W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:07 AM GMT

PDB ID	:	3HAB
Title	:	The structure of DPP4 in complex with piperidine fused benzimidazole 25
Authors	:	Scapin, G.
Deposited on	:	2009-05-01
Resolution	:	2.10 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 2.10 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		0.219
Clashscore		2
Ramachandran outliers		0.1%
Sidechain outliers		1.7%
RSRZ outliers		4.8%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
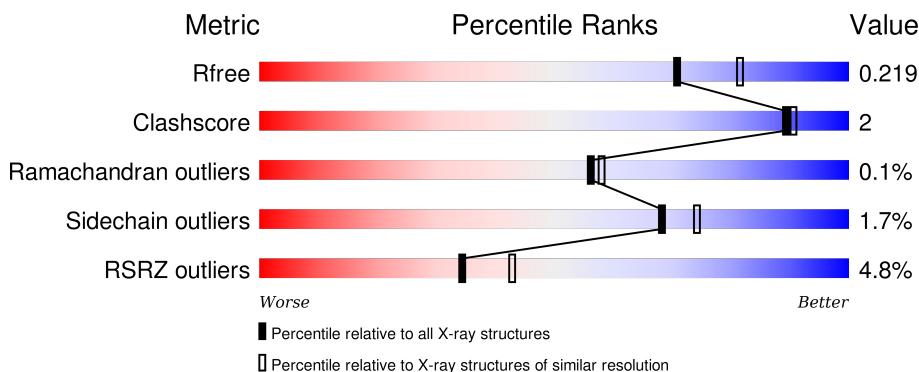
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	728	5% ██ 94% 6%
1	B	728	5% ██ 93% 7%

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	1219	-	-	-	X
3	NAG	A	1321	-	-	-	X
3	NAG	B	2085	-	-	-	X
3	NAG	B	2219	-	-	-	X
3	NAG	B	2220	-	-	-	X
3	NAG	B	2281	-	-	-	X
4	NAG	B	2321	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 13644 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total 6014	C 3860	N 990	O 1137	S 27	0	12	0
1	B	728	Total 6023	C 3865	N 993	O 1138	S 27	0	13	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	THR	SER	ENGINEERED	UNP P27487
B	39	THR	SER	ENGINEERED	UNP P27487

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

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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
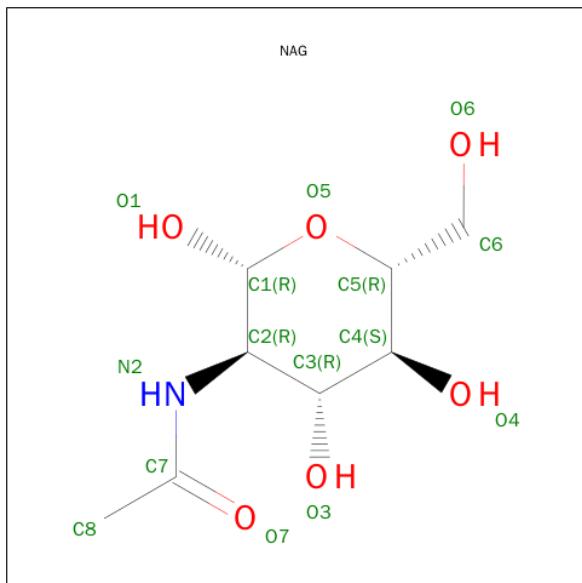
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is (2R,3R)-7-(METHYLSULFONYL)-3-(2,4,5-TRIFLUOROPHENYL)-1,2,3 ,4-TETRAHYDROPYRIDO[1,2-A]BENZIMIDAZOL-2-AMINE (three-letter code: 677) (formula: $C_{18}H_{16}F_3N_3O_2S$).
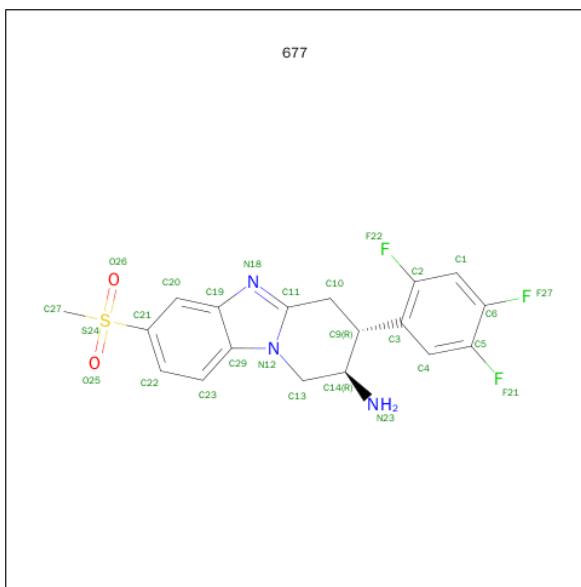
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	S	0	0
			27	18	3	3	2	1		
6	B	1	Total	C	F	N	O	S	0	0
			27	18	3	3	2	1		

