



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:31 AM GMT

PDB ID : 2HHA
Title : The structure of DPP4 in complex with an oxadiazole inhibitor
Authors : Scapin, G.
Deposited on : 2006-06-28
Resolution : 2.35 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

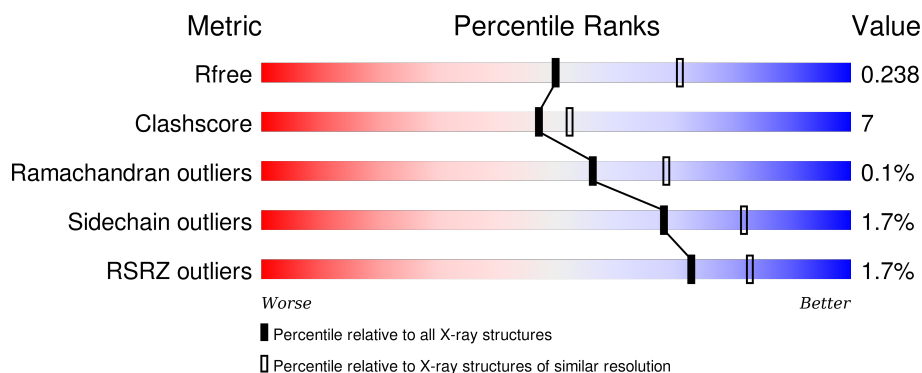
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	728	<div> <div></div> <div>84%</div> <div>15%</div> <div></div> </div>
1	B	728	<div> <div></div> <div>82%</div> <div>17%</div> <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
3	NAG	A	1520	-	-	-	X
3	NAG	B	2321	-	-	-	X
5	NAG	A	1220	-	-	-	X
5	NAG	A	1321	-	-	-	X
5	NAG	B	2219	-	-	-	X
5	NAG	B	2281	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13209 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 Hypothetical protein DPP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	B	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	THR	SER	ENGINEERED	UNP Q53TN1
B	39	THR	SER	ENGINEERED	UNP Q53TN1

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		

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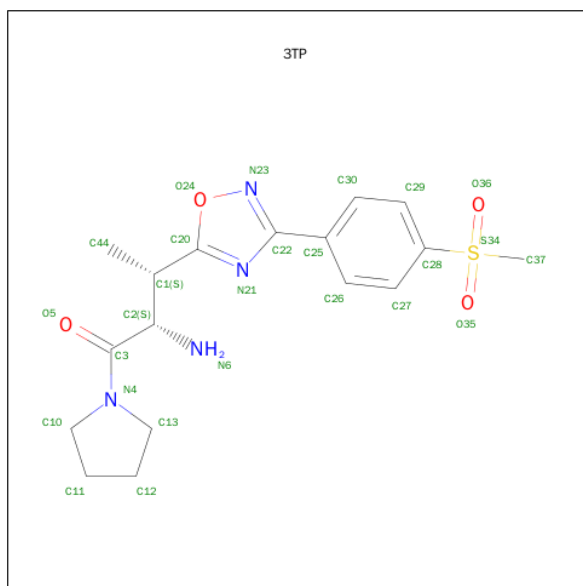
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is (2S,3S)-3-{3-[4-(METHYLSULFONYL)PHENYL]-1,2,4-OXADIAZOL-5-YL}-1-OXO-1-PYRROLIDIN-1-YLBUTAN-2-AMINE (three-letter code: 3TP) (formula: C₁₇H₂₂N₄O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			26	17	4	4	1		
7	B	1	Total	C	N	O	S	0	0
			26	17	4	4	1		

