.44	1.41
4	B	506	ADQ	C5-N7	-2.37	1.31	1.39
4	B	506	ADQ	C4'-C5'	2.29	1.57	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	506	ADQ	O3B-C1'-C2'	14.47	134.89	108.38
4	B	506	ADQ	O5'-C1'-O3B	-10.98	97.01	111.36
4	B	506	ADQ	PB-O3B-C1'	8.84	153.90	119.74
4	B	506	ADQ	N3-C2-N1	-6.66	118.26	128.68
4	B	506	ADQ	O3A-PB-O3B	6.40	115.39	102.48
3	A	557	ADP	C5-C6-N6	3.95	126.35	120.35
3	C	558	ADP	C5-C6-N6	3.78	126.09	120.35
3	C	558	ADP	N3-C2-N1	-3.55	123.13	128.68
3	A	557	ADP	N3-C2-N1	-3.37	123.42	128.68
3	A	557	ADP	C5-C6-N1	-2.85	113.89	120.35
4	B	506	ADQ	C2D-C3D-C4D	2.74	107.97	102.64
3	C	558	ADP	C5-C6-N1	-2.66	114.32	120.35
3	C	558	ADP	C2-N1-C6	2.61	123.22	118.75
4	B	506	ADQ	C1'-O5'-C5'	2.59	118.78	113.69
3	A	557	ADP	C2-N1-C6	2.53	123.08	118.75
4	B	506	ADQ	C3D-C2D-C1D	2.44	104.65	100.98
4	B	506	ADQ	O4'-C4'-C3'	2.17	115.36	110.35
4	B	506	ADQ	C4-C5-N7	-2.11	107.20	109.40
3	C	558	ADP	O5'-C5'-C4'	2.09	116.19	108.99

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	558	ADP	PA-O3A-PB-O3B
3	A	557	ADP	PA-O3A-PB-O3B
4	B	506	ADQ	C1'-O3B-PB-O3A
4	B	506	ADQ	C2'-C1'-O3B-PB
4	B	506	ADQ	O5'-C1'-O3B-PB
4	B	506	ADQ	PB-O3A-PA-O5D
4	B	506	ADQ	O4D-C4D-C5D-O5D
3	A	557	ADP	C3'-C4'-C5'-O5'
4	B	506	ADQ	C3D-C4D-C5D-O5D
3	C	558	ADP	PA-O3A-PB-O2B
3	A	557	ADP	PA-O3A-PB-O2B
4	B	506	ADQ	C5D-O5D-PA-O1A
3	C	558	ADP	PA-O3A-PB-O1B

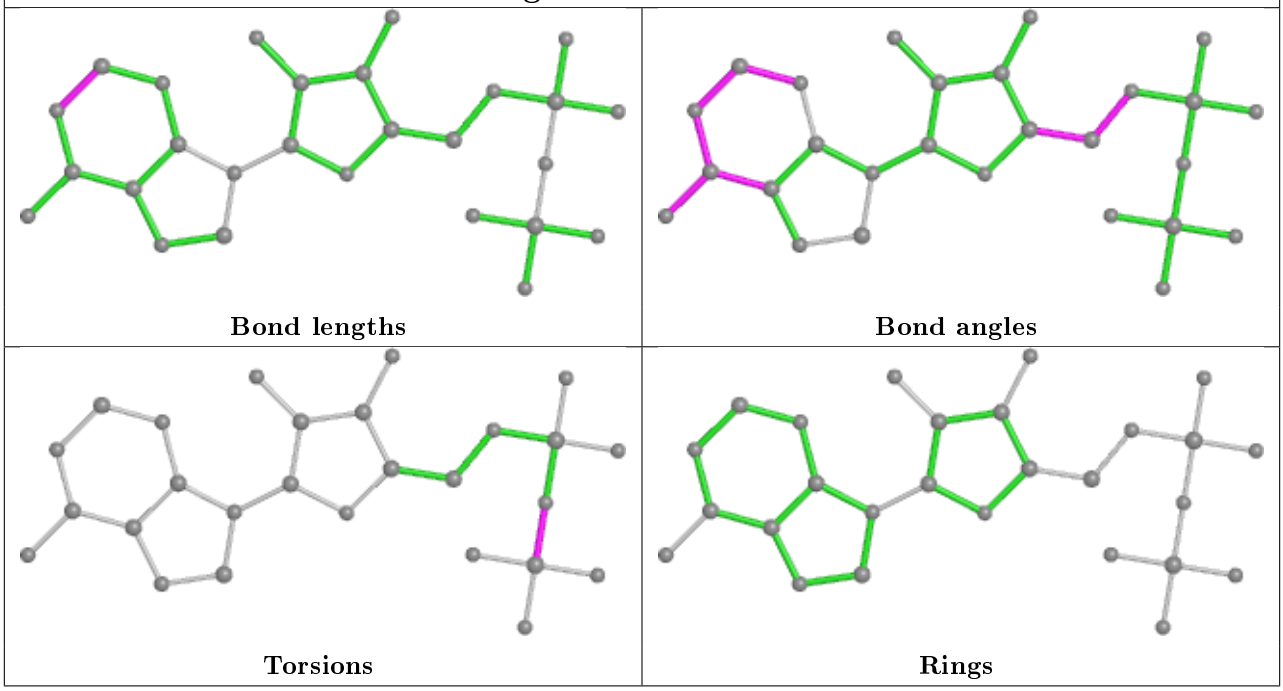
There are no ring outliers.

