



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:36 PM UTC

PDB ID : 4ZM9 / pdb_00004zm9
Title : Crystal structure of circularly permuted human asparaginase-like protein 1
Authors : Li, W.Z.; Zhang, Y.
Deposited on : 2015-05-02
Resolution : 2.51 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

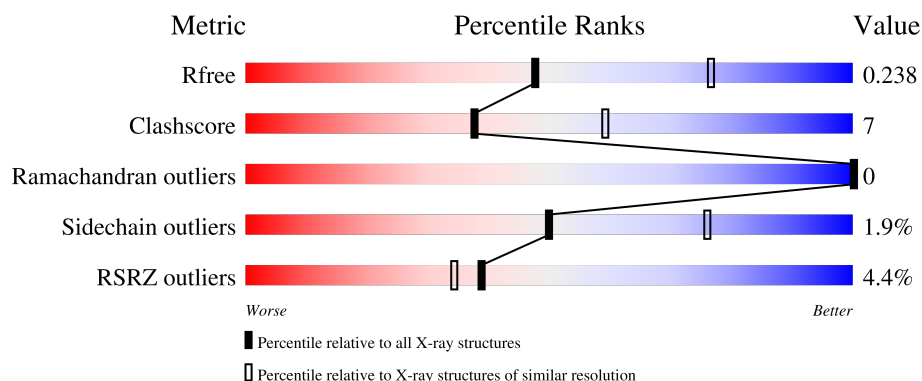
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

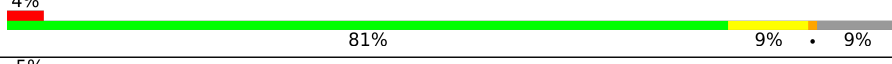
The reported resolution of this entry is 2.51 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	327	
1	B	327	
1	C	327	
1	D	327	

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	GLY	B	402	-	X	-	-
4	BME	A	405	-	-	X	-
4	BME	A	406	-	-	X	-
4	BME	C	406	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8838 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 Isoaspartyl peptidase/L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	3	0
			2163	1346	379	423	15			
1	B	296	Total	C	N	O	S	0	3	0
			2166	1347	380	424	15			
1	C	296	Total	C	N	O	S	0	3	0
			2163	1346	379	423	15			
1	D	296	Total	C	N	O	S	0	3	0
			2166	1347	380	424	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	linker	UNP Q7L266
A	154N	HIS	-	expression tag	UNP Q7L266
A	154O	HIS	-	expression tag	UNP Q7L266
A	154P	HIS	-	expression tag	UNP Q7L266
A	154Q	HIS	-	expression tag	UNP Q7L266
A	154R	HIS	-	expression tag	UNP Q7L266
A	154S	HIS	-	expression tag	UNP Q7L266
A	154T	MET	-	SEE REMARK 999	UNP Q7L266
A	309	GLY	-	linker	UNP Q7L266
A	310	ALA	-	linker	UNP Q7L266
A	311	GLY	-	linker	UNP Q7L266
A	312	SER	-	linker	UNP Q7L266
A	313	GLY	-	linker	UNP Q7L266
A	314	ALA	-	linker	UNP Q7L266
A	315	GLY	-	linker	UNP Q7L266
A	316	SER	-	linker	UNP Q7L266
A	317	GLY	-	linker	UNP Q7L266
A	318	ALA	-	linker	UNP Q7L266
A	319	GLY	-	linker	UNP Q7L266
A	320	GLY	-	linker	UNP Q7L266
B	1	GLY	-	linker	UNP Q7L266

