



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:18 PM UTC

PDB ID : 3JWR / pdb_00003jwr
Title : Crystal structure of chimeric PDE5/PDE6 catalytic domain complexed with 3-isobutyl-1-methylxanthine (IBMX) and PDE6 gamma-subunit inhibitory peptide 70-87.
Authors : Barren, B.; Gakhar, L.; Muradov, H.; Boyd, K.K.; Ramaswamy, S.; Artemyev, N.O.
Deposited on : 2009-09-18
Resolution : 2.99 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

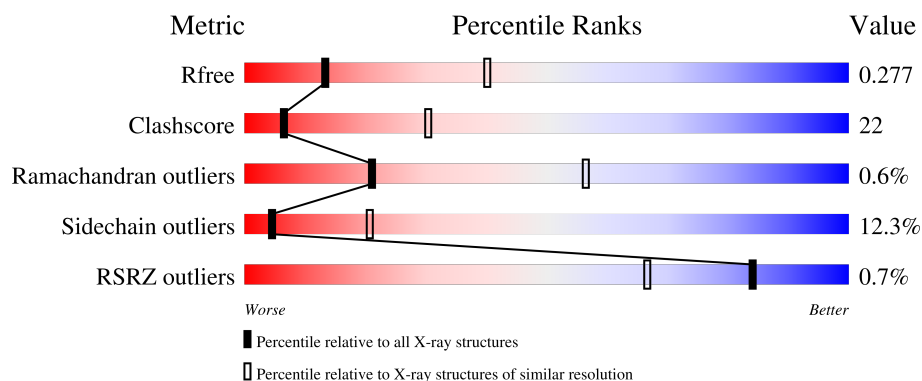
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	330	55% 38% 5%
1	B	330	57% 36% 6%
2	C	18	6% 61% 28% 6% 6%
2	D	18	6% 61% 28% 6% 6%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5683 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-specific 3',5'-cyclic phosphodiesterase catalytic domain, Cone cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2629	1676	458	477	18			
1	B	328	Total	C	N	O	S	0	0	0
			2671	1700	465	487	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	GLY	-	expression tag	UNP O76074
A	532	SER	-	expression tag	UNP O76074
A	533	HIS	-	expression tag	UNP O76074
A	534	MET	-	expression tag	UNP O76074
B	531	GLY	-	expression tag	UNP O76074
B	532	SER	-	expression tag	UNP O76074
B	533	HIS	-	expression tag	UNP O76074
B	534	MET	-	expression tag	UNP O76074

- Molecule 2 is a protein called Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit gamma.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	0	0	0
			141	92	23	26			
2	D	17	Total	C	N	O	0	0	0
			141	92	23	26			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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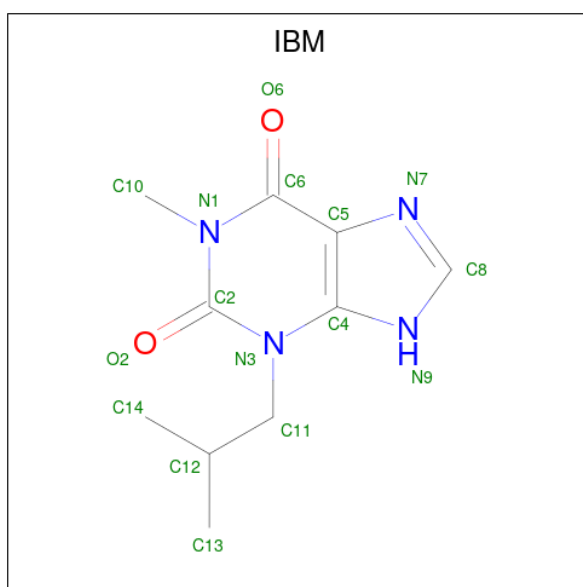
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is 3-ISOBUTYL-1-METHYLBXANTHINE (CCD ID: IBM) (formula: C₁₀H₁₄N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			16	10	4	2		
5	A	1	Total	C	N	O	0	0
			16	10	4	2		
5	A	1	Total	C	N	O	0	0
			16	10	4	2		
5	B	1	Total	C	N	O	0	0
			16	10	4	2		
5	B	1	Total	C	N	O	0	0
			16	10	4	2		

