Full wwPDB X-ray Structure Validation Report (i)

May 29, 2016 – 08:40 AM EDT

PDB ID	:	5FH6
Title	:	Crystal structure of the fifth bromodomain of human PB1 in complex with compound 10
Authors	:	Tallant, C.; Sutherell, C.L.; Siejka, P.; Krojer, T.; Picaud, S.; Fonseca, M.; Fedorov, O.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Brennan, P.E.; Ley, S.V.; Knapp, S.
Deposited on	:	2015-12-21
Resolution	:	2.30 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:

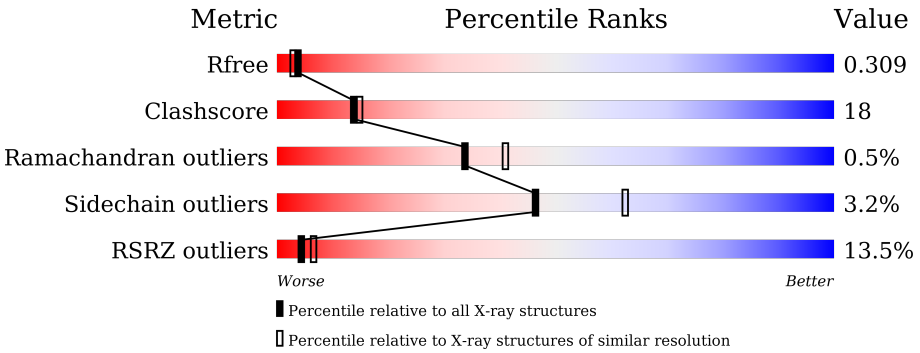
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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	124	8% 65% 23% 10%
1	B	124	16% 56% 28% 10%
1	C	124	12% 55% 31% 12%
1	D	124	11% 58% 26% 14%

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
2	5XM	B	801	X	-	-	-
2	5XM	C	801	X	-	-	-
2	5XM	D	801	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3743 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.

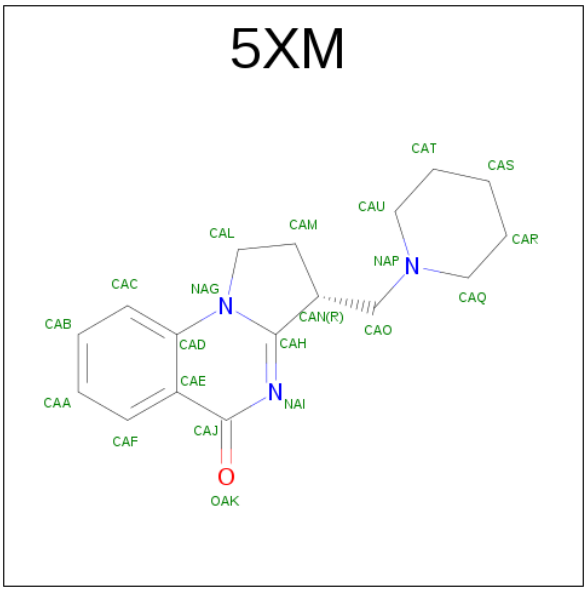
- Molecule 1 is a protein called Protein polybromo-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			929	590	158	171	10			
1	B	111	Total	C	N	O	S	0	0	0
			918	583	156	169	10			
1	C	109	Total	C	N	O	S	0	0	0
			908	575	155	168	10			
1	D	107	Total	C	N	O	S	0	0	0
			893	566	153	165	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	643	SER	-	expression tag	UNP Q86U86
A	644	MET	-	expression tag	UNP Q86U86
B	643	SER	-	expression tag	UNP Q86U86
B	644	MET	-	expression tag	UNP Q86U86
C	643	SER	-	expression tag	UNP Q86U86
C	644	MET	-	expression tag	UNP Q86U86
D	643	SER	-	expression tag	UNP Q86U86
D	644	MET	-	expression tag	UNP Q86U86

- Molecule 2 is (3 {R})-3-(piperidin-1-ylmethyl)-2,3-dihydro-1 {H}-pyrrolo[1,2-a]quinazolin-5 -one (three-letter code: 5XM) (formula: $C_{17}H_{21}N_3O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 21 17 3 1	0	0
2	B	1	Total C N O 21 17 3 1	0	0
2	C	1	Total C N O 21 17 3 1	0	0
2	D	1	Total C N O 19 15 3 1	0	0

- Molecule 3 is water.

