Full wwPDB X-ray Structure Validation Report

Feb 12, 2017 – 09:08 PM EST

PDB ID	:	5TZC
Title	:	Crystal Structure of human PDE2a in complex with (5S)-1-[(3-bromo-4-fluorophenyl)carbonyl]-3,3-difluoro-5-{5-methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl}piperidine
Authors	:	Xu, R.; Aertgeerts, K.
Deposited on	:	2016-11-21
Resolution	:	2.36 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

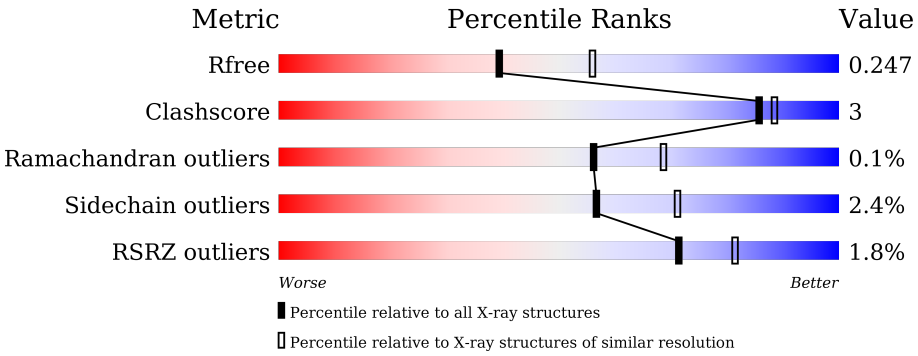
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.36 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 <=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	344	93% 6%
1	B	344	2% 90% 9%
1	C	344	3% 92% 6%
1	D	344	90% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11475 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.

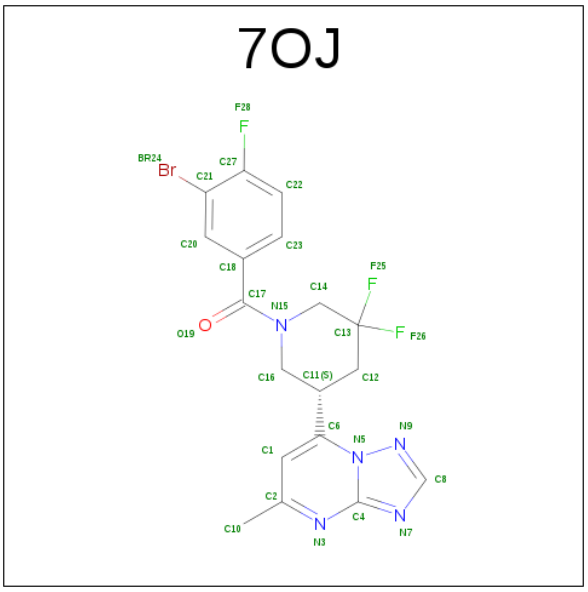
- Molecule 1 is a protein called cGMP-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	3	0
			2820	1794	482	518	26			
1	B	343	Total	C	N	O	S	0	3	0
			2814	1791	479	517	27			
1	C	340	Total	C	N	O	S	0	1	0
			2786	1774	476	510	26			
1	D	336	Total	C	N	O	S	0	3	0
			2765	1765	474	501	25			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	576	SER	-	expression tag	UNP O00408
A	577	ALA	-	expression tag	UNP O00408
A	578	MET	-	expression tag	UNP O00408
B	576	SER	-	expression tag	UNP O00408
B	577	ALA	-	expression tag	UNP O00408
B	578	MET	-	expression tag	UNP O00408
C	576	SER	-	expression tag	UNP O00408
C	577	ALA	-	expression tag	UNP O00408
C	578	MET	-	expression tag	UNP O00408
D	576	SER	-	expression tag	UNP O00408
D	577	ALA	-	expression tag	UNP O00408
D	578	MET	-	expression tag	UNP O00408

- Molecule 2 is (3-bromo-4-fluorophenyl)[(5S)-3,3-difluoro-5-(5-methyl[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)piperidin-1-yl]methanone (three-letter code: 7OJ) (formula: $C_{18}H_{15}BrF_3N_5O$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	F	N	O	0	0
			28	1	18	3	5	1		
2	B	1	Total	Br	C	F	N	O	0	0
			28	1	18	3	5	1		
2	C	1	Total	Br	C	F	N	O	0	0
			28	1	18	3	5	1		
2	D	1	Total	Br	C	F	N	O	0	0
			28	1	18	3	5	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

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

- Molecule 5 is water.