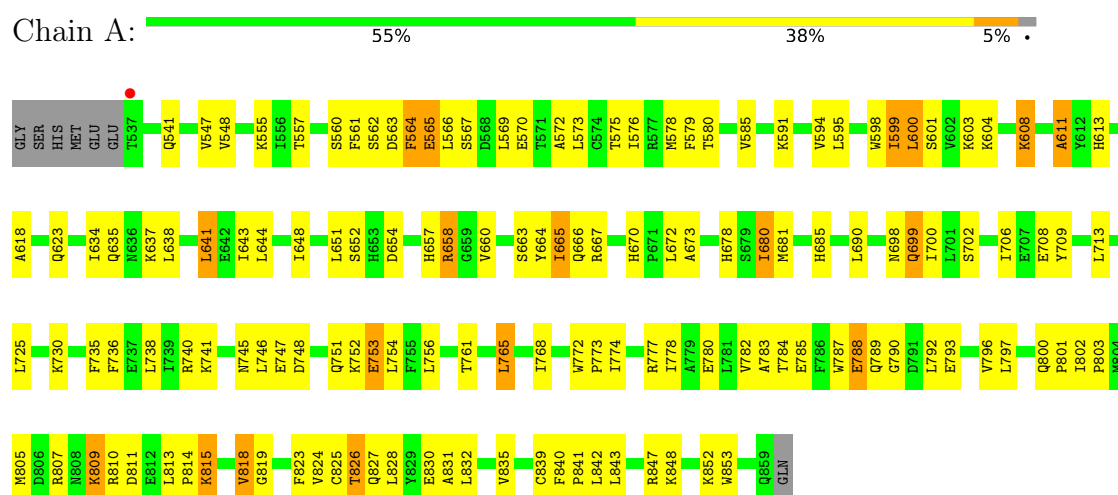
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total 5	O 5	0	0
6	B	11	Total 11	O 11	0	0
6	D	1	Total 1	O 1	0	0

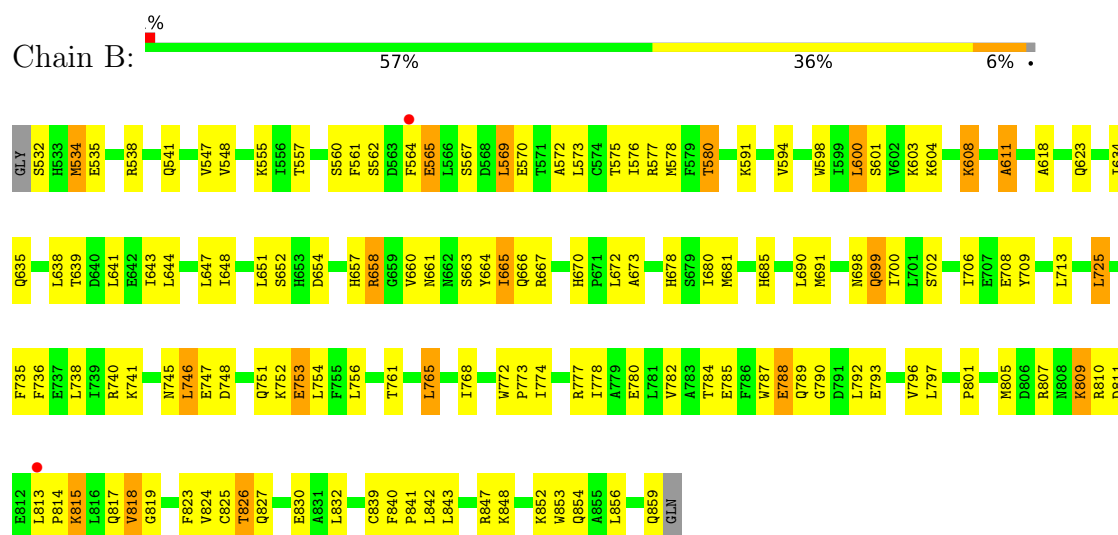
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: cGMP-specific 3',5'-cyclic phosphodiesterase catalytic domain, Cone cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha chimera



- Molecule 1: cGMP-specific 3',5'-cyclic phosphodiesterase catalytic domain, Cone cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha chimera



- Molecule 2: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit gamma



- Molecule 2: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.26Å 125.65Å 153.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.41 – 2.99 40.41 – 2.99	Depositor EDS
% Data completeness (in resolution range)	93.1 (40.41-2.99) 93.1 (40.41-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_161)	Depositor
R, R_{free}	0.212 , 0.280 0.209 , 0.277	Depositor DCC
R_{free} test set	921 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5683	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.49	0/2683	0.85	2/3628 (0.1%)
1	B	0.51	0/2726	0.83	1/3685 (0.0%)
2	C	0.40	0/144	0.79	0/194
2	D	0.48	0/144	0.86	0/194
All	All	0.50	0/5697	0.84	3/7701 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	611	ALA	N-CA-C	5.88	117.38	110.97
1	B	611	ALA	N-CA-C	5.38	116.83	110.97
1	A	599	ILE	CB-CA-C	-5.24	105.18	111.88

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	2629	0	2638	117	0
1	B	2671	0	2671	119	0
2	C	141	0	131	6	0
2	D	141	0	131	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	48	0	42	9	0
5	B	32	0	28	4	0
6	A	5	0	0	0	0
6	B	11	0	0	2	0
6	D	1	0	0	0	0
All	All	5683	0	5641	247	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 22.

