



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:26 pm GMT

PDB ID : 5JDC
Title : Trypanosoma brucei PTR1 in complex with inhibitor NP-13 (Hesperetin)
Authors : Mangani, S.; Pozzi, C.; Di Pisa, F.; Landi, G.; Dello Iacono, L.
Deposited on : 2016-04-16
Resolution : 1.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : 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

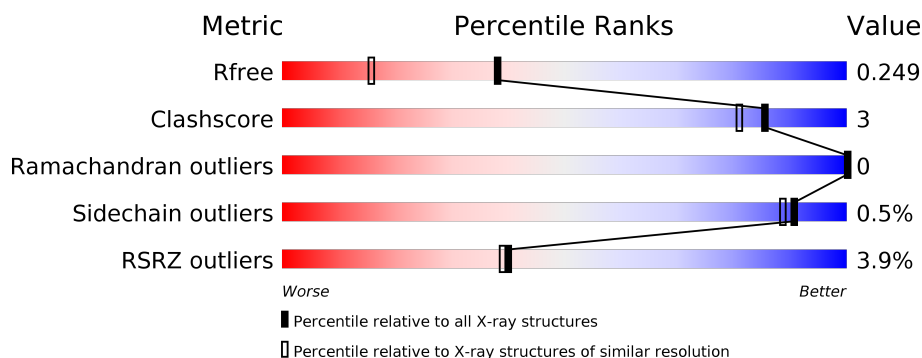
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	7172 (1.80-1.76)
Clashscore	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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 $\leq 5\%$. 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	288	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>5%</div> <div>14%</div> </div> </div>
1	B	288	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>•</div> <div>15%</div> </div> </div>
1	D	288	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>14%</div> </div> </div>
2	C	288	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>6%</div> <div>17%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAP	C	301	-	-	-	X
4	6JP	A	302	-	-	-	X
4	6JP	B	302	-	-	-	X
4	6JP	D	302	-	-	-	X
5	ACT	C	303	-	-	-	X
6	GOL	C	304	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7836 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 Pteridine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1845	1161	326	347	11			
1	B	246	Total	C	N	O	S	0	3	0
			1838	1156	320	350	12			
1	D	248	Total	C	N	O	S	0	2	0
			1831	1152	325	343	11			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O76290
A	-18	GLY	-	expression tag	UNP O76290
A	-17	SER	-	expression tag	UNP O76290
A	-16	SER	-	expression tag	UNP O76290
A	-15	HIS	-	expression tag	UNP O76290
A	-14	HIS	-	expression tag	UNP O76290
A	-13	HIS	-	expression tag	UNP O76290
A	-12	HIS	-	expression tag	UNP O76290
A	-11	HIS	-	expression tag	UNP O76290
A	-10	HIS	-	expression tag	UNP O76290
A	-9	SER	-	expression tag	UNP O76290
A	-8	SER	-	expression tag	UNP O76290
A	-7	GLY	-	expression tag	UNP O76290
A	-6	LEU	-	expression tag	UNP O76290
A	-5	VAL	-	expression tag	UNP O76290
A	-4	PRO	-	expression tag	UNP O76290
A	-3	ARG	-	expression tag	UNP O76290
A	-2	GLY	-	expression tag	UNP O76290
A	-1	SER	-	expression tag	UNP O76290
A	0	HIS	-	expression tag	UNP O76290
B	-19	MET	-	initiating methionine	UNP O76290
B	-18	GLY	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression tag	UNP O76290
B	-13	HIS	-	expression tag	UNP O76290
B	-12	HIS	-	expression tag	UNP O76290
B	-11	HIS	-	expression tag	UNP O76290
B	-10	HIS	-	expression tag	UNP O76290
B	-9	SER	-	expression tag	UNP O76290
B	-8	SER	-	expression tag	UNP O76290
B	-7	GLY	-	expression tag	UNP O76290
B	-6	LEU	-	expression tag	UNP O76290
B	-5	VAL	-	expression tag	UNP O76290
B	-4	PRO	-	expression tag	UNP O76290
B	-3	ARG	-	expression tag	UNP O76290
B	-2	GLY	-	expression tag	UNP O76290
B	-1	SER	-	expression tag	UNP O76290
B	0	HIS	-	expression tag	UNP O76290
D	-19	MET	-	initiating methionine	UNP O76290
D	-18	GLY	-	expression tag	UNP O76290
D	-17	SER	-	expression tag	UNP O76290
D	-16	SER	-	expression tag	UNP O76290
D	-15	HIS	-	expression tag	UNP O76290
D	-14	HIS	-	expression tag	UNP O76290
D	-13	HIS	-	expression tag	UNP O76290
D	-12	HIS	-	expression tag	UNP O76290
D	-11	HIS	-	expression tag	UNP O76290
D	-10	HIS	-	expression tag	UNP O76290
D	-9	SER	-	expression tag	UNP O76290
D	-8	SER	-	expression tag	UNP O76290
D	-7	GLY	-	expression tag	UNP O76290
D	-6	LEU	-	expression tag	UNP O76290
D	-5	VAL	-	expression tag	UNP O76290
D	-4	PRO	-	expression tag	UNP O76290
D	-3	ARG	-	expression tag	UNP O76290
D	-2	GLY	-	expression tag	UNP O76290
D	-1	SER	-	expression tag	UNP O76290
D	0	HIS	-	expression tag	UNP O76290