6 monomers are involved in 10 short contacts:

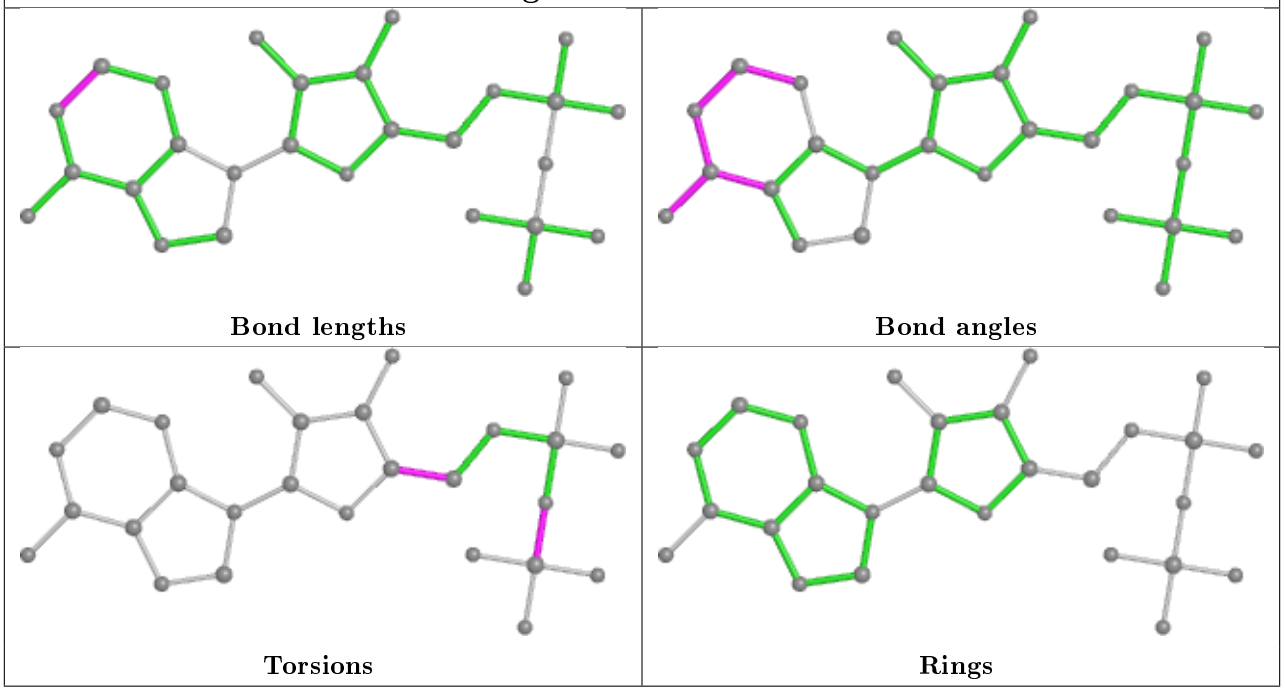
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1009	SO4	1	0
2	C	1010	SO4	1	0
2	D	1023	SO4	1	0
4	B	506	ADQ	4	0
2	B	1021	SO4	2	0
2	D	1011	SO4	1	0

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.