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Chain	Residue	Modelled	Actual	Comment	Reference
B	154N	HIS	-	expression tag	UNP Q7L266
B	154O	HIS	-	expression tag	UNP Q7L266
B	154P	HIS	-	expression tag	UNP Q7L266
B	154Q	HIS	-	expression tag	UNP Q7L266
B	154R	HIS	-	expression tag	UNP Q7L266
B	154S	HIS	-	expression tag	UNP Q7L266
B	154T	MET	-	SEE REMARK 999	UNP Q7L266
B	309	GLY	-	linker	UNP Q7L266
B	310	ALA	-	linker	UNP Q7L266
B	311	GLY	-	linker	UNP Q7L266
B	312	SER	-	linker	UNP Q7L266
B	313	GLY	-	linker	UNP Q7L266
B	314	ALA	-	linker	UNP Q7L266
B	315	GLY	-	linker	UNP Q7L266
B	316	SER	-	linker	UNP Q7L266
B	317	GLY	-	linker	UNP Q7L266
B	318	ALA	-	linker	UNP Q7L266
B	319	GLY	-	linker	UNP Q7L266
B	320	GLY	-	linker	UNP Q7L266
C	1	GLY	-	linker	UNP Q7L266
C	154N	HIS	-	expression tag	UNP Q7L266
C	154O	HIS	-	expression tag	UNP Q7L266
C	154P	HIS	-	expression tag	UNP Q7L266
C	154Q	HIS	-	expression tag	UNP Q7L266
C	154R	HIS	-	expression tag	UNP Q7L266
C	154S	HIS	-	expression tag	UNP Q7L266
C	154T	MET	-	SEE REMARK 999	UNP Q7L266
C	309	GLY	-	linker	UNP Q7L266
C	310	ALA	-	linker	UNP Q7L266
C	311	GLY	-	linker	UNP Q7L266
C	312	SER	-	linker	UNP Q7L266
C	313	GLY	-	linker	UNP Q7L266
C	314	ALA	-	linker	UNP Q7L266
C	315	GLY	-	linker	UNP Q7L266
C	316	SER	-	linker	UNP Q7L266
C	317	GLY	-	linker	UNP Q7L266
C	318	ALA	-	linker	UNP Q7L266
C	319	GLY	-	linker	UNP Q7L266
C	320	GLY	-	linker	UNP Q7L266
D	1	GLY	-	linker	UNP Q7L266
D	154N	HIS	-	expression tag	UNP Q7L266
D	154O	HIS	-	expression tag	UNP Q7L266

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Chain	Residue	Modelled	Actual	Comment	Reference
D	154P	HIS	-	expression tag	UNP Q7L266
D	154Q	HIS	-	expression tag	UNP Q7L266
D	154R	HIS	-	expression tag	UNP Q7L266
D	154S	HIS	-	expression tag	UNP Q7L266
D	154T	MET	-	SEE REMARK 999	UNP Q7L266
D	309	GLY	-	linker	UNP Q7L266
D	310	ALA	-	linker	UNP Q7L266
D	311	GLY	-	linker	UNP Q7L266
D	312	SER	-	linker	UNP Q7L266
D	313	GLY	-	linker	UNP Q7L266
D	314	ALA	-	linker	UNP Q7L266
D	315	GLY	-	linker	UNP Q7L266
D	316	SER	-	linker	UNP Q7L266
D	317	GLY	-	linker	UNP Q7L266
D	318	ALA	-	linker	UNP Q7L266
D	319	GLY	-	linker	UNP Q7L266
D	320	GLY	-	linker	UNP Q7L266

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

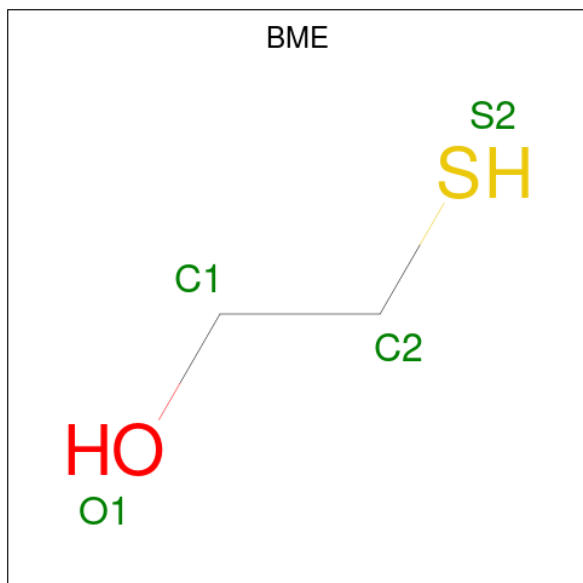
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0
2	B	1	Total Na 1 1	0	0
2	C	3	Total Na 3 3	0	0
2	D	1	Total Na 1 1	0	0