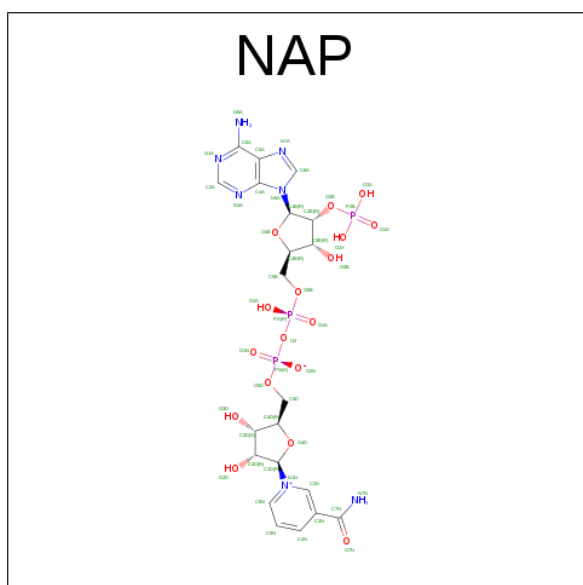
- Molecule 2 is a protein called Pteridine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	239	Total	C	N	O	S	0	0	0
			1771	1114	313	334	10			

There are 20 discrepancies between the modelled and reference sequences:

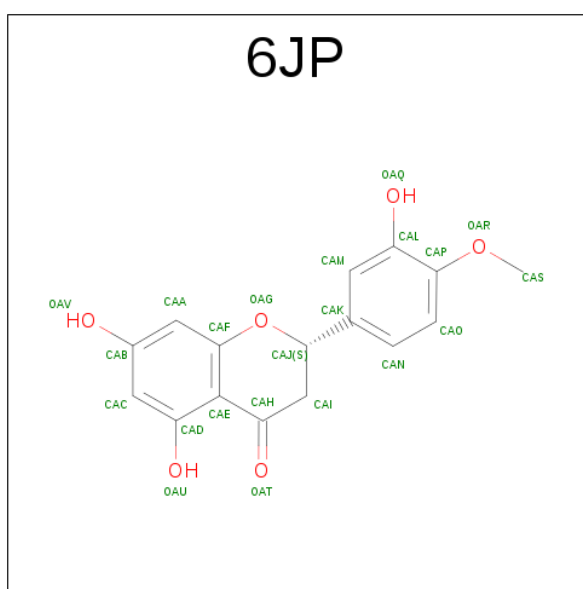
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP O76290
C	-18	GLY	-	expression tag	UNP O76290
C	-17	SER	-	expression tag	UNP O76290
C	-16	SER	-	expression tag	UNP O76290
C	-15	HIS	-	expression tag	UNP O76290
C	-14	HIS	-	expression tag	UNP O76290
C	-13	HIS	-	expression tag	UNP O76290
C	-12	HIS	-	expression tag	UNP O76290
C	-11	HIS	-	expression tag	UNP O76290
C	-10	HIS	-	expression tag	UNP O76290
C	-9	SER	-	expression tag	UNP O76290
C	-8	SER	-	expression tag	UNP O76290
C	-7	GLY	-	expression tag	UNP O76290
C	-6	LEU	-	expression tag	UNP O76290
C	-5	VAL	-	expression tag	UNP O76290
C	-4	PRO	-	expression tag	UNP O76290
C	-3	ARG	-	expression tag	UNP O76290
C	-2	GLY	-	expression tag	UNP O76290
C	-1	SER	-	expression tag	UNP O76290
C	0	HIS	-	expression tag	UNP O76290