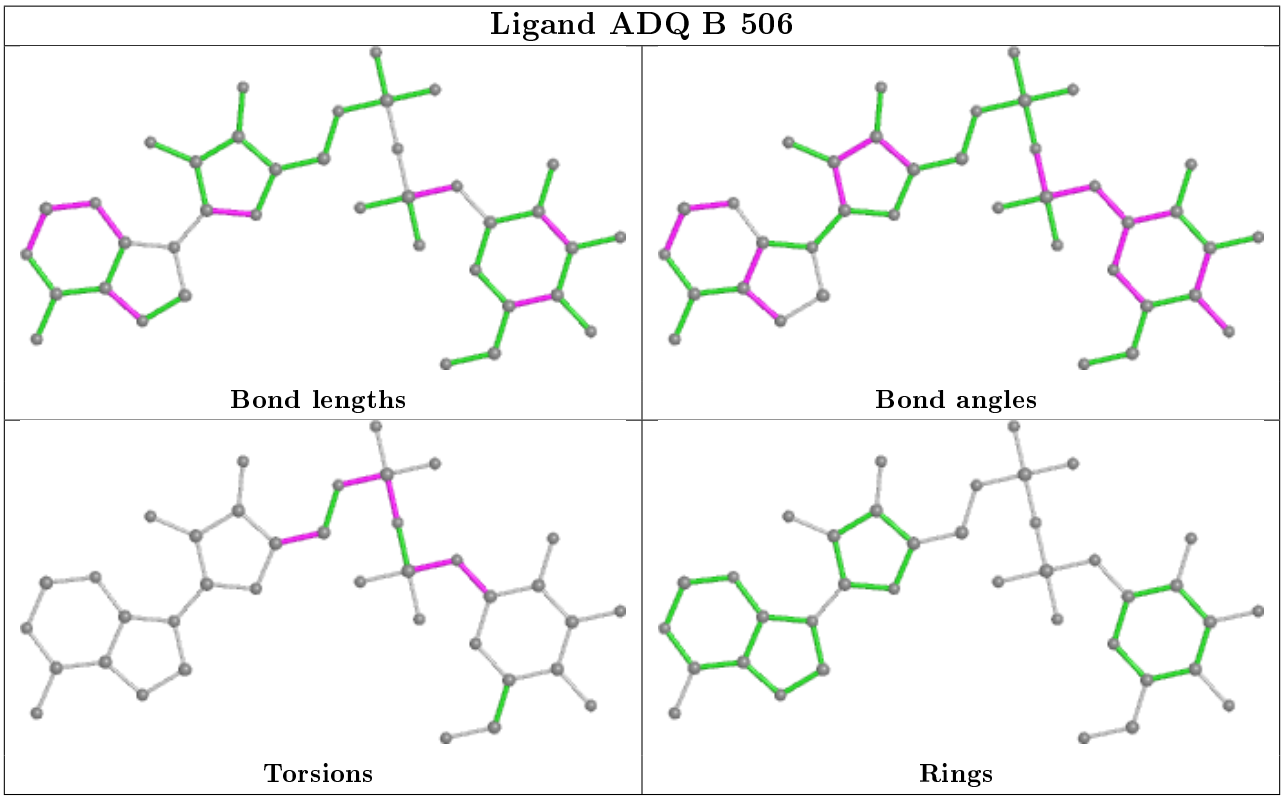
Ligand ADP C 558



Ligand ADP A 557



Ligand ADQ B 506



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	432/451 (95%)	0.32	28 (6%) 18 24	23, 42, 72, 91	0
1	B	433/451 (96%)	0.43	41 (9%) 8 11	22, 45, 81, 91	0
1	C	434/451 (96%)	0.24	19 (4%) 34 41	20, 40, 71, 91	0
1	D	426/451 (94%)	0.64	53 (12%) 4 5	22, 49, 86, 91	0
All	All	1725/1804 (95%)	0.41	141 (8%) 11 15	20, 44, 80, 91	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	299	VAL	6.9
1	D	298	PRO	6.9
1	D	30	ALA	6.6
1	C	297	LYS	6.6
1	D	299	VAL	6.5
1	D	383	ALA	5.8
1	A	299	VAL	5.7
1	D	12	CYS	5.4
1	C	298	PRO	5.1
1	D	385	GLY	4.9
1	D	297	LYS	4.6
1	B	418	ASP	4.3
1	D	29	GLY	4.3
1	A	11	THR	4.2
1	B	112	GLU	4.1
1	B	299	VAL	4.0
1	B	233	TYR	3.8
1	B	117	PHE	3.7
1	D	31	GLY	3.7
1	B	220	ARG	3.7
1	D	365	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	32	THR	3.6
1	D	14	ASP	3.5
1	B	213	ILE	3.4
1	D	366	LEU	3.4
1	A	349	VAL	3.4
1	A	374	THR	3.3
1	D	252	ASN	3.3
1	A	367	MET	3.3
1	D	181	PHE	3.3
1	A	380	LEU	3.2
1	C	217	ASP	3.2
1	A	366	LEU	3.2
1	B	232	ILE	3.2
1	B	217	ASP	3.2
1	C	418	ASP	3.2
1	B	91	SER	3.1
1	A	350	GLY	3.1
1	B	29	GLY	3.1
1	D	401	ILE	3.1
1	D	439	VAL	3.0
1	A	383	ALA	3.0
1	A	298	PRO	3.0
1	D	384	LYS	3.0
1	B	298	PRO	3.0
1	B	380	LEU	2.9
1	D	241	LEU	2.9
1	A	188	GLU	2.9
1	B	113	ASN	2.9
1	B	30	ALA	2.9
1	A	385	GLY	2.9
1	B	141	ILE	2.8
1	B	235	ILE	2.8
1	A	141	ILE	2.8
1	D	402	ILE	2.8
1	A	365	LEU	2.8
1	B	367	MET	2.8
1	D	234	VAL	2.8
