WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 12:09 am GMT

PDB ID : 1QIP

Title : HUMAN GLYOXALASE I COMPLEXED WITH S-P-NITROBENZYLOXY CARBONYLGLUTATHIONE

Authors : Cameron, A.D.; Ridderstrom, M.; Olin, B.; Mannervik, B.

Deposited on : 1999-06-14

Resolution : 1.72 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 (i)) 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 1.72 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	Percentile Ranks	Value
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		2.7%
RSRZ outliers		3.8%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
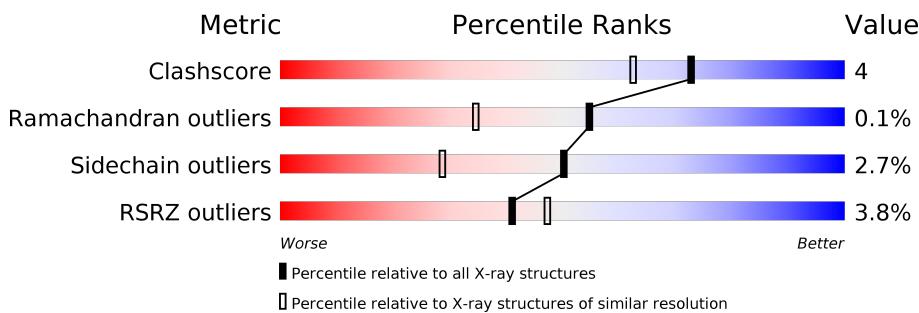
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4841 (1.74-1.70)
Ramachandran outliers	110173	4771 (1.74-1.70)
Sidechain outliers	110143	4771 (1.74-1.70)
RSRZ outliers	101464	4426 (1.74-1.70)

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	183	% 87% 9% ·
1	B	183	5% 89% 10% ·
1	C	183	2% 89% 7% · ·
1	D	183	7% 92% 7% ·
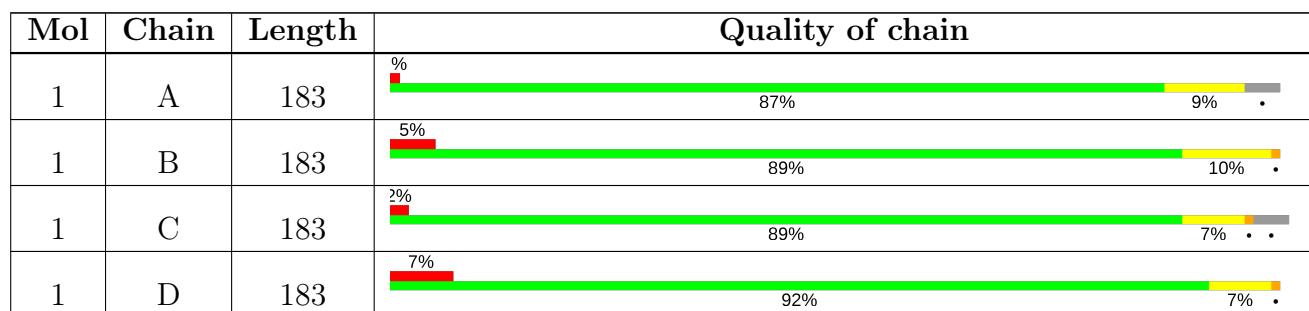
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GNB	A	1002	X	-	-	X
3	GNB	B	1001	X	-	-	X
3	GNB	C	1004	X	-	-	X
3	GNB	D	1003	X	-	-	X
4	BME	D	204	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6756 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 (LACTOYLGLUTATHIONE LYASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	15	0	0
			1400	892	229	269	10			
1	B	183	Total	C	N	O	S	28	0	0
			1450	923	237	280	10			
1	C	176	Total	C	N	O	S	16	0	0
			1399	892	229	268	10			
1	D	183	Total	C	N	O	S	16	0	0
			1450	923	237	280	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	GLU	ALA	VARIANT	UNP Q04760
B	110	GLU	ALA	VARIANT	UNP Q04760
C	110	GLU	ALA	VARIANT	UNP Q04760
D	110	GLU	ALA	VARIANT	UNP Q04760

