W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:42 am GMT

PDB ID	:	5BRN
Title	:	Human HGPRT in complex with (S)-HPEPHx, an acyclic nucleoside phosphonate
Authors	:	Keough, D.T.; Guddat, L.W.; Kaiser, M.M.; Hockova, D.; Wang, T.-H.; Janeba, Z.
Deposited on	:	2015-05-31
Resolution	:	2.30 Å(reported)

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	:	trunk28620
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)	:	recalc28949

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
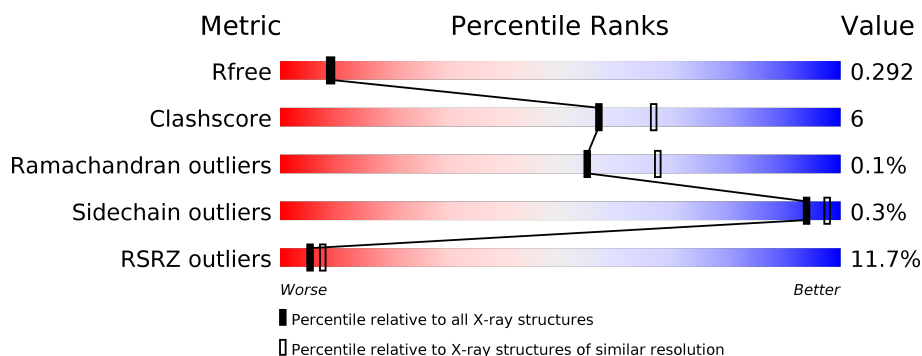
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	218	6% / 76% 13% 11%
1	B	218	12% / 79% 10% 11%
1	C	218	11% / 78% 12% 11%
1	D	218	13% / 76% 14% 10%

2   Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6437 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 Hypoxanthine-guanine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total 1527	C 983	N 254	O 283	S 7	0	0	0
1	B	194	Total 1498	C 965	N 249	O 278	S 6	0	0	0
1	C	195	Total 1525	C 983	N 253	O 282	S 7	0	0	0
1	D	197	Total 1534	C 990	N 251	O 286	S 7	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	CYS	engineered mutation	UNP P00492
A	105	ALA	CYS	engineered mutation	UNP P00492
A	205	ALA	CYS	engineered mutation	UNP P00492
B	22	ALA	CYS	engineered mutation	UNP P00492
B	105	ALA	CYS	engineered mutation	UNP P00492
B	205	ALA	CYS	engineered mutation	UNP P00492
C	22	ALA	CYS	engineered mutation	UNP P00492
C	105	ALA	CYS	engineered mutation	UNP P00492
C	205	ALA	CYS	engineered mutation	UNP P00492
D	22	ALA	CYS	engineered mutation	UNP P00492
D	105	ALA	CYS	engineered mutation	UNP P00492
D	205	ALA	CYS	engineered mutation	UNP P00492

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).
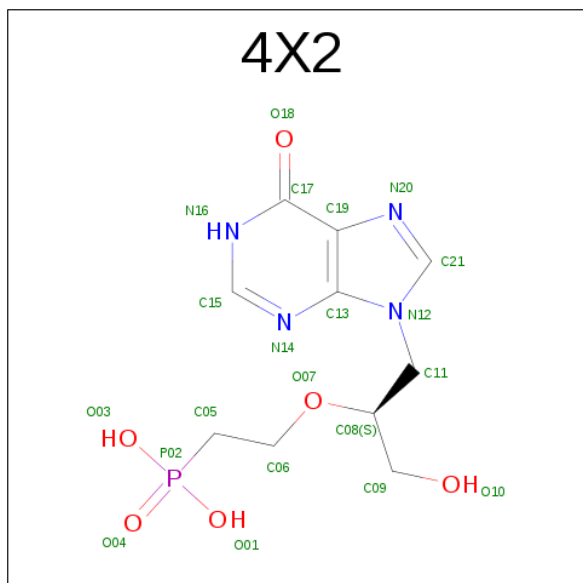
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mg 1	0	0
2	A	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total Mg	1　1	0	0
2	C	1	Total Mg	1　1	0	0