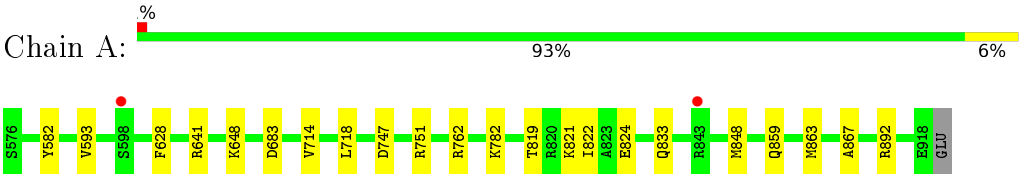
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	47	Total O 47 47	0	0
5	B	48	Total O 48 48	0	0
5	C	38	Total O 38 38	0	0
5	D	37	Total O 37 37	0	0

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.

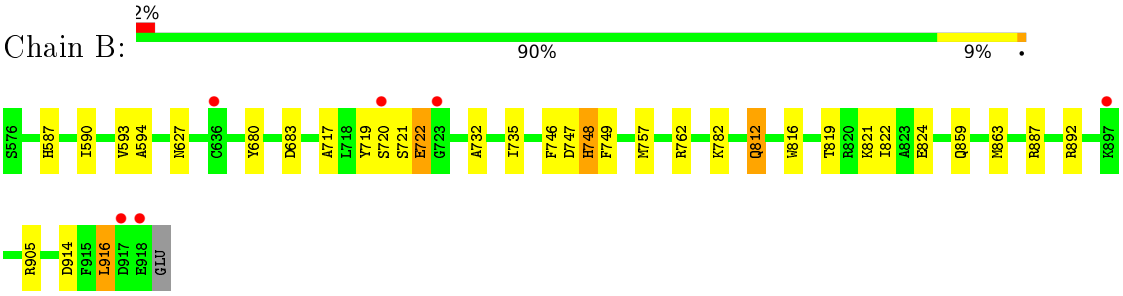
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

Chain A:



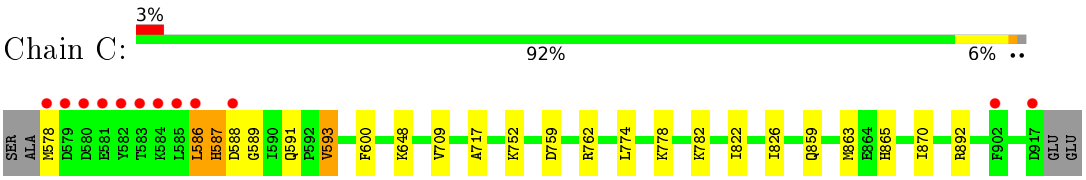
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

Chain B:



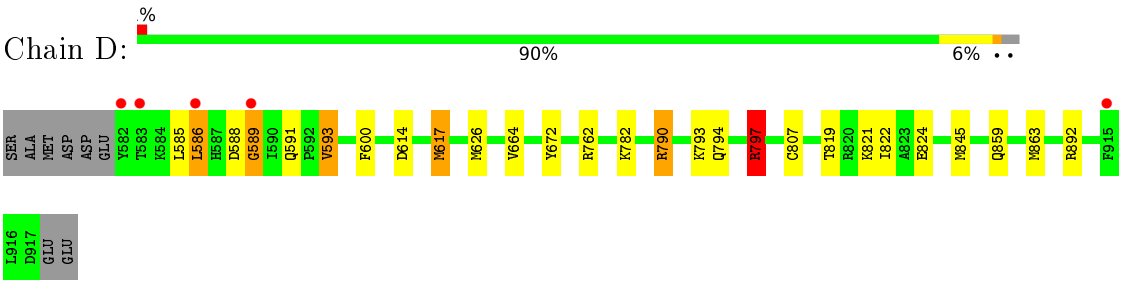
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