1	B	417	LYS	2.8
1	D	180	ALA	2.7
1	D	379	LYS	2.7
1	A	307	ARG	2.7
1	A	24	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	383	ALA	2.7
1	D	417	LYS	2.7
1	B	419	ASN	2.7
1	B	12	CYS	2.6
1	A	402	ILE	2.6
1	D	86	SER	2.6
1	A	375	ASP	2.6
1	B	200	GLN	2.6
1	D	219	LYS	2.6
1	D	382	ALA	2.6
1	A	297	LYS	2.6
1	D	89	TYR	2.5
1	B	222	LYS	2.5
1	B	231	GLY	2.5
1	D	307	ARG	2.5
1	C	11	THR	2.5
1	D	200	GLN	2.5
1	A	381	LEU	2.5
1	D	377	ASP	2.5
1	B	142	LEU	2.5
1	B	28	GLY	2.5
1	D	87	ARG	2.5
1	D	176	LYS	2.4
1	D	28	GLY	2.4
1	B	219	LYS	2.4
1	C	380	LEU	2.4
1	D	140	LEU	2.4
1	A	12	CYS	2.4
1	B	143	ALA	2.4
1	B	174	ASP	2.4
1	D	233	TYR	2.4
1	D	301	ASP	2.4
1	C	141	ILE	2.4
1	B	93	MET	2.4
1	D	308	SER	2.4
1	B	385	GLY	2.3
1	D	235	ILE	2.3
1	B	309	ALA	2.3
1	C	349	VAL	2.3
1	B	333	ILE	2.3
1	D	419	ASN	2.3
1	D	198	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	245	ARG	2.2
1	C	214	LEU	2.2
1	D	266	GLY	2.2
1	D	380	LEU	2.2
1	A	217	ASP	2.2
1	C	419	ASN	2.2
1	D	218	ASP	2.2
1	D	118	GLN	2.2
1	B	176	LYS	2.2
1	C	296	LYS	2.2
1	C	250	GLY	2.2
1	B	14	ASP	2.1
1	C	366	LEU	2.1
1	D	420	VAL	2.1
1	A	187	ASP	2.1
1	A	176	LYS	2.1
1	A	382	ALA	2.1
1	B	31	GLY	2.1
1	A	415	ILE	2.1
1	A	451	ILE	2.1
1	D	367	MET	2.1
1	D	424	ALA	2.1
1	D	248	PHE	2.1
1	D	451	ILE	2.1
1	B	384	LYS	2.1
1	C	90	ALA	2.1
1	D	296	LYS	2.1
1	C	87	ARG	2.0
1	B	23	GLY	2.0
1	D	161	GLU	2.0
1	C	161	GLU	2.0
1	D	217	ASP	2.0
1	A	337	CYS	2.0
1	B	275	ASP	2.0
1	B	377	ASP	2.0
1	C	417	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