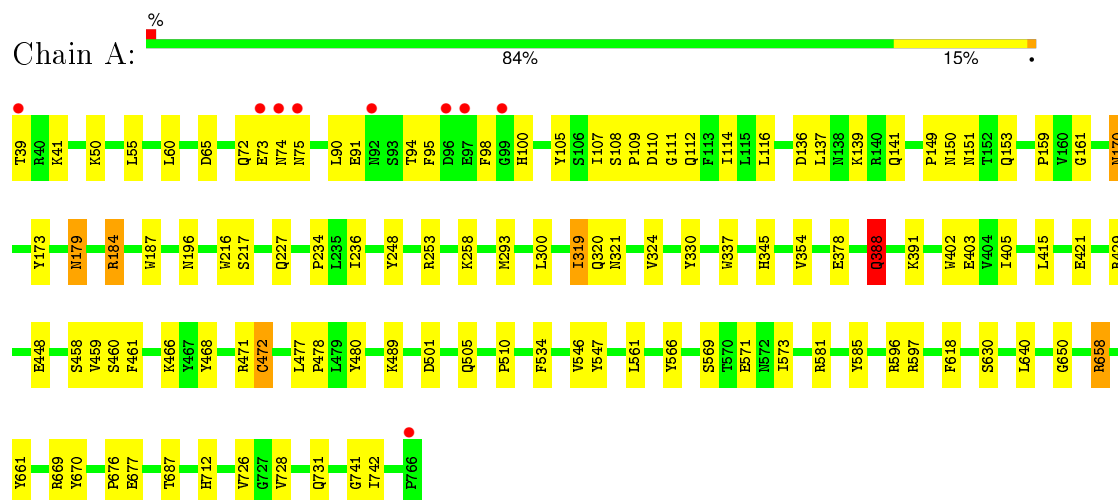
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	442	Total 442	O 442	0	0
8	B	448	Total 448	O 448	0	0

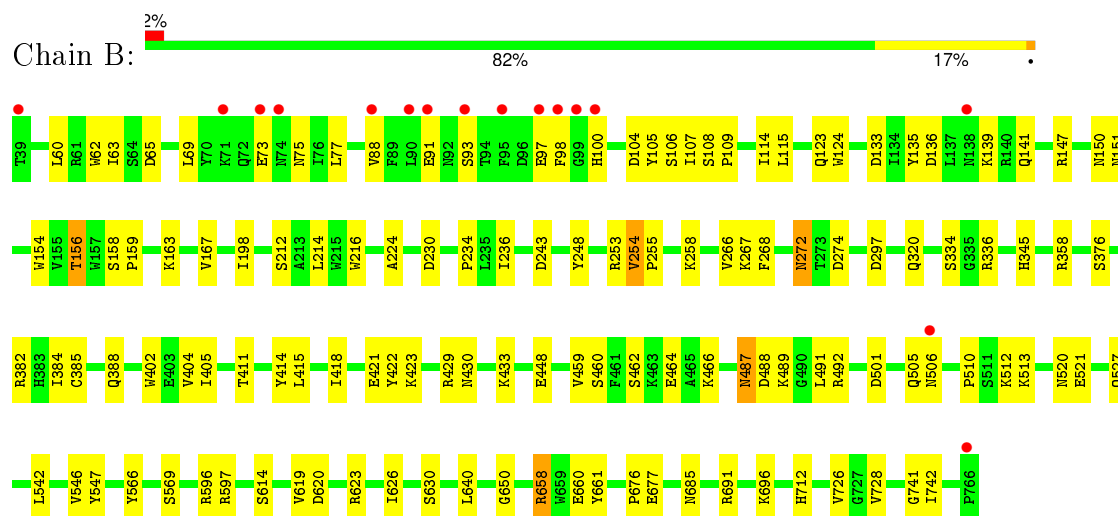
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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: Hypothetical protein DPP4



• Molecule 1: Hypothetical protein DPP4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.97Å 125.58Å 136.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35 43.05 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-2.35) 99.1 (43.05-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.185 , 0.233 0.192 , 0.238	Depositor DCC
R_{free} test set	4262 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.3	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 83919 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13209	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 3TP, NAG, NDG

