WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:37 PM GMT

PDB ID : 4M6P

Title : Identification of Amides Derived From 1H-Pyrazolo[3,4-b]pyridine-5-carboxylic Acid as Potent Inhibitors of Human Nicotinamide Phosphoribosyltransferase (NAMPT)

Authors : Giannetti, A.M.; Zheng, X.; Skelton, N.; Wang, W.; Bravo, B.; Feng, Y.; Gunzner-Toste, J.; Ho, Y.; Hua, R.; Wang, C.; Zhao, Q.; Liederer, B.M.; Liu, Y.; O' Brien, T.; Oeh, J.; Sampath, D.; Shen, Y.; Wang, L.; Wu, H.; Xiao, Y.; Yuen, P.; Zak, M.; Zhao, G.; Dragovich, P.S.

Deposited on : 2013-08-10

Resolution : 1.75 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

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

The reported resolution of this entry is 1.75 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		0.244
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		2.4%
RSRZ outliers		4.8%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
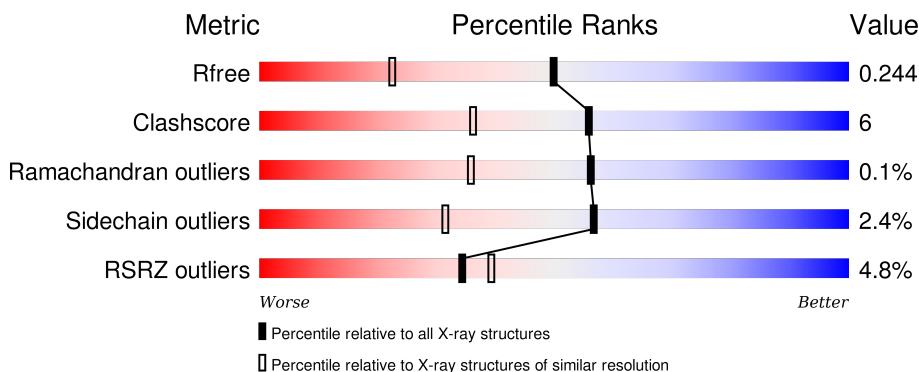
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	501	5% / 82% / 11% / · 6%
1	B	501	4% / 80% / 13% / · 6%
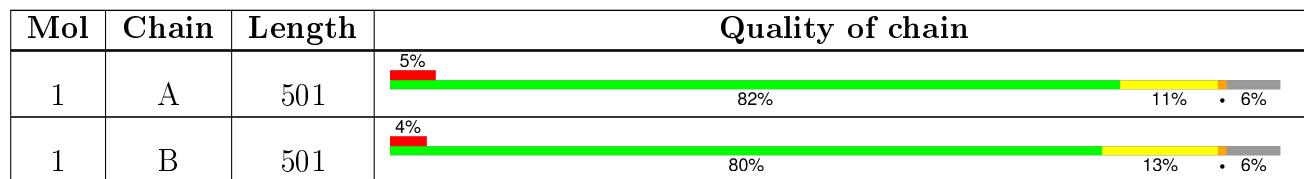
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8808 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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total 3769	C 2424	N 622	O 716	S 7	0	1	0
1	B	471	Total 3773	C 2427	N 622	O 717	S 7	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	492	LEU	-	EXPRESSION TAG	UNP P43490
A	493	GLU	-	EXPRESSION TAG	UNP P43490
A	494	HIS	-	EXPRESSION TAG	UNP P43490
A	495	HIS	-	EXPRESSION TAG	UNP P43490
A	496	HIS	-	EXPRESSION TAG	UNP P43490
A	497	HIS	-	EXPRESSION TAG	UNP P43490
A	498	HIS	-	EXPRESSION TAG	UNP P43490
A	499	HIS	-	EXPRESSION TAG	UNP P43490
A	500	HIS	-	EXPRESSION TAG	UNP P43490
A	501	HIS	-	EXPRESSION TAG	UNP P43490
B	492	LEU	-	EXPRESSION TAG	UNP P43490
B	493	GLU	-	EXPRESSION TAG	UNP P43490
B	494	HIS	-	EXPRESSION TAG	UNP P43490
B	495	HIS	-	EXPRESSION TAG	UNP P43490
B	496	HIS	-	EXPRESSION TAG	UNP P43490
B	497	HIS	-	EXPRESSION TAG	UNP P43490
B	498	HIS	-	EXPRESSION TAG	UNP P43490
B	499	HIS	-	EXPRESSION TAG	UNP P43490
B	500	HIS	-	EXPRESSION TAG	UNP P43490
B	501	HIS	-	EXPRESSION TAG	UNP P43490