All (247) 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)
5:A:903:IBM:HN9	5:A:903:IBM:H142	1.21	1.02
2:D:86:ILE:O	2:D:87:ILE:HG12	1.62	0.97
2:C:86:ILE:O	2:C:87:ILE:HG12	1.64	0.96
5:A:902:IBM:HN9	5:A:902:IBM:H12	1.31	0.92
1:A:773:PRO:HB3	1:B:840:PHE:CE1	2.05	0.91
1:A:565:GLU:HG2	1:B:847:ARG:HB2	1.60	0.83
1:A:809:LYS:HE3	1:A:809:LYS:HA	1.62	0.82
1:B:532:SER:HA	1:B:535:GLU:OE1	1.81	0.81
1:A:735:PHE:HB2	1:A:754:LEU:HD21	1.61	0.81
5:A:902:IBM:H12	5:A:902:IBM:N9	1.94	0.80
1:A:565:GLU:CG	1:B:847:ARG:HB2	2.12	0.80
1:B:809:LYS:HE3	1:B:809:LYS:HA	1.63	0.79
1:B:761:THR:O	1:B:765:LEU:HD22	1.84	0.78
1:A:736:PHE:CE1	1:A:827:GLN:HG3	2.18	0.77
1:A:761:THR:O	1:A:765:LEU:HD22	1.85	0.77
1:B:735:PHE:HB2	1:B:754:LEU:HD21	1.64	0.77
1:B:611:ALA:HB3	1:B:785:GLU:HB2	1.68	0.76
1:B:736:PHE:CE1	1:B:827:GLN:HG3	2.22	0.75
5:A:901:IBM:HN9	5:A:901:IBM:H142	1.52	0.74
1:B:608:LYS:H	1:B:608:LYS:CD	2.01	0.73
1:A:565:GLU:HG2	1:B:847:ARG:CB	2.19	0.73
1:B:780:GLU:O	1:B:784:THR:HG23	1.89	0.72
1:A:608:LYS:CD	1:A:608:LYS:H	2.03	0.72
1:A:780:GLU:O	1:A:784:THR:HG23	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:ALA:HB3	1:A:785:GLU:HB2	1.71	0.72
1:A:748:ASP:HB3	1:A:751:GLN:HB2	1.72	0.72
1:A:738:LEU:HD13	1:A:751:GLN:HE21	1.54	0.71
1:B:813:LEU:HB3	1:B:814:PRO:HD3	1.72	0.70
1:B:738:LEU:HD13	1:B:751:GLN:HE21	1.55	0.70
1:B:567:SER:OG	1:B:570:GLU:HG3	1.93	0.69
1:B:748:ASP:HB3	1:B:751:GLN:HB2	1.74	0.69
5:A:903:IBM:H142	5:A:903:IBM:N9	2.05	0.67
1:A:843:LEU:O	1:A:847:ARG:HG2	1.94	0.67
1:A:813:LEU:HB3	1:A:814:PRO:HD3	1.76	0.66
1:B:787:TRP:CD1	1:B:807:ARG:HA	2.30	0.66
1:A:608:LYS:H	1:A:608:LYS:HE3	1.60	0.65
1:A:608:LYS:H	1:A:608:LYS:CE	2.10	0.65
1:B:644:LEU:O	1:B:648:ILE:HG13	1.96	0.64
1:A:814:PRO:HD2	1:A:815:LYS:HE3	1.80	0.64
1:A:678:HIS:HD2	2:C:71:GLU:CD	2.06	0.63
1:A:807:ARG:HG3	1:A:807:ARG:HH11	1.63	0.63
1:B:843:LEU:O	1:B:847:ARG:HG2	1.98	0.63
1:A:644:LEU:O	1:A:648:ILE:HG13	2.00	0.62
1:B:665:ILE:HD11	1:B:680:ILE:HG21	1.82	0.62
1:B:608:LYS:H	1:B:608:LYS:CE	2.13	0.62
1:B:725:LEU:HD22	6:B:14:HOH:O	1.99	0.61
1:B:608:LYS:H	1:B:608:LYS:HD3	1.64	0.61
1:B:740:ARG:NH1	1:B:741:LYS:HE2	2.16	0.61
1:B:608:LYS:H	1:B:608:LYS:HE3	1.65	0.60
1:A:787:TRP:CD1	1:A:807:ARG:HA	2.35	0.60
1:A:788:GLU:O	1:A:792:LEU:HD13	2.01	0.60
1:B:788:GLU:O	1:B:792:LEU:HD13	2.00	0.59
1:A:608:LYS:H	1:A:608:LYS:HD3	1.66	0.59
1:B:814:PRO:HD2	1:B:815:LYS:HE3	1.82	0.59
1:B:664:TYR:HB2	1:B:789:GLN:NE2	2.18	0.59
1:A:664:TYR:HB2	1:A:789:GLN:NE2	2.17	0.59
1:A:567:SER:OG	1:A:570:GLU:HG3	2.01	0.58
1:A:690:LEU:O	1:A:690:LEU:HD23	2.02	0.58
1:B:564:PHE:HD1	1:B:777:ARG:CZ	2.17	0.58
1:B:702:SER:HA	5:B:902:IBM:O6	2.03	0.58
1:A:740:ARG:NH1	1:A:741:LYS:HE2	2.19	0.58
1:A:793:GLU:O	1:A:797:LEU:HB2	2.03	0.57
1:A:830:GLU:HA	1:A:843:LEU:HD22	1.84	0.57
1:B:807:ARG:HG3	1:B:807:ARG:HH11	1.70	0.57
1:A:565:GLU:HG3	1:B:847:ARG:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:LEU:HD23	1:B:690:LEU:O	2.05	0.57
1:A:772:TRP:HB3	1:A:773:PRO:HD3	1.86	0.56
5:A:903:IBM:HN9	5:A:903:IBM:C14	2.08	0.56
1:B:608:LYS:HD3	1:B:608:LYS:N	2.21	0.56
1:A:570:GLU:OE1	1:B:854:GLN:HG2	2.06	0.56
1:A:608:LYS:HD3	1:A:608:LYS:N	2.21	0.56
1:A:665:ILE:HD11	1:A:680:ILE:HG21	1.88	0.56
1:A:690:LEU:HD23	1:A:690:LEU:C	2.31	0.56
1:A:572:ALA:O	1:A:576:ILE:HG13	2.05	0.55
5:A:901:IBM:H142	5:A:901:IBM:N9	2.19	0.55
1:A:564:PHE:HD1	1:A:777:ARG:CZ	2.19	0.55
1:B:709:TYR:CZ	1:B:713:LEU:HD11	2.42	0.55
1:B:736:PHE:CZ	1:B:827:GLN:HG3	2.42	0.55
1:B:772:TRP:HB3	1:B:773:PRO:HD3	1.90	0.54
1:A:665:ILE:HG13	1:A:666:GLN:N	2.22	0.54
1:A:753:GLU:HG2	1:A:753:GLU:O	2.07	0.54
1:A:608:LYS:CD	1:A:608:LYS:N	2.68	0.54
1:A:736:PHE:CZ	1:A:827:GLN:HG3	2.41	0.54
1:A:765:LEU:HD22	1:A:765:LEU:H	1.72	0.54