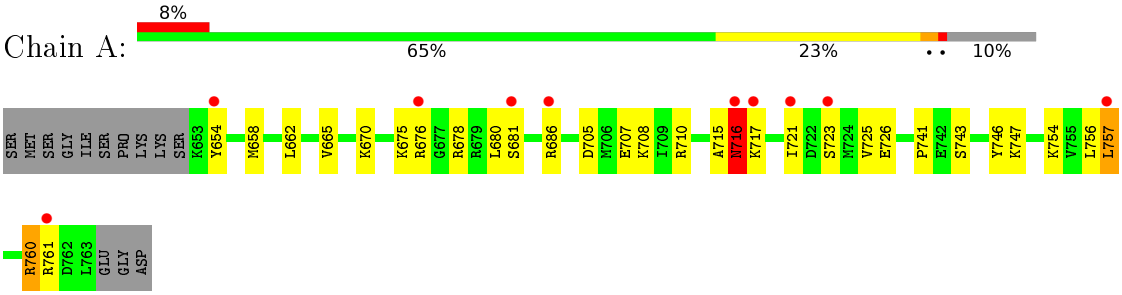
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0
3	B	4	Total O 4 4	0	0
3	C	3	Total O 3 3	0	0
3	D	3	Total O 3 3	0	0

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.

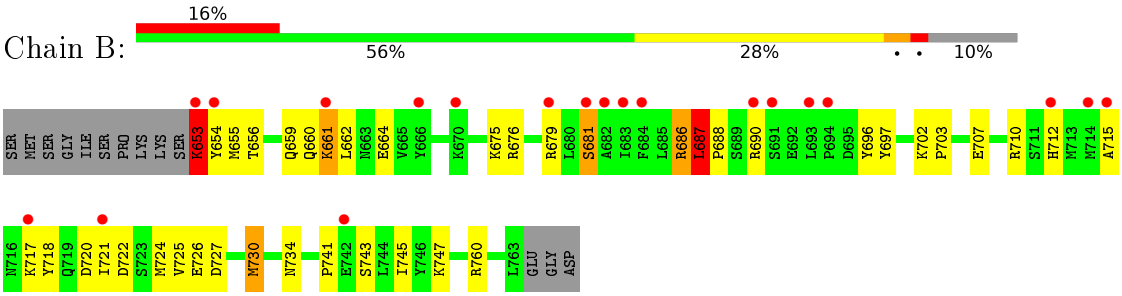
- Molecule 1: Protein polybromo-1

Chain A:



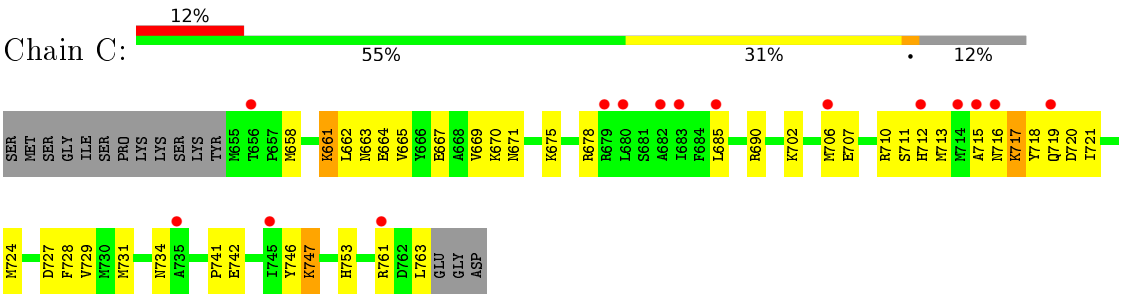
- Molecule 1: Protein polybromo-1

Chain B:



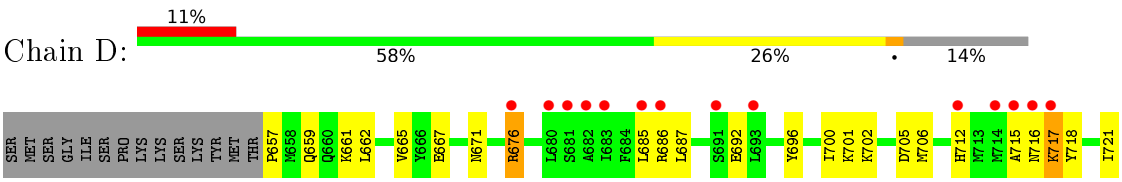
- Molecule 1: Protein polybromo-1

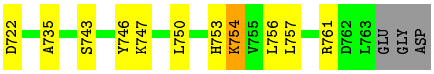
Chain C:



- Molecule 1: Protein polybromo-1

Chain D:




D722
A735
S743
Y746
K747
L750
H753
K754
V755
L756
L757
R761
D762
L763
GLU
GLY
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	41.87Å 136.42Å 56.75Å 90.00° 92.33° 90.00°	Depositor
Resolution (Å)	29.73 – 2.30 29.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.73-2.30) 92.4 (29.73-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1682)	Depositor
R, R_{free}	0.254 , 0.310 0.255 , 0.309	Depositor DCC
R_{free} test set	1292 reflections (4.95%)	DCC
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.767	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.078 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3743	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.34% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5XM

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	0.58	3/946 (0.3%)	1.24	5/1270 (0.4%)
1	B	0.66	1/935 (0.1%)	0.89	5/1258 (0.4%)
1	C	0.41	0/924	0.79	1/1241 (0.1%)
1	D	0.65	3/909 (0.3%)	0.95	6/1220 (0.5%)
All	All	0.58	7/3714 (0.2%)	0.98	17/4989 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	653	LYS	CD-CE	9.70	1.75	1.51
1	D	676	ARG	CG-CD	9.18	1.74	1.51
1	D	676	ARG	CZ-NH1	7.75	1.43	1.33
1	A	686	ARG	CZ-NH1	7.63	1.43	1.33
1	D	676	ARG	CB-CG	7.30	1.72	1.52
1	A	654	TYR	CD1-CE1	-6.78	1.29	1.39
1	A	686	ARG	CB-CG	5.56	1.67	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	686	ARG	NE-CZ-NH1	26.94	133.77	120.30
1	A	686	ARG	NE-CZ-NH2	-18.91	110.85	120.30
1	D	676	ARG	NE-CZ-NH1	17.04	128.82	120.30
1	B	686	ARG	NE-CZ-NH1	-10.30	115.15	120.30
1	D	676	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	A	716	ASN	CB-CA-C	-8.69	93.02	110.40
1	A	757	LEU	CB-CG-CD2	-8.36	96.78	111.00
1	D	676	ARG	CD-NE-CZ	8.31	135.24	123.60
1	B	730	MET	CG-SD-CE	-7.35	88.44	100.20
1	C	690	ARG	NE-CZ-NH1	-7.31	116.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	687	LEU	CB-CG-CD1	-7.20	98.76	111.00
1	B	653	LYS	CD-CE-NZ	6.95	127.68	111.70
1	D	717	LYS	CD-CE-NZ	6.43	126.48	111.70
1	D	717	LYS	CA-CB-CG	6.02	126.64	113.40
1	B	686	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	D	676	ARG	CB-CG-CD	5.60	126.17	111.60
1	A	716	ASN	N-CA-C	5.01	124.53	111.00

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	929	0	941	30	0
1	B	918	0	917	42	0
1	C	908	0	919	40	0
1	D	893	0	904	29	0
2	A	21	0	0	0	0
2	B	21	0	0	1	0
2	C	21	0	0	0	0
2	D	19	0	0	1	0
3	A	3	0	0	0	0
3	B	4	0	0	1	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
All	All	3743	0	3681	137	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 18.