- Molecule 2 is N-[4-(PHENYLSULFONYL)BENZYL]-2H-PYRAZOLO[3,4-B]PYRIDINE-5-CARBOXAMIDE (three-letter code: 20R) (formula: $C_{20}H_{16}N_4O_3S$).
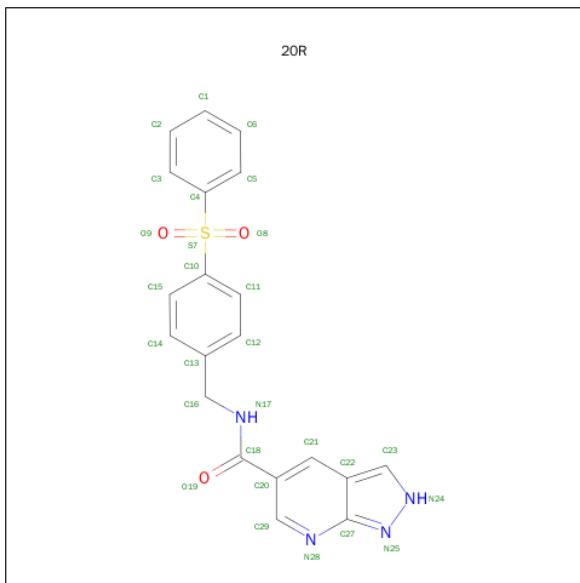
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	20	4	3	1		
2	B	1	Total	C	N	O	S	0	0
			28	20	4	3	1		

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
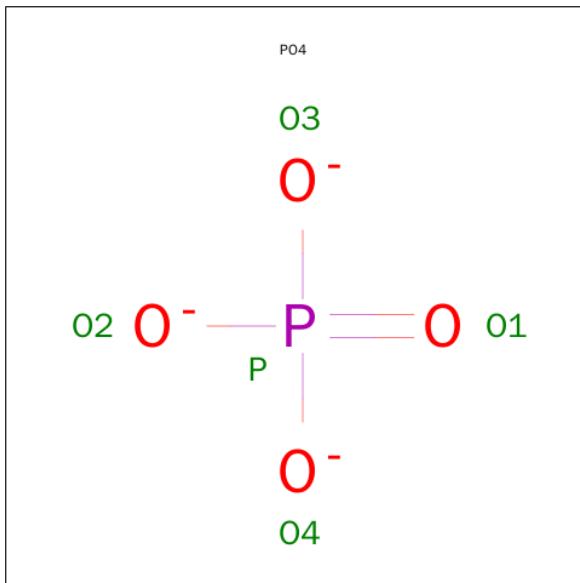
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	601	Total 601	O 601	0	0
4	B	599	Total 599	O 599	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 errors 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: Nicotinamide phosphoribosyltransferase
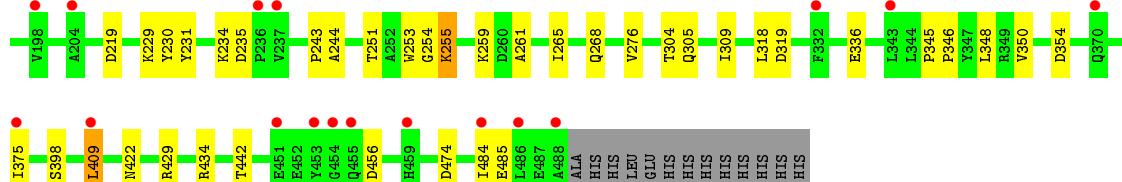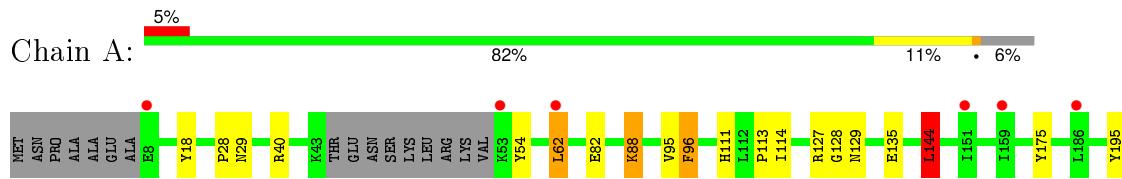
- Molecule 1: Nicotinamide phosphoribosyltransferase
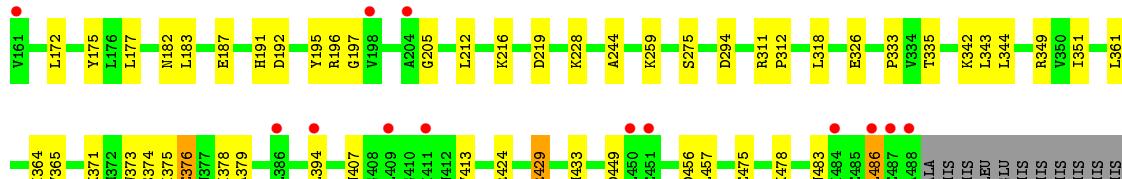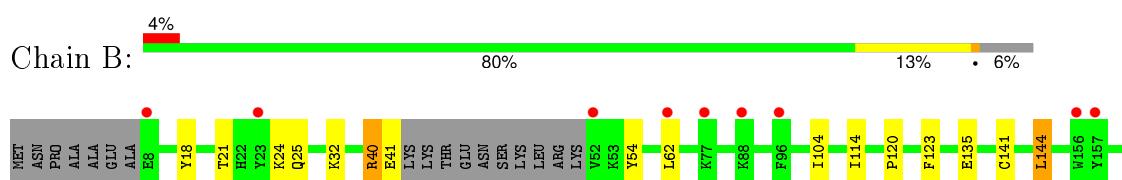
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.63Å 106.36Å 83.11Å 90.00° 96.43° 90.00°	Depositor
Resolution (Å)	46.35 – 1.75 46.35 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.35-1.75) 99.7 (46.35-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.54 (at 1.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.192 , 0.241 0.195 , 0.244	Depositor DCC
R_{free} test set	5259 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	15.4	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	0 of 105479 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8808	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.35% 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, 0.375 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: PO4, 20R