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



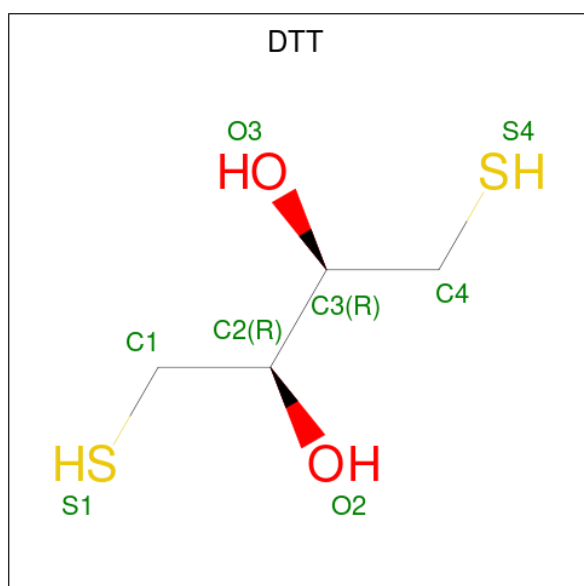
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	2	1	2		
3	B	1	Total	C	N	O	0	0
			5	2	1	2		
3	C	1	Total	C	N	O	0	0
			5	2	1	2		
3	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$).



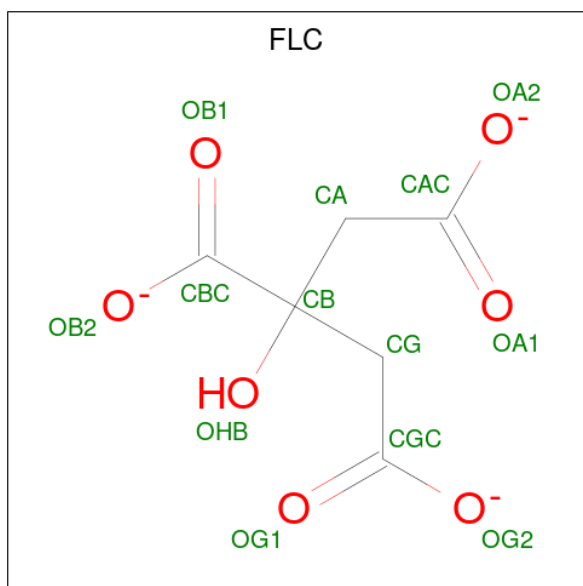
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			8	4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	S	
			8	4	2	2	
						0	0

- Molecule 6 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7^-$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O		
			13	6	7		
						0	0
6	D	1	Total	C	O		
			13	6	7		
						0	0

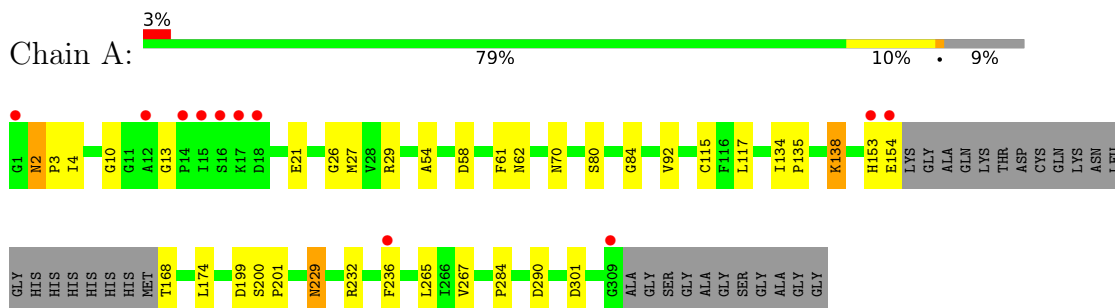
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	21	Total	O		
			21	21		
					0	0
7	B	19	Total	O		
			19	19		
					0	0
7	C	15	Total	O		
			15	15		
					0	0
7	D	16	Total	O		
			16	16		
					0	0