- Molecule 7 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).
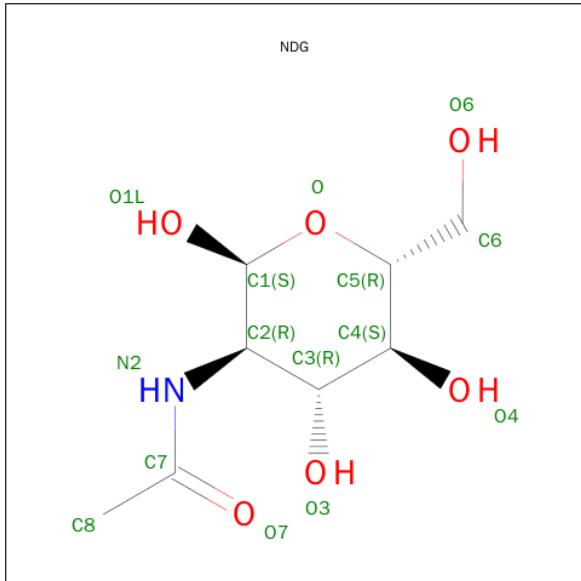
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	617	Total 617	O 617	0	0
8	B	627	Total 627	O 627	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Dipeptidyl peptidase 4
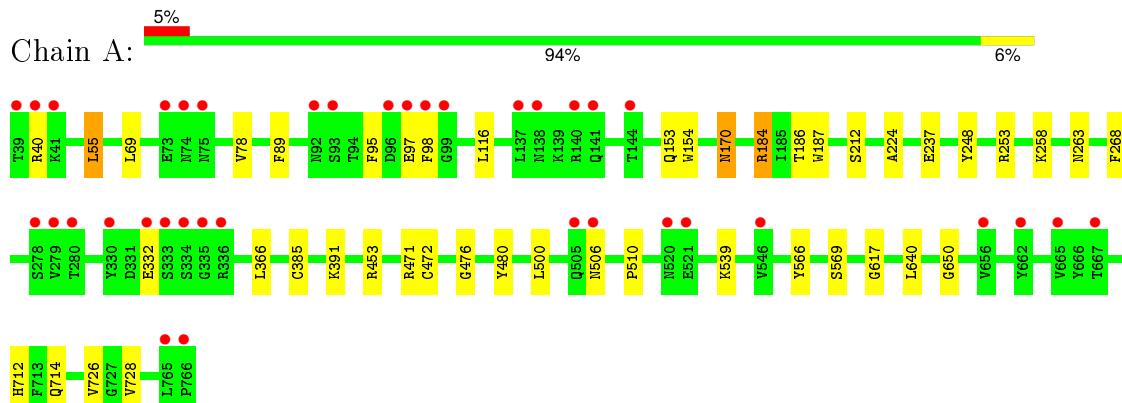
- Molecule 1: Dipeptidyl peptidase 4
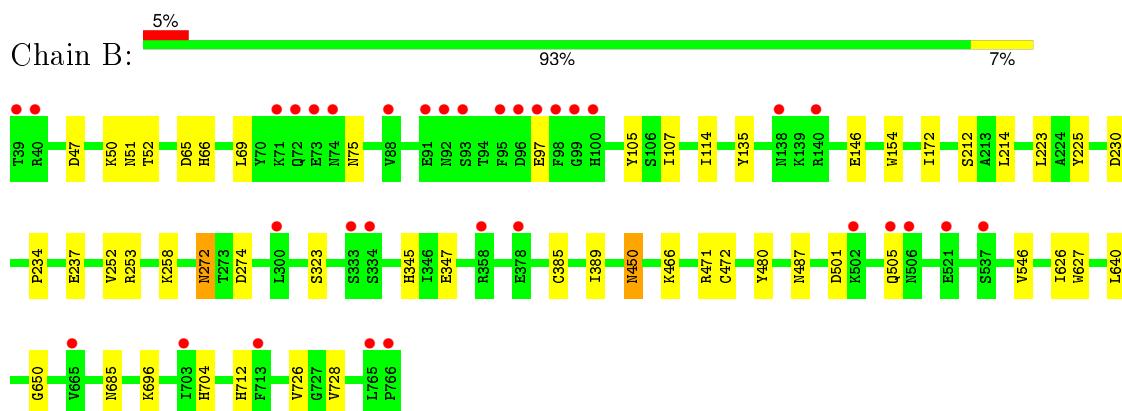
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.91Å 125.64Å 136.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.10) 99.9 (29.96-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.89 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.169 , 0.211 0.184 , 0.219	Depositor DCC
R_{free} test set	5950 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	1 of 118795 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13644	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 2.80% 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, 0.375 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: NA, 677, 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	0.57	0/6231	0.63	1/8472 (0.0%)
1	B	0.56	0/6247	0.61	0/8495
All	All	0.56	0/12478	0.62	1/16967 (0.0%)

