WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2017 – 06:24 PM EDT

PDB ID	:	5CQZ
Title	:	Human cytosolic 5'-nucleotidase II in complex with 3-(3-Imidazol-1-ylphenyl)-N-(9H-purin-6-yl)benzamide
Authors	:	Preeti, P.; Aghajari, N.
Deposited on	:	unknown
Resolution	:	2.90 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

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 2.90 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	Percentile Ranks	Value
Rfree		0.251
Clashscore		7
Ramachandran outliers		1.0%
Sidechain outliers		1.8%
RSRZ outliers		2.7%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
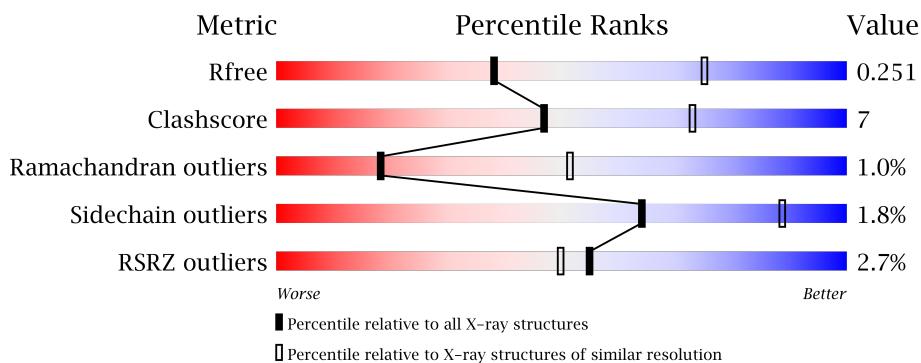
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 <=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	555	2% · 68% · 14% · 16%
1	B	555	2% · 71% · 10% · 18%
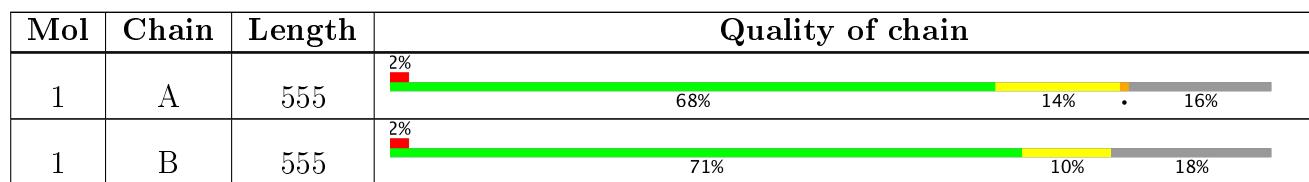
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	601	-	-	-	X
2	GOL	B	601	-	-	-	X
3	SO4	A	604	-	-	X	-
3	SO4	A	605	-	-	-	X
3	SO4	A	606	-	-	-	X
3	SO4	A	607	-	-	-	X
3	SO4	A	608	-	-	-	X
3	SO4	A	609	-	-	-	X
3	SO4	B	604	-	-	X	-
3	SO4	B	605	-	-	-	X
3	SO4	B	606	-	-	-	X
5	53O	A	612	-	-	-	X
5	53O	B	609	-	-	X	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7702 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 Cytosolic purine 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total 3806	C 2460	N 632	O 695	S 19	0	1	0
1	B	453	Total 3699	C 2393	N 611	O 676	S 19	0	1	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P49902
A	-17	GLY	-	expression tag	UNP P49902
A	-16	SER	-	expression tag	UNP P49902
A	-15	SER	-	expression tag	UNP P49902
A	-14	HIS	-	expression tag	UNP P49902
A	-13	HIS	-	expression tag	UNP P49902
A	-12	HIS	-	expression tag	UNP P49902
A	-11	HIS	-	expression tag	UNP P49902
A	-10	HIS	-	expression tag	UNP P49902
A	-9	HIS	-	expression tag	UNP P49902
A	-8	SER	-	expression tag	UNP P49902
A	-7	SER	-	expression tag	UNP P49902
A	-6	GLY	-	expression tag	UNP P49902
A	-5	LEU	-	expression tag	UNP P49902
A	-4	VAL	-	expression tag	UNP P49902
A	-3	PRO	-	expression tag	UNP P49902
A	-2	ARG	-	expression tag	UNP P49902
A	-1	GLY	-	expression tag	UNP P49902
A	0	SER	-	expression tag	UNP P49902
B	-18	MET	-	initiating methionine	UNP P49902
B	-17	GLY	-	expression tag	UNP P49902
B	-16	SER	-	expression tag	UNP P49902
B	-15	SER	-	expression tag	UNP P49902
B	-14	HIS	-	expression tag	UNP P49902
B	-13	HIS	-	expression tag	UNP P49902