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



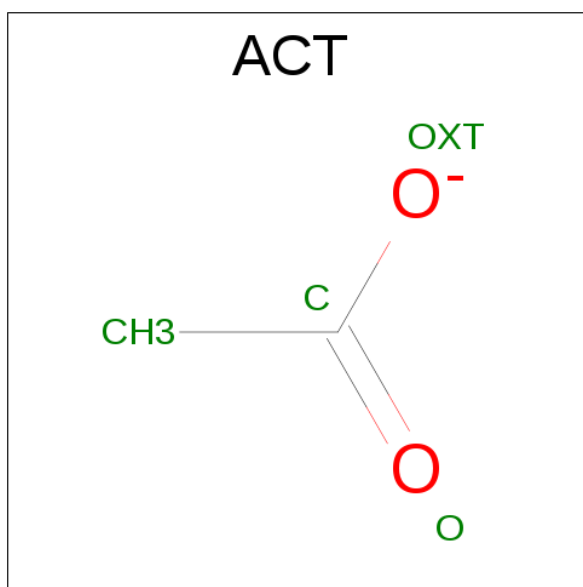
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	
			48	21	7	17	3	
3	B	1	Total	C	N	O	P	
			48	21	7	17	3	
3	C	1	Total	C	N	O	P	
			48	21	7	17	3	
3	D	1	Total	C	N	O	P	
			48	21	7	17	3	

- Molecule 4 is (2S)-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-2,3-dihydro-4H-1-benzopyran-4-one (three-letter code: 6JP) (formula: C₁₆H₁₄O₆).



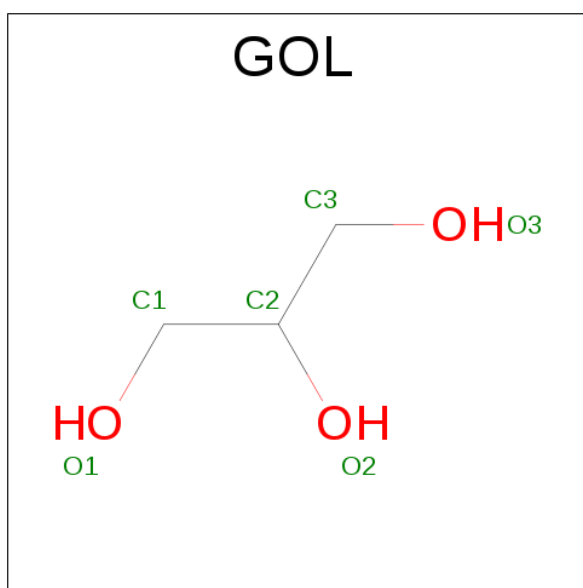
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			22	16 6		
4	B	1	Total	C O	0	0
			22	16 6		
4	C	1	Total	C O	0	0
			22	16 6		
4	D	1	Total	C O	0	0
			22	16 6		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		

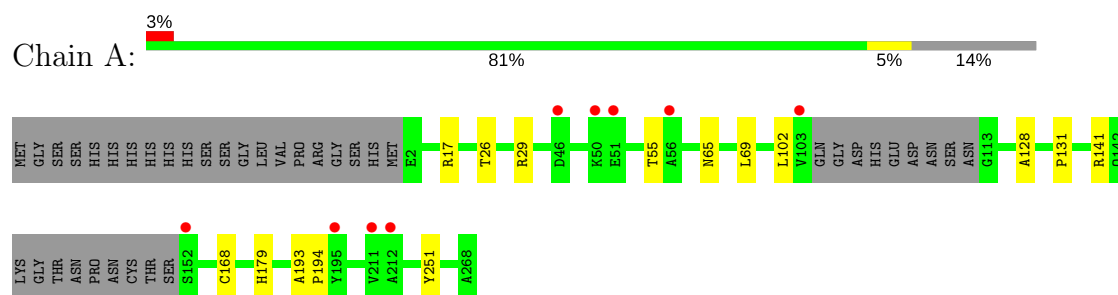
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	66	Total 66	O 66	0	0
7	B	86	Total 86	O 86	0	0
7	C	54	Total 54	O 54	0	0
7	D	51	Total 51	O 51	0	0