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	A	184	ARG	NE-CZ-NH1	5.55	123.08	120.30

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	6014	0	5723	28	0
1	B	6023	0	5738	31	0
2	A	56	0	50	0	0
3	A	84	0	75	1	0
3	B	112	0	100	1	0
4	A	14	0	13	0	0
4	B	28	0	26	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	27	0	16	0	0
6	B	27	0	16	0	0
7	B	14	0	13	1	0
8	A	617	0	0	2	0
8	B	627	0	0	4	0
All	All	13644	0	11770	59	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 2.

All (59) 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:258:LYS:HZ1	1:B:712:HIS:HD2	1.06	0.92
1:B:214[B]:LEU:HD23	1:B:225:TYR:HB3	1.56	0.87
1:A:69:LEU:HD23	1:A:78:VAL:HG22	1.61	0.82
1:A:184:ARG:HD2	1:A:186:THR:O	1.88	0.74
1:B:466:LYS:HE2	8:B:1085:HOH:O	1.90	0.71
1:A:258:LYS:HZ1	1:A:712:HIS:HD2	1.39	0.70
1:B:172:ILE:HD13	1:B:214[B]:LEU:HD21	1.76	0.68
1:A:258:LYS:NZ	1:A:712:HIS:HD2	1.92	0.68
1:B:258:LYS:HZ1	1:B:712:HIS:CD2	1.99	0.68
1:B:47:ASP:HA	1:B:52[B]:THR:HG23	1.78	0.64
1:A:78:VAL:HG23	1:A:89:PHE:HB2	1.78	0.64
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.78	0.64
1:B:47:ASP:HA	1:B:52[B]:THR:CG2	2.28	0.63
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.81	0.62
1:B:75:ASN:HD21	7:B:2092:NDG:HA	1.46	0.62
1:B:272:ASN:C	1:B:272:ASN:HD22	2.02	0.62
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.81	0.62
1:A:69:LEU:HD23	1:A:78:VAL:CG2	2.31	0.60
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.66	0.60
1:A:69:LEU:CD2	1:A:78:VAL:HG22	2.33	0.59
1:A:153:GLN:HE22	1:A:170:ASN:ND2	2.01	0.59
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.86	0.58
1:A:184:ARG:HG2	1:A:187:TRP:CE2	2.39	0.57
1:A:237:GLU:OE1	1:A:253[B]:ARG:HD2	2.05	0.56
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.90	0.54
1:A:55:LEU:HD12	1:A:500:LEU:CD2	2.37	0.54
1:A:253[A]:ARG:HH21	1:B:253[A]:ARG:HH21	1.56	0.54
1:A:471[A]:ARG:HD2	8:A:972:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2219:NAG:H82	8:B:1282:HOH:O	2.10	0.51
1:A:539:LYS:HE2	1:A:617:GLY:O	2.12	0.49
1:A:154:TRP:CE2	1:A:212[A]:SER:HB3	2.48	0.48
1:B:471[B]:ARG:HG3	1:B:480:TYR:CE2	2.47	0.48
1:B:50:LYS:HD3	8:B:848:HOH:O	2.14	0.48
3:A:1150:NAG:H4	3:A:1151:NAG:H2	1.66	0.47
1:A:471[B]:ARG:HD2	1:A:480:TYR:HE2	1.80	0.47
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.50	0.46
1:A:471[A]:ARG:HG3	1:A:480:TYR:CE2	2.51	0.46
1:B:546:VAL:HG21	1:B:626:ILE:HD11	1.98	0.46
1:B:214[B]:LEU:HD22	1:B:223:LEU:HD21	1.96	0.46
1:B:154:TRP:CE2	1:B:212[A]:SER:HB2	2.51	0.46
1:B:146:GLU:OE2	8:B:998:HOH:O	2.20	0.45
1:B:69:LEU:HD11	1:B:107:ILE:HG13	1.98	0.45
1:A:170:ASN:N	1:A:170:ASN:HD22	2.15	0.44
1:B:501:ASP:O	1:B:505:GLN:HG2	2.18	0.44
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.98	0.44
1:B:237:GLU:HA	1:B:252:VAL:O	2.17	0.44
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.18	0.43
1:A:154:TRP:CE2	1:A:212[B]:SER:HB2	2.53	0.43
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.99	0.43
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.53	0.43
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.99	0.43
1:A:332:GLU:HG3	8:A:1142:HOH:O	2.19	0.43
1:B:640:LEU:HD11	1:B:650:GLY:HA3	2.01	0.42
1:A:40:ARG:HB2	1:A:506:ASN:O	2.19	0.42
1:B:272:ASN:HD22	1:B:274:ASP:H	1.68	0.41
1:A:453:ARG:HG3	1:A:476:GLY:HA3	2.03	0.41
1:B:323[A]:SER:OG	1:B:347:GLU:HB3	2.20	0.41
1:B:345:HIS:HE1	1:B:389:ILE:O	2.03	0.41