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	0.47	0/6137	0.69	4/8346 (0.0%)
1	B	0.48	0/6137	0.68	1/8346 (0.0%)
All	All	0.48	0/12274	0.68	5/16692 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	GLN	N-CA-C	-5.58	95.93	111.00
1	A	458	SER	N-CA-C	-5.13	97.16	111.00
1	A	388	GLN	N-CA-C	-5.06	97.34	111.00
1	A	300	LEU	N-CA-C	-5.05	97.38	111.00
1	A	319	ILE	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5965	0	5677	82	0
1	B	5965	0	5679	98	0
2	A	56	0	50	2	0
3	A	42	0	39	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	0	39	6	0
4	A	28	0	25	3	0
5	A	56	0	50	1	0
5	B	112	0	100	2	0
6	A	1	0	0	0	0
7	A	26	0	22	1	0
7	B	26	0	22	1	0
8	A	442	0	0	5	0
8	B	448	0	0	7	0
All	All	13209	0	11703	180	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 (180) 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:149:PRO:HA	4:A:1150:NDG:H8C1	1.40	1.04
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.01	0.90
1:B:139:LYS:HB3	1:B:141:GLN:HE21	1.46	0.81
5:B:2085:NAG:H4	5:B:2086:NAG:N2	1.94	0.81
1:B:75:ASN:HD21	3:B:2092:NAG:HN2	1.30	0.78
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.20	0.75
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.69	0.73
1:A:676:PRO:HG2	1:A:677:GLU:OE2	1.90	0.72
1:A:596:ARG:O	1:A:597:ARG:HD2	1.89	0.72
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.55	0.71
1:A:581:ARG:CZ	3:A:1520:NAG:H62	2.21	0.71
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.74	0.69
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.72	0.69
1:A:173:TYR:CE2	1:A:184:ARG:HG2	2.27	0.69
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.84	0.69
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.85	0.68
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.76	0.67
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.77	0.67
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.92	0.67
1:B:620:ASP:OD2	1:B:623:ARG:HD3	1.95	0.66
1:B:597:ARG:HG2	8:B:2701:HOH:O	1.95	0.66
1:A:258:LYS:NZ	1:A:712:HIS:HD2	1.92	0.65
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.31	0.65
1:A:149:PRO:HA	4:A:1150:NDG:C8	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ARG:NH1	3:A:1520:NAG:H62	2.12	0.65
1:B:272:ASN:C	1:B:272:ASN:HD22	2.00	0.64
1:A:65:ASP:OD2	1:A:466:LYS:HB2	1.98	0.64
1:A:170:ASN:N	1:A:170:ASN:HD22	1.96	0.63
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.79	0.63
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.28	0.63
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.96	0.63
1:A:184:ARG:NH1	1:A:187:TRP:HA	2.14	0.62
1:B:691:ARG:HD2	8:B:2335:HOH:O	2.00	0.61
1:A:184:ARG:HH11	1:A:187:TRP:HA	1.66	0.61
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.36	0.60
1:B:676:PRO:HG2	1:B:677:GLU:OE2	2.01	0.60
1:B:596:ARG:O	1:B:597:ARG:HD2	2.03	0.59
1:B:139:LYS:HE2	1:B:141:GLN:NE2	2.18	0.58
1:B:422:TYR:CE2	1:B:423:LYS:HE2	2.39	0.58
1:A:630:SER:OG	7:A:1000:3TP:H13	2.03	0.58
1:A:345:HIS:HE1	1:A:391:LYS:O	1.87	0.57
2:A:1230:NDG:O7	2:A:1230:NDG:H3	2.05	0.57
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.86	0.57
1:B:487:ASN:C	1:B:487:ASN:HD22	2.08	0.56