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP P49902
B	-11	HIS	-	expression tag	UNP P49902
B	-10	HIS	-	expression tag	UNP P49902
B	-9	HIS	-	expression tag	UNP P49902
B	-8	SER	-	expression tag	UNP P49902
B	-7	SER	-	expression tag	UNP P49902
B	-6	GLY	-	expression tag	UNP P49902
B	-5	LEU	-	expression tag	UNP P49902
B	-4	VAL	-	expression tag	UNP P49902
B	-3	PRO	-	expression tag	UNP P49902
B	-2	ARG	-	expression tag	UNP P49902
B	-1	GLY	-	expression tag	UNP P49902
B	0	SER	-	expression tag	UNP P49902

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
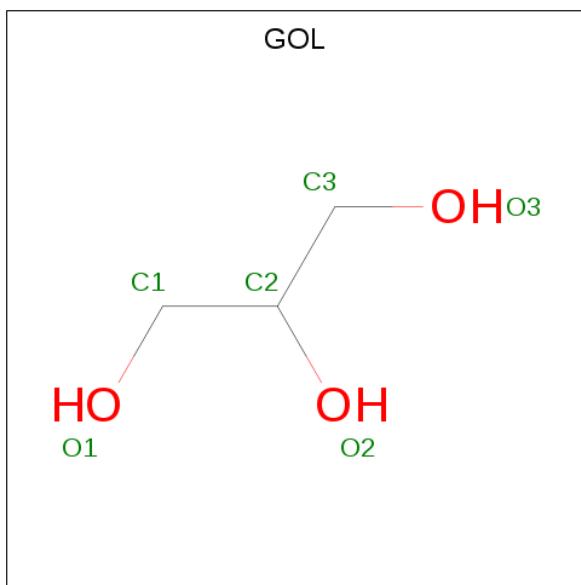
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
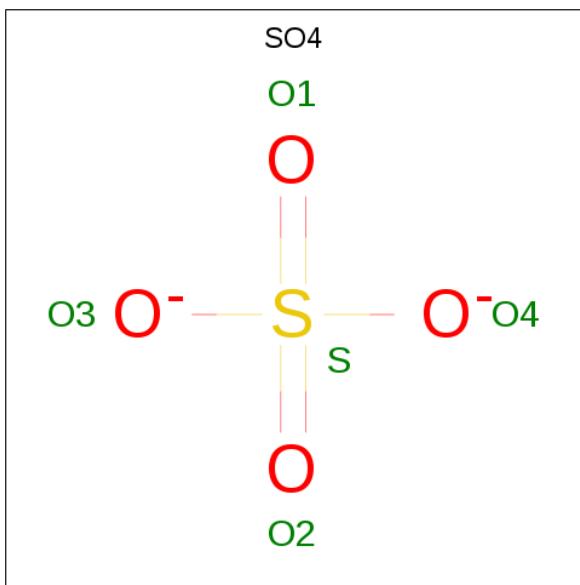
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mg 2	0	0