All (137) 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:676:ARG:CG	1:D:676:ARG:CD	1.74	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:653:LYS:CD	1:B:653:LYS:CE	1.75	1.58
1:B:712:HIS:HE1	1:B:717:LYS:HD2	1.14	1.06
1:A:716:ASN:HB2	1:A:717:LYS:HD2	1.34	1.04
1:B:712:HIS:CE1	1:B:717:LYS:HD2	1.97	0.99
1:B:686:ARG:HH12	1:C:678:ARG:NE	1.59	0.99
1:A:715:ALA:O	1:A:716:ASN:ND2	2.01	0.93
1:C:729:VAL:HG22	1:C:753:HIS:HE1	1.35	0.92
1:D:712:HIS:CD2	1:D:717:LYS:HG3	2.05	0.90
1:D:667:GLU:OE1	1:D:671:ASN:ND2	2.05	0.90
1:C:661:LYS:HA	1:C:664:GLU:H	1.42	0.85
1:A:757:LEU:HD23	1:A:761:ARG:HH12	1.43	0.83
1:B:662:LEU:HD23	1:B:721:ILE:HD13	1.66	0.77
1:A:757:LEU:HD21	1:A:761:ARG:HH22	1.51	0.75
1:B:702:LYS:HB3	1:B:730:MET:CE	2.16	0.75
1:B:687:LEU:HD11	1:B:697:TYR:OH	1.91	0.70
1:B:702:LYS:HB3	1:B:730:MET:HE1	1.73	0.70
1:B:697:TYR:HD1	1:B:703:PRO:HG2	1.57	0.69
1:B:661:LYS:HE3	1:B:664:GLU:OE1	1.92	0.68
1:C:662:LEU:HD23	1:C:721:ILE:HD13	1.75	0.68
1:C:675:LYS:HD3	1:C:675:LYS:N	2.08	0.68
1:C:675:LYS:HD3	1:C:675:LYS:H	1.60	0.67
1:B:697:TYR:CD1	1:B:703:PRO:HG2	2.32	0.65
1:A:716:ASN:CB	1:A:717:LYS:HD2	2.21	0.65
1:C:761:ARG:O	1:C:761:ARG:NH1	2.31	0.64
1:A:757:LEU:CD2	1:A:761:ARG:HH12	2.10	0.64
1:C:715:ALA:HB1	1:C:717:LYS:HE2	1.79	0.63
1:D:685:LEU:HA	1:D:706:MET:HB2	1.81	0.62
1:D:712:HIS:CG	1:D:717:LYS:HE3	2.35	0.62
1:C:715:ALA:O	1:C:717:LYS:NZ	2.19	0.61
1:C:661:LYS:O	1:C:665:VAL:HG12	2.01	0.61
1:A:708:LYS:HD2	1:A:708:LYS:O	2.02	0.59
1:C:712:HIS:CE1	1:C:717:LYS:HB2	2.37	0.59
1:D:712:HIS:CG	1:D:717:LYS:HG3	2.36	0.59
1:B:718:TYR:CE2	1:B:724:MET:HA	2.37	0.59
1:B:712:HIS:CE1	1:B:717:LYS:CD	2.82	0.59
1:C:658:MET:CE	1:C:720:ASP:HA	2.33	0.59
1:D:662:LEU:HD21	1:D:721:ILE:HA	1.84	0.58
1:B:722:ASP:HA	1:B:725:VAL:HB	1.85	0.58
1:B:686:ARG:HH12	1:C:678:ARG:CD	2.15	0.58
1:B:686:ARG:NH2	1:B:707:GLU:OE2	2.36	0.58
1:B:712:HIS:HE1	1:B:717:LYS:CD	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:ALA:O	1:A:716:ASN:CG	2.43	0.58
1:A:678:ARG:HH22	1:A:680:LEU:HG	1.69	0.57
1:C:715:ALA:HB1	1:C:717:LYS:CE	2.33	0.57
1:C:729:VAL:HG22	1:C:753:HIS:CE1	2.27	0.57
1:B:722:ASP:O	1:B:726:GLU:HG3	2.05	0.57