- Molecule 3 is (2-{[(2S)-1-hydroxy-3-(6-oxo-1,6-dihydro-9H-purin-9-yl)propan-2-yl]oxy}ethyl)phosphonic acid (three-letter code: 4X2) (formula: $C_{10}H_{15}N_4O_6P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 21	C 10	N 4	O 6	P 1	0	0
3	B	1	Total 21	C 10	N 4	O 6	P 1	0	0
3	C	1	Total 21	C 10	N 4	O 6	P 1	0	0
3	D	1	Total 21	C 10	N 4	O 6	P 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	80	Total O	80　80	0	0
4	B	46	Total O	46　46	0	0
4	C	80	Total O	80　80	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	59	Total O 59 59		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: Hypoxanthine-guanine phosphoribosyltransferase
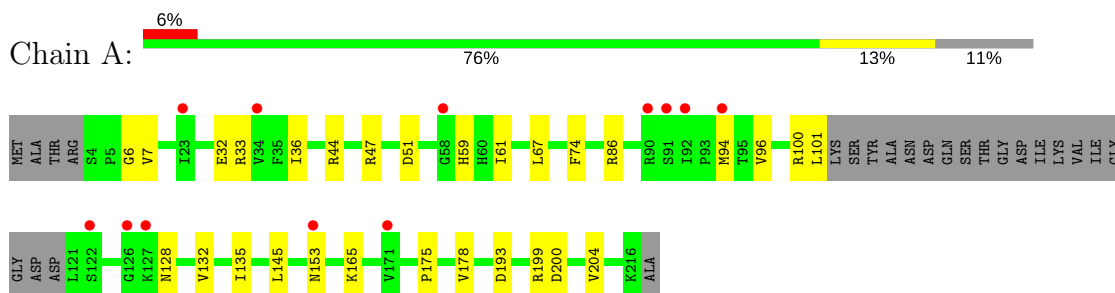
• Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

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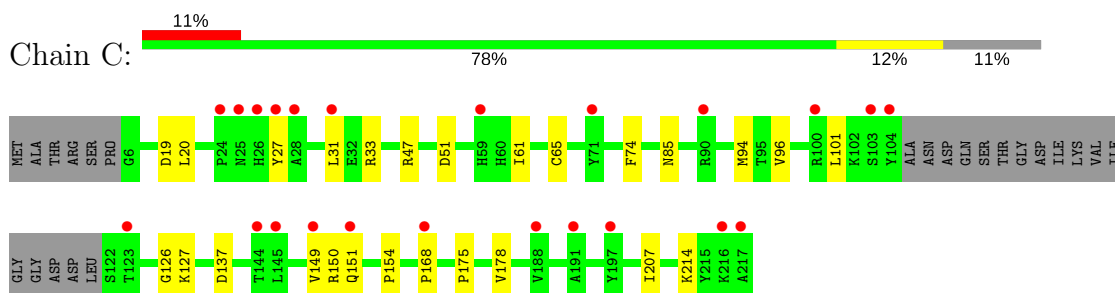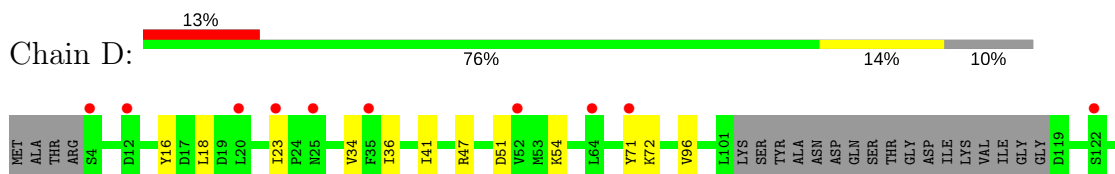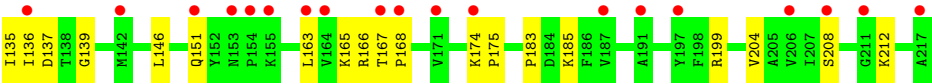I135 I136 D137 T138 G139 M142 L146 Q151 Y152 N153 P154 K155 L163 V164 K165 R166 T167 P168 V171 K174 P175 P183 D184 K185 F186 V187 A191 Y197 F198 R199 V204 A205 V206 I207 S208 G211 K212 A217
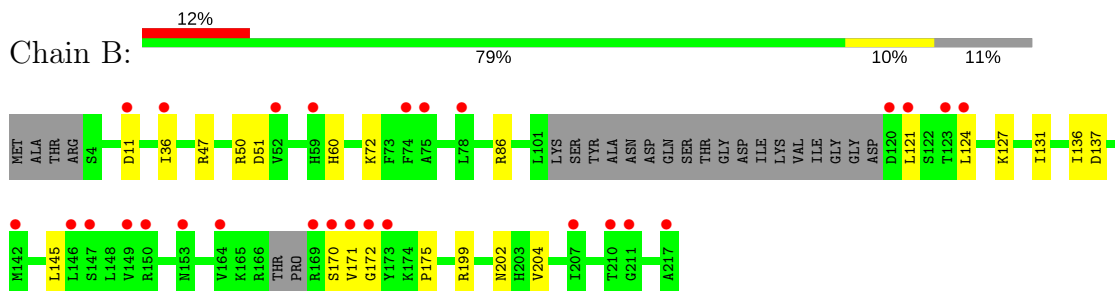
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.53Å 94.31Å 139.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.33 – 2.30 53.26 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.4 (47.33-2.30) 92.1 (53.26-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.239 , 0.292 0.240 , 0.292	Depositor DCC
R_{free} test set	2001 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.8	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6437	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 4X2