1:A:107:ILE:HG22	1:A:108:SER:O	2.06	0.56
1:B:75:ASN:ND2	3:B:2092:NAG:HN2	2.02	0.56
5:B:2085:NAG:H4	5:B:2086:NAG:HN2	1.71	0.56
1:B:109:PRO:HG2	1:B:158:SER:O	2.06	0.56
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.52	0.55
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.36	0.55
1:A:75:ASN:HD21	3:A:1092:NAG:HN2	1.54	0.55
1:A:489:LYS:HE3	8:A:3219:HOH:O	2.07	0.54
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.07	0.54
1:B:266:VAL:HG22	1:B:267:LYS:N	2.22	0.54
1:B:156:THR:HG21	1:B:214:LEU:HD11	1.90	0.54
1:A:150:ASN:O	1:A:151:ASN:HB2	2.08	0.54
1:A:258:LYS:HZ3	1:A:712:HIS:CD2	2.26	0.53
2:A:1229:NAG:H61	2:A:1230:NDG:O	2.08	0.53
1:A:571:GLU:HB2	1:A:573:ILE:HD12	1.89	0.53
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.89	0.53
1:B:60:LEU:HD12	1:B:60:LEU:C	2.29	0.53
1:B:91:GLU:HG3	1:B:93:SER:H	1.74	0.52
1:B:62:TRP:CG	1:B:462:SER:HA	2.45	0.52
1:A:136:ASP:CG	1:A:139:LYS:HG2	2.29	0.52
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:HD23	1:B:88:VAL:HA	1.93	0.51
1:B:147:ARG:HE	3:B:2150:NAG:H83	1.76	0.51
1:A:459:VAL:HG22	1:A:460:SER:N	2.26	0.50
1:A:41:LYS:HD2	8:A:3227:HOH:O	2.11	0.50
1:A:258:LYS:HZ3	1:A:712:HIS:HD2	1.54	0.50
1:B:258:LYS:HZ3	1:B:712:HIS:CD2	2.30	0.50
1:B:158:SER:HB3	1:B:163:LYS:HB2	1.93	0.50
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.93	0.50
1:B:150:ASN:O	1:B:151:ASN:HB2	2.12	0.50
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.41	0.49
1:B:542:LEU:HD23	1:B:542:LEU:C	2.33	0.49
1:B:405:ILE:HG13	1:B:429:ARG:CD	2.41	0.49
1:A:153:GLN:HE22	1:A:170:ASN:HD21	1.60	0.49
1:B:501:ASP:O	1:B:505:GLN:HG2	2.12	0.49
1:B:334:SER:O	1:B:336:ARG:HG2	2.13	0.49
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.48	0.48
1:B:487:ASN:ND2	1:B:489:LYS:H	2.11	0.48
1:B:741:GLY:O	1:B:742:ILE:C	2.51	0.48
1:B:98:PHE:CD2	1:B:100:HIS:HB2	2.48	0.48
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.49	0.48
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.96	0.48
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.14	0.47
1:B:411:THR:HG21	8:B:2764:HOH:O	2.13	0.47
1:B:345:HIS:HD2	8:B:2377:HOH:O	1.97	0.47
1:B:107:ILE:HD12	1:B:107:ILE:N	2.30	0.47
1:B:236:ILE:CG2	1:B:254:VAL:HG13	2.45	0.47
1:B:658:ARG:HD2	1:B:661:TYR:CE1	2.50	0.46
1:A:388:GLN:HB3	1:A:391:LYS:HB2	1.96	0.46
1:B:107:ILE:HG22	1:B:108:SER:O	2.15	0.46
1:B:487:ASN:HD22	1:B:488:ASP:N	2.13	0.46
1:A:60:LEU:HD12	1:A:60:LEU:C	2.35	0.46
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.97	0.46
1:A:330:TYR:CE2	5:A:1220:NAG:H83	2.50	0.46
1:B:546:VAL:CG2	1:B:547:TYR:N	2.79	0.46
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.51	0.46
1:A:415:LEU:HD23	1:A:415:LEU:C	2.36	0.46
1:A:293:MET:CE	1:A:324:VAL:HG23	2.45	0.46
1:B:358:ARG:HD2	8:B:2546:HOH:O	2.15	0.46
1:B:136:ASP:OD2	1:B:139:LYS:HD3	2.17	0.45
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.99	0.45
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:GLY:O	1:A:742:ILE:C	2.55	0.45
1:A:109:PRO:HD2	1:A:161:GLY:O	2.17	0.45
1:A:184:ARG:HD2	1:A:187:TRP:CE2	2.52	0.45
1:B:415:LEU:HD23	1:B:415:LEU:C	2.36	0.45