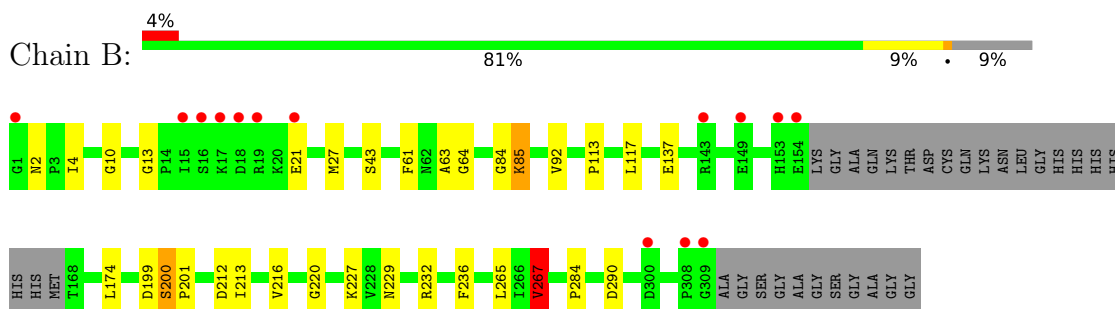
3 Residue-property plots

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.

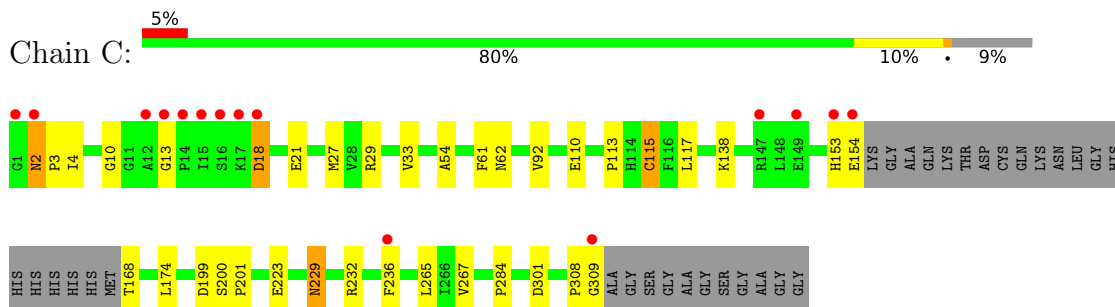
- Molecule 1: Isoaspartyl peptidase/L-asparaginase



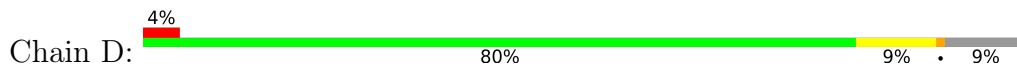
- Molecule 1: Isoaspartyl peptidase/L-asparaginase

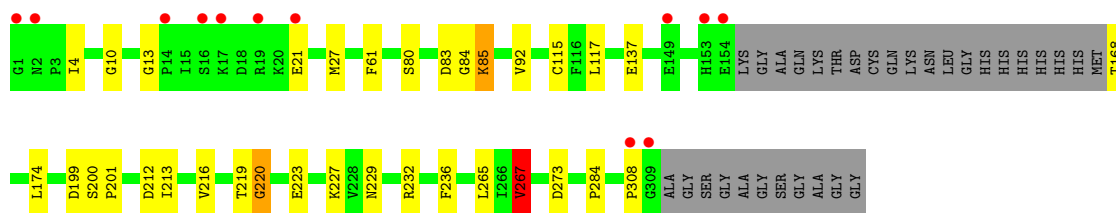


- Molecule 1: Isoaspartyl peptidase/L-asparaginase



- Molecule 1: Isoaspartyl peptidase/L-asparaginase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.31Å 111.11Å 122.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.74 – 2.51 39.74 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.74-2.51) 99.5 (39.74-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.204 , 0.233 0.209 , 0.238	Depositor DCC
R_{free} test set	2485 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtrriage
Anisotropy	0.851	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8838	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8273e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: DTT, NA, BME, FLC