- Molecule 5 is 1-(biphenyl-3-yl)-1H-imidazole (three-letter code: 53O) (formula: $C_{15}H_{12}N_2$).
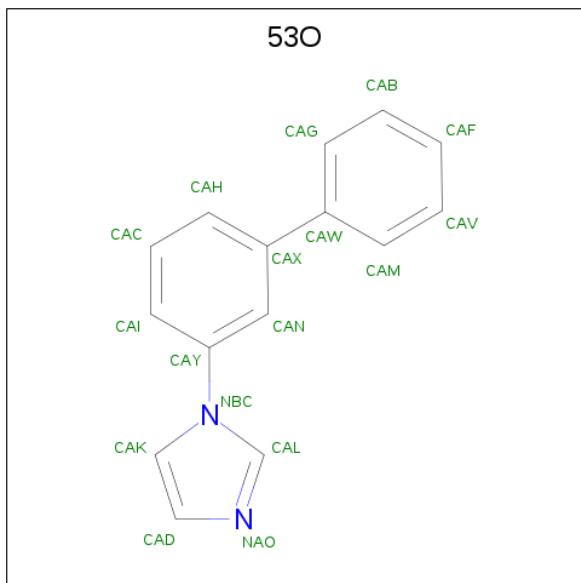
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 17	C 15	N 2	0	0
5	B	1	Total 17	C 15	N 2	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total 44	O 44	0	0
6	B	36	Total 36	O 36	0	0

3 Residue-property plots ⓘ

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: Cytosolic purine 5'-nucleotidase
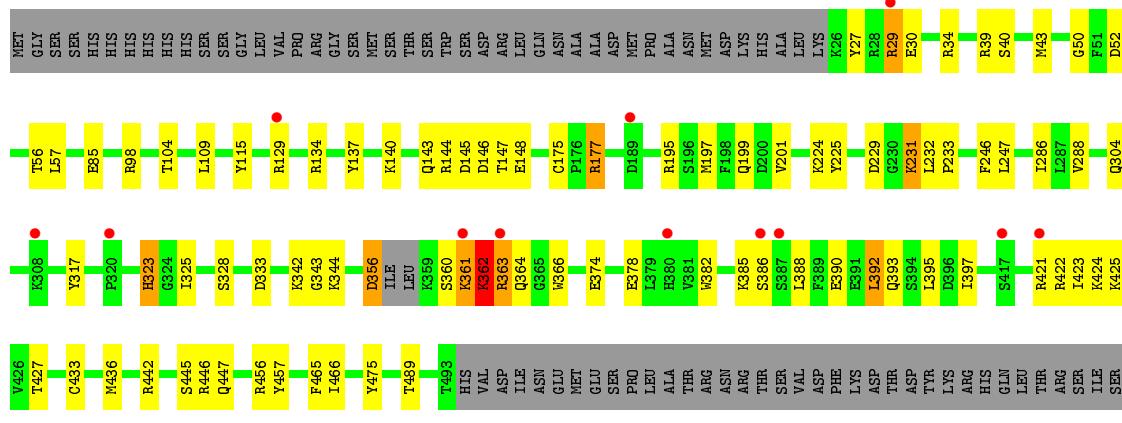
- Molecule 1: Cytosolic purine 5'-nucleotidase
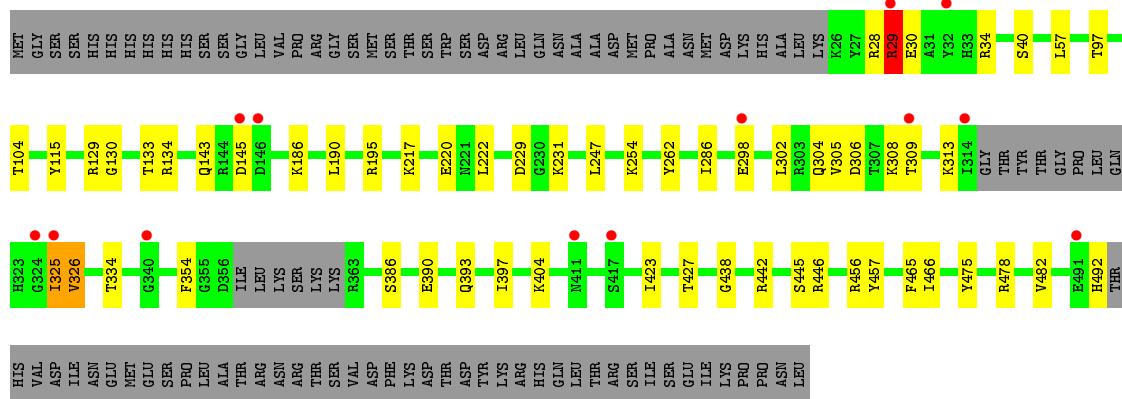
4　Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	143.89Å　　121.98Å　　90.15Å	Depositor
a, b, c, α, β, γ	90.00°　　114.29°　　90.00°	
Resolution (Å)	19.88　–　2.90	Depositor
	19.88　–　2.90	EDS
% Data completeness	98.6 (19.88-2.90)	Depositor
(in resolution range)	98.6 (19.88-2.90)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.14 (at 2.88Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.190　,　0.251	Depositor
	0.190　,　0.251	DCC
R_{free} test set	1548 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 59.7	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	0.92	EDS
Total number of atoms	7702	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 53O, GOL, MG, 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	0.51	0/3908	0.69	0/5278
1	B	0.52	0/3797	0.68	1/5126 (0.0%)
All	All	0.52	0/7705	0.69	1/10404 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	130	GLY	N-CA-C	-6.15	97.72	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	HIS	Peptide