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	0.22	0/1558	0.41	0/2111
1	B	0.22	0/1527	0.39	0/2070
1	C	0.22	0/1555	0.40	0/2105
1	D	0.22	0/1565	0.39	0/2121
All	All	0.22	0/6205	0.40	0/8407

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1527	0	1520	19	0
1	B	1498	0	1463	14	0
1	C	1525	0	1509	19	0
1	D	1534	0	1521	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	21	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	15	1	0
3	C	21	0	14	1	0
3	D	21	0	15	2	0
4	A	80	0	0	2	0
4	B	46	0	0	3	0
4	C	80	0	0	7	0
4	D	59	0	0	2	0
All	All	6437	0	6072	70	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 6.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ILE:HD12	1:D:175:PRO:HG3	1.69	0.74
1:D:47:ARG:NH1	1:D:51:ASP:OD1	2.23	0.72
1:C:31:LEU:HA	1:C:207:ILE:HA	1.72	0.71
1:A:135:ILE:HD11	1:A:165:LYS:HE3	1.72	0.70
1:D:185:LYS:NZ	4:D:401:HOH:O	2.23	0.69
1:B:47:ARG:NH1	1:B:51:ASP:OD1	2.26	0.68
1:C:175:PRO:HG2	1:C:178:VAL:HG22	1.75	0.67
1:B:136:ILE:HD12	1:B:175:PRO:HG3	1.76	0.67
1:B:86:ARG:NH1	4:B:403:HOH:O	2.30	0.64
1:A:86:ARG:O	1:B:50:ARG:NH1	2.31	0.64
1:C:137:ASP:HB3	3:C:302:4X2:O01	1.98	0.63
1:C:61:ILE:HB	1:C:94:MET:HG2	1.80	0.63
1:B:72:LYS:NZ	1:B:202:ASN:OD1	2.32	0.63
1:D:151:GLN:NE2	4:D:404:HOH:O	2.32	0.62
1:C:214:LYS:NZ	4:C:412:HOH:O	2.33	0.61
1:A:7:VAL:HG22	1:C:20:LEU:HD13	1.83	0.59
1:C:168:PRO:O	4:C:401:HOH:O	2.16	0.58
3:A:302:4X2:O03	4:A:401:HOH:O	2.16	0.57
1:C:150:ARG:HA	1:C:154:PRO:HD2	1.86	0.57
1:A:101:LEU:HD11	1:A:145:LEU:HD13	1.87	0.56
1:A:6:GLY:HA2	1:A:44:ARG:HH21	1.71	0.55
1:A:47:ARG:NH1	1:A:51:ASP:OD1	2.40	0.54
1:D:137:ASP:HB3	3:D:302:4X2:O03	2.09	0.53
1:A:175:PRO:HG2	1:A:178:VAL:HG22	1.91	0.53
1:A:32:GLU:HG3	1:A:33:ARG:HG2	1.91	0.52
1:C:85:ASN:ND2	4:C:404:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASN:ND2	4:B:408:HOH:O	2.43	0.51
1:A:47:ARG:NH2	4:C:402:HOH:O	2.42	0.50
1:C:47:ARG:NH1	1:C:51:ASP:OD1	2.45	0.50
1:B:170:SER:O	1:B:172:GLY:N	2.45	0.50
1:B:36:ILE:HB	1:B:204:VAL:HB	1.93	0.50