1:A:111:GLY:O	1:A:137:LEU:HD12	2.17	0.45
1:B:62:TRP:CD2	1:B:462:SER:HA	2.52	0.44
1:B:513:LYS:O	1:B:527:GLN:HA	2.17	0.44
1:B:123:GLN:HG2	1:B:124:TRP:N	2.33	0.44
1:B:65:ASP:CG	1:B:464:GLU:HB2	2.38	0.44
1:B:266:VAL:CG2	1:B:267:LYS:N	2.80	0.44
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.52	0.44
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.99	0.44
1:A:90:LEU:HD21	1:A:95:PHE:HE2	1.82	0.44
1:A:405:ILE:HG13	1:A:429:ARG:CD	2.48	0.44
1:B:158:SER:CB	1:B:163:LYS:HB2	2.48	0.43
1:B:167:VAL:HG21	1:B:198:ILE:HG23	2.00	0.43
1:A:110:ASP:OD2	1:A:112:GLN:HB2	2.18	0.43
1:A:91:GLU:HB2	1:A:94:THR:OG1	2.18	0.43
1:B:254:VAL:HA	1:B:255:PRO:HD3	1.91	0.43
1:B:75:ASN:HD21	3:B:2092:NAG:C1	2.31	0.43
1:A:731:GLN:NE2	8:A:3166:HOH:O	2.51	0.43
1:A:72:GLN:O	1:A:73:GLU:HB2	2.18	0.43
1:A:159:PRO:CD	1:A:216:TRP:HB3	2.47	0.43
1:B:60:LEU:HD12	1:B:60:LEU:O	2.17	0.43
1:B:418:ILE:HA	1:B:430:ASN:O	2.19	0.43
1:B:546:VAL:HG22	1:B:547:TYR:N	2.33	0.43
1:A:95:PHE:CE1	1:A:116:LEU:HD11	2.53	0.43
1:A:55:LEU:CD1	1:A:561:LEU:HD12	2.49	0.43
1:A:501:ASP:O	1:A:505:GLN:HG3	2.18	0.42
1:B:512:LYS:HD3	8:B:2717:HOH:O	2.18	0.42
1:B:614:SER:HA	1:B:619:VAL:HB	2.00	0.42
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.54	0.42
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.54	0.42
1:B:459:VAL:HG22	1:B:460:SER:N	2.34	0.42
1:A:159:PRO:HG3	1:A:217:SER:O	2.19	0.42
1:B:520:ASN:O	1:B:521:GLU:HB2	2.19	0.42
1:A:378:GLU:HG2	8:A:3051:HOH:O	2.18	0.42
1:B:658:ARG:HG2	1:B:661:TYR:CZ	2.55	0.42
1:A:546:VAL:CG2	1:A:547:TYR:N	2.82	0.42
1:B:658:ARG:HG3	1:B:658:ARG:O	2.19	0.42
1:A:546:VAL:HG22	1:A:547:TYR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.53	0.42
1:A:677:GLU:CD	1:A:677:GLU:H	2.23	0.42
4:A:1150:NDG:H4	4:A:1151:NAG:H2	1.67	0.42
1:A:534:PHE:HZ	1:A:618:PHE:CG	2.38	0.42
1:B:104:ASP:OD1	1:B:105:TYR:N	2.51	0.42
1:B:65:ASP:OD1	1:B:464:GLU:N	2.42	0.42
1:B:658:ARG:HD3	1:B:660:GLU:HB2	2.02	0.41
1:B:297:ASP:HB3	8:B:2437:HOH:O	2.20	0.41
1:B:491:LEU:O	1:B:492:ARG:HB3	2.20	0.41
1:B:384:ILE:HG13	1:B:404:VAL:HG21	2.01	0.41
1:B:630:SER:OG	7:B:2000:3TP:H13	2.20	0.41
1:B:63:ILE:HG21	1:B:69:LEU:HG	2.02	0.41
1:A:73:GLU:O	1:A:74:ASN:HB2	2.20	0.41
1:B:272:ASN:HD22	1:B:274:ASP:H	1.67	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.20	0.41
1:A:50:LYS:HA	1:A:50:LYS:HD3	1.86	0.41
1:A:184:ARG:HD2	1:A:187:TRP:CD2	2.56	0.41
1:B:73:GLU:HB3	3:B:2092:NAG:H3	2.02	0.41
1:A:330:TYR:HB2	1:A:337:TRP:CH2	2.55	0.41
1:B:73:GLU:O	3:B:2092:NAG:H5	2.20	0.41
1:A:477:LEU:HD12	1:A:501:ASP:HB2	2.03	0.41
1:A:139:LYS:HG3	1:A:141:GLN:HB3	2.03	0.41
1:B:414:TYR:CE2	1:B:433:LYS:HE2	2.56	0.41
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.21	0.41
1:A:179:ASN:H	1:A:179:ASN:HD22	1.69	0.41
1:A:319:ILE:HG12	8:A:3211:HOH:O	2.21	0.41
1:A:321:ASN:HA	1:A:354:VAL:HG23	2.02	0.40
1:B:133:ASP:OD1	1:B:147:ARG:NH1	2.54	0.40
1:A:471:ARG:HD2	1:A:480:TYR:CE2	2.57	0.40
1:B:272:ASN:ND2	1:B:274:ASP:H	2.20	0.40
1:A:472:CYS:O	1:A:478:PRO:HA	2.21	0.40
1:B:376:SER:HA	1:B:382:ARG:HA	2.04	0.40
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.57	0.40