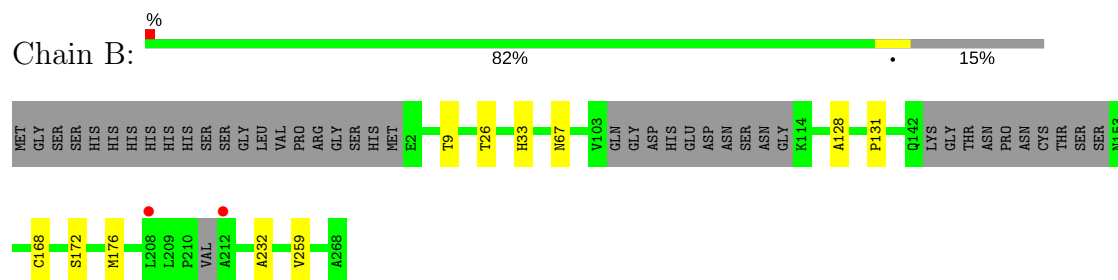
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

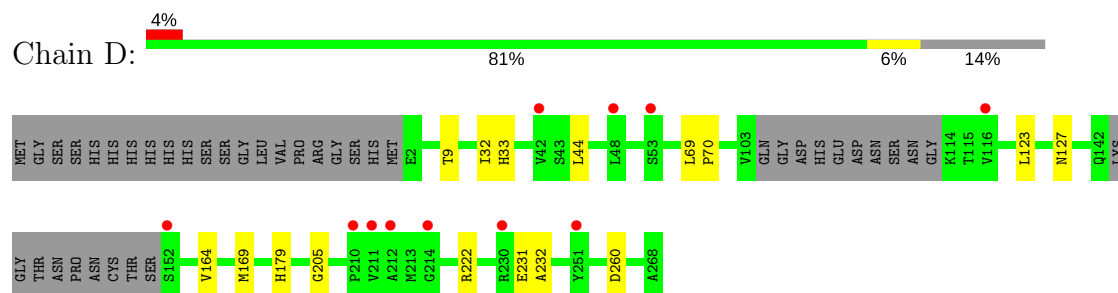
• Molecule 1: Pteridine reductase



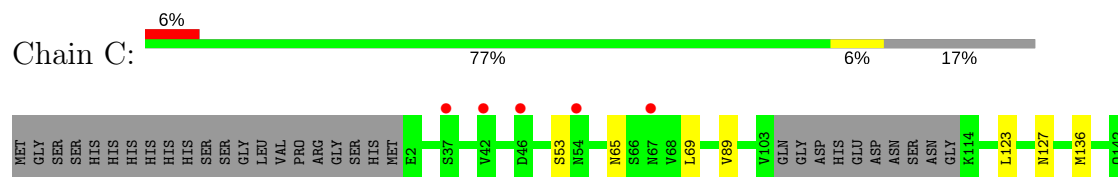
• Molecule 1: Pteridine reductase

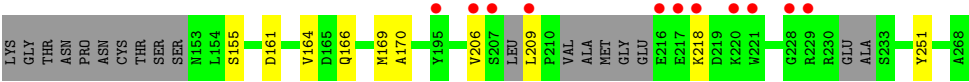


• Molecule 1: Pteridine reductase



• Molecule 2: Pteridine reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.84Å 90.04Å 82.94Å 90.00° 115.78° 90.00°	Depositor
Resolution (Å)	53.68 – 1.78 53.95 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.1 (53.68-1.78) 99.1 (53.95-1.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.208 , 0.241 0.222 , 0.249	Depositor DCC
R_{free} test set	4615 reflections (5.17%)	DCC
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7836	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.38 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.7194e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 6JP, NAP, CSX, ACT, OCS

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	0.84	0/1864	0.86	0/2528
1	B	0.95	1/1855 (0.1%)	0.90	0/2516
1	D	0.86	0/1856	0.91	0/2520
2	C	0.87	0/1777	0.86	0/2408
All	All	0.88	1/7352 (0.0%)	0.88	0/9972

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	VAL	C-N	13.19	1.64	1.34

There are no bond angle outliers.

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	1845	0	1867	13	0
1	B	1838	0	1846	9	0
1	D	1831	0	1846	10	0
2	C	1771	0	1776	10	0
3	A	48	0	25	0	0
3	B	48	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	48	0	25	0	0
3	D	48	0	25	1	0
4	A	22	0	0	1	0
4	B	22	0	0	3	0
4	C	22	0	0	0	0
4	D	22	0	0	0	0
5	A	4	0	3	1	0
5	C	4	0	3	0	0
6	C	6	0	8	0	0
7	A	66	0	0	1	0
7	B	86	0	0	1	0
7	C	54	0	0	0	0
7	D	51	0	0	0	0
All	All	7836	0	7449	39	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 3.