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	737/728 (101%)	715 (97%)	21 (3%)	1 (0%)	56	58
1	B	739/728 (102%)	714 (97%)	25 (3%)	0	100	100
All	All	1476/1456 (101%)	1429 (97%)	46 (3%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	714	GLN

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	664/653 (102%)	654 (98%)	10 (2%)	72	78
1	B	666/653 (102%)	653 (98%)	13 (2%)	63	68
All	All	1330/1306 (102%)	1307 (98%)	23 (2%)	68	74

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	97	GLU
1	A	116	LEU
1	A	170	ASN
1	A	263	ASN
1	A	366	LEU
1	A	385	CYS
1	A	391	LYS
1	A	472	CYS
1	A	566	TYR
1	B	51	ASN
1	B	66	HIS

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Mol	Chain	Res	Type
1	B	97	GLU
1	B	230	ASP
1	B	272	ASN
1	B	385	CYS
1	B	450[A]	ASN
1	B	450[B]	ASN
1	B	472	CYS
1	B	487	ASN
1	B	627	TRP
1	B	685	ASN
1	B	704	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	141	GLN
1	A	169	ASN
1	A	170	ASN
1	A	263	ASN
1	A	388	GLN
1	A	435	GLN
1	A	572	ASN
1	A	694	ASN
1	A	712	HIS
1	B	74	ASN
1	B	169	ASN
1	B	272	ASN
1	B	345	HIS
1	B	388	GLN
1	B	487	ASN
1	B	533	HIS
1	B	572	ASN
1	B	685	ASN
1	B	694	ASN
1	B	712	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)