1:B:653:LYS:HB2	1:B:654:TYR:CD1	2.38	0.57
1:B:712:HIS:CE1	1:B:717:LYS:HB2	2.40	0.56
1:C:718:TYR:CE2	1:C:724:MET:HA	2.40	0.56
1:A:760:ARG:NH1	1:A:761:ARG:HG3	2.21	0.56
1:A:716:ASN:HB2	1:A:717:LYS:CD	2.23	0.56
1:B:712:HIS:NE2	1:B:717:LYS:HB2	2.21	0.56
1:C:670:LYS:NZ	1:C:671:ASN:OD1	2.39	0.56
1:A:675:LYS:O	1:A:676:ARG:HG3	2.06	0.55
1:C:718:TYR:CE2	1:C:724:MET:HG3	2.42	0.55
1:A:658:MET:O	1:A:662:LEU:HD13	2.07	0.54
1:A:678:ARG:NH1	1:A:680:LEU:HA	2.21	0.54
1:A:757:LEU:HG	1:A:760:ARG:NH1	2.22	0.54
1:B:687:LEU:HD11	1:B:697:TYR:CZ	2.42	0.54
1:B:718:TYR:OH	1:B:727:ASP:OD2	2.16	0.54
1:C:718:TYR:HE2	1:C:724:MET:HG3	1.73	0.54
1:B:718:TYR:HE2	1:B:724:MET:HA	1.73	0.53
1:C:707:GLU:OE2	1:C:710:ARG:NH1	2.41	0.53
1:C:702:LYS:O	1:C:734:ASN:ND2	2.38	0.53
1:B:715:ALA:HB1	1:B:717:LYS:HZ3	1.73	0.53
1:D:661:LYS:NZ	1:D:721:ILE:HG21	2.24	0.53
1:D:661:LYS:O	1:D:665:VAL:HG23	2.10	0.52
1:A:662:LEU:HD12	1:A:721:ILE:HD13	1.91	0.52
1:B:679:ARG:HG2	1:B:681:SER:HB3	1.91	0.51
1:A:707:GLU:HG2	1:A:710:ARG:HD3	1.92	0.51
1:B:655:MET:HG2	1:B:660:GLN:HG3	1.93	0.51
1:D:721:ILE:HG13	1:D:722:ASP:OD1	2.10	0.51
1:A:741:PRO:HA	1:A:746:TYR:CD2	2.46	0.51
1:C:675:LYS:CD	1:C:675:LYS:H	2.21	0.51
1:B:687:LEU:C	1:B:687:LEU:HD12	2.32	0.50
1:B:656:THR:HG23	1:B:659:GLN:HB2	1.94	0.49
1:C:715:ALA:O	1:C:716:ASN:HB2	2.12	0.49
1:A:662:LEU:CD1	1:A:721:ILE:HD13	2.43	0.49
1:C:741:PRO:HA	1:C:746:TYR:CG	2.47	0.49
1:C:663:ASN:HB2	1:C:713:MET:HE1	1.94	0.49
1:A:743:SER:O	1:A:747:LYS:HD2	2.13	0.48
1:C:741:PRO:HG2	1:D:702:LYS:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:ARG:HH12	1:C:678:ARG:HE	1.53	0.48
1:D:696:TYR:CE2	1:D:700:ILE:HD11	2.49	0.47
1:A:760:ARG:HG2	1:A:761:ARG:N	2.29	0.47
1:D:753:HIS:O	1:D:757:LEU:HD13	2.14	0.47
1:A:705:ASP:OD1	1:A:708:LYS:HB3	2.14	0.47
1:B:690:ARG:NH1	3:B:901:HOH:O	2.48	0.46
1:D:712:HIS:CB	1:D:717:LYS:HE3	2.45	0.46
1:B:696:TYR:OH	2:B:801:5XM:OAK	2.26	0.46
1:B:653:LYS:HB2	1:B:654:TYR:CE1	2.51	0.46
1:B:720:ASP:CG	1:B:721:ILE:N	2.69	0.46
1:B:730:MET:HG2	1:B:734:ASN:HD21	1.81	0.46
1:D:715:ALA:O	1:D:716:ASN:HB2	2.15	0.46
1:C:669:VAL:HG11	1:C:728:PHE:HE2	1.81	0.46