All (39) 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:168[A]:CSX:HG	4:B:302:6JP:CAS	1.81	0.94
2:C:161:ASP:HB3	2:C:164:VAL:HG13	1.76	0.67
1:A:141:ARG:HG2	7:A:465:HOH:O	1.95	0.66
1:A:193:ALA:HB3	1:A:194:PRO:HD3	1.82	0.60
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.37	0.59
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.88	0.56
2:C:209:LEU:HD13	2:C:218:LYS:HG3	1.88	0.56
1:A:168:CSX:HG	4:A:302:6JP:CAP	2.19	0.55
2:C:209:LEU:HD13	2:C:218:LYS:CG	2.38	0.54
2:C:65:ASN:HA	2:C:69:LEU:HD22	1.91	0.52
1:D:205:GLY:HA3	1:D:260:ASP:HB2	1.92	0.51
1:B:168[A]:CSX:SG	4:B:302:6JP:CAS	2.94	0.51
1:A:17:ARG:HD3	5:A:303:ACT:H3	1.93	0.50
1:B:128:ALA:C	1:B:131:PRO:HD2	2.32	0.50
2:C:251:TYR:CE2	1:D:232:ALA:HB2	2.47	0.49
1:D:69:LEU:N	1:D:70:PRO:HD2	2.27	0.49
1:A:128:ALA:C	1:A:131:PRO:HD2	2.33	0.49
1:A:251:TYR:CD2	1:B:232:ALA:HB2	2.48	0.48
1:A:193:ALA:N	1:A:194:PRO:CD	2.76	0.48
1:D:69:LEU:N	1:D:70:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:SER:O	1:B:176:MET:HG3	2.15	0.46
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.52	0.44
2:C:123:LEU:O	2:C:127:ASN:HB2	2.17	0.44
1:D:205:GLY:O	3:D:301:NAP:H4N	2.16	0.44
1:A:102:LEU:O	2:C:136:MET:HG3	2.17	0.44
2:C:169:MET:O	2:C:170:ALA:HB3	2.19	0.43
4:B:302:6JP:OAT	4:B:302:6JP:OAU	2.37	0.42
2:C:89:VAL:HA	2:C:155:SER:O	2.19	0.42
1:A:29:ARG:HG2	1:A:55:THR:HG22	2.01	0.42
1:B:9:THR:HA	1:B:33:HIS:HB3	2.02	0.42
2:C:206:VAL:O	2:C:206:VAL:HG23	2.19	0.41
1:D:9:THR:HA	1:D:33:HIS:HB3	2.02	0.41
1:D:123:LEU:O	1:D:127:ASN:HB2	2.19	0.41
1:B:26:THR:O	1:B:26:THR:HG22	2.21	0.41
1:A:26:THR:O	1:A:26:THR:HG22	2.21	0.41
1:D:32:ILE:HD13	1:D:44:LEU:HD23	2.03	0.41
1:B:67:ASN:HB2	7:B:461:HOH:O	2.20	0.41
1:A:193:ALA:N	1:A:194:PRO:HD2	2.36	0.40
1:D:222:ARG:HD3	1:D:231:GLU:OE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/288 (84%)	234 (97%)	8 (3%)	0	100	100
1	B	239/288 (83%)	233 (98%)	6 (2%)	0	100	100
1	D	243/288 (84%)	234 (96%)	9 (4%)	0	100	100
2	C	225/288 (78%)	218 (97%)	7 (3%)	0	100	100
All	All	949/1152 (82%)	919 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	193/230 (84%)	192 (100%)	1 (0%)	91	89
1	B	192/230 (84%)	192 (100%)	0	100	100
1	D	191/230 (83%)	190 (100%)	1 (0%)	91	89
2	C	184/229 (80%)	182 (99%)	2 (1%)	78	70
All	All	760/919 (83%)	756 (100%)	4 (0%)	91	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	HIS
2	C	53	SER
2	C	166	GLN
1	D	169	MET

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 ⓘ

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSX	A	168	1	4,6,7	0.55	0	2,6,8	1.14	0
1	CSX	B	168[A]	1	4,6,7	0.80	0	2,6,8	0.74	0
1	CSX	B	168[B]	1	4,6,7	1.57	1 (25%)	2,6,8	2.57	1 (50%)
2	CSX	C	168	2	4,6,7	0.64	0	2,6,8	0.96	0
2	OCS	C	59	2	8,8,9	1.90	1 (12%)	7,11,13	2.37	1 (14%)
1	CSX	D	168	1	4,6,7	0.47	0	2,6,8	1.05	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
1	CSX	A	168	1	-	0/1/5/7	0/0/0/0
1	CSX	B	168[A]	1	-	0/1/5/7	0/0/0/0
1	CSX	B	168[B]	1	-	0/1/5/7	0/0/0/0
2	CSX	C	168	2	-	0/1/5/7	0/0/0/0
2	OCS	C	59	2	-	1/4/7/9	0/0/0/0
1	CSX	D	168	1	-	0/1/5/7	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168[B]	CSX	CA-C	2.25	1.53	1.50
2	C	59	OCS	OD3-SG	4.83	1.59	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168[B]	CSX	CA-CB-SG	3.40	121.10	113.47
2	C	59	OCS	OD3-SG-CB	5.32	111.38	106.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	59	OCS	SG-CB-CA-N

