



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

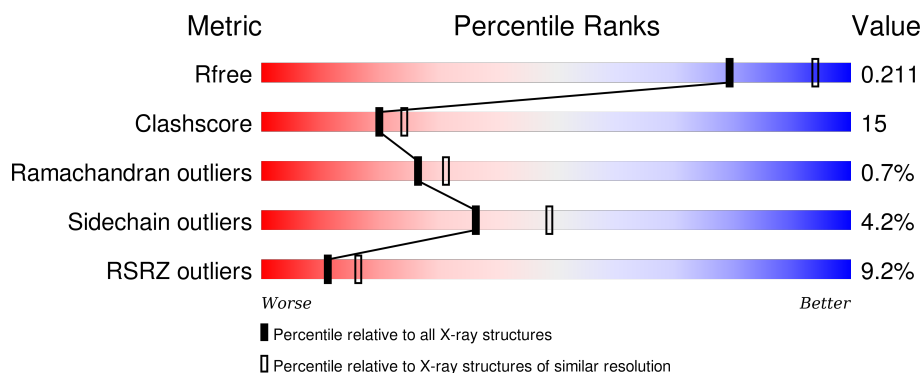
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>• •</div> </div> </div>
1	B	451	<div> <div>10%</div> <div> <div></div> <div>64%</div> <div>31%</div> <div>• •</div> </div> </div>
1	C	451	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• •</div> </div> </div>
1	D	451	<div> <div>13%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>• 6%</div> </div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	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.

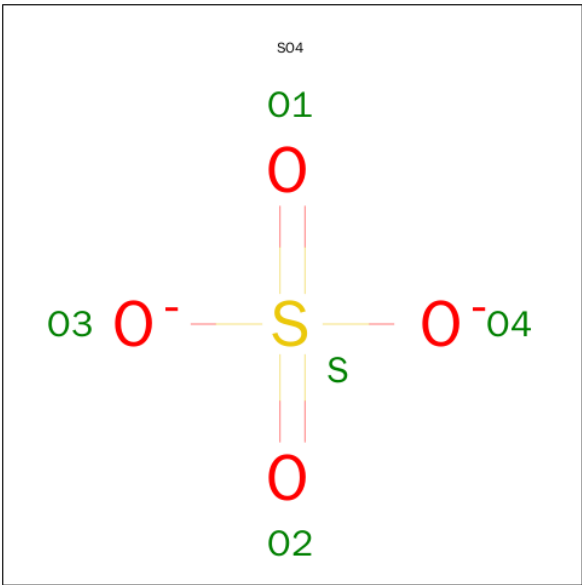
- Molecule 1 is a protein called Glucose-1-phosphate adenylyltransferase small subunit.

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: O₄S).



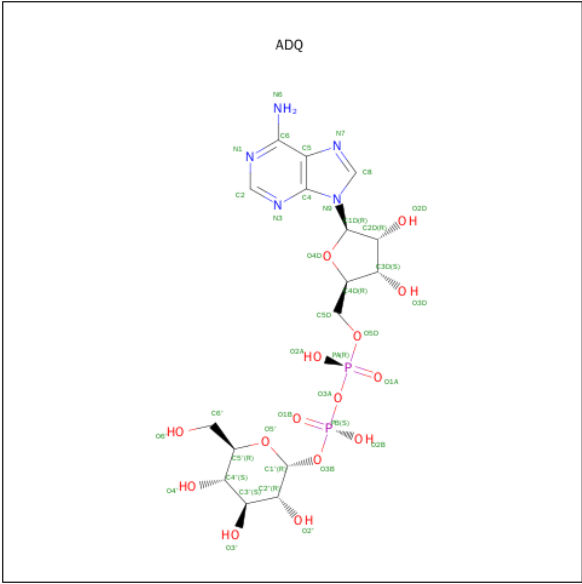
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total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

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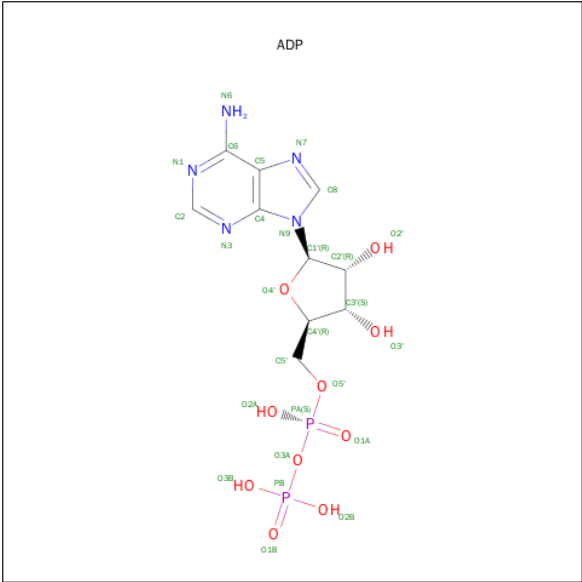
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: ADQ) (formula: C₁₆H₂₅N₅O₁₅P₂).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.86 Å 137.96 Å 90.83 Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.31 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.244 0.206 , 0.211	Depositor DCC
R_{free} test set	3933 reflections (5.28%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 78406 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 [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	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	B	38	0	22	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	27	0	12	0	0
4	C	27	0	12	0	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:C:367:MET:HG3	1:C:403:ASP:HA	1.52	0.90
1:B:367:MET:HG3	1:B:403:ASP:HA	1.53	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:D:297:LYS:CB	1:D:298:PRO:HD2	2.06	0.86
1:A:378:ARG:HA	1:A:381:LEU:HD12	1.57	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:HE3	1:B:173:MET:HA	1.66	0.76
1:B:384:LYS:HB3	1:B:384:LYS:NZ	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:341:ASN:OD1	1:C:357:GLU:HG3	1.88	0.73
1:C:125:ARG:HD2	5:C:1114:HOH:O	1.89	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:86:SER:O	1:C:90:ALA:HB3	1.94	0.68
1:C:377:ASP:O	1:C:381:LEU:HD23	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:341:ASN:OD1	1:B:357:GLU:HG3	2.00	0.61
1:B:192:ILE:HD12	1:B:269:VAL:HG12	1.83	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:C:446:PRO:HG2	1:C:449:ILE:HG13	1.83	0.60