1:A:74:PHE:HA	1:A:132:VAL:HG11	1.93	0.50
1:D:18:LEU:HB3	1:D:23:ILE:HD13	1.93	0.49
1:A:96:VAL:HG22	1:D:199:ARG:HD2	1.95	0.49
1:C:127:LYS:NZ	4:C:421:HOH:O	2.46	0.47
1:A:67:LEU:HB2	1:A:100:ARG:HG2	1.97	0.47
1:C:126:GLY:H	1:C:154:PRO:HA	1.79	0.46
1:D:139:GLY:N	3:D:302:4X2:O01	2.24	0.46
1:D:36:ILE:HB	1:D:204:VAL:HB	1.97	0.46
1:D:167:THR:HA	1:D:168:PRO:HD2	1.77	0.46
1:D:18:LEU:HD23	1:D:34:VAL:HG23	1.97	0.45
1:B:121:LEU:HD13	1:B:124:LEU:HD12	1.99	0.44
1:C:149:VAL:HG12	1:C:150:ARG:H	1.83	0.44
1:D:174:LYS:HA	1:D:175:PRO:HD3	1.83	0.44
1:B:199:ARG:HD2	1:C:96:VAL:HG22	1.99	0.43
1:D:208:SER:O	1:D:212:LYS:HB2	2.18	0.43
1:C:65:CYS:HB2	1:C:74:PHE:CD1	2.53	0.43
1:A:36:ILE:HB	1:A:204:VAL:HB	2.01	0.43
1:D:135:ILE:HG13	1:D:163:LEU:HB2	2.00	0.43
1:A:61:ILE:HB	1:A:94:MET:HG2	2.00	0.43
1:B:131:ILE:HD13	1:B:145:LEU:HD22	2.01	0.43
1:A:59:HIS:HB3	1:A:128:ASN:ND2	2.34	0.42
1:C:27:TYR:HB3	1:C:31:LEU:HD12	2.00	0.42
1:D:135:ILE:HD11	1:D:165:LYS:HE3	2.01	0.42
1:C:19:ASP:OD1	4:C:402:HOH:O	2.22	0.42
1:A:199:ARG:HD2	1:D:96:VAL:HG22	2.00	0.42
1:A:200:ASP:OD1	1:A:200:ASP:N	2.53	0.42
1:A:193:ASP:HB3	1:A:199:ARG:CZ	2.50	0.41
1:D:166:ARG:NH2	1:D:183:PRO:HG3	2.36	0.41
1:D:16:TYR:HB2	1:D:34:VAL:HB	2.02	0.41
1:A:153:ASN:ND2	4:A:421:HOH:O	2.49	0.41
1:B:137:ASP:HB3	3:B:302:4X2:O01	2.19	0.41
1:D:54:LYS:HE3	1:D:54:LYS:HB2	1.89	0.41
1:B:60:HIS:HB3	1:B:127:LYS:HG2	2.02	0.41
1:B:50:ARG:NE	4:B:413:HOH:O	2.51	0.41
1:C:33:ARG:NH2	4:C:428:HOH:O	2.53	0.41
1:D:71:TYR:CZ	1:D:72:LYS:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ILE:HD11	1:D:204:VAL:HG23	2.02	0.41
1:C:149:VAL:C	1:C:151:GLN:H	2.24	0.41
1:D:146:LEU:HA	1:D:146:LEU:HD23	1.97	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	190/218 (87%)	184 (97%)	6 (3%)	0	100	100
1	B	188/218 (86%)	176 (94%)	11 (6%)	1 (0%)	32	39
1	C	191/218 (88%)	178 (93%)	13 (7%)	0	100	100
1	D	193/218 (88%)	186 (96%)	7 (4%)	0	100	100
All	All	762/872 (87%)	724 (95%)	37 (5%)	1 (0%)	55	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	171	VAL