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	168	CSX	1	0
1	B	168[A]	CSX	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 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
3	NAP	A	301	-	44,52,52	1.09	3 (6%)	51,80,80	1.57	6 (11%)
4	6JP	A	302	-	24,24,24	1.88	4 (16%)	35,35,35	1.62	6 (17%)
5	ACT	A	303	-	1,3,3	3.79	1 (100%)	0,3,3	0.00	-
3	NAP	B	301	-	44,52,52	1.07	3 (6%)	51,80,80	1.80	10 (19%)
4	6JP	B	302	-	24,24,24	1.89	5 (20%)	35,35,35	2.28	9 (25%)
3	NAP	C	301	-	44,52,52	1.06	2 (4%)	51,80,80	1.82	8 (15%)
4	6JP	C	302	-	24,24,24	1.72	3 (12%)	35,35,35	1.78	7 (20%)
5	ACT	C	303	-	1,3,3	1.35	0	0,3,3	0.00	-
6	GOL	C	304	-	5,5,5	0.77	0	5,5,5	0.72	0
3	NAP	D	301	-	44,52,52	1.18	5 (11%)	51,80,80	1.89	9 (17%)
4	6JP	D	302	-	24,24,24	2.01	5 (20%)	35,35,35	1.50	5 (14%)

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	NAP	A	301	-	-	0/27/67/67	0/5/5/5
4	6JP	A	302	-	-	0/6/18/18	0/3/3/3
5	ACT	A	303	-	-	0/0/0/0	0/0/0/0
3	NAP	B	301	-	-	0/27/67/67	0/5/5/5
4	6JP	B	302	-	-	0/6/18/18	0/3/3/3
3	NAP	C	301	-	-	0/27/67/67	0/5/5/5
4	6JP	C	302	-	-	0/6/18/18	0/3/3/3
5	ACT	C	303	-	-	0/0/0/0	0/0/0/0
6	GOL	C	304	-	-	0/4/4/4	0/0/0/0
3	NAP	D	301	-	-	0/27/67/67	0/5/5/5
4	6JP	D	302	-	-	0/6/18/18	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	6JP	CAK-CAJ	-5.62	1.42	1.51
4	D	302	6JP	CAI-CAH	-5.13	1.41	1.50
4	B	302	6JP	CAI-CAH	-4.96	1.41	1.50
4	B	302	6JP	CAK-CAJ	-4.75	1.43	1.51
4	D	302	6JP	CAK-CAJ	-4.74	1.43	1.51
4	C	302	6JP	CAK-CAJ	-4.69	1.43	1.51
4	A	302	6JP	CAI-CAH	-4.47	1.42	1.50
4	C	302	6JP	CAI-CAH	-4.28	1.43	1.50
5	A	303	ACT	CH3-C	-3.79	1.43	1.48
4	B	302	6JP	OAG-CAF	-2.51	1.34	1.37
4	B	302	6JP	CAE-CAH	-2.29	1.41	1.46
4	D	302	6JP	CAE-CAH	-2.19	1.41	1.46
3	A	301	NAP	PA-O2A	-2.03	1.44	1.55
4	A	302	6JP	CAM-CAK	2.01	1.42	1.39
4	A	302	6JP	OAR-CAP	2.09	1.40	1.37
3	D	301	NAP	O2D-C2D	2.10	1.47	1.43
3	D	301	NAP	C5A-C4A	2.21	1.45	1.40
3	B	301	NAP	C2A-N3A	2.23	1.35	1.32
4	D	302	6JP	CAC-CAD	2.35	1.42	1.38
4	B	302	6JP	CAL-CAP	2.37	1.44	1.40
4	D	302	6JP	CAM-CAK	2.67	1.43	1.39
4	C	302	6JP	CAN-CAK	2.71	1.43	1.39
3	A	301	NAP	C5A-C4A	2.81	1.46	1.40
3	C	301	NAP	P2B-O2B	2.81	1.64	1.59
3	D	301	NAP	C7N-N7N	2.88	1.38	1.33
3	B	301	NAP	C5A-C4A	2.90	1.47	1.40
3	D	301	NAP	O4D-C1D	3.35	1.45	1.41
3	B	301	NAP	P2B-O2B	3.48	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	NAP	C5A-C4A	3.55	1.48	1.40
3	A	301	NAP	P2B-O2B	3.82	1.66	1.59
3	D	301	NAP	P2B-O2B	3.86	1.66	1.59