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	0.88	1/3857 (0.0%)	0.85	6/5229 (0.1%)
1	B	0.84	1/3861 (0.0%)	0.84	4/5232 (0.1%)
All	All	0.86	2/7718 (0.0%)	0.85	10/10461 (0.1%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	ARG	CG-CD	-5.45	1.38	1.51
1	B	376	GLU	CB-CG	-5.39	1.42	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	ASP	CB-CG-OD2	7.48	125.03	118.30
1	A	409	LEU	CA-CB-CG	7.42	132.37	115.30
1	B	429	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	127	ARG	CA-CB-CG	-6.75	98.55	113.40
1	A	62	LEU	CB-CG-CD2	6.04	121.28	111.00
1	B	429	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	192	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	144	LEU	CB-CG-CD2	5.59	120.51	111.00
1	B	456	ASP	CB-CG-OD1	5.17	122.96	118.30

Continued on next page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	ASP	CB-CG-OD1	-5.17	113.65	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	ARG	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	3769	0	3730	43	0
1	B	3773	0	3745	51	0
2	A	28	0	16	0	0
2	B	28	0	16	1	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
4	A	601	0	0	25	3
4	B	599	0	0	26	3
All	All	8808	0	7507	94	3

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 6.

All (94) 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:B:343:LEU:HB3	4:B:1162:HOH:O	1.65	0.97
1:B:40:ARG:NH2	4:B:864:HOH:O	2.05	0.88
1:A:40:ARG:HD3	1:A:422:ASN:O	1.75	0.86
1:A:276:VAL:N	4:A:1263:HOH:O	2.11	0.83
1:B:343:LEU:HD13	1:B:376:GLU:HG3	1.59	0.81
1:A:128:GLY:O	4:A:1258:HOH:O	1.99	0.81
1:A:251:THR:O	4:A:1269:HOH:O	2.04	0.76