1:B:830:GLU:HA	1:B:843:LEU:HD22	1.90	0.53
1:A:823:PHE:HD2	1:A:824:VAL:HG23	1.73	0.53
1:B:815:LYS:CE	1:B:815:LYS:H	2.20	0.53
1:B:572:ALA:O	1:B:576:ILE:HG13	2.08	0.53
1:A:815:LYS:H	1:A:815:LYS:CE	2.21	0.53
1:B:670:HIS:ND1	1:B:672:LEU:HB2	2.24	0.53
1:B:793:GLU:O	1:B:797:LEU:HB2	2.08	0.53
1:B:608:LYS:CD	1:B:608:LYS:N	2.69	0.53
1:A:601:SER:O	1:A:604:LYS:HG2	2.09	0.52
1:B:777:ARG:O	1:B:780:GLU:HB2	2.09	0.52
1:B:690:LEU:HD23	1:B:690:LEU:C	2.35	0.52
1:A:562:SER:HB2	1:A:774:ILE:CD1	2.41	0.51
1:A:670:HIS:ND1	1:A:672:LEU:HB2	2.25	0.51
1:B:663:SER:O	1:B:667:ARG:HD3	2.10	0.51
1:B:745:ASN:OD1	1:B:747:GLU:HG2	2.09	0.51
1:B:765:LEU:HD22	1:B:765:LEU:H	1.76	0.51
5:B:901:IBM:H12	5:B:901:IBM:O2	2.11	0.51
1:A:745:ASN:OD1	1:A:747:GLU:HG2	2.10	0.51
1:A:809:LYS:HA	1:A:809:LYS:CE	2.34	0.50
1:A:809:LYS:HD2	1:A:809:LYS:N	2.26	0.50
2:D:81:LEU:HB3	2:D:87:ILE:HD13	1.93	0.50
1:A:699:GLN:HB3	1:A:702:SER:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ARG:HG2	1:B:681:MET:HE1	1.93	0.50
1:B:823:PHE:HD2	1:B:824:VAL:HG23	1.76	0.50
1:A:777:ARG:O	1:A:780:GLU:HB2	2.10	0.50
2:C:86:ILE:HG22	2:C:87:ILE:H	1.76	0.50
1:A:826:THR:O	1:A:827:GLN:C	2.55	0.50
1:A:839:CYS:C	1:A:841:PRO:HD2	2.36	0.50
1:B:562:SER:HB2	1:B:774:ILE:CD1	2.41	0.50
1:B:809:LYS:N	1:B:809:LYS:HD2	2.27	0.50
1:A:570:GLU:HA	1:A:573:LEU:HD12	1.94	0.49
1:A:591:LYS:HB2	1:A:594:VAL:HG23	1.94	0.49
1:A:709:TYR:CZ	1:A:713:LEU:HD11	2.47	0.49
1:A:807:ARG:HG3	1:A:807:ARG:NH1	2.27	0.49
1:B:761:THR:O	1:B:765:LEU:CD2	2.58	0.49
5:B:902:IBM:HN9	5:B:902:IBM:H133	1.78	0.49
1:A:790:GLY:HA3	1:A:805:MET:O	2.12	0.49
1:A:840:PHE:N	1:A:841:PRO:CD	2.76	0.48
1:B:753:GLU:O	1:B:753:GLU:HG2	2.13	0.48
1:B:562:SER:HB2	1:B:774:ILE:HD13	1.95	0.48
1:A:613:HIS:CE1	5:A:901:IBM:H131	2.49	0.48
1:B:765:LEU:O	1:B:768:ILE:HG22	2.14	0.48
1:B:534:MET:HE2	1:B:534:MET:HB3	1.80	0.48
1:B:601:SER:O	1:B:604:LYS:HG2	2.14	0.47
1:B:809:LYS:HA	1:B:809:LYS:CE	2.36	0.47
2:C:81:LEU:HB3	2:C:87:ILE:HD13	1.96	0.47
1:A:598:TRP:HA	1:A:698:ASN:OD1	2.15	0.47
1:B:793:GLU:OE2	1:B:801:PRO:HA	2.15	0.47
1:B:825:CYS:O	1:B:826:THR:C	2.57	0.47
1:B:839:CYS:C	1:B:841:PRO:HD2	2.39	0.47
1:A:578:MET:HE1	1:A:623:GLN:HB2	1.96	0.47
1:A:658:ARG:HG2	1:A:681:MET:HE1	1.95	0.47
2:D:86:ILE:HG22	2:D:87:ILE:H	1.80	0.47
1:A:765:LEU:HD22	1:A:765:LEU:N	2.30	0.47
1:B:658:ARG:HG2	1:B:658:ARG:H	1.54	0.47
1:B:665:ILE:HD12	1:B:673:ALA:HB2	1.97	0.47
1:A:658:ARG:HG2	1:A:658:ARG:H	1.53	0.46
1:B:840:PHE:N	1:B:841:PRO:CD	2.78	0.46
1:A:761:THR:O	1:A:765:LEU:CD2	2.59	0.46
1:B:618:ALA:HB1	1:B:651:LEU:O	2.16	0.46
1:B:778:ILE:O	1:B:782:VAL:HG23	2.15	0.46
2:C:86:ILE:HG22	2:C:87:ILE:N	2.31	0.46
1:B:813:LEU:HD22	1:B:853:TRP:CZ3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:ILE:O	1:A:782:VAL:HG23	2.16	0.46
1:B:790:GLY:HA3	1:B:805:MET:O	2.16	0.46
1:A:736:PHE:CE1	1:A:827:GLN:CG	2.96	0.46
1:A:818:VAL:HG12	1:A:819:GLY:N	2.30	0.46
1:B:534:MET:HE3	1:B:538:ARG:NH1	2.31	0.46
1:B:654:ASP:HA	1:B:685:HIS:CD2	2.51	0.46
1:B:702:SER:C	5:B:902:IBM:H103	2.41	0.46
1:A:765:LEU:H	1:A:765:LEU:CD2	2.29	0.46
1:A:825:CYS:O	1:A:826:THR:C	2.57	0.46
1:B:665:ILE:HG13	1:B:666:GLN:N	2.31	0.46
1:A:746:LEU:O	1:A:747:GLU:C	2.60	0.45
1:B:813:LEU:HB3	1:B:814:PRO:CD	2.45	0.45
1:B:708:GLU:O	1:B:709:TYR:C	2.60	0.45
1:B:826:THR:O	1:B:827:GLN:C	2.60	0.45
1:A:562:SER:HB2	1:A:774:ILE:HD11	1.98	0.45
1:A:793:GLU:OE2	1:A:801:PRO:HA	2.17	0.45
2:D:86:ILE:HG22	2:D:87:ILE:N	2.31	0.45
1:A:780:GLU:O	1:A:783:ALA:HB3	2.17	0.45
1:A:813:LEU:HD22	1:A:853:TRP:CZ3	2.52	0.45
1:B:570:GLU:HA	1:B:573:LEU:HD12	1.98	0.45
1:B:746:LEU:HD13	1:B:746:LEU:HA	1.76	0.45
1:B:832:LEU:O	1:B:832:LEU:HG	2.18	0.44
1:A:814:PRO:HD2	1:A:815:LYS:CE	2.45	0.44