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	NAP	N3A-C2A-N1A	-8.42	121.53	128.86
3	C	301	NAP	N3A-C2A-N1A	-7.49	122.33	128.86
3	B	301	NAP	N3A-C2A-N1A	-6.65	123.06	128.86
3	A	301	NAP	N3A-C2A-N1A	-6.37	123.31	128.86
3	D	301	NAP	C1B-N9A-C4A	-5.90	116.44	126.64
3	A	301	NAP	C1B-N9A-C4A	-4.71	118.50	126.64
4	B	302	6JP	OAR-CAP-CAO	-4.46	116.89	124.37
3	A	301	NAP	C4B-O4B-C1B	-4.15	105.36	109.77
4	A	302	6JP	OAG-CAF-CAE	-3.98	117.39	121.62
4	B	302	6JP	OAG-CAF-CAE	-3.75	117.63	121.62
3	D	301	NAP	C4B-O4B-C1B	-3.39	106.16	109.77
4	D	302	6JP	OAG-CAF-CAE	-3.38	118.03	121.62
3	B	301	NAP	C1B-N9A-C4A	-3.35	120.84	126.64
4	B	302	6JP	OAU-CAD-CAE	-3.29	114.86	121.14
3	B	301	NAP	O7N-C7N-C3N	-3.27	115.80	119.62
3	C	301	NAP	C1B-N9A-C4A	-3.25	121.02	126.64
3	B	301	NAP	C4A-C5A-N7A	-3.16	106.36	109.41
3	B	301	NAP	C4B-O4B-C1B	-3.07	106.50	109.77
3	C	301	NAP	C4B-O4B-C1B	-2.84	106.75	109.77
3	B	301	NAP	O2B-P2B-O1X	-2.69	98.70	109.26
3	A	301	NAP	O7N-C7N-C3N	-2.64	116.53	119.62
3	C	301	NAP	C4A-C5A-N7A	-2.64	106.86	109.41
4	C	302	6JP	OAR-CAP-CAO	-2.61	120.00	124.37
3	D	301	NAP	C4A-C5A-N7A	-2.60	106.89	109.41
4	C	302	6JP	OAG-CAF-CAE	-2.37	119.10	121.62
4	C	302	6JP	CAJ-CAI-CAH	-2.32	105.47	112.98
4	A	302	6JP	CAJ-CAI-CAH	-2.30	105.55	112.98
4	B	302	6JP	CAJ-CAI-CAH	-2.27	105.64	112.98
3	C	301	NAP	O7N-C7N-N7N	-2.24	119.39	122.58
3	C	301	NAP	O7N-C7N-C3N	-2.21	117.04	119.62
4	A	302	6JP	OAU-CAD-CAE	-2.20	116.94	121.14
3	D	301	NAP	O7N-C7N-C3N	-2.18	117.08	119.62
3	D	301	NAP	C3N-C7N-N7N	2.00	120.06	117.77
3	B	301	NAP	O5B-PA-O1A	2.01	117.37	109.25
3	A	301	NAP	O3X-P2B-O2X	2.04	115.86	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	302	6JP	CAD-CAE-CAH	2.05	123.64	120.57
3	A	301	NAP	C4D-O4D-C1D	2.15	112.05	109.77
3	D	301	NAP	O2X-P2B-O1X	2.19	119.06	110.50
4	B	302	6JP	CAD-CAC-CAB	2.23	121.67	119.65
4	A	302	6JP	CAI-CAH-CAE	2.24	121.35	117.23
4	D	302	6JP	CAF-OAG-CAJ	2.28	119.50	115.68
3	D	301	NAP	O4B-C1B-C2B	2.35	110.71	106.59
4	C	302	6JP	CAD-CAC-CAB	2.40	121.82	119.65
3	B	301	NAP	O3X-P2B-O2X	2.42	117.37	107.61
4	B	302	6JP	CAF-OAG-CAJ	2.43	119.75	115.68
4	D	302	6JP	CAI-CAH-CAE	2.45	121.75	117.23
4	B	302	6JP	CAF-CAE-CAH	2.58	122.89	120.41
3	B	301	NAP	O2A-PA-O1A	2.73	126.39	112.28
3	D	301	NAP	C2A-N1A-C6A	2.87	123.80	118.77
4	D	302	6JP	CAD-CAC-CAB	3.07	122.44	119.65
4	A	302	6JP	CAF-OAG-CAJ	3.31	121.22	115.68
3	C	301	NAP	C2A-N1A-C6A	3.50	124.89	118.77
4	A	302	6JP	CAS-OAR-CAP	3.85	123.08	117.54
4	D	302	6JP	CAS-OAR-CAP	4.43	123.91	117.54
4	B	302	6JP	CAS-OAR-CAP	4.76	124.38	117.54
4	C	302	6JP	OAR-CAP-CAL	4.88	120.49	114.55
3	C	301	NAP	C3N-C7N-N7N	5.01	123.50	117.77
3	B	301	NAP	C3N-C7N-N7N	5.36	123.89	117.77
4	C	302	6JP	CAS-OAR-CAP	5.77	125.84	117.54
4	B	302	6JP	OAR-CAP-CAL	7.58	123.78	114.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	6JP	1	0
5	A	303	ACT	1	0
4	B	302	6JP	3	0
3	D	301	NAP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	259:VAL	C	260:ASP	N	1.64