There are no symmetry-related clashes.

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	726/728 (100%)	692 (95%)	33 (4%)	1 (0%)	56	69
1	B	726/728 (100%)	693 (96%)	32 (4%)	1 (0%)	56	69
All	All	1452/1456 (100%)	1385 (95%)	65 (4%)	2 (0%)	56	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	320	GLN
1	A	320	GLN

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	653/653 (100%)	644 (99%)	9 (1%)	74	86
1	B	653/653 (100%)	640 (98%)	13 (2%)	63	77
All	All	1306/1306 (100%)	1284 (98%)	22 (2%)	68	82

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	170	ASN
1	A	179	ASN
1	A	184	ARG

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Mol	Chain	Res	Type
1	A	388	GLN
1	A	448	GLU
1	A	472	CYS
1	A	566	TYR
1	A	658	ARG
1	B	97	GLU
1	B	156	THR
1	B	230	ASP
1	B	243	ASP
1	B	254	VAL
1	B	272	ASN
1	B	385	CYS
1	B	448	GLU
1	B	487	ASN
1	B	506	ASN
1	B	566	TYR
1	B	658	ARG
1	B	685	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	170	ASN
1	A	179	ASN
1	A	345	HIS
1	A	505	GLN
1	A	572	ASN
1	A	712	HIS
1	A	731	GLN
1	B	66	HIS
1	B	74	ASN
1	B	75	ASN
1	B	141	GLN
1	B	169	ASN
1	B	272	ASN
1	B	345	HIS
1	B	487	ASN
1	B	533	HIS
1	B	572	ASN
1	B	712	HIS
1	B	731	GLN

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 ⓘ

18 carbohydrates 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	NAG	A	1085	1,2	14,14,15	1.02	1 (7%)	15,19,21	1.71	3 (20%)
2	NDG	A	1086	2	14,14,15	0.93	1 (7%)	15,19,21	0.94	2 (13%)
4	NDG	A	1150	1,4	14,14,15	0.79	1 (7%)	15,19,21	0.88	0
4	NAG	A	1151	4	14,14,15	0.90	1 (7%)	15,19,21	0.74	0
5	NAG	A	1219	1,5	14,14,15	0.59	0	15,19,21	0.65	0
5	NAG	A	1220	5	14,14,15	0.79	0	15,19,21	0.86	1 (6%)
2	NAG	A	1229	1,2	14,14,15	0.73	0	15,19,21	1.03	1 (6%)
2	NDG	A	1230	2	14,14,15	0.71	0	15,19,21	0.75	1 (6%)
5	NAG	A	1321	1,5	14,14,15	0.71	0	15,19,21	0.99	1 (6%)
5	NAG	A	1322	5	14,14,15	0.67	0	15,19,21	0.64	0
5	NAG	B	2085	1,5	14,14,15	0.77	0	15,19,21	0.70	0
5	NAG	B	2086	5	14,14,15	1.08	1 (7%)	15,19,21	0.62	0
5	NAG	B	2219	1,5	14,14,15	0.50	0	15,19,21	0.62	0
5	NAG	B	2220	5	14,14,15	0.61	0	15,19,21	0.85	0
5	NAG	B	2229	1,5	14,14,15	0.52	0	15,19,21	0.88	1 (6%)
5	NAG	B	2230	5	14,14,15	0.62	0	15,19,21	0.66	0
5	NAG	B	2281	1,5	14,14,15	0.52	0	15,19,21	1.06	2 (13%)
5	NAG	B	2282	5	14,14,15	0.70	0	15,19,21	0.87	1 (6%)