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	3806	0	3740	67	0
1	B	3699	0	3626	45	0
2	A	12	0	16	1	0
2	B	12	0	16	1	0
3	A	35	0	0	2	0
3	B	20	0	0	3	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	17	0	12	5	0
5	B	17	0	12	11	0
6	A	44	0	0	1	0
6	B	36	0	0	0	0
All	All	7702	0	7422	106	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 7.

All (106) 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:446:ARG:HH21	5:B:609:53O:H11	1.27	1.00
5:A:612:53O:H9	1:B:445:SER:H	1.38	0.89
1:A:344:LYS:NZ	3:B:604:SO4:O1	2.08	0.86
1:B:456:ARG:HH21	1:B:457:TYR:HB2	1.47	0.79
1:A:344:LYS:NZ	3:B:604:SO4:S	2.61	0.73
1:A:446:ARG:HE	5:B:609:53O:H10	1.55	0.71
1:A:343:GLY:HA2	1:A:366:TRP:HD1	1.56	0.70
1:B:478:ARG:HH21	5:B:609:53O:H5	1.56	0.68
1:A:144:ARG:NH2	6:A:701:HOH:O	2.22	0.68
1:A:442:ARG:NH1	1:A:445:SER:O	2.24	0.67
1:A:445:SER:OG	5:B:609:53O:H9	1.94	0.67
1:A:360:SER:OG	1:A:361:LYS:N	2.25	0.67
1:B:478:ARG:NH2	5:B:609:53O:H5	2.10	0.65
1:B:29[B]:ARG:HB2	1:B:34:ARG:HG2	1.79	0.64
1:A:115:TYR:CD1	1:B:456:ARG:HG3	2.34	0.63
1:B:134:ARG:NH1	3:B:604:SO4:O4	2.32	0.63
1:B:478:ARG:HH21	5:B:609:53O:H3	1.64	0.62
1:A:343:GLY:HA2	1:A:366:TRP:CD1	2.34	0.62
1:B:386:SER:O	1:B:390:GLU:HG2	2.00	0.61
1:A:386:SER:O	1:A:390:GLU:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:612:53O:H11	1:B:446:ARG:CZ	2.31	0.61
5:A:612:53O:H10	1:B:446:ARG:HG3	1.83	0.60
1:A:85:GLU:OE2	1:A:177:ARG:NH2	2.35	0.59
1:A:247:LEU:HD23	1:A:286:ILE:HG23	1.84	0.59
1:A:342:LYS:HG2	1:A:364:GLN:HB3	1.85	0.59
1:A:356:ASP:OD1	1:A:356:ASP:N	2.36	0.59
1:B:97:THR:HG21	1:B:438:GLY:O	2.03	0.58
1:B:217:LYS:HA	1:B:220:GLU:HG2	1.84	0.58
1:A:446:ARG:HE	5:B:609:53O:CAB	2.15	0.58
1:A:29[B]:ARG:HH11	1:A:34:ARG:HE	1.51	0.58