1:A:678:ARG:HH12	1:A:680:LEU:HA	1.81	0.45
1:C:658:MET:HE3	1:C:720:ASP:HA	1.97	0.45
1:B:687:LEU:HD12	1:B:688:PRO:O	2.16	0.45
1:C:761:ARG:C	1:C:763:LEU:N	2.68	0.45
1:D:657:PRO:HD2	1:D:659:GLN:HE21	1.82	0.45
1:A:707:GLU:HA	1:A:710:ARG:HB3	1.99	0.45
1:A:670:LYS:HA	1:A:681:SER:HB2	1.99	0.45
1:D:735:ALA:HA	2:D:801:5XM:OAK	2.17	0.45
1:C:742:GLU:OE1	1:C:747:LYS:NZ	2.30	0.44
1:A:754:LYS:NZ	1:A:754:LYS:HB2	2.32	0.44
1:D:676:ARG:O	1:D:676:ARG:HG3	2.16	0.44
1:D:743:SER:O	1:D:747:LYS:HG3	2.17	0.44
1:B:745:ILE:H	1:B:745:ILE:HD12	1.81	0.44
1:D:746:TYR:O	1:D:750:LEU:HD13	2.18	0.44
1:C:712:HIS:HD1	1:C:718:TYR:HE1	1.66	0.44
1:C:761:ARG:O	1:C:761:ARG:HG3	2.18	0.44
1:D:686:ARG:HA	1:D:705:ASP:OD2	2.17	0.44
1:C:685:LEU:HA	1:C:706:MET:HB2	2.00	0.43
1:C:663:ASN:O	1:C:667:GLU:HB2	2.18	0.43
1:A:723:SER:O	1:A:726:GLU:HG2	2.18	0.43
1:C:706:MET:HG3	1:C:731:MET:HE1	1.99	0.43
1:D:692:GLU:HG2	1:D:692:GLU:O	2.18	0.42
1:A:662:LEU:HA	1:A:665:VAL:HG12	2.00	0.42
1:A:725:VAL:HG13	1:A:756:LEU:HD21	2.02	0.42
1:B:743:SER:O	1:B:747:LYS:HG3	2.19	0.42
1:B:653:LYS:CE	1:B:653:LYS:CG	2.82	0.42
1:C:715:ALA:C	1:C:717:LYS:HD3	2.39	0.42
1:B:675:LYS:HG3	1:B:676:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:LYS:HD2	1:A:708:LYS:C	2.40	0.42
1:C:718:TYR:OH	1:C:727:ASP:OD2	2.22	0.42
1:D:701:LYS:H	1:D:701:LYS:HG2	1.68	0.41
1:D:686:ARG:HD2	1:D:686:ARG:HH11	1.68	0.41
1:B:718:TYR:HD2	1:B:724:MET:HB2	1.85	0.41
1:C:742:GLU:HA	1:C:742:GLU:OE1	2.20	0.41
1:D:712:HIS:CD2	1:D:718:TYR:CE2	3.09	0.41
1:B:686:ARG:HH11	1:B:686:ARG:HD2	1.54	0.41
1:D:661:LYS:HZ2	1:D:721:ILE:HG21	1.85	0.41
1:D:754:LYS:HE2	1:D:754:LYS:HB2	1.88	0.41
1:C:711:SER:O	1:C:715:ALA:HB2	2.22	0.40
1:D:753:HIS:O	1:D:756:LEU:HB3	2.21	0.40
1:D:687:LEU:HG	1:D:705:ASP:HB3	2.03	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	109/124 (88%)	106 (97%)	2 (2%)	1 (1%)	21	24
1	B	109/124 (88%)	105 (96%)	3 (3%)	1 (1%)	21	24
1	C	107/124 (86%)	105 (98%)	2 (2%)	0	100	100
1	D	105/124 (85%)	102 (97%)	3 (3%)	0	100	100
All	All	430/496 (87%)	418 (97%)	10 (2%)	2 (0%)	34	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	716	ASN
1	B	741	PRO