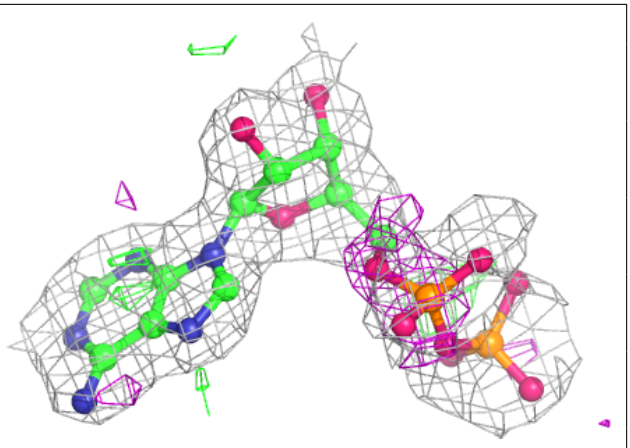
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

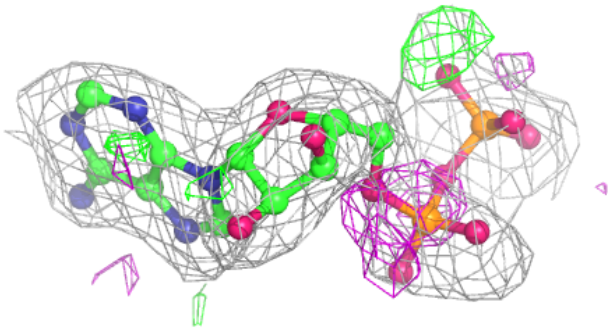
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	C	558	27/27	0.81	0.18	42,53,78,79	0
2	SO4	B	1006	5/5	0.83	0.22	96,96,96,96	0
3	ADP	A	557	27/27	0.86	0.16	43,50,85,85	0
2	SO4	D	1023	5/5	0.88	0.24	96,96,96,96	0
4	ADQ	B	506	38/38	0.88	0.15	47,54,61,62	0
2	SO4	C	1022	5/5	0.90	0.18	90,91,91,91	0
2	SO4	D	1011	5/5	0.91	0.16	62,65,66,67	0
2	SO4	D	1004	5/5	0.92	0.19	96,96,96,96	0
2	SO4	D	1003	5/5	0.94	0.17	43,45,48,49	0
2	SO4	A	1020	5/5	0.95	0.16	66,67,68,69	0
2	SO4	B	1021	5/5	0.95	0.20	96,96,96,96	0
2	SO4	C	1005	5/5	0.95	0.14	77,78,79,79	0
2	SO4	A	1007	5/5	0.96	0.15	70,71,71,71	0
2	SO4	B	1009	5/5	0.96	0.14	62,62,65,66	0
2	SO4	C	1010	5/5	0.97	0.15	54,58,58,58	0
2	SO4	A	1008	5/5	0.97	0.14	54,56,57,59	0
2	SO4	A	1000	5/5	0.99	0.16	43,46,47,49	0
2	SO4	C	1002	5/5	0.99	0.17	38,39,41,41	0
2	SO4	B	1001	5/5	0.99	0.10	36,37,39,41	0