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	1.06	0/2201	1.06	7/2975 (0.2%)
1	B	1.11	4/2201 (0.2%)	1.06	4/2975 (0.1%)
1	C	1.11	1/2201 (0.0%)	1.05	4/2975 (0.1%)
1	D	1.08	3/2201 (0.1%)	1.06	5/2975 (0.2%)
All	All	1.09	8/8804 (0.1%)	1.06	20/11900 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	PRO	CA-C	5.51	1.57	1.52
1	B	85	LYS	C-O	-5.45	1.17	1.24
1	C	113	PRO	CA-C	5.44	1.57	1.52
1	D	85	LYS	C-O	-5.38	1.17	1.24
1	D	220	GLY	N-CA	5.36	1.51	1.45
1	B	200	SER	C-O	-5.27	1.19	1.24
1	D	308	PRO	CA-C	5.23	1.58	1.52
1	B	43	SER	C-O	5.06	1.30	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	267	VAL	CB-CA-C	-9.44	93.82	110.71
1	B	267	VAL	CB-CA-C	-9.44	93.82	110.71
1	C	301	ASP	N-CA-C	7.48	121.69	109.72
1	A	301	ASP	N-CA-C	7.14	121.14	109.72
1	A	2	ASN	CA-C-O	7.03	126.30	119.55
1	C	13	GLY	CA-C-N	-7.01	113.44	120.31
1	C	13	GLY	C-N-CA	-7.01	113.44	120.31
1	D	273	ASP	CB-CA-C	6.83	121.08	109.53
1	D	13	GLY	CA-C-N	-6.60	113.19	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	GLY	C-N-CA	-6.60	113.19	119.85
1	C	2	ASN	CA-C-O	6.59	125.87	119.55
1	B	13	GLY	CA-C-N	-6.57	113.21	119.85
1	B	13	GLY	C-N-CA	-6.57	113.21	119.85
1	A	13	GLY	CA-C-N	-6.46	113.98	120.31
1	A	13	GLY	C-N-CA	-6.46	113.98	120.31
1	D	84	GLY	N-CA-C	6.35	121.84	114.16
1	A	84	GLY	N-CA-C	6.01	121.44	114.16
1	B	84	GLY	N-CA-C	5.63	120.97	114.16
1	A	134	ILE	CA-C-N	-5.37	114.19	119.99
1	A	134	ILE	C-N-CA	-5.37	114.19	119.99

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	2163	0	2168	40	0
1	B	2166	0	2167	34	0
1	C	2163	0	2168	37	0
1	D	2166	0	2167	32	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	2	1	0
3	B	5	0	2	1	0
3	C	5	0	2	1	0
3	D	5	0	2	1	0
4	A	16	0	24	16	0
4	B	4	0	6	0	0
4	C	16	0	24	8	0
4	D	4	0	6	0	0
5	A	8	0	10	0	0
5	C	8	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	13	0	5	2	0
6	D	13	0	5	3	0
7	A	21	0	0	0	0
7	B	19	0	0	0	0
7	C	15	0	0	0	0
7	D	16	0	0	1	0
All	All	8838	0	8768	123	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 7.