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	166/189 (88%)	166 (100%)	0	100	100
1	B	157/189 (83%)	156 (99%)	1 (1%)	89	95
1	C	162/189 (86%)	161 (99%)	1 (1%)	89	95
1	D	165/189 (87%)	165 (100%)	0	100	100
All	All	650/756 (86%)	648 (100%)	2 (0%)	94	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	11	ASP
1	C	101	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6   Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#|Z| > 2$
3	4X2	A	302	-	18,22,22	2.38	2 (11%)	14,31,31	2.29	4 (28%)
3	4X2	B	302	-	18,22,22	2.38	2 (11%)	14,31,31	2.27	4 (28%)
3	4X2	C	302	2	18,22,22	2.38	2 (11%)	14,31,31	2.31	4 (28%)
3	4X2	D	302	2	18,22,22	2.35	2 (11%)	14,31,31	2.23	4 (28%)

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
3	4X2	A	302	-	-	0/11/13/13	0/2/2/2
3	4X2	B	302	-	-	0/11/13/13	0/2/2/2
3	4X2	C	302	2	-	0/11/13/13	0/2/2/2
3	4X2	D	302	2	-	0/11/13/13	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	4X2	P02-C05	5.75	1.84	1.78
3	B	302	4X2	P02-C05	5.94	1.84	1.78
3	C	302	4X2	P02-C05	5.97	1.84	1.78
3	A	302	4X2	P02-C05	5.98	1.84	1.78
3	C	302	4X2	O18-C17	7.29	1.42	1.24
3	A	302	4X2	O18-C17	7.30	1.42	1.24
3	D	302	4X2	O18-C17	7.33	1.43	1.24
3	B	302	4X2	O18-C17	7.33	1.43	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	4X2	N14-C15-N16	-6.44	123.25	128.86
3	C	302	4X2	N14-C15-N16	-6.41	123.28	128.86
3	B	302	4X2	N14-C15-N16	-6.31	123.36	128.86
3	D	302	4X2	N14-C15-N16	-6.29	123.38	128.86
3	A	302	4X2	C17-C19-C13	-3.41	117.45	120.84
3	B	302	4X2	C17-C19-C13	-3.40	117.46	120.84
3	C	302	4X2	C17-C19-C13	-3.30	117.56	120.84
3	D	302	4X2	C17-C19-C13	-3.19	117.67	120.84
3	D	302	4X2	C13-C19-N20	-2.74	106.76	109.41
3	B	302	4X2	C13-C19-N20	-2.74	106.76	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	4X2	C13-C19-N20	-2.64	106.86	109.41
3	C	302	4X2	C13-C19-N20	-2.55	106.95	109.41
3	D	302	4X2	C15-N16-C17	2.18	119.55	115.91
3	B	302	4X2	C15-N16-C17	2.23	119.63	115.91
3	A	302	4X2	C15-N16-C17	2.33	119.80	115.91
3	C	302	4X2	C15-N16-C17	2.38	119.87	115.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	4X2	1	0
3	B	302	4X2	1	0
3	C	302	4X2	1	0
3	D	302	4X2	2	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(Å²)	Q<0.9
1	A	194/218 (88%)	0.78	12 (6%)	21	28	20, 35, 60, 87	0