1:A:815:LYS:HE3	1:A:815:LYS:H	1.82	0.44
1:B:577:ARG:NH1	1:B:580:THR:HG21	2.32	0.44
1:A:802:ILE:HB	1:A:803:PRO:HD2	1.98	0.44
1:A:842:LEU:HD23	1:A:842:LEU:HA	1.77	0.44
1:B:842:LEU:HA	1:B:842:LEU:HD23	1.78	0.44
2:C:71:GLU:OE1	2:C:71:GLU:N	2.51	0.44
1:A:765:LEU:N	1:A:765:LEU:CD2	2.81	0.43
1:A:765:LEU:O	1:A:768:ILE:HG22	2.18	0.43
1:B:634:ILE:O	1:B:635:GLN:C	2.61	0.43
1:A:618:ALA:HB1	1:A:651:LEU:O	2.19	0.43
1:A:813:LEU:N	1:A:814:PRO:CD	2.80	0.43
1:B:814:PRO:HD2	1:B:815:LYS:CE	2.48	0.43
1:A:634:ILE:O	1:A:635:GLN:C	2.61	0.43
1:A:708:GLU:O	1:A:709:TYR:C	2.61	0.43
1:B:699:GLN:HB3	1:B:702:SER:HB3	2.01	0.43
1:A:654:ASP:HA	1:A:685:HIS:CD2	2.53	0.43
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.70	0.43
1:A:756:LEU:HD23	1:A:756:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:ILE:CD1	1:B:673:ALA:HB2	2.48	0.43
1:A:802:ILE:HG12	1:A:805:MET:HE2	2.01	0.43
1:A:773:PRO:HB3	1:B:840:PHE:CD1	2.52	0.43
1:A:773:PRO:CB	1:B:840:PHE:CE1	2.90	0.43
1:B:661:ASN:O	1:B:665:ILE:HG23	2.19	0.43
1:B:740:ARG:HH12	1:B:741:LYS:HE2	1.83	0.43
1:B:807:ARG:HG3	1:B:807:ARG:NH1	2.32	0.43
1:A:561:PHE:CD2	1:A:561:PHE:C	2.97	0.42
1:B:746:LEU:O	1:B:747:GLU:C	2.62	0.42
1:B:768:ILE:O	1:B:768:ILE:HG13	2.19	0.42
1:A:813:LEU:HB3	1:A:814:PRO:CD	2.49	0.42
1:A:563:ASP:HA	1:A:566:LEU:HD12	2.02	0.42
1:A:665:ILE:HD12	1:A:673:ALA:HB2	2.02	0.42
1:A:663:SER:O	1:A:667:ARG:HD3	2.20	0.42
1:B:578:MET:HE1	1:B:623:GLN:HB2	2.01	0.42
1:B:598:TRP:HA	1:B:698:ASN:OD1	2.20	0.41
1:A:575:THR:O	1:A:578:MET:HB2	2.20	0.41
1:B:600:LEU:HD12	1:B:600:LEU:HA	1.74	0.41
1:B:815:LYS:HE3	1:B:815:LYS:H	1.85	0.41
1:B:818:VAL:HG12	1:B:819:GLY:N	2.33	0.41
1:A:635:GLN:HG3	1:A:643:ILE:HD13	2.02	0.41
1:B:635:GLN:HG3	1:B:643:ILE:HD13	2.02	0.41
1:B:765:LEU:H	1:B:765:LEU:CD2	2.33	0.41
1:B:772:TRP:N	1:B:773:PRO:CD	2.83	0.41
1:B:575:THR:O	1:B:578:MET:HB2	2.21	0.41
1:B:591:LYS:HB2	1:B:594:VAL:HG23	2.02	0.41
1:B:678:HIS:HD2	2:D:71:GLU:OE2	2.03	0.41
1:B:756:LEU:HD23	1:B:756:LEU:HA	1.82	0.41
1:A:654:ASP:O	1:A:657:HIS:HB2	2.21	0.41
1:A:831:ALA:O	1:A:835:VAL:HG23	2.20	0.41
1:B:817:GLN:OE1	1:B:817:GLN:HA	2.20	0.41
2:D:71:GLU:N	2:D:71:GLU:OE1	2.53	0.41
1:B:565:GLU:H	1:B:565:GLU:CD	2.28	0.41
1:B:569:LEU:HD22	1:B:569:LEU:HA	1.81	0.41
1:A:672:LEU:HD12	1:A:672:LEU:HA	1.84	0.41
1:A:813:LEU:C	1:A:813:LEU:HD23	2.45	0.41
1:B:639:THR:O	1:B:643:ILE:HG13	2.21	0.41
1:B:859:GLN:O	6:B:8:HOH:O	2.21	0.41
1:A:595:LEU:O	1:A:599:ILE:HG13	2.21	0.41
1:A:730:LYS:O	1:A:730:LYS:HG3	2.20	0.41
1:A:740:ARG:HH12	1:A:741:LYS:HE2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:CYS:O	1:A:828:LEU:N	2.54	0.41
1:B:601:SER:HA	1:B:604:LYS:HE2	2.03	0.41
1:B:654:ASP:O	1:B:657:HIS:HB2	2.20	0.41
1:B:856:LEU:HA	1:B:856:LEU:HD23	1.79	0.41
1:A:579:PHE:C	1:A:585:VAL:HG23	2.46	0.41
1:A:600:LEU:HD12	1:A:600:LEU:HA	1.74	0.41
1:A:635:GLN:C	1:A:637:LYS:H	2.28	0.41
1:A:832:LEU:O	1:A:832:LEU:HG	2.20	0.41
1:A:800:GLN:HA	1:A:801:PRO:HD3	1.85	0.40
1:B:647:LEU:HD12	1:B:647:LEU:HA	1.92	0.40
1:A:665:ILE:CD1	1:A:673:ALA:HB2	2.51	0.40
1:B:698:ASN:O	1:B:700:ILE:N	2.54	0.40
1:A:699:GLN:HG2	5:A:902:IBM:C10	2.51	0.40
1:B:765:LEU:HD22	1:B:765:LEU:N	2.36	0.40
1:B:673:ALA:HA	1:B:680:ILE:HD13	2.03	0.40
1:B:736:PHE:CE1	1:B:827:GLN:CG	2.98	0.40
1:A:595:LEU:HA	1:A:700:ILE:CG2	2.51	0.40
1:B:561:PHE:CD2	1:B:561:PHE:C	2.99	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	321/330 (97%)	291 (91%)	27 (8%)	3 (1%)	14	48
1	B	326/330 (99%)	295 (90%)	30 (9%)	1 (0%)	36	70
2	C	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
2	D	15/18 (83%)	15 (100%)	0	0	100	100
All	All	677/696 (97%)	615 (91%)	58 (9%)	4 (1%)	21	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	699	GLN
1	A	564	PHE
1	B	699	GLN
1	A	680	ILE