All (123) 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:54:ALA:O	4:C:406:BME:H22	1.69	0.93
1:C:29:ARG:HH21	4:C:406:BME:H11	1.37	0.89
4:A:405:BME:C1	4:A:406:BME:S2	2.61	0.89
1:A:236[A]:PHE:CE1	1:B:236[A]:PHE:CD2	2.64	0.86
1:A:2:ASN:ND2	1:A:290:ASP:OD1	2.10	0.83
4:A:403:BME:O1	1:B:236[A]:PHE:HE2	1.62	0.83
1:A:54:ALA:O	4:A:406:BME:H22	1.79	0.82
4:A:403:BME:HO1	1:B:236[A]:PHE:HE2	0.83	0.81
1:C:236[A]:PHE:CE1	1:D:236[A]:PHE:CD2	2.74	0.76
6:B:403:FLC:OG2	6:B:403:FLC:OB1	2.03	0.75
1:B:27:MET:HE3	1:B:61:PHE:CE1	2.23	0.74
1:D:27:MET:HE3	1:D:61:PHE:CE1	2.23	0.74
1:C:29:ARG:HD2	4:C:406:BME:H11	1.69	0.73
1:A:236[A]:PHE:HE1	1:B:236[A]:PHE:CD2	2.06	0.73
1:C:27:MET:HE3	1:C:61:PHE:CE1	2.24	0.72
1:A:236[A]:PHE:CE1	1:B:236[A]:PHE:CG	2.77	0.72
1:A:27:MET:HE3	1:A:61:PHE:CE1	2.25	0.71
1:D:232:ARG:HG3	1:D:236[B]:PHE:CE2	2.28	0.69
4:A:405:BME:H12	4:A:406:BME:S2	2.34	0.67
1:B:232:ARG:HG3	1:B:236[B]:PHE:CE2	2.31	0.65
1:A:236[A]:PHE:HD1	1:B:236[A]:PHE:CZ	2.16	0.64
1:A:236[A]:PHE:CD1	1:B:236[A]:PHE:CD1	2.84	0.64
1:D:219:THR:OG1	6:D:403:FLC:OA1	2.11	0.64
1:A:236[A]:PHE:CD1	1:B:236[A]:PHE:CE1	2.87	0.62
1:C:236[A]:PHE:HE1	1:D:236[A]:PHE:CD2	2.16	0.61
1:A:29:ARG:NH2	4:A:406:BME:H11	2.15	0.61
1:A:29:ARG:HH21	4:A:406:BME:H11	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:404:BME:O1	1:B:227:LYS:NZ	2.32	0.61
1:D:216:VAL:HG22	1:D:267:VAL:HG13	1.81	0.60
1:C:236[A]:PHE:CE1	1:D:236[A]:PHE:CG	2.89	0.60
1:A:232:ARG:HG3	1:A:236[A]:PHE:CE2	2.36	0.60
1:C:18:ASP:OD1	1:C:18:ASP:N	2.34	0.60
1:A:58:ASP:HB2	4:A:406:BME:H12	1.83	0.60
1:C:232:ARG:HG3	1:C:236[A]:PHE:CE2	2.36	0.60
1:B:216:VAL:HG22	1:B:267:VAL:HG13	1.83	0.59
1:C:29:ARG:HH21	4:C:406:BME:C1	2.13	0.58
4:A:405:BME:O1	4:A:406:BME:S2	2.62	0.57
1:D:199:ASP:OD1	3:D:402:GLY:N	2.38	0.57
1:A:29:ARG:HH21	4:A:406:BME:C1	2.18	0.56
1:C:236[A]:PHE:CD1	1:D:236[A]:PHE:CE1	2.94	0.55
1:C:236[A]:PHE:HD1	1:D:236[A]:PHE:CZ	2.24	0.55
1:B:199:ASP:OD1	3:B:402:GLY:N	2.38	0.55
1:A:236[A]:PHE:CD1	1:B:236[A]:PHE:CG	2.95	0.55
1:A:236[B]:PHE:CD2	1:B:236[B]:PHE:CE1	2.95	0.54
1:C:199:ASP:OD1	3:C:402:GLY:N	2.41	0.54
1:A:153:HIS:O	1:A:154:GLU:HB2	2.08	0.54
1:D:27:MET:HE3	1:D:61:PHE:CZ	2.43	0.53
1:A:236[A]:PHE:HD1	1:B:236[A]:PHE:CE1	2.26	0.53
1:B:10:GLY:O	1:B:284:PRO:HD2	2.08	0.53
1:C:153:HIS:O	1:C:154:GLU:HB2	2.09	0.53
1:C:236[A]:PHE:CD1	1:D:236[A]:PHE:CD1	2.97	0.53