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 Counts	Bond lengths RMSZ	Bond lengths #$|Z| > 2$	Bond angles Counts	Bond angles RMSZ	Bond angles #$|Z| > 2$
2	NAG	A	1085	1,2	14,14,15	0.61	0	15,19,21	1.99	6 (40%)
2	NDG	A	1086	2	14,14,15	0.55	0	15,19,21	0.88	1 (6%)
3	NAG	A	1150	1,3	14,14,15	0.53	0	15,19,21	1.66	2 (13%)
3	NAG	A	1151	3	14,14,15	0.82	0	15,19,21	1.62	4 (26%)
3	NAG	A	1219	1,3	14,14,15	0.53	0	15,19,21	0.67	0
3	NAG	A	1220	3	14,14,15	0.46	0	15,19,21	0.92	1 (6%)
2	NAG	A	1229	1,2	14,14,15	0.61	0	15,19,21	1.12	1 (6%)
2	NDG	A	1230	2	14,14,15	0.80	0	15,19,21	1.32	2 (13%)
3	NAG	A	1321	1,3	14,14,15	0.62	0	15,19,21	1.43	3 (20%)
3	NAG	A	1322	3	14,14,15	0.73	0	15,19,21	1.37	3 (20%)
3	NAG	B	2085	1,3	14,14,15	0.60	0	15,19,21	1.24	1 (6%)
3	NAG	B	2086	3	14,14,15	0.75	0	15,19,21	1.53	3 (20%)
3	NAG	B	2219	1,3	14,14,15	0.57	0	15,19,21	0.87	0
3	NAG	B	2220	3	14,14,15	0.58	0	15,19,21	1.17	2 (13%)
3	NAG	B	2229	1,3	14,14,15	0.60	0	15,19,21	0.86	0
3	NAG	B	2230	3	14,14,15	0.55	0	15,19,21	1.25	1 (6%)
3	NAG	B	2281	1,3	14,14,15	0.62	0	15,19,21	1.00	1 (6%)
3	NAG	B	2282	3	14,14,15	0.48	0	15,19,21	1.30	2 (13%)

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
3	NAG	A	1150	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1151	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1219	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1220	3	-	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
3	NAG	A	1321	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1322	3	-	2/6/23/26	0/1/1/1
3	NAG	B	2085	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2086	3	-	0/6/23/26	0/1/1/1
3	NAG	B	2219	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2220	3	-	0/6/23/26	0/1/1/1
3	NAG	B	2229	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2230	3	-	0/6/23/26	0/1/1/1
3	NAG	B	2281	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2282	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1150	NAG	O4-C4-C3	-3.47	102.53	110.34
2	A	1085	NAG	C4-C3-C2	-3.36	106.01	111.23
3	A	1321	NAG	O4-C4-C3	-3.26	103.01	110.34
2	A	1085	NAG	C3-C4-C5	-2.30	106.19	110.20
3	B	2281	NAG	C2-N2-C7	-2.01	120.45	123.04
3	B	2086	NAG	C2-N2-C7	2.03	125.64	123.04
2	A	1086	NDG	C3-C4-C5	2.05	113.77	110.20
3	B	2220	NAG	C3-C4-C5	2.12	113.89	110.20
3	B	2282	NAG	O5-C5-C6	2.15	112.01	107.35
3	B	2220	NAG	C4-C3-C2	2.20	114.64	111.23
2	A	1085	NAG	O4-C4-C5	2.23	115.15	109.24
2	A	1085	NAG	C1-O5-C5	2.26	115.12	112.25
3	A	1321	NAG	C4-C3-C2	2.29	114.78	111.23
3	A	1151	NAG	C3-C4-C5	2.47	114.50	110.20
3	A	1220	NAG	C1-O5-C5	2.54	115.47	112.25
3	A	1151	NAG	C4-C3-C2	2.56	115.22	111.23
3	A	1321	NAG	C1-O5-C5	2.59	115.53	112.25
3	A	1322	NAG	C2-N2-C7	2.61	126.39	123.04
2	A	1230	NDG	C4-C3-C2	2.65	115.35	111.23
2	A	1085	NAG	O5-C5-C6	2.74	113.27	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1322	NAG	C4-C3-C2	2.86	115.68	111.23
3	A	1322	NAG	C3-C4-C5	2.89	115.23	110.20
3	B	2282	NAG	C1-O5-C5	2.98	116.03	112.25
3	A	1151	NAG	C1-O5-C5	3.14	116.24	112.25
3	B	2230	NAG	C1-O5-C5	3.19	116.30	112.25
3	A	1151	NAG	C2-N2-C7	3.25	127.21	123.04
2	A	1229	NAG	C1-O5-C5	3.28	116.41	112.25
3	B	2085	NAG	C4-C3-C2	3.30	116.35	111.23
3	B	2086	NAG	C3-C4-C5	3.39	116.10	110.20
2	A	1230	NDG	C2-N2-C7	3.40	127.40	123.04
3	A	1150	NAG	C1-O5-C5	3.85	117.13	112.25
3	B	2086	NAG	C4-C3-C2	3.92	117.33	111.23
2	A	1085	NAG	O4-C4-C3	4.25	119.92	110.34