Chain C:



- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.85Å 73.44Å 91.32Å 109.60° 90.90° 91.24°	Depositor
Resolution (Å)	46.81 – 2.36 46.76 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.81-2.36) 87.2 (46.76-2.36)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.37Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.240 0.205 , 0.247	Depositor DCC
R_{free} test set	2821 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11475	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: ZN, MG, 7OJ

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	0.65	0/2896	0.72	1/3906 (0.0%)
1	B	0.66	0/2890	0.76	7/3898 (0.2%)
1	C	0.60	0/2856	0.68	1/3853 (0.0%)
1	D	0.66	0/2841	0.76	4/3832 (0.1%)
All	All	0.64	0/11483	0.73	13/15489 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	790	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	D	586	LEU	CA-CB-CG	5.90	128.88	115.30
1	B	887	ARG	CG-CD-NE	-5.84	99.52	111.80
1	D	797	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	586	LEU	CA-CB-CG	5.43	127.79	115.30
1	D	797	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	B	762	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	747	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	916	LEU	N-CA-C	-5.08	97.28	111.00
1	B	905	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	905	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	747	ASP	CB-CG-OD1	-5.04	113.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	762	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	721	SER	Peptide

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	2820	0	2762	22	0
1	B	2814	0	2757	22	0
1	C	2786	0	2727	14	0
1	D	2765	0	2725	16	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
2	C	28	0	0	1	0
2	D	28	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	47	0	0	3	0
5	B	48	0	0	0	0
5	C	38	0	0	1	0
5	D	37	0	0	2	0
All	All	11475	0	10971	63	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 (63) 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:C:578:MET:SD	1:C:648:LYS:HE3	2.02	1.00
1:A:683:ASP:HB3	5:A:1146:HOH:O	1.68	0.93
1:A:751[B]:ARG:HH11	1:A:751[B]:ARG:CG	1.94	0.81
1:A:648:LYS:HG3	1:D:790:ARG:HD3	1.64	0.76
1:A:751[B]:ARG:HH11	1:A:751[B]:ARG:HG2	1.54	0.73
1:C:578:MET:SD	1:C:648:LYS:CE	2.78	0.70
1:A:863:MET:HA	1:A:863:MET:HE3	1.73	0.70
1:D:794[B]:GLN:HE21	1:D:794[B]:GLN:HA	1.58	0.68
1:A:863:MET:HE3	1:A:867:ALA:HB3	1.78	0.66
1:B:720:SER:HA	1:B:722:GLU:OE1	1.97	0.64
1:B:812:GLN:HG2	1:B:863:MET:SD	2.42	0.60
1:B:719:TYR:O	1:B:722:GLU:OE1	2.20	0.59
1:A:718:LEU:HD22	1:B:732:ALA:CB	2.34	0.57
1:D:819:THR:HG23	5:D:1105:HOH:O	2.05	0.57
1:A:751[B]:ARG:NH1	1:A:751[B]:ARG:CG	2.60	0.56
1:A:819:THR:HG23	5:A:1116:HOH:O	2.06	0.55
1:A:833:GLN:NE2	1:A:848:MET:CE	2.70	0.55
1:D:588:ASP:O	1:D:589:GLY:O	2.28	0.52