1:B:305:VAL:HB	1:B:326:VAL:HG12	1.86	0.57
1:B:393:GLN:O	1:B:397:ILE:HG12	2.05	0.56
1:A:229:ASP:OD2	1:A:231:LYS:HG3	2.07	0.55
1:A:143:GLN:OE1	1:A:145:ASP:HB2	2.06	0.55
1:A:361:LYS:HD3	1:A:363:ARG:HH12	1.71	0.55
1:A:39:ARG:HD2	1:B:446:ARG:HH21	1.72	0.54
1:A:140:LYS:NZ	3:A:604:SO4:O1	2.41	0.54
1:A:393:GLN:O	1:A:397:ILE:HG12	2.08	0.54
1:A:195:ARG:NH1	1:A:199:GLN:OE1	2.38	0.54
1:A:57:LEU:HD23	1:A:465:PHE:CZ	2.43	0.53
1:A:447:GLN:NE2	1:B:482:VAL:O	2.36	0.53
1:B:143:GLN:HG3	1:B:145:ASP:HB2	1.90	0.52
1:A:304:GLN:NE2	1:A:325:ILE:HG23	2.24	0.52
1:B:354:PHE:O	1:B:456:ARG:NH2	2.41	0.52
1:A:378:GLU:HB3	2:A:601:GOL:H12	1.91	0.51
1:A:456:ARG:HG3	1:B:115:TYR:CD1	2.45	0.51
1:B:423:ILE:O	1:B:427:THR:HG23	2.10	0.51
1:A:395:LEU:HD21	1:A:422:ARG:HG3	1.93	0.51
1:A:232:LEU:HB3	1:A:233:PRO:HD3	1.93	0.50
1:B:104:THR:HB	1:B:195:ARG:HA	1.92	0.50
1:A:175:CYS:SG	1:A:177:ARG:HG3	2.52	0.50
1:B:302:LEU:HD13	1:B:334:THR:HG21	1.94	0.49
1:A:445:SER:HB3	5:B:609:53O:H7	1.93	0.49
1:A:456:ARG:NH2	1:A:457:TYR:HB2	2.28	0.49
1:B:304:GLN:HG2	1:B:313:LYS:HD2	1.94	0.48
1:A:333:ASP:OD2	1:A:363:ARG:HD3	2.14	0.48
1:B:390:GLU:HA	1:B:393:GLN:HB2	1.95	0.48
1:A:385:LYS:HE3	1:A:388:LEU:HD13	1.97	0.47
1:A:382:TRP:CD2	1:B:492:HIS:HE1	2.33	0.46
1:B:475:TYR:CZ	2:B:602:GOL:H32	2.50	0.46
1:A:385:LYS:HE2	1:A:433:CYS:SG	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HA	1:B:133:THR:OG1	2.16	0.46
1:B:40:SER:HB2	5:B:609:53O:CAM	2.45	0.46
1:A:146:ASP:C	1:A:148:GLU:H	2.19	0.46
1:A:52:ASP:O	1:A:56:THR:HB	2.15	0.46
1:A:134:ARG:HA	1:A:137:TYR:O	2.16	0.46
1:B:306:ASP:OD2	1:B:309:THR:HG23	2.16	0.45
1:A:104:THR:HB	1:A:195:ARG:HA	1.97	0.45
1:A:98:ARG:NE	1:A:374:GLU:OE2	2.33	0.45
1:A:442:ARG:NH2	1:B:482:VAL:O	2.41	0.44