1:B:73:LEU:HD23	1:B:105:LEU:HB2	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:D:268:ARG:HH11	1:D:268:ARG:HG3	1.68	0.59
1:A:87:ARG:HD2	1:A:314:GLN:OE1	2.02	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:D:147:LEU:O	1:D:148:TYR:HB3	2.03	0.58
1:C:277:TYR:CD2	1:C:302:PHE:HB2	2.38	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: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: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:D:346:HIS:HD2	1:D:363:ASP:OD1	1.90	0.55
1:C:444:LEU:CD1	1:C:444:LEU:C	2.75	0.55
1:A:421:GLN:NE2	5:A:1149:HOH:O	2.40	0.55
1:D:362:GLU:O	1:D:398:LYS:HA	2.08	0.54
1:D:137:LEU:HD12	1:D:160:ARG:NH2	2.22	0.54
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: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:C:296:LYS:NZ	1:C:301:ASP:H	2.06	0.54
1:B:185:LYS:HB2	1:B:194:GLU:HB2	1.90	0.54
1:B:87:ARG:HG2	1:B:314:GLN:HG3	1.90	0.53
1:B:243:LEU:HD21	1:B:267:MET:SD	2.48	0.53
1:A:57:ILE:HB	1:A:58:PRO:CD	2.38	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:C:259:ILE:HG13	5:C:1153:HOH:O	2.09	0.52
1:A:409:GLY:O	1:A:412:VAL:HG23	2.10	0.52
1:A:242:ASN:ND2	1:A:246:ASP:HB2	2.24	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:324:LEU:O	1:D:329:THR:HA	2.10	0.52
1:C:166:ILE:HG12	1:C:235:ILE:HG12	1.92	0.52
1:A:305:TYR:CB	1:B:319:PRO:HD3	2.40	0.52
1:B:273:LEU:HD22	1:B:273:LEU:N	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	3: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: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:B:217:ASP:OD2	1:B:218:ASP:N	2.42	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: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:B:31:GLY:HA3	2:B:1021:SO4:S	2.51	0.51
1:D:341:ASN:ND2	1:D:357:GLU:HG3	2.26	0.50
1:D:330:ASP:O	1:D:346:HIS:HA	2.11	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: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: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:B:222:LYS:CA	1:B:222:LYS:HE2	2.41	0.50
1:B:29:GLY:O	1:B:30:ALA:HB3	2.12	0.50
1:A:186:ILE:HD13	1:A:214:LEU:HD21	1.92	0.50
1:D:201:GLY:O	1:D:205:GLN:HG2	2.12	0.50
1:B:150:MET:CE	1:B:155:PHE:HB2	2.42	0.50
1:A:159:HIS:HD2	1:A:167:THR:OG1	1.95	0.50
1:B:120:THR:CG2	3: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:D:268:ARG:HG3	1:D:268:ARG:NH1	2.28	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: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:C:86:SER:HA	1:C:90:ALA:HB2	1.94	0.49
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:D:83:ARG:HG3	1:D:83:ARG:HH21	1.78	0.49