4:A:405:BME:H11	4:A:406:BME:S2	2.49	0.53
1:A:58:ASP:HB2	4:A:406:BME:C1	2.39	0.52
1:A:236[A]:PHE:CD1	1:B:236[A]:PHE:CZ	2.98	0.52
1:D:10:GLY:O	1:D:284:PRO:HD2	2.10	0.52
5:C:407:DTT:S4	5:C:407:DTT:O2	2.67	0.52
1:B:2:ASN:ND2	1:B:290:ASP:OD1	2.44	0.50
1:D:83:ASP:OD1	7:D:501:HOH:O	2.20	0.50
1:B:27:MET:HE3	1:B:61:PHE:CZ	2.46	0.50
1:A:10:GLY:O	1:A:284:PRO:HD2	2.12	0.49
1:C:10:GLY:O	1:C:284:PRO:HD2	2.13	0.49
1:C:223:GLU:HG3	1:D:115[B]:CYS:SG	2.53	0.48
1:A:27:MET:HE3	1:A:61:PHE:CZ	2.48	0.48
1:C:27:MET:HE3	1:C:61:PHE:CZ	2.48	0.48
1:C:29:ARG:HD2	4:C:406:BME:C1	2.43	0.48
1:A:236[A]:PHE:CD1	1:B:236[A]:PHE:CD2	3.03	0.47
1:B:4:ILE:HD12	1:B:174:LEU:HB3	1.96	0.47
1:A:153:HIS:O	1:A:154:GLU:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ALA:HB1	4:C:406:BME:H21	1.95	0.47
1:C:153:HIS:O	1:C:154:GLU:CB	2.62	0.46
1:A:26:GLY:HA2	4:A:406:BME:O1	2.16	0.46
1:D:4:ILE:HD12	1:D:174:LEU:HB3	1.97	0.46
1:A:200:SER:N	1:A:201:PRO:CD	2.79	0.46
1:A:265:LEU:HD12	1:A:265:LEU:C	2.40	0.46
1:A:236[B]:PHE:CG	1:B:236[B]:PHE:CE1	3.04	0.46
1:C:229:ASN:OD1	1:D:229:ASN:ND2	2.49	0.46
1:C:4:ILE:HD12	1:C:174:LEU:HB3	1.98	0.45
1:C:236[A]:PHE:CD1	1:D:236[A]:PHE:CZ	3.03	0.45
1:A:236[A]:PHE:CD1	1:B:236[A]:PHE:CE2	3.05	0.45
4:A:404:BME:HO1	1:B:227:LYS:HZ1	1.63	0.45
1:C:33:VAL:HG21	4:C:405:BME:H21	1.98	0.45
1:A:4:ILE:HD12	1:A:174:LEU:HB3	1.99	0.44
1:D:220:GLY:O	6:D:403:FLC:OA2	2.35	0.44
1:D:92:VAL:HA	1:D:117:LEU:O	2.18	0.44
1:C:200:SER:N	1:C:201:PRO:CD	2.81	0.44
1:A:62:ASN:O	1:A:168:THR:N	2.51	0.44
1:B:265:LEU:C	1:B:265:LEU:HD12	2.43	0.43
1:D:232:ARG:CZ	1:D:236[B]:PHE:CZ	3.01	0.43
1:D:168:THR:HB	6:D:403:FLC:OA1	2.18	0.43
1:A:80:SER:HB3	1:A:201:PRO:HA	2.00	0.43
1:B:92:VAL:HA	1:B:117:LEU:O	2.19	0.43
1:D:80:SER:HB3	1:D:201:PRO:HA	2.00	0.43
1:A:92:VAL:HA	1:A:117:LEU:O	2.19	0.43
1:A:135:PRO:HG2	1:A:138:LYS:HG3	2.00	0.43
1:C:115[A]:CYS:SG	1:D:223:GLU:HG3	2.59	0.42
1:C:168:THR:N	5:C:407:DTT:H42	2.34	0.42
1:D:265:LEU:C	1:D:265:LEU:HD12	2.44	0.42
1:C:92:VAL:HA	1:C:117:LEU:O	2.19	0.42
1:A:229:ASN:OD1	1:B:229:ASN:ND2	2.53	0.42
1:C:2:ASN:HA	1:C:3:PRO:HD3	1.85	0.42
4:A:403:BME:O1	1:B:236[A]:PHE:CE2	2.48	0.42
1:C:232:ARG:CZ	1:C:236[A]:PHE:CZ	3.02	0.42
1:C:308:PRO:O	1:C:309:GLY:C	2.62	0.42
1:C:110:GLU:OE1	1:C:110:GLU:HA	2.20	0.42
1:B:63:ALA:O	1:B:64:GLY:C	2.62	0.42
1:D:200:SER:N	1:D:201:PRO:CD	2.83	0.41