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is S-P-NITROBENZYLOXYCARBONYLGLUTATHIONE (three-letter code: GNB) (formula: $C_{18}H_{24}N_4O_{10}S$).
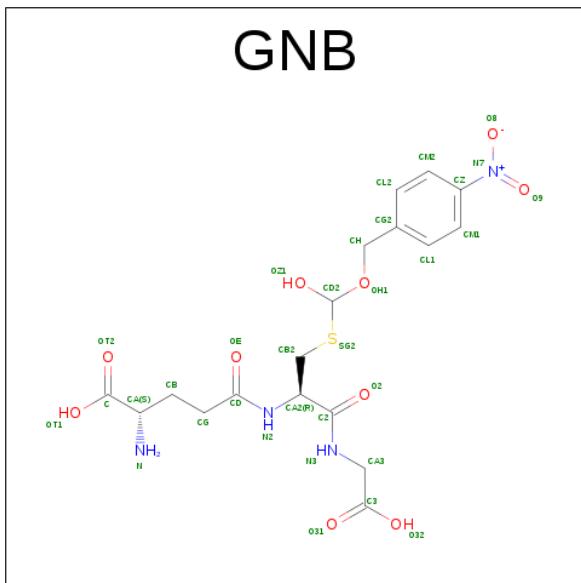
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			33	18	4	10	1		
3	A	1	Total	C	N	O	S	0	0
			33	18	4	10	1		
3	D	1	Total	C	N	O	S	0	0
			33	18	4	10	1		
3	C	1	Total	C	N	O	S	0	0
			33	18	4	10	1		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).
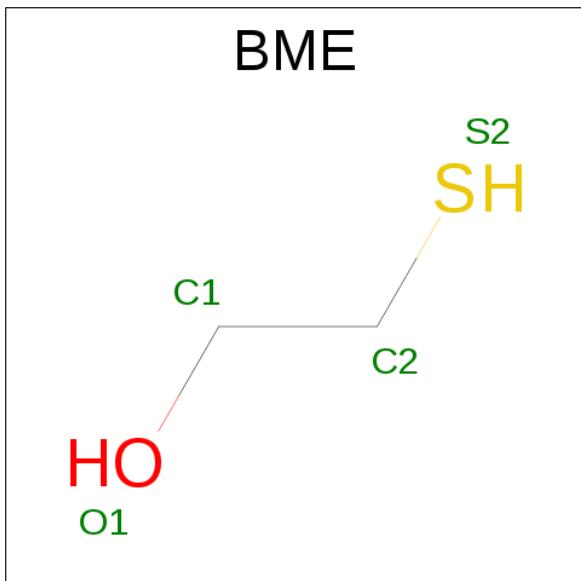
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	227	Total 227	O 227	0	0
5	B	224	Total 224	O 224	0	0
5	C	229	Total 229	O 229	0	0
5	D	225	Total 225	O 225	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PROTEIN (LACTOYLGLUTATHIONE LYASE)
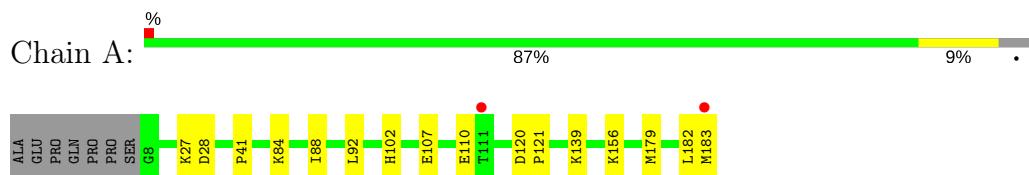
• Molecule 1: PROTEIN (LACTOYLGLUTATHIONE LYASE)
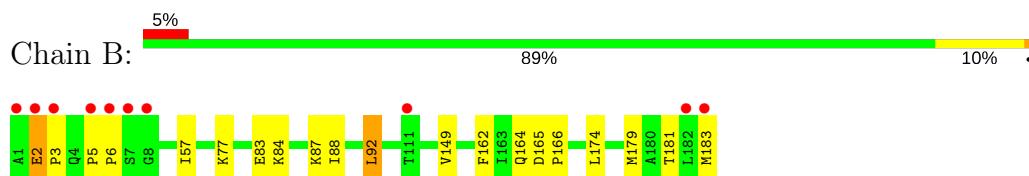
• Molecule 1: PROTEIN (LACTOYLGLUTATHIONE LYASE)
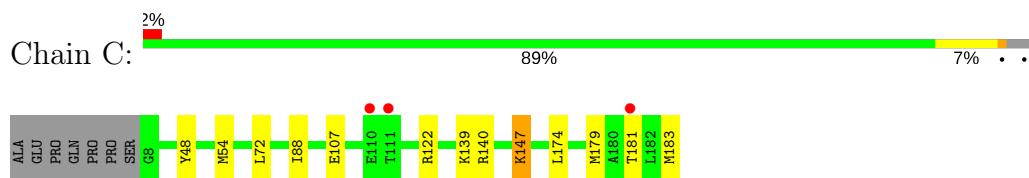
• Molecule 1: PROTEIN (LACTOYLGLUTATHIONE LYASE)
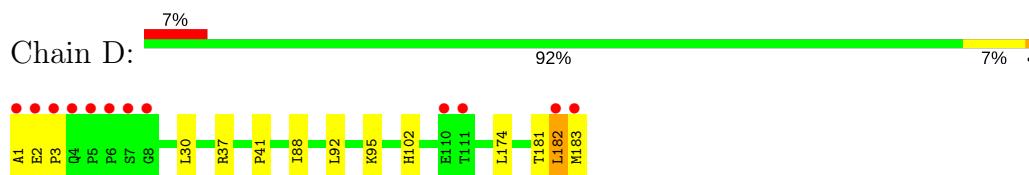
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	67.30Å 67.30Å 167.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.72 28.83 – 1.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-1.72) 99.8 (28.83-1.72)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 1.72Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.210 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	15.3	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6756	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.43	0/1432	0.96	0/1930
1	B	0.51	1/1485 (0.1%)	0.91	0/2005
1	C	0.41	0/1431	0.94	2/1930 (0.1%)
1	D	0.52	1/1485 (0.1%)	1.09	3/2005 (0.1%)
All	All	0.47	2/5833 (0.0%)	0.98	5/7870 (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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	182	LEU	C-N	11.91	1.61	1.34
1	B	83	GLU	CB-CG	8.67	1.68	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	182	LEU	O-C-N	-25.06	82.61	122.70
1	D	182	LEU	CA-C-N	-8.11	99.36	117.20
1	C	140	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	D	37	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	C	122	ARG	NE-CZ-NH2	-5.44	117.58	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	182	LEU	Mainchain