1:B:325:ASP:HB3	1:B:341:ASN:HA	1.95	0.48
1:B:222:LYS:HE2	1:B:222:LYS: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:D:297:LYS:O	1:D:298:PRO:C	2.53	0.47
1:B:415:ILE:HG22	1:B:415:ILE:O	2.12	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:D:211:THR:HB	1:D:216:LEU:HD12	1.96	0.47
1:C:245:ARG:HD3	1:C:246:ASP:OD1	2.15	0.47
1:B:177:ARG:HB3	1:B:181:PHE:HE1	1.80	0.47
1:C:377:ASP:O	1:C:381:LEU:CD2	2.63	0.47
1:C:296:LYS:HZ1	1:C:301:ASP:N	2.08	0.47
1:B:314:GLN:HA	1:B:315:PRO:HD3	1.81	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:A:415:ILE:HD13	1:A:415:ILE:N	2.29	0.47
1:D:57:ILE:HB	1:D:58:PRO:CD	2.44	0.47
1:A:296:LYS:HD3	1:A:299:VAL:O	2.14	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:D:155:PHE:CE2	1:D:232:ILE:HG22	2.50	0.47
1:C:241:LEU:O	1:C:245:ARG:HB3	2.15	0.47
1:B:152:TYR:O	1:B:156:ILE:HD12	2.14	0.47
1:A:13:LEU:CD2	1:A:157:GLN:HG2	2.44	0.47
5:B:1112:HOH:O	1:C:82:ASN:HB3	2.14	0.47
1:B:157:GLN:O	1:B:161:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLU:OE1	1:B:198:LYS:HE2	2.14	0.46
1:A:242:ASN:HD22	1:A:246:ASP:HB2	1.79	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: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: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:67:ILE:HD12	1:D:140:LEU:HD12	1.96	0.46
1:B:200:GLN:HA	1:B:204:LEU:HB2	1.97	0.46
1:B:137:LEU:O	1:B:138:GLU:HG3	2.15	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:B:197:GLU:HG3	1:B:198:LYS:HD2	1.98	0.45
1:A:307:ARG:HG3	1:A:308:SER:N	2.31	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	3: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:129:TRP:CG	1:C:111:PRO:HD3	2.51	0.45
1:B:444:LEU:HD23	1:B:445:ILE:N	2.32	0.45
1:A:375:ASP:OD2	1:A:376:ALA:N	2.49	0.44
1:B:351:LEU:CD2	1:B:351:LEU:H	2.30	0.44
1:C:330:ASP:O	1:C:346:HIS:HA	2.17	0.44
1:B:46:VAL:HA	1:B:47:PRO:HD3	1.86	0.44
1:B:112:GLU:OE1	1:B:112:GLU:HA	2.16	0.44
1:B:74:THR:O	1:B:106:ALA:HA	2.18	0.44
1:A:143:ALA:HB3	1:A:146:HIS:CE1	2.52	0.44
1:D:342:CYS:HB2	1:D:359:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:THR:O	1:C:106:ALA:HA	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:444:LEU:C	1:B:444:LEU:HD23	2.38	0.44
1:B:246:ASP:O	1:B:249:PRO:HD3	2.18	0.44
1:A:90:ALA:HB2	1:A:102:VAL:H	1.81	0.44
1:D:380:LEU:HD23	1:D:380:LEU:O	2.18	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: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:D:155:PHE:CE1	1:D:167:THR:HG22	2.53	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:A:426:GLU:HG2	1:A:431:PHE:CE1	2.33	0.43