1:A:718:LEU:HD22	1:B:732:ALA:HB2	1.91	0.52
1:C:859:GLN:O	1:C:863:MET:HG2	2.10	0.52
1:C:759:ASP:OD1	1:C:762:ARG:NH2	2.43	0.52
1:D:859:GLN:O	1:D:863:MET:HG2	2.10	0.51
1:D:845:MET:HG2	5:D:1123:HOH:O	2.11	0.51
1:C:593:VAL:HG22	1:C:600:PHE:CD2	2.46	0.50
1:D:593:VAL:HG22	1:D:600:PHE:CD2	2.46	0.50
1:B:746:PHE:HB3	1:B:749:PHE:HD2	1.77	0.49
1:B:859:GLN:O	1:B:863:MET:HG2	2.12	0.49
1:B:627:ASN:OD1	1:C:778:LYS:HD2	2.13	0.48
1:A:859:GLN:O	1:A:863:MET:HG2	2.13	0.48
1:B:720:SER:O	1:B:722:GLU:HB2	2.13	0.47
1:B:590:ILE:O	1:C:774:LEU:HD13	2.15	0.47
1:B:914:ASP:O	1:B:916:LEU:O	2.33	0.47
1:A:582:TYR:CE1	1:A:641:ARG:HG3	2.50	0.46
1:B:816:TRP:O	1:B:819:THR:HG22	2.15	0.46
1:A:833:GLN:NE2	1:A:848:MET:HE1	2.30	0.46
1:B:749:PHE:CE2	1:B:757:MET:HG3	2.52	0.45
1:B:594:ALA:HB1	1:C:865:HIS:CE1	2.52	0.45
1:B:812:GLN:HB2	1:B:812:GLN:HE21	1.62	0.45
1:A:628:PHE:HE1	5:A:1146:HOH:O	2.00	0.45
1:C:587:HIS:C	1:C:589:GLY:H	2.21	0.44
1:D:588:ASP:C	1:D:589:GLY:O	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:ARG:HG3	1:B:717:ALA:HB1	1.99	0.44
1:A:863:MET:HA	1:A:863:MET:CE	2.44	0.43
1:A:863:MET:HE3	1:A:867:ALA:CB	2.45	0.43
1:B:748:HIS:C	1:B:748:HIS:CD2	2.91	0.43
1:C:587:HIS:O	1:C:588:ASP:HB2	2.19	0.43
1:D:821:LYS:O	1:D:824:GLU:HB2	2.19	0.42
1:D:585:LEU:O	1:D:588:ASP:O	2.37	0.42
1:A:714:VAL:HG13	1:B:735:ILE:HG21	2.01	0.42
1:B:587:HIS:CD2	1:C:709:VAL:HG21	2.54	0.42
1:A:718:LEU:HD21	1:B:732:ALA:HA	2.02	0.42
1:B:680:TYR:CD1	1:B:680:TYR:N	2.87	0.42
1:A:821:LYS:O	1:A:824[A]:GLU:HB2	2.20	0.42
1:A:751[B]:ARG:HG3	1:A:751[B]:ARG:NH1	2.35	0.41
1:D:664:VAL:HG13	1:D:807:CYS:HB3	2.02	0.41
1:D:797:ARG:HG2	1:D:797:ARG:HH11	1.84	0.41
1:C:826:ILE:HD13	2:C:1001:7OJ:N5	2.36	0.41
1:B:821:LYS:O	1:B:824:GLU:HB2	2.20	0.41
1:D:626:MET:HG2	1:D:672:TYR:CD2	2.55	0.41
1:D:614:ASP:O	1:D:617:MET:HG3	2.21	0.41
1:C:870:ILE:HG13	5:C:1103:HOH:O	2.22	0.40
1:D:794[B]:GLN:CA	1:D:794[B]:GLN:HE21	2.25	0.40
1:C:717:ALA:O	1:D:762:ARG:NH2	2.54	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	344/344 (100%)	340 (99%)	4 (1%)	0	100	100
1	B	344/344 (100%)	337 (98%)	7 (2%)	0	100	100
1	C	339/344 (98%)	334 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	337/344 (98%)	332 (98%)	4 (1%)	1 (0%)	46 55
All	All	1364/1376 (99%)	1343 (98%)	20 (2%)	1 (0%)	56 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	589	GLY

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	312/310 (101%)	308 (99%)	4 (1%)	76 87
1	B	312/310 (101%)	304 (97%)	8 (3%)	54 68
1	C	308/310 (99%)	300 (97%)	8 (3%)	54 68
1	D	306/310 (99%)	297 (97%)	9 (3%)	50 64
All	All	1238/1240 (100%)	1209 (98%)	29 (2%)	57 73

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	593	VAL
1	A	782	LYS
1	A	822	ILE
1	A	892	ARG
1	B	593	VAL
1	B	683	ASP
1	B	722	GLU
1	B	748	HIS
1	B	782	LYS
1	B	812	GLN
1	B	822	ILE
1	B	892	ARG
1	C	586	LEU