1	B	194/218 (88%)	1.17	27 (13%)	3	5	30, 48, 88, 123	0
1	C	195/218 (89%)	1.01	23 (11%)	5	7	23, 38, 67, 95	0
1	D	197/218 (90%)	1.06	29 (14%)	3	4	25, 45, 74, 92	0
All	All	780/872 (89%)	1.00	91 (11%)	5	7	20, 42, 75, 123	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	ARG	10.0
1	C	103	SER	9.2
1	B	171	VAL	8.1
1	C	104	TYR	8.1
1	C	217	ALA	7.5
1	B	217	ALA	6.4
1	D	217	ALA	6.3
1	D	174	LYS	6.1
1	B	173	TYR	5.0
1	B	121	LEU	5.0
1	B	170	SER	4.6
1	D	211	GLY	4.5
1	B	78	LEU	4.4
1	B	123	THR	4.3
1	C	123	THR	4.3
1	A	90	ARG	4.2
1	C	31	LEU	4.1
1	D	171	VAL	4.0
1	D	208	SER	4.0
1	D	4	SER	4.0
1	B	172	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	59	HIS	4.0
1	B	59	HIS	3.9
1	A	92	ILE	3.7
1	D	71	TYR	3.6
1	D	167	THR	3.5
1	B	153	ASN	3.4
1	B	124	LEU	3.4
1	B	120	ASP	3.4
1	A	126	GLY	3.3
1	D	168	PRO	3.3
1	C	151	GLN	3.2
1	D	136	ILE	3.2
1	C	90	ARG	3.2
1	D	191	ALA	3.1
1	A	153	ASN	3.1
1	C	27	TYR	3.1
1	B	147	SER	3.1
1	A	23	ILE	3.0
1	C	191	ALA	3.0
1	C	216	LYS	2.9
1	D	12	ASP	2.9
1	D	151	GLN	2.8
1	A	34	VAL	2.8
1	C	28	ALA	2.8
1	A	91	SER	2.8
1	A	94	MET	2.7
1	B	210	THR	2.7
1	B	142	MET	2.7
1	C	26	HIS	2.7
1	D	154	PRO	2.6
1	A	58	GLY	2.6
1	D	52	VAL	2.5
1	D	197	TYR	2.5
1	C	149	VAL	2.5
1	D	122	SER	2.5
1	C	145	LEU	2.5
1	B	150	ARG	2.4
1	C	144	THR	2.4
1	D	206	VAL	2.4
1	B	149	VAL	2.3
1	A	122	SER	2.3
1	D	25	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	207	ILE	2.3
1	A	127	LYS	2.3
1	D	35	PHE	2.2
1	B	146	LEU	2.2
1	C	168	PRO	2.2
1	B	52	VAL	2.2
1	C	188	VAL	2.2
1	D	20	LEU	2.2
1	D	163	LEU	2.2
1	A	171	VAL	2.2
1	B	74	PHE	2.2
1	D	155	LYS	2.2
1	D	64	LEU	2.2
1	B	164	VAL	2.1
1	C	24	PRO	2.1
1	D	153	ASN	2.1
1	B	75	ALA	2.1
1	B	11	ASP	2.1
1	D	23	ILE	2.1
1	B	36	ILE	2.1
1	D	142	MET	2.1
1	C	197	TYR	2.1
1	C	25	ASN	2.1
1	D	187	VAL	2.1
1	B	211	GLY	2.0
1	D	164	VAL	2.0
1	C	71	TYR	2.0
1	C	100	ARG	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	4X2	C	302	21/21	0.88	0.18	-0.03	27,38,44,49	0
3	4X2	D	302	21/21	0.83	0.19	-0.26	44,48,80,81	0
3	4X2	B	302	21/21	0.87	0.17	-0.42	47,59,60,62	0
3	4X2	A	302	21/21	0.91	0.14	-0.91	25,30,38,43	0
2	MG	D	301	1/1	0.99	0.10	-	27,27,27,27	0
2	MG	A	301	1/1	0.96	0.09	-	21,21,21,21	0
2	MG	C	301	1/1	0.93	0.10	-	25,25,25,25	0
2	MG	B	301	1/1	0.96	0.07	-	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.