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	1400	0	1374	15	0
1	B	1450	0	1422	14	0
1	C	1399	0	1374	9	0
1	D	1450	0	1422	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	33	0	20	5	0
3	B	33	0	20	4	0
3	C	33	0	20	1	0
3	D	33	0	20	3	0
4	A	4	0	5	0	0
4	B	4	0	5	0	0
4	C	4	0	5	0	0
4	D	4	0	5	0	0
5	A	227	0	0	0	0
5	B	224	0	0	0	0
5	C	229	0	0	1	0
5	D	225	0	0	0	0
All	All	6756	0	5692	44	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 4.

All (44) 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:48:TYR:HB3	1:C:54:MET:HE2	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:MET:HE3	1:C:72:LEU:HB3	1.45	0.96
1:A:179:MET:HG3	1:B:92:LEU:HD12	1.51	0.90
1:A:183:MET:OXT	1:A:183:MET:HG3	1.78	0.84
1:A:88:ILE:HG12	3:A:1002:GNB:O8	1.92	0.70
1:A:92:LEU:HD13	1:B:179:MET:HG3	1.74	0.69
1:C:54:MET:HE3	1:C:72:LEU:CB	2.25	0.66
1:C:179:MET:HG3	1:D:92:LEU:HD13	1.76	0.66
1:B:88:ILE:HG23	3:B:1001:GNB:O9	1.95	0.66
1:D:88:ILE:HG12	3:D:1003:GNB:O8	1.97	0.65
1:C:48:TYR:CB	1:C:54:MET:HE2	2.23	0.64
1:C:48:TYR:HB3	1:C:54:MET:CE	2.23	0.62
1:B:2:GLU:H	1:B:3:PRO:HD2	1.64	0.62
1:A:110:GLU:CD	1:A:110:GLU:H	2.06	0.58
1:B:2:GLU:HB3	1:B:3:PRO:HD3	1.86	0.57
1:D:88:ILE:HG23	3:D:1003:GNB:O9	2.05	0.56
1:D:1:ALA:O	1:D:2:GLU:HB2	2.05	0.56
1:B:165:ASP:HB2	1:B:166:PRO:CD	2.39	0.53
1:A:88:ILE:HG23	3:A:1002:GNB:O9	2.09	0.52
1:B:88:ILE:HG12	3:B:1001:GNB:O8	2.09	0.52
1:D:2:GLU:N	1:D:3:PRO:CD	2.74	0.50
1:A:182:LEU:O	1:A:183:MET:CB	2.61	0.49
1:D:30:LEU:HD13	1:D:95:LYS:HB3	1.95	0.49
1:B:2:GLU:HB3	1:B:3:PRO:CD	2.43	0.48
1:C:147:LYS:N	1:C:147:LYS:HD2	2.28	0.48
1:D:2:GLU:N	1:D:3:PRO:HD3	2.30	0.47
1:C:139:LYS:HD3	5:C:1193:HOH:O	2.14	0.47
1:A:92:LEU:HD11	3:A:1002:GNB:CM1	2.45	0.46
1:B:88:ILE:HG23	3:B:1001:GNB:N7	2.31	0.46
1:D:88:ILE:HG23	3:D:1003:GNB:N7	2.31	0.46
1:A:88:ILE:HG23	3:A:1002:GNB:N7	2.32	0.45
1:A:27:LYS:O	1:A:28:ASP:HB2	2.15	0.45
3:A:1002:GNB:HA32	1:B:162:PHE:CE1	2.50	0.45
1:C:88:ILE:HG23	3:C:1004:GNB:O9	2.18	0.44
1:A:156:LYS:HG3	1:A:183:MET:CE	2.48	0.43
1:A:182:LEU:HD12	3:B:1001:GNB:HC1	2.00	0.43
1:A:120:ASP:HA	1:A:121:PRO:HA	1.85	0.42
1:A:41:PRO:HD3	1:A:102:HIS:CD2	2.54	0.42
1:B:57:ILE:O	1:B:87:LYS:HE2	2.20	0.41
1:B:149:VAL:HG23	1:B:164:GLN:HG3	2.02	0.41
1:B:5:PRO:HA	1:B:6:PRO:HD3	1.91	0.41
1:D:41:PRO:HD3	1:D:102:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LYS:HG3	1:A:183:MET:HE1	2.03	0.40
1:B:165:ASP:HB2	1:B:166:PRO:HD2	2.00	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	174/183 (95%)	171 (98%)	3 (2%)	0	100	100
1	B	181/183 (99%)	176 (97%)	4 (2%)	1 (1%)	28	11
1	C	174/183 (95%)	171 (98%)	3 (2%)	0	100	100
1	D	181/183 (99%)	175 (97%)	6 (3%)	0	100	100
All	All	710/732 (97%)	693 (98%)	16 (2%)	1 (0%)	55	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	GLU