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Mol	Chain	Res	Type
1	C	587	HIS
1	C	591	GLN
1	C	593	VAL
1	C	752	LYS
1	C	782	LYS
1	C	822	ILE
1	C	892	ARG
1	D	586	LEU
1	D	591	GLN
1	D	593	VAL
1	D	617	MET
1	D	782	LYS
1	D	793	LYS
1	D	797	ARG
1	D	822	ILE
1	D	892	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	894	HIS
1	B	748	HIS
1	B	812	GLN
1	C	791	ASN
1	C	894	HIS
1	D	791	ASN
1	D	894	HIS

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 (i)

Of 12 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
2	7OJ	A	1001	-	24,31,31	1.81	5 (20%)	31,47,47	3.50	13 (41%)
2	7OJ	B	1001	-	24,31,31	1.63	3 (12%)	31,47,47	1.69	8 (25%)
2	7OJ	C	1001	-	24,31,31	1.86	5 (20%)	31,47,47	2.60	9 (29%)
2	7OJ	D	1001	-	24,31,31	1.96	6 (25%)	31,47,47	1.79	7 (22%)

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	7OJ	A	1001	-	-	0/12/26/26	0/4/4/4
2	7OJ	B	1001	-	-	0/12/26/26	0/4/4/4
2	7OJ	C	1001	-	-	0/12/26/26	0/4/4/4
2	7OJ	D	1001	-	-	0/12/26/26	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	7OJ	C1-C6	-4.05	1.33	1.38
2	D	1001	7OJ	C1-C6	-3.81	1.34	1.38
2	D	1001	7OJ	C4-N7	-3.30	1.30	1.35
2	C	1001	7OJ	C4-N7	-3.26	1.30	1.35
2	A	1001	7OJ	C18-C17	-3.07	1.45	1.50
2	B	1001	7OJ	C1-C6	-2.87	1.35	1.38
2	C	1001	7OJ	C1-C6	-2.81	1.35	1.38
2	A	1001	7OJ	C4-N7	-2.46	1.32	1.35
2	D	1001	7OJ	C12-C11	-2.46	1.51	1.53
2	B	1001	7OJ	C4-N7	-2.06	1.32	1.35
2	A	1001	7OJ	C17-N15	2.00	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	7OJ	F26-C13	2.32	1.41	1.38
2	D	1001	7OJ	F25-C13	2.54	1.41	1.38
2	C	1001	7OJ	C17-N15	2.73	1.40	1.34
2	D	1001	7OJ	C17-N15	3.01	1.41	1.34
2	A	1001	7OJ	C1-C2	5.39	1.48	1.38
2	D	1001	7OJ	C1-C2	5.69	1.48	1.38
2	B	1001	7OJ	C1-C2	5.89	1.48	1.38
2	C	1001	7OJ	C1-C2	6.19	1.49	1.38