1:A:40:SER:HB2	5:A:612:53O:H8	1.99	0.44
1:A:140:LYS:NZ	3:A:604:SO4:S	2.91	0.44
1:B:229:ASP:OD2	1:B:231:LYS:HE2	2.18	0.44
1:B:30:GLU:O	1:B:34:ARG:HG3	2.17	0.44
1:A:489:THR:CB	1:B:34:ARG:HH12	2.31	0.43
1:B:222:LEU:HD13	1:B:262:TYR:HB2	1.99	0.43
1:A:29[B]:ARG:HB2	1:A:34:ARG:HG2	2.01	0.43
5:B:609:53O:H8	5:B:609:53O:H4	1.66	0.43
1:A:342:LYS:CG	1:A:343:GLY:H	2.31	0.43
1:A:109:LEU:HA	1:A:109:LEU:HD23	1.80	0.43
1:A:288:VAL:O	1:A:328:SER:HA	2.19	0.43
1:A:43:MET:HB2	1:A:475:TYR:O	2.19	0.42
1:B:186:LYS:HA	1:B:190:LEU:O	2.19	0.42
1:B:286:ILE:HG13	1:B:325:ILE:HG21	2.01	0.42
1:B:325:ILE:HG22	1:B:326:VAL:N	2.34	0.42
1:A:423:ILE:O	1:A:427:THR:HG23	2.19	0.42
5:A:612:53O:H4	5:A:612:53O:H8	1.62	0.42
1:A:421:ARG:HA	1:A:424:LYS:HD2	2.00	0.42
1:B:57:LEU:HD23	1:B:465:PHE:CZ	2.54	0.42
1:A:29[B]:ARG:NH1	1:A:34:ARG:HH21	2.17	0.42
1:A:323:HIS:CE1	1:A:325:ILE:O	2.72	0.42
1:A:50:GLY:HA3	1:A:246:PHE:CZ	2.55	0.42
1:A:342:LYS:HG3	1:A:343:GLY:H	1.85	0.42
1:B:247:LEU:HD23	1:B:286:ILE:HG23	2.02	0.42
1:A:197:MET:O	1:A:201:VAL:HG23	2.20	0.41
1:B:28:ARG:HG2	1:B:29[B]:ARG:HH11	1.85	0.41
1:A:361:LYS:O	1:A:363:ARG:N	2.53	0.41
5:B:609:53O:H1	5:B:609:53O:H4	1.65	0.41
1:B:57:LEU:HA	1:B:57:LEU:HD23	1.84	0.41
1:A:29[B]:ARG:HG3	1:A:29[B]:ARG:H	1.53	0.40
1:A:224:LYS:HD3	1:A:225:TYR:CZ	2.57	0.40
1:A:362:LYS:HD2	1:A:362:LYS:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LEU:HD21	1:A:427:THR:HG22	2.03	0.40
1:B:466:ILE:HG23	1:B:466:ILE:HD12	1.77	0.40
1:A:489:THR:HB	1:B:34:ARG:HH12	1.85	0.40
1:A:27:TYR:CG	1:B:404:LYS:HG3	2.56	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	463/555 (83%)	438 (95%)	18 (4%)	7 (2%)	12	39
1	B	448/555 (81%)	430 (96%)	14 (3%)	4 (1%)	20	54
All	All	911/1110 (82%)	868 (95%)	32 (4%)	11 (1%)	18	46