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:SER:OG	3:A:602:PO4:O3	2.02	0.76
1:B:196:ARG:HG2	4:B:1168:HOH:O	1.85	0.76
1:B:475:GLU:OE1	4:B:1161:HOH:O	2.06	0.73
3:B:602:PO4:O1	4:B:845:HOH:O	2.07	0.72
1:B:343:LEU:CD1	1:B:376:GLU:HG3	2.18	0.72
1:A:135:GLU:OE1	4:A:1255:HOH:O	2.08	0.71
1:B:429:ARG:NH2	1:B:449:ASP:OD2	2.20	0.71
1:A:54:TYR:N	4:A:1064:HOH:O	2.13	0.69
1:A:319:ASP:OD2	4:A:1225:HOH:O	2.10	0.69
1:B:374:SER:OG	1:B:376:GLU:HG2	1.93	0.68
1:A:254:GLY:HA2	1:A:255:LYS:HZ1	1.63	0.64
1:A:309:ILE:O	4:A:1263:HOH:O	2.15	0.63
1:B:433:HIS:HA	1:B:457:LEU:HD13	1.80	0.62
1:A:229:LYS:HG3	1:A:230:TYR:CD1	2.36	0.61
1:A:354:ASP:OD1	4:A:730:HOH:O	2.16	0.59
1:B:182:ASN:O	4:B:1101:HOH:O	2.15	0.58
1:B:373:TRP:O	4:B:1188:HOH:O	2.17	0.58
1:B:335:THR:C	4:B:1162:HOH:O	2.42	0.57
1:A:231:TYR:O	4:A:1295:HOH:O	2.17	0.57
1:B:483:ASN:HA	1:B:486:LEU:HD22	1.85	0.57
1:A:82:GLU:HG2	4:A:1249:HOH:O	2.03	0.57
1:A:345:PRO:O	4:A:1254:HOH:O	2.17	0.56
1:A:350:VAL:O	4:A:1073:HOH:O	2.18	0.56
1:A:304:THR:HG22	1:A:346:PRO:HB2	1.87	0.56
1:B:407:ASN:ND2	4:B:1271:HOH:O	2.39	0.55
1:B:342:LYS:NZ	4:B:978:HOH:O	2.24	0.55
1:A:348:LEU:HB3	4:A:1254:HOH:O	2.05	0.55
1:B:378:ILE:HG13	1:B:379:ALA:N	2.21	0.54
1:B:424:ARG:NH1	4:B:1063:HOH:O	2.40	0.54
1:B:104:ILE:HD11	1:B:141:CYS:SG	2.47	0.54
1:A:255:LYS:HE3	4:A:842:HOH:O	2.08	0.53
1:B:394[B]:LEU:HG	4:B:1157:HOH:O	2.08	0.53
1:A:129:ASN:HA	4:A:1258:HOH:O	2.09	0.53
1:A:235:ASP:OD1	4:A:934:HOH:O	2.19	0.53
1:B:259:LYS:HD2	1:B:294:ASP:HB3	1.91	0.52
1:A:243:PRO:HA	4:B:884:HOH:O	2.09	0.52
1:B:228:LYS:NZ	4:B:1193:HOH:O	2.43	0.52
1:A:336:GLU:OE2	4:A:1182:HOH:O	2.19	0.51
1:A:484:ILE:HD12	1:A:485:GLU:N	2.26	0.51
1:A:268:GLN:OE1	4:A:1078:HOH:O	2.19	0.51
1:A:255:LYS:CD	1:A:255:LYS:H	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLY:N	4:B:1168:HOH:O	2.44	0.49
1:A:429:ARG:NE	4:A:1194:HOH:O	2.46	0.49
1:A:254:GLY:HA2	1:A:255:LYS:NZ	2.26	0.48
1:A:265:ILE:HG12	1:B:25:GLN:HB3	1.95	0.48
1:B:333:PRO:HA	4:B:1229:HOH:O	2.13	0.48
1:A:304:THR:OG1	1:A:305:GLN:OE1	2.24	0.48
1:B:196:ARG:N	4:B:1168:HOH:O	2.47	0.47
1:A:234:LYS:HE3	1:A:474:ASP:OD2	2.15	0.46
1:A:175:TYR:HB3	1:A:375:ILE:HG13	1.98	0.46
1:B:187:GLU:CD	1:B:216:LYS:HD2	2.35	0.46
1:A:305:GLN:HA	4:A:1271:HOH:O	2.15	0.46
1:B:32:LYS:NZ	1:B:135:GLU:OE2	2.37	0.46
1:B:114:ILE:HG12	1:B:144:LEU:HD13	1.98	0.46
1:A:254:GLY:HA2	4:A:1269:HOH:O	2.17	0.45
1:B:191:HIS:CG	2:B:601:20R:H9	2.51	0.45
1:A:442:THR:HB	4:A:1258:HOH:O	2.16	0.45
4:A:1269:HOH:O	1:B:413:VAL:HG12	2.17	0.45
1:A:348:LEU:CB	4:A:1254:HOH:O	2.64	0.44
1:B:172:LEU:HD21	1:B:361:LEU:HD11	2.00	0.44
1:B:205:GLY:HA3	4:B:984:HOH:O	2.17	0.44
1:B:478:LYS:NZ	4:B:1148:HOH:O	2.23	0.44
1:B:374:SER:HG	1:B:376:GLU:HG2	1.81	0.43
1:B:326:GLU:HG2	4:B:918:HOH:O	2.17	0.43
1:B:394[B]:LEU:HD23	1:B:394[B]:LEU:HA	1.89	0.43
1:B:365:VAL:HG12	1:B:375:ILE:HD12	2.00	0.43
1:B:349:ARG:NE	4:B:1257:HOH:O	2.51	0.43
1:B:371:LYS:HE3	4:B:1266:HOH:O	2.18	0.43
1:B:120:PRO:HB2	1:B:123:PHE:CD1	2.55	0.42
1:A:244:ALA:N	4:B:884:HOH:O	2.38	0.42
1:A:114:ILE:HG12	1:A:144:LEU:HD13	2.02	0.42
1:B:40:ARG:O	1:B:41:GLU:HB3	2.20	0.42
1:B:21:THR:OG1	4:B:884:HOH:O	2.01	0.42
1:A:28:PRO:O	1:A:29:ASN:HB2	2.19	0.42
1:B:175:TYR:HB3	1:B:375:ILE:HG13	2.02	0.42
1:B:114:ILE:CG1	1:B:144:LEU:HD13	2.50	0.41
1:A:95:VAL:O	1:A:96:PHE:HB2	2.21	0.41
1:B:312:PRO:HD2	1:B:351:ILE:O	2.21	0.41
1:A:88:LYS:HE3	4:A:1277:HOH:O	2.21	0.41
1:B:54:TYR:CE1	1:B:394[A]:LEU:HD11	2.56	0.41
1:A:253:TRP:CG	1:A:261:ALA:HB2	2.56	0.41
1:A:111:HIS:O	1:A:113:PRO:HD3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LEU:HD13	1:B:364:ILE:HA	2.02	0.40
1:B:24:LYS:NZ	4:B:931:HOH:O	2.51	0.40
1:B:177:LEU:HA	1:B:177:LEU:HD12	1.87	0.40
1:B:244:ALA:CB	1:B:275:SER:HB3	2.50	0.40
1:B:311:ARG:NH1	4:B:1255:HOH:O	2.55	0.40