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	7OJ	F26-C13-C12	-10.65	102.09	109.39
2	C	1001	7OJ	F26-C13-C12	-7.82	104.03	109.39
2	C	1001	7OJ	C10-C2-C1	-5.53	114.13	121.76
2	A	1001	7OJ	O19-C17-C18	-4.69	111.24	120.16
2	D	1001	7OJ	O19-C17-C18	-4.14	112.29	120.16
2	A	1001	7OJ	C10-C2-C1	-4.04	116.19	121.76
2	A	1001	7OJ	C18-C20-C21	-3.86	115.18	119.69
2	A	1001	7OJ	BR24-C21-C27	-3.72	114.04	119.53
2	C	1001	7OJ	C2-N3-C4	-3.58	113.74	117.61
2	D	1001	7OJ	C10-C2-C1	-3.50	116.93	121.76
2	C	1001	7OJ	O19-C17-N15	-3.27	117.16	122.40
2	B	1001	7OJ	O19-C17-C18	-3.06	114.33	120.16
2	A	1001	7OJ	C2-N3-C4	-2.86	114.52	117.61
2	B	1001	7OJ	C10-C2-C1	-2.65	118.11	121.76
2	B	1001	7OJ	F25-C13-C12	-2.44	107.72	109.39
2	A	1001	7OJ	F28-C27-C21	-2.24	116.24	119.54
2	B	1001	7OJ	C14-N15-C17	-2.17	116.23	121.81
2	B	1001	7OJ	F26-C13-C14	2.10	111.23	109.17
2	D	1001	7OJ	C23-C18-C20	2.21	121.90	119.25
2	B	1001	7OJ	BR24-C21-C27	2.34	122.99	119.53
2	D	1001	7OJ	F25-C13-C14	2.37	111.51	109.17
2	C	1001	7OJ	C13-C12-C11	2.41	115.95	109.58
2	C	1001	7OJ	F26-C13-C14	2.60	111.73	109.17
2	A	1001	7OJ	F25-C13-F26	2.72	108.85	105.21
2	A	1001	7OJ	BR24-C21-C20	2.83	123.38	118.41
2	C	1001	7OJ	C18-C17-N15	3.02	122.77	118.77
2	D	1001	7OJ	C1-C2-N3	3.02	125.57	122.76
2	A	1001	7OJ	C23-C18-C20	3.20	123.08	119.25
2	A	1001	7OJ	C18-C17-N15	3.31	123.16	118.77
2	D	1001	7OJ	F25-C13-F26	3.42	109.78	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1001	7OJ	C18-C17-N15	3.53	123.44	118.77
2	B	1001	7OJ	C1-C2-N3	3.65	126.14	122.76
2	C	1001	7OJ	F25-C13-F26	4.08	110.66	105.21
2	B	1001	7OJ	C18-C17-N15	4.65	124.94	118.77
2	C	1001	7OJ	C1-C2-N3	5.45	127.82	122.76
2	A	1001	7OJ	C1-C2-N3	5.78	128.13	122.76
2	A	1001	7OJ	F25-C13-C12	9.48	115.89	109.39

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
2	C	1001	7OJ	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	343/344 (99%)	-0.06	2 (0%) 90 95	13, 26, 48, 77	0
1	B	343/344 (99%)	0.03	6 (1%) 73 83	15, 28, 51, 82	0
1	C	340/344 (98%)	0.09	12 (3%) 48 61	15, 29, 58, 124	0
1	D	336/344 (97%)	-0.02	5 (1%) 76 85	14, 28, 52, 76	0
All	All	1362/1376 (98%)	0.01	25 (1%) 71 81	13, 28, 53, 124	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	578	MET	9.5
1	C	579	ASP	9.2
1	C	581	GLU	6.5
1	C	586	LEU	4.1
1	C	584	LYS	3.8
1	C	917	ASP	3.6
1	D	582	TYR	3.5
1	C	580	ASP	3.3
1	A	843	ARG	3.1
1	C	588	ASP	3.0
1	D	586	LEU	3.0
1	B	918	GLU	2.9
1	D	589	GLY	2.7
1	C	583	THR	2.7
1	B	917	ASP	2.7
1	B	723	GLY	2.4
1	D	583	THR	2.4
1	B	897	LYS	2.3
1	D	915	PHE	2.3
1	A	598	SER	2.3
1	C	585	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	902	PHE	2.1
1	B	720	SER	2.1
1	B	636	CYS	2.1
1	C	582	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	7OJ	B	1001	28/28	0.98	0.13	0.00	20,23,27,34	0
2	7OJ	A	1001	28/28	0.97	0.10	-0.71	16,19,25,27	0
2	7OJ	C	1001	28/28	0.97	0.10	-0.90	15,18,23,28	0
4	MG	A	1003	1/1	0.98	0.09	-1.07	15,15,15,15	0
2	7OJ	D	1001	28/28	0.98	0.09	-1.26	17,18,25,33	0
3	ZN	B	1002	1/1	1.00	0.07	-1.84	24,24,24,24	0
3	ZN	C	1002	1/1	1.00	0.08	-2.50	23,23,23,23	0
4	MG	B	1003	1/1	0.94	0.06	-2.71	10,10,10,10	0
3	ZN	D	1002	1/1	1.00	0.08	-2.94	23,23,23,23	0
4	MG	D	1003	1/1	0.99	0.06	-4.36	4,4,4,4	0
4	MG	C	1003	1/1	0.96	0.06	-4.41	10,10,10,10	0
3	ZN	A	1002	1/1	0.99	0.04	-6.42	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.