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	TYR
1	A	362	LYS
1	B	29[A]	ARG
1	B	29[B]	ARG
1	B	325	ILE
1	B	326	VAL
1	A	29[A]	ARG
1	A	29[B]	ARG
1	A	129	ARG
1	A	147	THR
1	A	361	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	415/497 (84%)	405 (98%)	10 (2%)	54	84
1	B	403/497 (81%)	397 (98%)	6 (2%)	70	91
All	All	818/994 (82%)	802 (98%)	16 (2%)	64	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	177	ARG
1	A	231	LYS
1	A	356	ASP
1	A	362	LYS
1	A	363	ARG
1	A	392	LEU
1	A	425	LYS
1	A	436	MET
1	A	466	ILE
1	B	29[A]	ARG
1	B	29[B]	ARG
1	B	254	LYS
1	B	298	GLU
1	B	308	LYS
1	B	442	ARG

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

Mol	Chain	Res	Type
1	A	304	GLN
1	A	405	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	GOL	A	601	-	5,5,5	0.38	0	5,5,5	0.21	0
2	GOL	A	602	-	5,5,5	0.41	0	5,5,5	0.36	0
3	SO4	A	603	4	4,4,4	0.20	0	6,6,6	0.14	0
3	SO4	A	604	-	4,4,4	0.17	0	6,6,6	0.35	0
3	SO4	A	605	-	4,4,4	0.25	0	6,6,6	0.20	0
3	SO4	A	606	-	4,4,4	0.31	0	6,6,6	0.15	0
3	SO4	A	607	-	4,4,4	0.36	0	6,6,6	0.40	0
3	SO4	A	608	-	4,4,4	0.23	0	6,6,6	0.24	0
3	SO4	A	609	-	4,4,4	0.20	0	6,6,6	0.30	0
5	53O	A	612	-	18,19,19	2.11	3 (16%)	21,25,25	1.74	5 (23%)
2	GOL	B	601	-	5,5,5	0.44	0	5,5,5	0.83	0
2	GOL	B	602	-	5,5,5	0.41	0	5,5,5	0.29	0
3	SO4	B	603	4	4,4,4	0.25	0	6,6,6	0.51	0
3	SO4	B	604	-	4,4,4	0.18	0	6,6,6	0.29	0
3	SO4	B	605	-	4,4,4	0.25	0	6,6,6	0.27	0
3	SO4	B	606	-	4,4,4	0.19	0	6,6,6	0.18	0
5	53O	B	609	-	18,19,19	2.04	3 (16%)	21,25,25	1.92	5 (23%)