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	NAG	A	1085	1,2	-	0/6/23/26	0/1/1/1
2	NDG	A	1086	2	-	0/6/23/26	0/1/1/1
4	NDG	A	1150	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1151	4	-	0/6/23/26	0/1/1/1
5	NAG	A	1219	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1220	5	-	0/6/23/26	0/1/1/1
2	NAG	A	1229	1,2	-	0/6/23/26	0/1/1/1
2	NDG	A	1230	2	-	0/6/23/26	0/1/1/1
5	NAG	A	1321	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1322	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2085	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2086	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2219	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2220	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2229	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2230	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2281	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2282	5	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1150	NDG	C1-C2	2.11	1.55	1.52
2	A	1086	NDG	C4-C5	2.21	1.57	1.53
4	A	1151	NAG	C1-C2	2.34	1.55	1.52
5	B	2086	NAG	C1-C2	2.91	1.56	1.52
2	A	1085	NAG	C1-C2	3.22	1.56	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1085	NAG	C4-C3-C2	-4.96	103.52	111.23
5	A	1321	NAG	C2-N2-C7	-2.74	119.51	123.04
2	A	1229	NAG	C2-N2-C7	-2.71	119.55	123.04
5	B	2281	NAG	C2-N2-C7	-2.67	119.60	123.04
5	B	2229	NAG	C2-N2-C7	-2.52	119.80	123.04
2	A	1085	NAG	C2-N2-C7	-2.47	119.86	123.04
2	A	1086	NDG	C2-N2-C7	-2.28	120.11	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2282	NAG	C2-N2-C7	-2.25	120.15	123.04
5	B	2281	NAG	C4-C3-C2	-2.20	107.80	111.23
2	A	1230	NDG	C2-N2-C7	-2.19	120.23	123.04
5	A	1220	NAG	C2-N2-C7	-2.04	120.42	123.04
2	A	1085	NAG	C1-O5-C5	2.09	114.90	112.25
2	A	1086	NDG	C3-C4-C5	2.16	113.97	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1150	NDG	3	0
4	A	1151	NAG	1	0
5	A	1220	NAG	1	0
2	A	1229	NAG	1	0
2	A	1230	NDG	2	0
5	B	2085	NAG	2	0
5	B	2086	NAG	2	0

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
7	3TP	A	1000	-	21,28,28	2.94	6 (28%)	29,41,41	1.28	4 (13%)
3	NAG	A	1092	1	14,14,15	0.98	1 (7%)	15,19,21	0.81	0
3	NAG	A	1281	1	14,14,15	0.90	1 (7%)	15,19,21	0.86	1 (6%)
3	NAG	A	1520	1	14,14,15	0.82	0	15,19,21	0.83	0
7	3TP	B	2000	-	21,28,28	3.15	10 (47%)	29,41,41	1.40	6 (20%)
3	NAG	B	2092	1	14,14,15	0.86	0	15,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	2150	1	14,14,15	0.89	1 (7%)	15,19,21	0.91	1 (6%)
3	NAG	B	2321	1	14,14,15	0.67	0	15,19,21	0.85	1 (6%)

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
7	3TP	A	1000	-	-	0/19/33/33	0/2/3/3
3	NAG	A	1092	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1281	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1520	1	-	0/6/23/26	0/1/1/1
7	3TP	B	2000	-	-	0/19/33/33	0/2/3/3
3	NAG	B	2092	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2150	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2321	1	-	0/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2000	3TP	C20-C1	2.00	1.54	1.50
3	B	2150	NAG	C1-C2	2.14	1.55	1.52
3	A	1281	NAG	C1-C2	2.21	1.55	1.52
7	B	2000	3TP	C30-C25	2.24	1.44	1.39
7	B	2000	3TP	C29-C28	2.62	1.43	1.38
7	A	1000	3TP	C29-C28	2.70	1.43	1.38
3	A	1092	NAG	C1-C2	2.82	1.56	1.52
7	B	2000	3TP	C30-C29	3.29	1.44	1.38
7	B	2000	3TP	C12-C11	3.42	1.53	1.40
7	A	1000	3TP	C12-C11	3.54	1.53	1.40
7	B	2000	3TP	C1-C2	3.72	1.57	1.54
7	A	1000	3TP	C13-N4	4.15	1.45	1.39
7	B	2000	3TP	C13-N4	4.97	1.46	1.39
7	B	2000	3TP	C10-N4	5.02	1.46	1.39
7	A	1000	3TP	C10-N4	5.85	1.47	1.39
7	A	1000	3TP	C13-C12	6.68	1.53	1.37
7	A	1000	3TP	C10-C11	6.69	1.53	1.37
7	B	2000	3TP	C10-C11	6.78	1.53	1.37
7	B	2000	3TP	C13-C12	6.82	1.53	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2321	NAG	C2-N2-C7	-2.74	119.52	123.04
7	B	2000	3TP	O36-S34-C28	-2.62	106.01	108.31
3	B	2150	NAG	C2-N2-C7	-2.30	120.08	123.04
3	A	1281	NAG	C2-N2-C7	-2.28	120.12	123.04
7	B	2000	3TP	C37-S34-C28	-2.15	102.08	104.68
7	B	2000	3TP	C26-C25-C22	-2.11	117.19	120.80
7	A	1000	3TP	C3-C2-N6	-2.01	104.61	108.84
7	B	2000	3TP	O35-S34-C37	2.00	111.80	108.53
7	B	2000	3TP	C1-C20-N21	2.07	128.23	124.27
7	A	1000	3TP	C1-C20-N21	2.09	128.27	124.27
7	A	1000	3TP	O35-S34-C37	2.60	112.78	108.53
7	A	1000	3TP	C25-C22-N23	2.81	122.65	119.11
7	B	2000	3TP	C25-C22-N23	3.00	122.90	119.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1000	3TP	1	0
3	A	1092	NAG	1	0
3	A	1520	NAG	2	0
7	B	2000	3TP	1	0
3	B	2092	NAG	5	0
3	B	2150	NAG	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	728/728 (100%)	-0.18	9 (1%) 81 89	13, 23, 45, 58	0
1	B	728/728 (100%)	-0.17	16 (2%) 65 77	13, 24, 43, 59	0
All	All	1456/1456 (100%)	-0.17	25 (1%) 73 83	13, 24, 44, 59	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	5.7
1	A	92	ASN	3.8
1	A	97	GLU	3.7
1	B	39	THR	3.6
1	B	91	GLU	3.6
1	B	88	VAL	3.5
1	B	138	ASN	3.5
1	A	99	GLY	3.4
1	A	766	PRO	3.4
1	B	74	ASN	3.0
1	B	73	GLU	3.0
1	B	95	PHE	3.0
1	A	73	GLU	3.0
1	B	90	LEU	2.8
1	A	96	ASP	2.8
1	B	98	PHE	2.8
1	B	766	PRO	2.7
1	A	74	ASN	2.7
1	A	75	ASN	2.6
1	B	100	HIS	2.5
1	B	71	LYS	2.5
1	B	93	SER	2.4
1	B	97	GLU	2.3
1	B	99	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	506	ASN	2.3