1:C:332:VAL:HA	1:D:321:SER:O	2.19	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: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: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:B:323:MET:HE2	1:B:333:ILE:HD13	1.99	0.43
1:C:277:TYR:CE2	1:C:302:PHE:HB2	2.54	0.43
1:D:346:HIS:CD2	1:D:363:ASP:OD1	2.69	0.43
1:C:20:SER:O	1:C:136:VAL:HB	2.19	0.43
1:C:29:GLY:HA2	1:C:75:GLN:HB2	2.00	0.43
1:C:357:GLU:H	1:C:357:GLU:CD	2.21	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:A:11:THR:OG1	1:A:12:CYS:N	2.51	0.43
1:C:259:ILE:HB	1:C:260:PRO:HD3	2.00	0.43
1:B:220:ARG:NH2	1:B:223:GLU:HB2	2.34	0.43
1:A:421:GLN:HA	1:A:421:GLN:OE1	2.18	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:78:SER:OG	1:C:81:LEU:HB2	2.19	0.43
1:C:409:GLY:O	1:C:412:VAL:HG23	2.19	0.43
1:C:294:ILE:HD13	5:C:1096:HOH:O	2.18	0.42
1:B:351:LEU:CD2	1:B:351:LEU:N	2.82	0.42
1:B:247:LYS:HE2	5:B:1116:HOH:O	2.17	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:B:163:ASP:O	1:B:268:ARG:HD3	2.19	0.42
1:A:425:ARG:HH11	1:A:425:ARG:HG3	1.84	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:B:133:GLU:HG2	1:C:79:ALA:CB	2.50	0.42
1:A:432:ILE:HA	1:A:436:ILE:O	2.20	0.42
1:C:77:ASN:HD22	1:C:78:SER:H	1.66	0.42
1:B:181:PHE:CD2	3:B:506:ADQ:H6'2	2.54	0.42
1:D:222:LYS:HE2	1:D:222:LYS:HA	2.02	0.42
1:C:268:ARG:NH2	1:C:268:ARG:HG3	2.32	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:B:110:SER:HB2	1:B:111:PRO:HD2	2.02	0.42
1:C:16:ASP:OD1	1:C:19:ARG:HG2	2.20	0.42
1:B:155:PHE:HE1	1:B:167:THR:HG22	1.84	0.42
1:A:46:VAL:HA	1:A:47:PRO:HD3	1.77	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:C:12:CYS:HB2	5:C:1127:HOH:O	2.20	0.41
1:A:40:LYS:N	1:A:113:ASN:HD21	2.07	0.41
1:D:341:ASN:H	1:D:341:ASN:ND2	2.10	0.41
1:D:155:PHE:CZ	1:D:234:VAL:HG23	2.54	0.41
1:A:387:VAL:HA	1:A:388:PRO:HD3	1.82	0.41
1:D:424:ALA:HA	1:D:431:PHE:CD1	2.55	0.41
1:C:367:MET:HG2	1:C:402:ILE:O	2.20	0.41
1:B:384:LYS:CB	1:B:384:LYS:NZ	2.78	0.41
1:C:241:LEU:HD21	1:C:245:ARG:NH1	2.35	0.41
1:B:245:ARG:CZ	5:B:1098:HOH:O	2.67	0.41
1:C:177:ARG:HG2	1:C:181:PHE:HE1	1.86	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:D:314:GLN:NE2	2:D:1011:SO4:O4	2.53	0.41
1:C:236:SER:HB2	1:C:239:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:214:LEU:HD11	1:B:227:ILE:HG12	2.03	0.41
1:C:446:PRO:HG2	1:C:449:ILE:CG1	2.48	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:A:433:LYS:C	1:A:433:LYS:HD3	2.40	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:B:14:ASP:HA	1:B:15:PRO:C	2.41	0.41
1:D:367:MET:HE3	1:D:403:ASP:OD1	2.21	0.41