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	289/295 (98%)	256 (89%)	33 (11%)	5	24
1	B	294/295 (100%)	258 (88%)	36 (12%)	5	21
2	C	14/15 (93%)	11 (79%)	3 (21%)	1	6
2	D	14/15 (93%)	11 (79%)	3 (21%)	1	6
All	All	611/620 (98%)	536 (88%)	75 (12%)	4	21

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	541	GLN
1	A	547	VAL
1	A	548	VAL
1	A	555	LYS
1	A	557	THR
1	A	560	SER
1	A	565	GLU
1	A	569	LEU
1	A	580	THR
1	A	600	LEU
1	A	603	LYS
1	A	608	LYS
1	A	638	LEU
1	A	641	LEU
1	A	652	SER
1	A	658	ARG
1	A	660	VAL
1	A	665	ILE

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Mol	Chain	Res	Type
1	A	706	ILE
1	A	725	LEU
1	A	752	LYS
1	A	753	GLU
1	A	765	LEU
1	A	788	GLU
1	A	796	VAL
1	A	809	LYS
1	A	810	ARG
1	A	811	ASP
1	A	815	LYS
1	A	818	VAL
1	A	826	THR
1	A	848	LYS
1	A	852	LYS
1	B	534	MET
1	B	541	GLN
1	B	547	VAL
1	B	548	VAL
1	B	555	LYS
1	B	557	THR
1	B	560	SER
1	B	565	GLU
1	B	569	LEU
1	B	580	THR
1	B	600	LEU
1	B	603	LYS
1	B	608	LYS
1	B	638	LEU
1	B	641	LEU
1	B	652	SER
1	B	658	ARG
1	B	660	VAL
1	B	665	ILE
1	B	691	MET
1	B	706	ILE
1	B	725	LEU
1	B	746	LEU
1	B	752	LYS
1	B	753	GLU
1	B	765	LEU
1	B	788	GLU