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](#)

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
5	NAG	A	1321	14/15	0.86	0.29	9.86	44,48,51,53	0
5	NAG	A	1220	14/15	0.84	0.22	2.54	46,48,50,52	0
5	NAG	B	2219	14/15	0.94	0.14	2.17	35,39,44,44	0
5	NAG	B	2281	14/15	0.95	0.12	2.17	30,33,40,43	0
5	NAG	A	1219	14/15	0.89	0.16	1.53	38,42,46,46	0
5	NAG	B	2220	14/15	0.92	0.19	1.47	43,45,47,47	0
2	NAG	A	1229	14/15	0.92	0.15	1.15	33,36,42,44	0
2	NAG	A	1085	14/15	0.83	0.17	1.01	42,45,50,53	0
5	NAG	B	2085	14/15	0.90	0.17	0.01	42,48,54,55	0
5	NAG	B	2229	14/15	0.96	0.09	-0.34	28,31,35,39	0
5	NAG	B	2086	14/15	0.41	0.42	-	58,61,66,66	0
5	NAG	A	1322	14/15	0.68	0.42	-	56,58,61,62	0
4	NDG	A	1150	14/15	0.80	0.36	-	54,58,61,62	0
4	NAG	A	1151	14/15	0.69	0.32	-	58,62,65,65	0
2	NDG	A	1230	14/15	0.81	0.30	-	49,52,55,56	0
2	NDG	A	1086	14/15	0.61	0.32	-	54,56,57,57	0
5	NAG	B	2282	14/15	0.73	0.21	-	42,48,50,51	0
5	NAG	B	2230	14/15	0.90	0.24	-	42,45,48,51	0

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(\AA^2)	Q<0.9
3	NAG	B	2321	14/15	0.84	0.24	5.76	38,41,43,44	0
3	NAG	A	1520	14/15	0.64	0.33	5.18	59,61,63,64	0
7	3TP	A	1000	26/26	0.95	0.19	1.49	18,24,30,31	0
7	3TP	B	2000	26/26	0.96	0.16	1.18	18,25,29,31	0
6	NA	A	3000	1/1	0.95	0.10	-0.26	30,30,30,30	0
3	NAG	A	1092	14/15	0.57	0.44	-	61,63,64,65	0
3	NAG	B	2092	14/15	0.72	0.38	-	57,59,60,62	0
3	NAG	A	1281	14/15	0.83	0.18	-	45,47,48,48	0
3	NAG	B	2150	14/15	0.83	0.38	-	52,55,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.