1:C:205:GLN:HA	1:C:205:GLN:OE1	2.21	0.41
1:B:78:SER:HA	5:B:1071:HOH:O	2.19	0.41
1:A:51:ASN:ND2	1:A:335:GLU:HG2	2.36	0.41
1:A:151:ASP:OD1	1:A:153:GLU:HG3	2.21	0.41
1:D:254:PHE:O	1:D:259:ILE:HG12	2.20	0.41
1:B:84:HIS:ND1	2:B:1009:SO4:O4	2.51	0.41
1:A:205:GLN:C	1:A:207:MET:H	2.24	0.41
1:D:277:TYR:CE1	1:D:279:GLU:HG2	2.56	0.41
1:D:33:ARG:HG3	2:D:1023:SO4:S	2.61	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:B:171:LEU:HB2	1:B:172:PRO:CD	2.51	0.41
1:D:247:LYS:HD2	1:D:265:LEU:CD1	2.50	0.41
1:C:43:LYS:N	1:C:44:PRO:CD	2.83	0.41
1:A:230:MET:N	5:A:1145:HOH:O	2.32	0.41
1:C:379:LYS:HE3	1:C:379:LYS:CA	2.51	0.41
1:B:31:GLY:HA3	2:B:1021:SO4:O2	2.21	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: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:D:13:LEU:HD13	1:D:17:ALA:HB2	2.03	0.40
1:D:49:GLY:O	1:D:50:ALA:CB	2.66	0.40
1:A:314:GLN:HA	1:A:315:PRO:HD3	1.89	0.40
1:D:34:LEU:HA	1:D:284:ILE:HD12	2.03	0.40
1:C:181:PHE:HB3	5:C:1098:HOH:O	2.22	0.40
1:D:152:TYR:O	1:D:156:ILE:HG13	2.21	0.40
1:C:342:CYS:HB2	1:C:359:ALA:O	2.20	0.40
1:D:248:PHE:HB3	1:D:251:ALA:HB2	2.04	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:D:296:LYS:O	1:D:297:LYS:O	2.39	0.40
1:A:189:GLU:N	1:A:189:GLU:OE1	2.55	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

5.3.1 Protein backbone

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%)	52	64
1	B	427/451 (95%)	393 (92%)	30 (7%)	4 (1%)	21	24
1	C	430/451 (95%)	406 (94%)	23 (5%)	1 (0%)	52	64
1	D	420/451 (93%)	386 (92%)	28 (7%)	6 (1%)	14	13
All	All	1705/1804 (94%)	1586 (93%)	107 (6%)	12 (1%)	26	31

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 ⓘ

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%)	39	53
1	B	358/375 (96%)	341 (95%)	17 (5%)	32	43
1	C	361/375 (96%)	349 (97%)	12 (3%)	45	61
1	D	353/375 (94%)	336 (95%)	17 (5%)	31	42
All	All	1431/1500 (95%)	1371 (96%)	60 (4%)	36	49

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	A	1000	-	4,4,4	0.06	0	6,6,6	0.24	0
2	SO4	A	1007	-	4,4,4	0.29	0	6,6,6	0.08	0
2	SO4	A	1008	-	4,4,4	0.19	0	6,6,6	0.12	0
2	SO4	A	1020	-	4,4,4	0.15	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	A	557	-	22,29,29	1.08	1 (4%)	27,45,45	1.79	3 (11%)
2	SO4	B	1001	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	B	1006	-	4,4,4	0.21	0	6,6,6	0.13	0
2	SO4	B	1009	-	4,4,4	0.11	0	6,6,6	0.15	0
2	SO4	B	1021	-	4,4,4	0.20	0	6,6,6	0.06	0
3	ADQ	B	506	-	33,41,41	1.87	10 (30%)	44,63,63	3.66	10 (22%)
2	SO4	C	1002	-	4,4,4	0.21	0	6,6,6	0.33	0