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Mol	Chain	Res	Type
1	B	796	VAL
1	B	809	LYS
1	B	810	ARG
1	B	811	ASP
1	B	815	LYS
1	B	818	VAL
1	B	826	THR
1	B	848	LYS
1	B	852	LYS
2	C	78	LEU
2	C	80	GLU
2	C	86	ILE
2	D	78	LEU
2	D	80	GLU
2	D	86	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	592	HIS
1	A	635	GLN
1	A	699	GLN
1	A	751	GLN
1	A	834	HIS
1	B	541	GLN
1	B	592	HIS
1	B	635	GLN
1	B	834	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
5	IBM	B	901	-	17,17,17	1.52	5 (29%)	19,25,25	2.18	10 (52%)
5	IBM	A	902	-	17,17,17	1.33	1 (5%)	19,25,25	2.12	8 (42%)
5	IBM	A	901	-	17,17,17	1.34	2 (11%)	19,25,25	1.89	5 (26%)
5	IBM	B	902	-	17,17,17	1.34	3 (17%)	19,25,25	1.95	7 (36%)
5	IBM	A	903	-	17,17,17	1.23	1 (5%)	19,25,25	2.07	6 (31%)

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
5	IBM	B	901	-	-	2/4/4/4	0/2/2/2
5	IBM	A	902	-	-	4/4/4/4	0/2/2/2
5	IBM	A	901	-	-	2/4/4/4	0/2/2/2
5	IBM	B	902	-	-	2/4/4/4	0/2/2/2
5	IBM	A	903	-	-	4/4/4/4	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	IBM	C4-N3	-3.01	1.33	1.38
5	A	902	IBM	C6-N1	-2.94	1.34	1.40
5	B	902	IBM	C6-N1	-2.49	1.35	1.40
5	B	901	IBM	C6-N1	-2.46	1.35	1.40
5	A	901	IBM	C6-N1	-2.34	1.35	1.40
5	B	901	IBM	C5-N7	-2.31	1.34	1.39
5	B	902	IBM	C2-N3	-2.22	1.35	1.38
5	A	901	IBM	C4-N3	-2.20	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	903	IBM	O2-C2	2.19	1.26	1.22
5	B	902	IBM	C2-N1	-2.16	1.34	1.39
5	B	901	IBM	C2-N1	-2.05	1.35	1.39
5	B	901	IBM	O2-C2	2.04	1.26	1.22