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1322	NAG	C8-C7-N2-C2
3	A	1322	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1150	NAG	1	0
3	A	1151	NAG	1	0
3	B	2219	NAG	1	0

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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
4	NAG	A	1281	1	14,14,15	0.51	0	15,19,21	1.29	2 (13%)
6	677	A	767	-	27,30,30	2.41	5 (18%)	35,47,47	1.90	6 (17%)
6	677	B	2	-	27,30,30	2.35	5 (18%)	35,47,47	2.18	9 (25%)
7	NDG	B	2092	1	14,14,15	0.53	0	15,19,21	1.35	1 (6%)
4	NAG	B	2150	1	14,14,15	0.51	0	15,19,21	0.83	0
4	NAG	B	2321	1	14,14,15	0.49	0	15,19,21	1.58	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
4	NAG	A	1281	1	-	0/6/23/26	0/1/1/1
6	677	A	767	-	-	0/10/22/22	0/3/4/4
6	677	B	2	-	-	0/10/22/22	0/3/4/4
7	NDG	B	2092	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2150	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2321	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2	677	C21-S24	-10.11	1.64	1.77
6	A	767	677	C21-S24	-10.08	1.64	1.77
6	B	2	677	C27-S24	-2.30	1.64	1.74
6	A	767	677	C27-S24	-2.22	1.64	1.74
6	A	767	677	C20-C21	2.30	1.40	1.36
6	B	2	677	C23-C22	2.57	1.42	1.36
6	B	2	677	C20-C21	2.64	1.41	1.36
6	A	767	677	C23-C22	2.68	1.42	1.36
6	B	2	677	C29-C19	3.14	1.46	1.40
6	A	767	677	C29-C19	4.28	1.49	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	2	677	O26-S24-O25	-5.06	107.17	117.73
6	A	767	677	O26-S24-O25	-4.94	107.43	117.73
6	A	767	677	O25-S24-C21	-3.51	105.24	108.31
6	B	2	677	C1-C2-C3	-3.46	120.10	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	2	677	O25-S24-C21	-3.28	105.43	108.31
6	B	2	677	C11-C10-C9	-3.23	109.34	114.00
6	B	2	677	C22-C21-C20	-2.10	118.43	121.01
6	A	767	677	C3-C9-C14	-2.01	108.44	114.55
4	A	1281	NAG	O5-C5-C6	2.17	112.05	107.35
6	A	767	677	O26-S24-C27	2.27	112.25	108.53
6	A	767	677	C23-C22-C21	2.28	122.53	119.73
6	B	2	677	O26-S24-C27	2.47	112.57	108.53
6	B	2	677	C4-C3-C2	2.70	119.82	116.17
4	A	1281	NAG	C1-O5-C5	3.07	116.14	112.25
6	B	2	677	O26-S24-C21	3.24	111.14	108.31
7	B	2092	NDG	C1-O-C5	4.36	117.79	112.25
4	B	2321	NAG	C1-O5-C5	4.83	118.37	112.25
6	A	767	677	C27-S24-C21	6.43	112.47	104.68
6	B	2	677	C27-S24-C21	6.96	113.11	104.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	2092	NDG	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	728/728 (100%)	0.09	37 (5%)	32	40	16, 24, 37, 51	0
1	B	728/728 (100%)	0.03	33 (4%)	37	46	17, 24, 38, 54	0
All	All	1456/1456 (100%)	0.06	70 (4%)	34	43	16, 24, 38, 54	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	7.7
1	B	39	THR	6.1
1	A	279	VAL	5.9
1	B	766	PRO	5.4
1	A	99	GLY	4.8
1	A	97	GLU	4.5
1	A	74	ASN	4.5
1	A	96	ASP	4.3
1	B	73	GLU	4.2
1	A	73	GLU	4.1
1	B	138	ASN	4.1
1	B	74	ASN	4.1
1	A	766	PRO	4.1
1	A	138	ASN	4.1
1	B	92	ASN	4.0
1	B	97	GLU	3.9
1	A	92	ASN	3.6
1	A	93	SER	3.4
1	A	333	SER	3.4
1	B	333	SER	3.3
1	B	96	ASP	3.3
1	A	75	ASN	3.2
1	A	280	THR	3.2
1	B	40	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	40	ARG	3.1
1	B	506	ASN	3.1
1	A	278	SER	3.0
1	A	140	ARG	2.9
1	B	71	LYS	2.9
1	A	546[A]	VAL	2.9
1	B	765	LEU	2.9
1	A	98	PHE	2.9
1	B	91	GLU	2.8
1	B	502	LYS	2.8
1	A	335	GLY	2.8
1	A	521	GLU	2.7
1	B	537	SER	2.7
1	B	98	PHE	2.7
1	B	99	GLY	2.7
1	B	140	ARG	2.6
1	B	93	SER	2.6
1	B	334	SER	2.6
1	B	95	PHE	2.6
1	B	521	GLU	2.5
1	A	336	ARG	2.5
1	B	100	HIS	2.5
1	A	656	VAL	2.5
1	B	88	VAL	2.5
1	A	141	GLN	2.5
1	A	144	THR	2.4
1	A	137	LEU	2.4
1	A	765	LEU	2.4
1	B	72	GLN	2.4
1	A	506	ASN	2.4
1	B	505	GLN	2.3
1	A	665	VAL	2.3
1	B	358[A]	ARG	2.3
1	B	378	GLU	2.2
1	A	520	ASN	2.2
1	A	667	THR	2.2
1	A	334	SER	2.2
1	A	332	GLU	2.2
1	A	330	TYR	2.1
1	B	665	VAL	2.1
1	B	300	LEU	2.1
1	B	713	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	662	TYR	2.1
1	B	703	ILE	2.0
1	A	505	GLN	2.0
1	A	41	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