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	105/116 (90%)	104 (99%)	1 (1%)	82	91
1	B	102/116 (88%)	96 (94%)	6 (6%)	24	32
1	C	103/116 (89%)	99 (96%)	4 (4%)	39	53
1	D	101/116 (87%)	99 (98%)	2 (2%)	63	79
All	All	411/464 (89%)	398 (97%)	13 (3%)	46	62

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	760	ARG
1	B	653	LYS
1	B	661	LYS
1	B	681	SER
1	B	687	LEU
1	B	710	ARG
1	B	760	ARG
1	C	661	LYS
1	C	717	LYS
1	C	719	GLN
1	C	747	LYS
1	D	754	LYS
1	D	761	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	712	HIS
1	B	734	ASN
1	C	753	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

4 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	$\#\|Z\| > 2$
2	5XM	A	801	-	22,24,24	4.51	8 (36%)	18,34,34	1.79	1 (5%)
2	5XM	B	801	-	22,24,24	4.57	9 (40%)	18,34,34	1.90	1 (5%)
2	5XM	C	801	-	22,24,24	4.93	8 (36%)	18,34,34	1.53	2 (11%)
2	5XM	D	801	-	19,21,24	5.15	8 (42%)	12,30,34	2.28	5 (41%)

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	5XM	A	801	-	-	0/4/21/21	0/4/4/4
2	5XM	B	801	-	1/1/2/2	0/4/21/21	0/4/4/4
2	5XM	C	801	-	1/1/2/2	0/4/21/21	0/4/4/4
2	5XM	D	801	-	1/1/2/2	0/6/15/21	0/3/3/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	5XM	CAO-CAN	-17.89	1.31	1.53
2	D	801	5XM	CAO-CAN	-17.00	1.32	1.53
2	B	801	5XM	CAO-CAN	-14.77	1.35	1.53
2	A	801	5XM	CAO-CAN	-14.70	1.35	1.53
2	C	801	5XM	CAH-CAN	-10.11	1.32	1.51
2	D	801	5XM	CAH-CAN	-9.95	1.32	1.51
2	B	801	5XM	CAH-CAN	-9.42	1.33	1.51
2	A	801	5XM	CAH-CAN	-9.15	1.34	1.51
2	C	801	5XM	CAO-NAP	-7.15	1.32	1.47
2	D	801	5XM	CAO-NAP	-6.70	1.32	1.47
2	B	801	5XM	CAO-NAP	-6.15	1.34	1.47
2	A	801	5XM	CAO-NAP	-6.04	1.34	1.47
2	B	801	5XM	CAD-NAG	-5.79	1.32	1.40
2	A	801	5XM	CAD-NAG	-5.42	1.32	1.40
2	D	801	5XM	CAM-CAN	-4.56	1.35	1.54
2	D	801	5XM	CAD-NAG	-4.31	1.34	1.40
2	A	801	5XM	CAM-CAN	-4.05	1.37	1.54
2	B	801	5XM	CAM-CAN	-4.00	1.38	1.54
2	C	801	5XM	CAD-NAG	-3.58	1.35	1.40
2	C	801	5XM	CAM-CAN	-3.51	1.40	1.54
2	D	801	5XM	CAM-CAL	-2.94	1.46	1.52
2	A	801	5XM	CAE-CAD	-2.56	1.39	1.41
2	D	801	5XM	CAJ-CAE	-2.34	1.37	1.41
2	B	801	5XM	CAE-CAD	-2.24	1.39	1.41
2	B	801	5XM	CAM-CAL	-2.11	1.48	1.52
2	C	801	5XM	CAM-CAL	-2.03	1.48	1.52
2	D	801	5XM	CAB-CAC	2.01	1.41	1.36
2	C	801	5XM	CAH-NAI	2.93	1.35	1.31
2	C	801	5XM	CAJ-NAI	3.02	1.38	1.33
2	B	801	5XM	CAJ-NAI	3.75	1.39	1.33
2	A	801	5XM	CAJ-NAI	3.86	1.40	1.33
2	A	801	5XM	CAH-NAI	5.56	1.39	1.31
2	B	801	5XM	CAH-NAI	5.84	1.39	1.31