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	902	IBM	N3-C2-N1	5.06	122.96	116.72
5	A	903	IBM	N3-C2-N1	4.65	122.46	116.72
5	B	902	IBM	N3-C2-N1	4.15	121.84	116.72
5	A	901	IBM	N3-C2-N1	4.15	121.83	116.72
5	B	901	IBM	N3-C2-N1	3.64	121.21	116.72
5	B	901	IBM	C12-C11-N3	-3.54	107.24	112.38
5	A	902	IBM	N9-C8-N7	-3.32	109.12	112.98
5	B	901	IBM	N9-C8-N7	-3.27	109.19	112.98
5	A	901	IBM	C6-C5-N7	3.20	136.46	129.36
5	B	901	IBM	C6-C5-N7	3.08	136.20	129.36
5	A	903	IBM	C6-N1-C2	-3.04	120.71	125.66
5	A	903	IBM	N9-C8-N7	-2.99	109.51	112.98
5	A	903	IBM	C6-C5-N7	2.90	135.80	129.36
5	B	902	IBM	C6-C5-N7	2.76	135.50	129.36
5	B	901	IBM	C6-N1-C2	-2.76	121.18	125.66
5	A	901	IBM	C6-N1-C2	-2.74	121.21	125.66
5	A	902	IBM	C6-C5-N7	2.73	135.42	129.36
5	A	902	IBM	C12-C11-N3	2.72	116.33	112.38
5	B	901	IBM	C8-N7-C5	2.71	108.05	104.38
5	B	901	IBM	O2-C2-N1	-2.71	117.59	121.33
5	B	902	IBM	C6-N1-C2	-2.70	121.27	125.66
5	A	903	IBM	C8-N7-C5	2.62	107.92	104.38
5	B	902	IBM	N9-C8-N7	-2.62	109.94	112.98
5	A	902	IBM	C8-N7-C5	2.61	107.91	104.38
5	A	902	IBM	C6-N1-C2	-2.58	121.46	125.66
5	A	903	IBM	O2-C2-N1	-2.58	117.77	121.33
5	A	901	IBM	N9-C8-N7	-2.52	110.06	112.98
5	A	902	IBM	O2-C2-N3	-2.42	118.72	121.98
5	A	901	IBM	C8-N7-C5	2.41	107.64	104.38
5	B	902	IBM	C12-C11-N3	-2.36	108.96	112.38
5	B	902	IBM	O6-C6-C5	-2.25	118.78	124.59
5	A	902	IBM	O2-C2-N1	-2.18	118.32	121.33
5	B	901	IBM	C10-N1-C6	2.17	121.00	117.64
5	B	902	IBM	C10-N1-C6	2.13	120.95	117.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	901	IBM	O6-C6-C5	-2.08	119.24	124.59
5	B	901	IBM	C11-N3-C2	2.02	121.78	117.67

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	902	IBM	C12-C11-N3-C4
5	A	902	IBM	C12-C11-N3-C2
5	A	901	IBM	N3-C11-C12-C13
5	A	902	IBM	N3-C11-C12-C14
5	A	903	IBM	N3-C11-C12-C13
5	A	901	IBM	N3-C11-C12-C14
5	A	902	IBM	N3-C11-C12-C13
5	A	903	IBM	N3-C11-C12-C14
5	B	902	IBM	N3-C11-C12-C13
5	B	902	IBM	N3-C11-C12-C14
5	A	903	IBM	C12-C11-N3-C4
5	A	903	IBM	C12-C11-N3-C2
5	B	901	IBM	C12-C11-N3-C2
5	B	901	IBM	C12-C11-N3-C4

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	901	IBM	1	0
5	A	902	IBM	3	0
5	A	901	IBM	3	0
5	B	902	IBM	3	0
5	A	903	IBM	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/330 (97%)	-0.30	1 (0%) 90 79	25, 44, 69, 92	0
1	B	328/330 (99%)	-0.23	2 (0%) 85 69	26, 44, 70, 90	0
2	C	17/18 (94%)	0.12	1 (5%) 28 14	34, 53, 75, 98	0
2	D	17/18 (94%)	0.35	1 (5%) 28 14	32, 56, 76, 98	0
All	All	685/696 (98%)	-0.24	5 (0%) 84 66	25, 44, 71, 98	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	564	PHE	2.7
1	B	813	LEU	2.5
2	D	71	GLU	2.4
2	C	87	ILE	2.2
1	A	537	THR	2.1

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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
5	IBM	B	902	16/16	0.83	0.13	66,85,100,103	0
5	IBM	A	903	16/16	0.89	0.11	31,54,64,72	0
5	IBM	A	902	16/16	0.89	0.12	55,70,81,94	0
3	ZN	A	899	1/1	0.93	0.07	43,43,43,43	0
4	MG	A	900	1/1	0.95	0.15	18,18,18,18	0
5	IBM	A	901	16/16	0.96	0.08	29,47,58,62	0
5	IBM	B	901	16/16	0.96	0.09	16,31,47,48	0
3	ZN	B	899	1/1	0.96	0.04	41,41,41,41	0
4	MG	B	900	1/1	0.98	0.07	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.