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	153/159 (96%)	150 (98%)	3 (2%)	60	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	159/159 (100%)	153 (96%)	6 (4%)	38	15
1	C	153/159 (96%)	148 (97%)	5 (3%)	43	20
1	D	159/159 (100%)	156 (98%)	3 (2%)	62	43
All	All	624/636 (98%)	607 (97%)	17 (3%)	50	29

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LYS
1	A	107	GLU
1	A	139	LYS
1	B	77	LYS
1	B	84	LYS
1	B	92	LEU
1	B	174	LEU
1	B	181	THR
1	B	183	MET
1	C	107	GLU
1	C	147	LYS
1	C	174	LEU
1	C	181	THR
1	C	183	MET
1	D	174	LEU
1	D	181	THR
1	D	183	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	115	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 ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	GNB	A	1002	-	21,33,33	1.87	3 (14%)	27,43,43	1.92	8 (29%)
4	BME	A	204	-	3,3,3	1.14	0	2,2,2	0.74	0
3	GNB	B	1001	-	21,33,33	1.75	3 (14%)	27,43,43	1.97	7 (25%)
4	BME	B	204	-	3,3,3	1.09	0	2,2,2	0.36	0
3	GNB	C	1004	-	21,33,33	1.82	2 (9%)	27,43,43	2.00	4 (14%)
4	BME	C	204	-	3,3,3	1.09	0	2,2,2	0.67	0
3	GNB	D	1003	-	21,33,33	1.83	3 (14%)	27,43,43	1.68	7 (25%)
4	BME	D	204	-	3,3,3	1.11	0	2,2,2	0.54	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
3	GNB	A	1002	-	1/1/8/10	0/24/36/36	0/1/1/1
4	BME	A	204	-	-	0/1/1/1	0/0/0/0
3	GNB	B	1001	-	1/1/8/10	0/24/36/36	0/1/1/1
4	BME	B	204	-	-	0/1/1/1	0/0/0/0
3	GNB	C	1004	-	1/1/8/10	0/24/36/36	0/1/1/1
4	BME	C	204	-	-	0/1/1/1	0/0/0/0
3	GNB	D	1003	-	1/1/8/10	0/24/36/36	0/1/1/1
4	BME	D	204	-	-	0/1/1/1	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1003	GNB	OZ1-CD2	-5.63	1.22	1.40
3	C	1004	GNB	OZ1-CD2	-5.52	1.23	1.40
3	A	1002	GNB	OZ1-CD2	-5.42	1.23	1.40
3	B	1001	GNB	OZ1-CD2	-5.09	1.24	1.40
3	D	1003	GNB	CA2-N2	2.06	1.50	1.45
3	A	1002	GNB	CA2-N2	2.14	1.50	1.45
3	B	1001	GNB	CA2-N2	2.24	1.50	1.45
3	B	1001	GNB	O9-N7	3.90	1.29	1.22
3	D	1003	GNB	O9-N7	4.10	1.30	1.22
3	C	1004	GNB	O9-N7	4.35	1.30	1.22
3	A	1002	GNB	O9-N7	4.46	1.30	1.22