All (3) 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)
4:A:1198:HOH:O	4:B:1229:HOH:O[1_554]	2.11	0.09
4:A:1274:HOH:O	4:B:1262:HOH:O[2_645]	2.12	0.08
4:A:1252:HOH:O	4:B:1273:HOH:O[2_646]	2.17	0.03

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	469/501 (94%)	459 (98%)	9 (2%)	1 (0%)	52	32
1	B	468/501 (93%)	455 (97%)	13 (3%)	0	100	100
All	All	937/1002 (94%)	914 (98%)	22 (2%)	1 (0%)	56	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PHE

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	412/440 (94%)	401 (97%)	11 (3%)	52	27
1	B	414/440 (94%)	405 (98%)	9 (2%)	60	35
All	All	826/880 (94%)	806 (98%)	20 (2%)	57	31

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	62	LEU
1	A	88	LYS
1	A	144	LEU
1	A	195	TYR
1	A	219	ASP
1	A	255	LYS
1	A	259	LYS
1	A	318	LEU
1	A	409	LEU
1	A	434	ARG
1	B	18	TYR
1	B	62	LEU
1	B	144	LEU
1	B	183	LEU
1	B	195	TYR
1	B	212	LEU
1	B	219	ASP
1	B	344	LEU
1	B	486	LEU