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	5XM	CAA-CAB-CAC	-2.41	116.97	120.45
2	D	801	5XM	CAF-CAE-CAD	2.11	120.75	117.72
2	D	801	5XM	CAU-NAP-CAQ	2.35	113.75	110.92
2	D	801	5XM	CAC-CAD-NAG	2.41	124.10	121.22
2	C	801	5XM	CAJ-CAE-CAD	2.42	120.66	118.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	5XM	CAN-CAO-NAP	4.99	121.89	113.59
2	D	801	5XM	CAN-CAO-NAP	5.57	122.18	113.68
2	A	801	5XM	CAN-CAO-NAP	6.64	124.64	113.59
2	B	801	5XM	CAN-CAO-NAP	6.99	125.21	113.59

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	801	5XM	CAN
2	C	801	5XM	CAN
2	D	801	5XM	CAN

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	5XM	1	0
2	D	801	5XM	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	111/124 (89%)	0.77	10 (9%)	12	17	47, 70, 113, 153	0
1	B	111/124 (89%)	1.04	20 (18%)	2	3	46, 74, 129, 162	0
1	C	109/124 (87%)	0.87	15 (13%)	4	6	47, 75, 106, 153	0
1	D	107/124 (86%)	0.79	14 (13%)	5	7	45, 75, 116, 141	0
All	All	438/496 (88%)	0.87	59 (13%)	4	6	45, 74, 120, 162	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	653	LYS	6.0
1	B	654	TYR	5.4
1	B	715	ALA	4.9
1	C	683	ILE	4.5
1	C	656	THR	4.2
1	B	681	SER	4.2
1	D	712	HIS	4.2
1	C	682	ALA	4.0
1	B	683	ILE	3.9
1	A	654	TYR	3.9
1	B	682	ALA	3.9
1	B	690	ARG	3.8
1	C	712	HIS	3.8
1	B	712	HIS	3.3
1	B	742	GLU	3.2
1	A	676	ARG	3.2
1	C	761	ARG	3.1
1	D	715	ALA	3.0
1	B	691	SER	2.9
1	B	684	PHE	2.9
1	A	717	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	714	MET	2.8
1	A	723	SER	2.8
1	A	761	ARG	2.8
1	D	681	SER	2.6
1	D	685	LEU	2.5
1	D	717	LYS	2.5
1	A	716	ASN	2.5
1	D	686	ARG	2.5
1	C	735	ALA	2.4
1	D	680	LEU	2.4
1	C	745	ILE	2.4
1	C	719	GLN	2.4
1	A	686	ARG	2.3
1	B	670	LYS	2.3
1	C	715	ALA	2.3
1	D	682	ALA	2.3
1	D	714	MET	2.3
1	A	681	SER	2.3
1	C	685	LEU	2.2
1	D	693	LEU	2.2
1	B	694	PRO	2.2
1	B	666	TYR	2.2
1	B	714	MET	2.2
1	C	679	ARG	2.2
1	D	676	ARG	2.2
1	C	680	LEU	2.2
1	D	716	ASN	2.1
1	A	721	ILE	2.1
1	B	721	ILE	2.1
1	A	757	LEU	2.1
1	B	661	LYS	2.1
1	B	717	LYS	2.1
1	C	706	MET	2.1
1	B	679	ARG	2.0
1	B	693	LEU	2.0
1	D	683	ILE	2.0
1	C	716	ASN	2.0
1	D	691	SER	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	5XM	A	801	21/21	0.90	0.21	0.33	46,57,80,87	0
2	5XM	C	801	21/21	0.86	0.22	0.19	53,79,90,92	0
2	5XM	D	801	19/21	0.90	0.16	-0.57	45,61,83,84	0
2	5XM	B	801	21/21	0.90	0.15	-0.79	45,68,88,92	0

6.5 Other polymers (i)

There are no such residues in this entry.