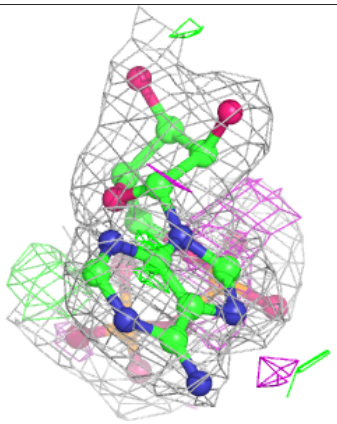
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP C 558:

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

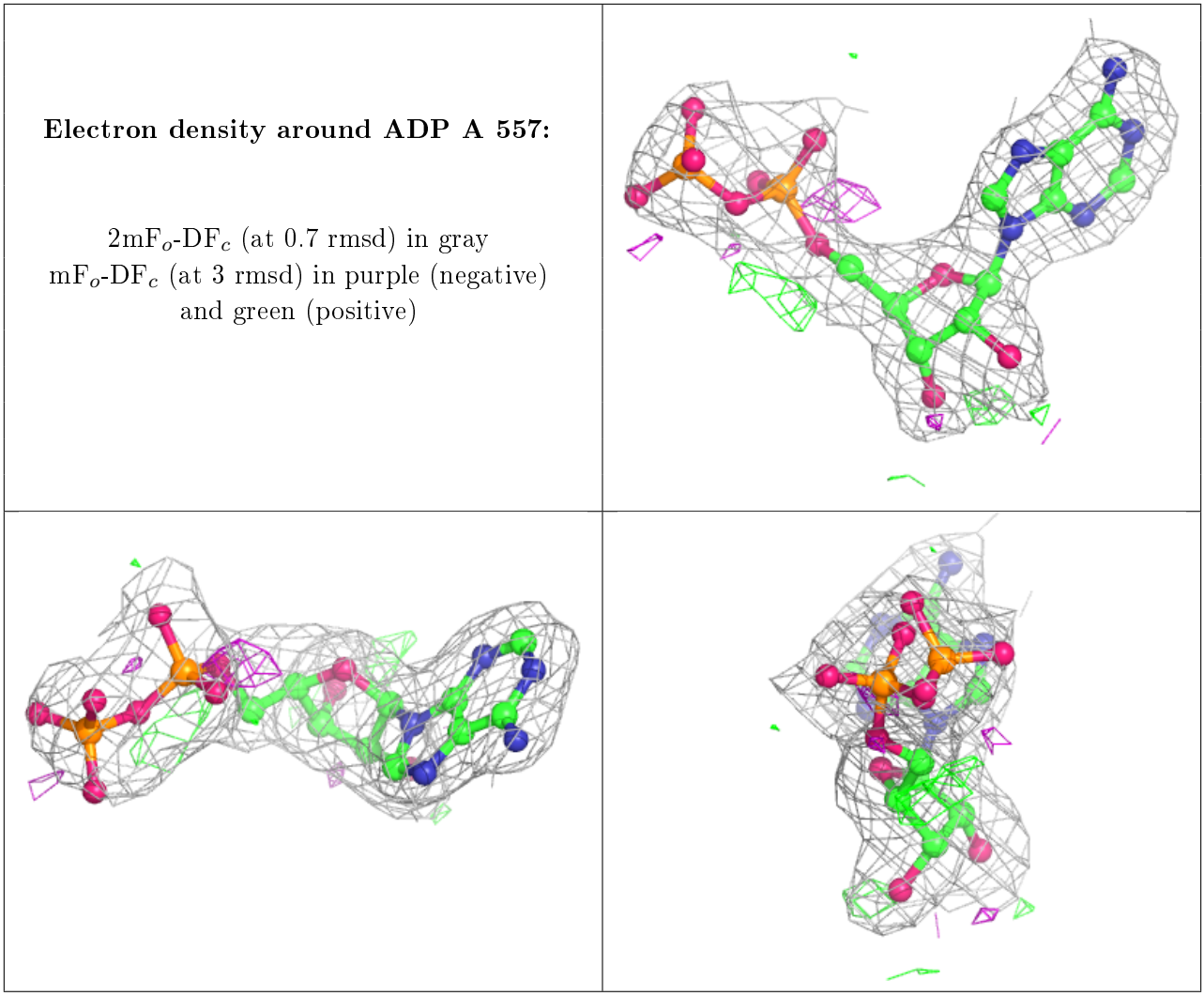