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	483	ASN
1	B	483	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	20R	A	601	-	31,31,31	1.07	1 (3%)	39,44,44	1.97	8 (20%)
3	PO4	A	602	-	4,4,4	0.40	0	6,6,6	0.33	0
2	20R	B	601	-	31,31,31	1.09	3 (9%)	39,44,44	2.25	10 (25%)
3	PO4	B	602	-	4,4,4	0.29	0	6,6,6	0.28	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	20R	A	601	-	-	0/21/21/21	0/4/4/4
3	PO4	A	602	-	-	0/0/0/0	0/0/0/0
2	20R	B	601	-	-	0/21/21/21	0/4/4/4
3	PO4	B	602	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	20R	C27-N28	-3.37	1.31	1.37
2	B	601	20R	C27-N28	-3.12	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	20R	C23-C22	2.24	1.45	1.40
2	B	601	20R	C21-C20	2.31	1.41	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	20R	C20-C29-N28	-6.91	119.79	125.26
2	B	601	20R	O8-S7-C4	-5.52	101.85	107.96
2	A	601	20R	C20-C29-N28	-5.24	121.11	125.26
2	A	601	20R	O8-S7-C4	-3.88	103.66	107.96
2	A	601	20R	C16-N17-C18	-3.24	113.38	121.84
2	B	601	20R	C15-C10-C11	-2.41	117.19	120.42
2	B	601	20R	C10-S7-C4	-2.33	100.39	104.47
2	A	601	20R	C20-C21-C22	-2.10	117.10	121.19
2	B	601	20R	C22-C23-N24	-2.09	106.19	111.38
2	B	601	20R	O8-S7-O9	2.28	122.55	119.15
2	A	601	20R	C5-C4-S7	2.49	123.09	119.58
2	B	601	20R	C14-C15-C10	2.71	122.47	119.48
2	A	601	20R	C29-N28-C27	3.86	121.47	116.93
2	B	601	20R	O8-S7-C10	3.95	112.34	107.96
2	A	601	20R	C21-C20-C29	4.09	120.44	116.57
2	B	601	20R	C21-C20-C29	4.34	120.68	116.57
2	B	601	20R	C29-N28-C27	4.65	122.41	116.93
2	A	601	20R	O9-S7-C10	4.89	113.38	107.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	PO4	1	0
2	B	601	20R	1	0
3	B	602	PO4	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 (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	472/501 (94%)	0.64	23 (4%)	33	38	6, 15, 29, 51	0
1	B	471/501 (94%)	0.65	22 (4%)	35	40	6, 14, 29, 66	0
All	All	943/1002 (94%)	0.64	45 (4%)	34	39	6, 14, 29, 66	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	VAL	6.9
1	A	53	LYS	4.8
1	B	486	LEU	4.6
1	A	486	LEU	4.5
1	A	488	ALA	3.7
1	A	484	ILE	3.7
1	B	409	LEU	3.6
1	B	488	ALA	3.6
1	B	394[A]	LEU	3.3
1	A	459	HIS	3.3
1	B	487	GLU	3.2
1	A	236	PRO	3.2
1	B	62	LEU	3.0
1	B	88	LYS	2.9
1	A	409	LEU	2.9
1	A	237	VAL	2.9
1	A	453	TYR	2.7
1	A	454	GLY	2.6
1	B	77	LYS	2.5
1	A	343	LEU	2.4
1	B	411	ILE	2.4
1	A	451	GLU	2.4
1	A	370	GLN	2.4
1	B	484	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	157	TYR	2.3
1	B	450	LEU	2.3
1	B	451	GLU	2.3
1	A	332	PHE	2.3
1	B	161	VAL	2.3
1	A	8	GLU	2.2
1	A	62	LEU	2.2
1	B	386	LEU	2.2
1	A	375	ILE	2.2
1	B	23	TYR	2.2
1	A	151	ILE	2.2
1	A	159	ILE	2.2
1	B	156	TRP	2.2
1	A	204	ALA	2.2
1	B	204	ALA	2.1
1	A	455	GLN	2.1
1	A	198	VAL	2.1
1	B	198	VAL	2.1
1	B	96	PHE	2.0
1	B	8	GLU	2.0
1	A	186	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
3	PO4	A	602	5/5	0.82	0.16	1.05	32,33,43,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PO4	B	602	5/5	0.86	0.14	0.67	26,34,36,42	0
2	20R	A	601	28/28	0.93	0.12	0.12	6,16,21,25	0
2	20R	B	601	28/28	0.93	0.12	-0.14	7,14,27,29	0

6.5 Other polymers (i)

There are no such residues in this entry.