2	SO4	C	1005	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	C	1010	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	C	1022	-	4,4,4	0.16	0	6,6,6	0.21	0
4	ADP	C	558	-	22,29,29	1.02	2 (9%)	27,45,45	1.91	3 (11%)
2	SO4	D	1003	-	4,4,4	0.35	0	6,6,6	0.30	0
2	SO4	D	1004	-	4,4,4	0.29	0	6,6,6	0.08	0
2	SO4	D	1011	-	4,4,4	0.24	0	6,6,6	0.15	0
2	SO4	D	1023	-	4,4,4	0.28	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
2	SO4	A	1000	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1007	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1008	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1020	-	-	0/0/0/0	0/0/0/0
4	ADP	A	557	-	-	0/12/32/32	0/3/3/3
2	SO4	B	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1006	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1009	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1021	-	-	0/0/0/0	0/0/0/0
3	ADQ	B	506	-	-	0/19/59/59	0/4/4/4
2	SO4	C	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1005	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1010	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1022	-	-	0/0/0/0	0/0/0/0
4	ADP	C	558	-	-	0/12/32/32	0/3/3/3
2	SO4	D	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1004	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1011	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1023	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	506	ADQ	PB-O3B	-4.87	1.47	1.60
3	B	506	ADQ	C5-N7	-2.44	1.31	1.39
4	C	558	ADP	C6-N6	-2.10	1.28	1.34
3	B	506	ADQ	PB-O2B	2.00	1.63	1.54
3	B	506	ADQ	C5-C4	2.17	1.45	1.40
3	B	506	ADQ	C4'-C5'	2.25	1.57	1.53
4	C	558	ADP	C2-N1	2.57	1.38	1.33
3	B	506	ADQ	O4D-C1D	2.61	1.44	1.41
3	B	506	ADQ	C3'-C2'	2.85	1.59	1.52
4	A	557	ADP	C2-N1	2.98	1.39	1.33
3	B	506	ADQ	C2-N1	3.03	1.39	1.33
3	B	506	ADQ	C4-N3	3.05	1.40	1.35
3	B	506	ADQ	C2-N3	3.58	1.38	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	506	ADQ	N3-C2-N1	-13.89	118.26	128.89
3	B	506	ADQ	O5'-C1'-O3B	-10.88	97.01	111.36
4	C	558	ADP	N3-C2-N1	-7.53	123.13	128.89
4	A	557	ADP	N3-C2-N1	-7.15	123.42	128.89
3	B	506	ADQ	C4-C5-N7	-2.48	107.20	109.48
3	B	506	ADQ	C1'-C2'-C3'	2.10	114.11	109.97
3	B	506	ADQ	O4'-C4'-C3'	2.23	115.36	110.34
4	A	557	ADP	C2-N1-C6	2.41	123.08	118.77
4	C	558	ADP	C2-N1-C6	2.49	123.22	118.77
4	C	558	ADP	C4'-O4'-C1'	2.57	112.54	109.72
3	B	506	ADQ	C1'-O5'-C5'	2.59	118.78	113.75
3	B	506	ADQ	C2D-C3D-C4D	2.61	107.97	102.61
4	A	557	ADP	C4'-O4'-C1'	2.72	112.70	109.72
3	B	506	ADQ	C4D-O4D-C1D	3.16	113.19	109.72
3	B	506	ADQ	O3A-PB-O3B	4.09	115.39	103.63
3	B	506	ADQ	O3B-C1'-C2'	14.19	134.89	108.39

There are no chirality outliers.