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	GNB	CH-CG2-CL1	-4.52	109.94	120.66
3	A	1002	GNB	CA3-N3-C2	-3.68	117.41	122.39
3	C	1004	GNB	CA3-N3-C2	-3.54	117.60	122.39
3	D	1003	GNB	CH-CG2-CL1	-3.44	112.50	120.66
3	B	1001	GNB	OH1-CH-CG2	-3.37	101.97	109.95
3	A	1002	GNB	O2-C2-N3	-3.30	116.72	123.07
3	B	1001	GNB	CA2-N2-CD	-2.68	114.55	121.62
3	A	1002	GNB	CH-CG2-CL1	-2.52	114.69	120.66
3	B	1001	GNB	CM2-CL2-CG2	-2.42	117.67	121.02
3	D	1003	GNB	OH1-CH-CG2	-2.14	104.88	109.95
3	D	1003	GNB	CA3-N3-C2	-2.14	119.50	122.39
3	D	1003	GNB	CM2-CL2-CG2	-2.06	118.18	121.02
3	A	1002	GNB	OE-CD-CG	-2.03	118.20	122.01
3	A	1002	GNB	CL2-CG2-CL1	2.10	121.49	118.16
3	A	1002	GNB	CB2-SG2-CD2	2.54	104.01	100.35
3	D	1003	GNB	CL2-CG2-CL1	2.65	122.37	118.16
3	B	1001	GNB	CL2-CG2-CL1	2.76	122.53	118.16
3	B	1001	GNB	CH-CG2-CL2	2.89	127.51	120.66
3	D	1003	GNB	CB2-SG2-CD2	2.89	104.52	100.35
3	D	1003	GNB	O9-N7-CZ	3.32	124.08	118.80
3	C	1004	GNB	CM1-CZ-N7	3.42	122.01	119.41
3	A	1002	GNB	O9-N7-CZ	3.65	124.62	118.80
3	A	1002	GNB	CA2-C2-N3	4.18	125.05	116.51
3	C	1004	GNB	O9-N7-CZ	4.19	125.48	118.80
3	B	1001	GNB	O9-N7-CZ	4.44	125.87	118.80
3	C	1004	GNB	CB2-SG2-CD2	6.79	110.14	100.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1004	GNB	CD2
3	B	1001	GNB	CD2
3	A	1002	GNB	CD2
3	D	1003	GNB	CD2

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	GNB	5	0
3	B	1001	GNB	4	0
3	C	1004	GNB	1	0
3	D	1003	GNB	3	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	176/183 (96%)	0.02	2 (1%)	80	84	9, 15, 29, 45	5 (2%)
1	B	183/183 (100%)	0.24	10 (5%)	26	29	9, 16, 36, 50	7 (3%)
1	C	175/183 (95%)	-0.04	3 (1%)	70	76	10, 17, 29, 49	2 (1%)
1	D	183/183 (100%)	0.32	12 (6%)	19	22	10, 16, 37, 51	3 (1%)
All	All	717/732 (97%)	0.14	27 (3%)	41	47	9, 16, 33, 51	17 (2%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	MET	20.2
1	B	1	ALA	16.1
1	A	183	MET	11.3
1	D	3	PRO	11.0
1	D	2	GLU	10.0
1	D	1	ALA	9.5
1	D	183	MET	8.9
1	D	6	PRO	7.2
1	D	5	PRO	7.1
1	D	7	SER	5.2
1	B	5	PRO	4.3
1	C	181	THR	4.2
1	B	3	PRO	4.2
1	D	8	GLY	4.0
1	B	2	GLU	3.9
1	B	8	GLY	3.7
1	D	182	LEU	3.7
1	D	4	GLN	3.4
1	B	182	LEU	3.4
1	C	110	GLU	3.4
1	B	111	THR	3.3

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Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	6	PRO	3.3
1	B	7	SER	3.2
1	D	111	THR	2.9
1	A	111	THR	2.3
1	D	110	GLU	2.1
1	C	111	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	GNB	B	1001	33/33	0.73	0.21	5.67	18,31,45,46	0
3	GNB	C	1004	33/33	0.84	0.17	4.12	15,30,43,44	0
3	GNB	D	1003	33/33	0.81	0.19	3.80	18,32,42,43	0
3	GNB	A	1002	33/33	0.79	0.21	3.63	15,28,41,43	0
4	BME	D	204	4/4	0.88	0.15	2.00	32,34,34,35	0
4	BME	C	204	4/4	0.92	0.18	1.21	34,35,35,35	0
4	BME	B	204	4/4	0.94	0.15	0.92	31,33,34,36	0
4	BME	A	204	4/4	0.92	0.14	-0.23	29,32,32,32	0
2	ZN	C	904	1/1	0.99	0.04	-2.84	13,13,13,13	0
2	ZN	A	902	1/1	1.00	0.05	-3.37	12,12,12,12	0
2	ZN	B	901	1/1	0.99	0.04	-4.30	13,13,13,13	0
2	ZN	D	903	1/1	0.99	0.04	-4.62	14,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.