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	GOL	A	601	-	-	0/4/4/4	0/0/0/0
2	GOL	A	602	-	-	0/4/4/4	0/0/0/0
3	SO4	A	603	4	-	0/0/0/0	0/0/0/0
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0
3	SO4	A	605	-	-	0/0/0/0	0/0/0/0
3	SO4	A	606	-	-	0/0/0/0	0/0/0/0
3	SO4	A	607	-	-	0/0/0/0	0/0/0/0
3	SO4	A	608	-	-	0/0/0/0	0/0/0/0
3	SO4	A	609	-	-	0/0/0/0	0/0/0/0
5	53O	A	612	-	-	0/8/8/8	0/3/3/3
2	GOL	B	601	-	-	0/4/4/4	0/0/0/0
2	GOL	B	602	-	-	0/4/4/4	0/0/0/0
3	SO4	B	603	4	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0
3	SO4	B	605	-	-	0/0/0/0	0/0/0/0
3	SO4	B	606	-	-	0/0/0/0	0/0/0/0
5	53O	B	609	-	-	0/8/8/8	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	609	53O	CAY-NBC	-6.49	1.33	1.45
5	A	612	53O	CAY-NBC	-6.31	1.34	1.45
5	A	612	53O	CAK-NBC	-4.23	1.33	1.39
5	A	612	53O	CAX-CAW	-4.06	1.38	1.49
5	B	609	53O	CAK-NBC	-3.81	1.33	1.39
5	B	609	53O	CAX-CAW	-3.78	1.39	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	609	53O	CAK-NBC-CAY	-3.63	120.44	126.33
5	B	609	53O	CAN-CAX-CAW	-3.03	115.74	120.88
5	B	609	53O	CAI-CAY-CAN	-3.01	118.57	121.55
5	B	609	53O	CAN-CAY-NBC	-2.91	115.68	118.85
5	A	612	53O	CAN-CAX-CAW	-2.79	116.16	120.88
5	A	612	53O	CAI-CAY-CAN	-2.57	119.00	121.55
5	A	612	53O	CAN-CAY-NBC	-2.36	116.29	118.85
5	A	612	53O	CAK-NBC-CAY	-2.35	122.52	126.33
5	A	612	53O	CAI-CAY-NBC	4.02	124.58	119.37
5	B	609	53O	CAI-CAY-NBC	4.86	125.68	119.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GOL	1	0
3	A	604	SO4	2	0
5	A	612	53O	5	0
2	B	602	GOL	1	0
3	B	604	SO4	3	0
5	B	609	53O	11	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 (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(Å²)	Q<0.9
1	A	466/555 (83%)	-0.15	12 (2%)	56	51	28, 40, 66, 90	0
1	B	453/555 (81%)	-0.10	13 (2%)	52	46	29, 43, 67, 80	0
All	All	919/1110 (82%)	-0.13	25 (2%)	55	50	28, 42, 67, 90	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	THR	3.7
1	A	361	LYS	3.7
1	A	29[A]	ARG	3.5
1	A	387	SER	3.2
1	A	363	ARG	3.1
1	B	145	ASP	2.8
1	B	314	ILE	2.8
1	B	32	TYR	2.7
1	A	417	SER	2.6
1	B	324	GLY	2.6
1	B	325	ILE	2.5
1	B	29[A]	ARG	2.5
1	B	340	GLY	2.5
1	A	189	ASP	2.5
1	A	129	ARG	2.5
1	B	491	GLU	2.5
1	A	308	LYS	2.3
1	B	411	ASN	2.3
1	A	386	SER	2.2
1	B	417	SER	2.1
1	A	380	HIS	2.1
1	A	320	PRO	2.1
1	B	298	GLU	2.1
1	B	146	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	421	ARG	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	GOL	B	601	6/6	0.98	0.30	6.44	36,38,39,41	0
3	SO4	A	606	5/5	0.93	0.33	4.65	51,52,65,77	0
3	SO4	A	605	5/5	0.93	0.26	4.19	61,63,77,90	0
3	SO4	A	608	5/5	0.95	0.42	4.01	51,54,76,77	0
5	53O	A	612	17/17	0.78	0.30	3.46	59,65,69,69	0
3	SO4	A	609	5/5	0.90	0.41	3.45	70,72,88,97	0
3	SO4	A	607	5/5	0.93	0.26	3.00	61,68,70,92	0
2	GOL	A	601	6/6	0.95	0.26	2.83	42,44,48,48	0
5	53O	B	609	17/17	0.86	0.30	2.79	50,64,69,69	0
3	SO4	B	606	5/5	0.95	0.46	2.44	81,82,100,102	0
3	SO4	B	605	5/5	0.95	0.34	2.38	58,63,72,85	0
4	MG	A	611	1/1	0.92	0.24	1.61	44,44,44,44	0
4	MG	A	610	1/1	0.98	0.18	0.68	28,28,28,28	0
2	GOL	B	602	6/6	0.95	0.25	0.25	41,45,49,53	0
2	GOL	A	602	6/6	0.94	0.20	-0.28	44,46,51,53	0
3	SO4	A	603	5/5	0.99	0.11	-1.25	30,31,36,38	0
3	SO4	B	603	5/5	0.99	0.08	-1.87	36,36,38,43	0
4	MG	B	607	1/1	0.98	0.07	-2.40	28,28,28,28	0
3	SO4	A	604	5/5	0.97	0.20	-	61,70,81,84	0
3	SO4	B	604	5/5	0.97	0.20	-	63,65,75,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	MG	B	608	1/1	0.95	0.30	-	41,41,41,41	0

6.5   Other polymers (i)

There are no such residues in this entry.