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	248/288 (86%)	0.58	9 (3%) 43 42	10, 19, 38, 51	0
1	B	245/288 (85%)	0.30	2 (0%) 86 86	9, 16, 33, 43	0
1	D	247/288 (85%)	0.57	11 (4%) 34 33	10, 20, 40, 55	0
2	C	237/288 (82%)	0.62	16 (6%) 18 18	10, 19, 42, 63	0
All	All	977/1152 (84%)	0.52	38 (3%) 40 39	9, 19, 38, 63	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	206	VAL	5.1
2	C	220	LYS	4.9
1	B	212	ALA	4.6
2	C	221	TRP	4.5
1	A	212	ALA	4.2
1	D	211	VAL	4.1
2	C	216	GLU	3.9
2	C	209	LEU	3.7
1	D	212	ALA	3.5
1	D	152	SER	3.4
2	C	228	GLY	3.0
1	A	211	VAL	2.8
1	B	208	LEU	2.8
2	C	217	GLU	2.7
2	C	195	TYR	2.7
1	A	56	ALA	2.6
2	C	67	ASN	2.6
2	C	218	LYS	2.6
1	A	50	LYS	2.5
2	C	46	ASP	2.5
2	C	54	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	42	VAL	2.4
1	A	152	SER	2.4
1	A	195	TYR	2.4
1	D	251	TYR	2.2
1	A	46	ASP	2.2
1	D	214	GLY	2.2
1	D	53[A]	SER	2.1
2	C	229	ARG	2.1
2	C	207	SER	2.1
1	A	103	VAL	2.1
1	D	210	PRO	2.1
1	D	230	ARG	2.1
2	C	37	SER	2.1
1	D	116	VAL	2.1
1	D	48	LEU	2.1
1	A	51	GLU	2.0
1	D	42	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	OCS	C	59	9/10	0.95	0.08	-	16,19,24,24	0
1	CSX	A	168	7/8	0.86	0.12	-	23,28,54,55	0
1	CSX	D	168	7/8	0.85	0.11	-	23,28,50,54	0
2	CSX	C	168	7/8	0.89	0.12	-	22,26,41,50	0
1	CSX	B	168[B]	7/8	0.87	0.14	-	20,23,27,30	7
1	CSX	B	168[A]	7/8	0.87	0.14	-	18,21,22,25	7

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
4	6JP	D	302	22/22	0.71	0.26	5.22	37,44,48,49	0
4	6JP	B	302	22/22	0.71	0.24	4.17	36,42,58,64	0
6	GOL	C	304	6/6	0.74	0.22	2.89	29,39,40,44	0
4	6JP	A	302	22/22	0.78	0.17	2.19	27,35,44,50	0
3	NAP	C	301	48/48	0.83	0.22	2.18	21,33,45,55	0
5	ACT	C	303	4/4	0.91	0.17	2.06	26,27,30,31	0
4	6JP	C	302	22/22	0.64	0.26	1.82	47,55,64,81	0
3	NAP	B	301	48/48	0.91	0.14	1.38	15,20,31,33	0
3	NAP	D	301	48/48	0.90	0.14	0.98	17,26,36,41	0
5	ACT	A	303	4/4	0.85	0.16	0.22	22,23,24,34	0
3	NAP	A	301	48/48	0.94	0.11	-0.24	16,21,33,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.