There are no torsion outliers.

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	B	1021	SO4	2	0
3	B	506	ADQ	4	0
2	C	1010	SO4	1	0
2	D	1011	SO4	1	0
2	D	1023	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	432/451 (95%)	0.38	32 (7%) 17 25	23, 42, 72, 91	0
1	B	433/451 (96%)	0.50	47 (10%) 7 11	22, 45, 81, 91	0
1	C	434/451 (96%)	0.30	23 (5%) 30 39	20, 40, 71, 91	0
1	D	426/451 (94%)	0.71	57 (13%) 4 7	22, 49, 86, 91	0
All	All	1725/1804 (95%)	0.47	159 (9%) 11 16	20, 44, 80, 91	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	299	VAL	7.2
1	D	298	PRO	7.2
1	D	30	ALA	6.9
1	D	299	VAL	6.8
1	C	297	LYS	6.7
1	D	383	ALA	5.9
1	A	299	VAL	5.9
1	D	12	CYS	5.7
1	C	298	PRO	5.2
1	D	385	GLY	5.1
1	D	297	LYS	4.7
1	D	29	GLY	4.5
1	B	418	ASP	4.5
1	A	11	THR	4.3
1	B	112	GLU	4.2
1	B	299	VAL	4.2
1	B	233	TYR	4.0
1	B	117	PHE	3.8
1	D	31	GLY	3.8
1	D	365	LEU	3.8
1	B	220	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	32	THR	3.7
1	D	14	ASP	3.7
1	D	366	LEU	3.6
1	A	349	VAL	3.6
1	B	213	ILE	3.5
1	A	374	THR	3.5
1	A	367	MET	3.4
1	D	252	ASN	3.4
1	D	181	PHE	3.4
1	A	380	LEU	3.4
1	C	217	ASP	3.4
1	B	232	ILE	3.3
1	A	366	LEU	3.3
1	C	418	ASP	3.3
1	B	217	ASP	3.3
1	A	350	GLY	3.2
1	B	29	GLY	3.2
1	B	91	SER	3.2
1	D	439	VAL	3.2
1	D	401	ILE	3.2
1	B	298	PRO	3.1
1	A	383	ALA	3.1
1	A	298	PRO	3.1
1	B	380	LEU	3.1
1	D	241	LEU	3.0
1	A	385	GLY	3.0
1	D	384	LYS	3.0
1	B	30	ALA	3.0
1	B	113	ASN	3.0
1	A	188	GLU	3.0
1	B	141	ILE	3.0
1	A	141	ILE	3.0
1	B	235	ILE	3.0
1	D	234	VAL	2.9
1	D	180	ALA	2.9
1	D	402	ILE	2.9
1	A	365	LEU	2.9
1	B	367	MET	2.9
1	B	417	LYS	2.9
1	C	383	ALA	2.9
1	A	24	ILE	2.9
1	B	12	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	419	ASN	2.8
1	D	379	LYS	2.8
1	D	417	LYS	2.8
1	A	402	ILE	2.8
1	A	307	ARG	2.8
1	D	382	ALA	2.7
1	D	86	SER	2.7
1	B	200	GLN	2.7
1	B	231	GLY	2.7
1	D	89	TYR	2.7
1	A	375	ASP	2.7
1	B	222	LYS	2.7
1	A	297	LYS	2.6
1	D	219	LYS	2.6
1	C	11	THR	2.6
1	D	307	ARG	2.6
1	B	28	GLY	2.6
1	B	142	LEU	2.6
1	D	377	ASP	2.6
1	A	381	LEU	2.6
1	A	12	CYS	2.6
1	D	200	GLN	2.6
1	D	28	GLY	2.6
1	B	143	ALA	2.6
1	D	140	LEU	2.6
1	D	87	ARG	2.5
1	B	174	ASP	2.5
1	D	176	LYS	2.5
1	C	141	ILE	2.5
1	D	301	ASP	2.5
1	D	233	TYR	2.5