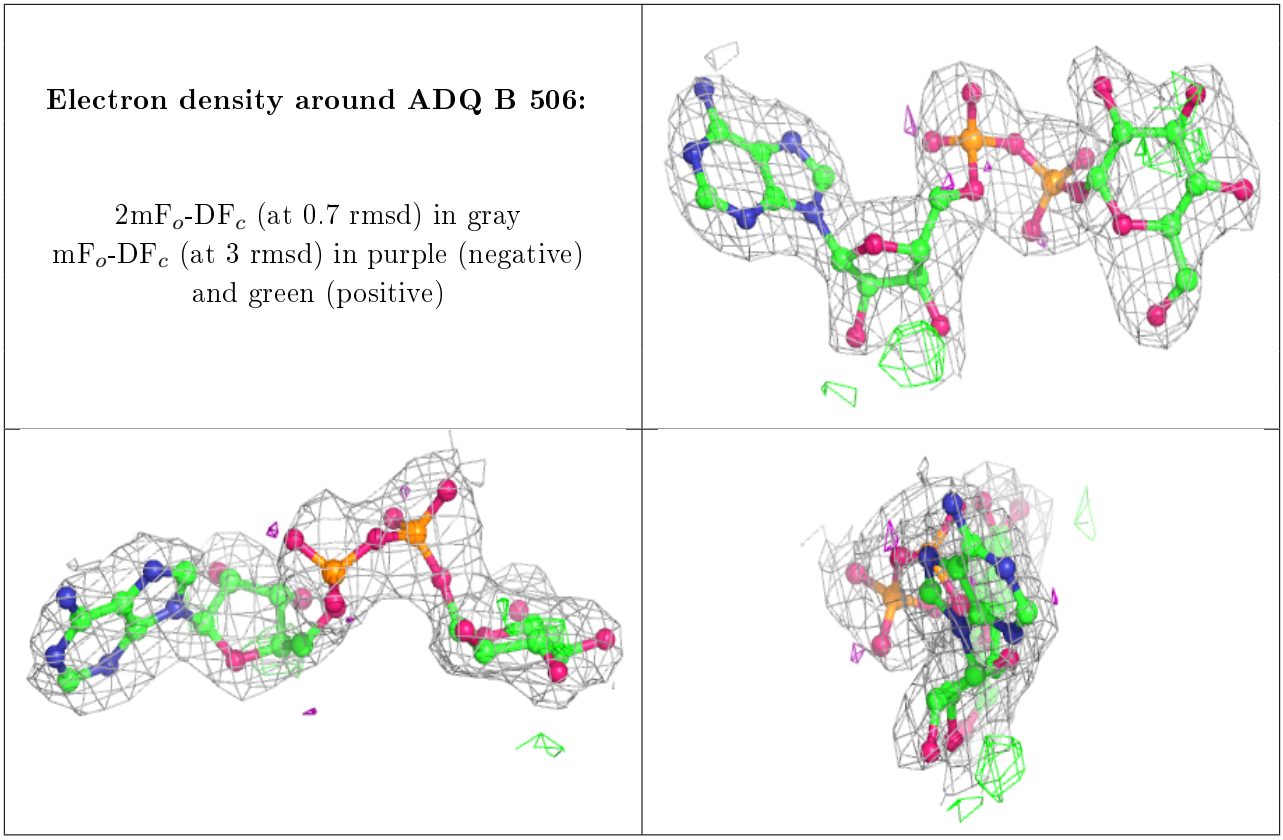
Electron density around ADP A 557:

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



Electron density around ADQ B 506:

$2mF_o$-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.