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	NAG	B	2219	14/15	0.94	0.20	5.88	30,37,41,43	0
3	NAG	A	1321	14/15	0.84	0.25	4.67	41,45,48,54	0
3	NAG	A	1219	14/15	0.88	0.21	3.67	37,43,47,47	0
3	NAG	B	2220	14/15	0.83	0.28	2.10	41,46,49,50	0
3	NAG	B	2281	14/15	0.90	0.13	2.09	30,33,40,44	0
3	NAG	B	2085	14/15	0.85	0.18	2.05	41,50,57,60	0
2	NAG	A	1085	14/15	0.88	0.17	1.85	44,48,55,60	0
3	NAG	A	1220	14/15	0.76	0.28	1.73	50,52,56,57	0
2	NAG	A	1229	14/15	0.93	0.15	1.35	35,39,44,51	0
3	NAG	B	2229	14/15	0.94	0.16	0.95	23,27,33,37	0
3	NAG	A	1322	14/15	0.60	0.41	-	58,61,62,63	0
3	NAG	B	2282	14/15	0.62	0.28	-	48,52,53,53	0
2	NDG	A	1230	14/15	0.69	0.33	-	56,60,65,65	0
3	NAG	B	2230	14/15	0.86	0.31	-	41,45,47,47	0
3	NAG	B	2086	14/15	0.43	0.38	-	65,68,70,71	0
2	NDG	A	1086	14/15	0.60	0.36	-	64,67,68,68	0
3	NAG	A	1150	14/15	0.77	0.32	-	51,56,59,64	0
3	NAG	A	1151	14/15	0.61	0.47	-	67,69,71,71	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(Å^2)	Q<0.9
4	NAG	B	2321	14/15	0.81	0.25	4.65	39,43,44,44	0
6	677	B	2	27/27	0.96	0.08	-1.38	15,20,23,26	0
6	677	A	767	27/27	0.96	0.08	-1.51	13,18,21,25	0
5	NA	A	1	1/1	0.94	0.06	-2.23	25,25,25,25	0
4	NAG	A	1281	14/15	0.79	0.22	-	42,46,48,48	0
7	NDG	B	2092	14/15	0.76	0.45	-	66,69,70,71	0
4	NAG	B	2150	14/15	0.68	0.36	-	49,53,55,56	0

6.5 Other polymers (i)

There are no such residues in this entry.