1	B	385	GLY	2.5
1	C	380	LEU	2.5
1	D	308	SER	2.5
1	B	219	LYS	2.5
1	D	235	ILE	2.4
1	B	93	MET	2.4
1	C	349	VAL	2.4
1	B	309	ALA	2.4
1	B	333	ILE	2.4
1	D	266	GLY	2.3
1	D	380	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	419	ASN	2.3
1	C	419	ASN	2.3
1	A	217	ASP	2.3
1	D	198	LYS	2.3
1	B	245	ARG	2.3
1	C	214	LEU	2.3
1	D	218	ASP	2.3
1	D	118	GLN	2.3
1	D	420	VAL	2.3
1	B	176	LYS	2.2
1	C	366	LEU	2.2
1	C	250	GLY	2.2
1	C	296	LYS	2.2
1	D	248	PHE	2.2
1	A	187	ASP	2.2
1	B	14	ASP	2.2
1	A	415	ILE	2.2
1	D	367	MET	2.2
1	A	382	ALA	2.2
1	B	23	GLY	2.2
1	C	90	ALA	2.2
1	D	424	ALA	2.2
1	A	451	ILE	2.2
1	A	176	LYS	2.2
1	A	337	CYS	2.2
1	D	451	ILE	2.1
1	B	31	GLY	2.1
1	B	275	ASP	2.1
1	D	217	ASP	2.1
1	C	188	GLU	2.1
1	D	161	GLU	2.1
1	B	401	ILE	2.1
1	D	199	PRO	2.1
1	D	296	LYS	2.1
1	C	161	GLU	2.1
1	A	105	LEU	2.1
1	B	384	LYS	2.1
1	C	87	ARG	2.1
1	A	216	LEU	2.1
1	B	212	THR	2.1
1	B	230	MET	2.1
1	B	349	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	92	ASN	2.1
1	A	376	ALA	2.1
1	B	377	ASP	2.1
1	C	417	LYS	2.1
1	D	24	ILE	2.1
1	C	246	ASP	2.0
1	A	379	LYS	2.0
1	D	154	LYS	2.0
1	B	140	LEU	2.0
1	C	140	LEU	2.0
1	C	367	MET	2.0
1	D	22	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	C	1022	5/5	0.90	0.18	1.41	90,91,91,91	0
4	ADP	C	558	27/27	0.81	0.18	1.29	42,53,78,79	0
2	SO4	C	1002	5/5	0.99	0.17	0.74	38,39,41,41	0
2	SO4	B	1006	5/5	0.83	0.22	0.58	96,96,96,96	0
2	SO4	D	1003	5/5	0.94	0.17	0.43	43,45,48,49	0
2	SO4	A	1000	5/5	0.99	0.16	0.37	43,46,47,49	0
2	SO4	C	1005	5/5	0.96	0.14	0.29	77,78,79,79	0
2	SO4	A	1020	5/5	0.95	0.16	0.26	66,67,68,69	0
4	ADP	A	557	27/27	0.87	0.16	0.21	43,50,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	D	1011	5/5	0.91	0.16	0.19	62,65,66,67	0
2	SO4	B	1009	5/5	0.96	0.14	-0.05	62,62,65,66	0
2	SO4	C	1010	5/5	0.97	0.15	-0.09	54,58,58,58	0
2	SO4	A	1007	5/5	0.96	0.15	-0.11	70,71,71,71	0
2	SO4	B	1021	5/5	0.95	0.20	-0.26	96,96,96,96	0
2	SO4	A	1008	5/5	0.97	0.14	-0.33	54,56,57,59	0
2	SO4	D	1023	5/5	0.88	0.23	-0.40	96,96,96,96	0
3	ADQ	B	506	38/38	0.88	0.15	-0.42	47,54,61,62	0
2	SO4	B	1001	5/5	0.99	0.10	-0.86	36,37,39,41	0
2	SO4	D	1004	5/5	0.92	0.20	-	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.