1:C:236[A]:PHE:CD1	1:D:236[A]:PHE:CG	3.08	0.41
1:B:220:GLY:N	6:B:403:FLC:OB1	2.50	0.41
1:D:85:LYS:HE2	1:D:85:LYS:HB3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:CZ	1:A:236[A]:PHE:CZ	3.02	0.41
1:B:200:SER:N	1:B:201:PRO:CD	2.84	0.41
1:D:232:ARG:NH1	1:D:236[B]:PHE:CE1	2.87	0.41
4:C:403:BME:O1	1:D:227:LYS:NZ	2.53	0.41
1:A:2:ASN:HA	1:A:3:PRO:HD3	1.85	0.41
1:C:62:ASN:O	1:C:168:THR:N	2.53	0.41
1:C:236[A]:PHE:HD1	1:D:236[A]:PHE:CE1	2.38	0.41
1:A:70:ASN:OD1	1:A:70:ASN:C	2.64	0.41
1:A:200:SER:N	1:A:201:PRO:HD2	2.36	0.41
1:B:212:ASP:C	1:B:213:ILE:HG13	2.46	0.41
1:C:265:LEU:HD12	1:C:265:LEU:C	2.45	0.41
1:B:85:LYS:HE2	1:B:85:LYS:HB3	1.89	0.41
1:A:199:ASP:OD1	3:A:402:GLY:N	2.54	0.40
1:D:212:ASP:C	1:D:213:ILE:HG13	2.46	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	295/327 (90%)	286 (97%)	9 (3%)	0	100	100
1	B	295/327 (90%)	287 (97%)	8 (3%)	0	100	100
1	C	295/327 (90%)	286 (97%)	9 (3%)	0	100	100
1	D	295/327 (90%)	287 (97%)	8 (3%)	0	100	100
All	All	1180/1308 (90%)	1146 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/242 (93%)	220 (97%)	6 (3%)	39	67
1	B	226/242 (93%)	223 (99%)	3 (1%)	61	82
1	C	226/242 (93%)	219 (97%)	7 (3%)	35	62
1	D	226/242 (93%)	223 (99%)	3 (1%)	61	82
All	All	904/968 (93%)	885 (98%)	19 (2%)	50	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	115[A]	CYS
1	A	115[B]	CYS
1	A	138	LYS
1	A	229	ASN
1	A	267	VAL
1	B	21	GLU
1	B	137	GLU
1	B	267	VAL
1	C	18	ASP
1	C	21	GLU
1	C	115[A]	CYS
1	C	115[B]	CYS
1	C	138	LYS
1	C	229	ASN
1	C	267	VAL
1	D	21	GLU
1	D	137	GLU
1	D	267	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	294	HIS
1	B	96	GLN
1	B	120	GLN
1	B	124	GLN
1	B	153	HIS
1	B	229	ASN
1	B	240	GLN
1	C	124	GLN
1	C	240	GLN
1	D	96	GLN
1	D	120	GLN
1	D	124	GLN
1	D	153	HIS
1	D	229	ASN
1	D	240	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 7 are monoatomic - leaving 18 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
4	BME	A	404	-	3,3,3	0.26	0	2,2,2	1.99	1 (50%)
3	GLY	A	402	-	4,4,4	0.82	0	3,4,4	1.60	1 (33%)
3	GLY	C	402	-	4,4,4	1.16	1 (25%)	3,4,4	1.37	0
4	BME	C	404	-	3,3,3	0.56	0	2,2,2	1.64	1 (50%)
3	GLY	B	402	-	4,4,4	1.04	0	3,4,4	1.75	2 (66%)
4	BME	C	405	-	3,3,3	0.67	0	2,2,2	1.00	0
4	BME	B	404	-	3,3,3	0.25	0	2,2,2	0.77	0
4	BME	D	404	-	3,3,3	0.11	0	2,2,2	1.87	1 (50%)
4	BME	C	403	-	3,3,3	0.13	0	2,2,2	1.97	1 (50%)
5	DTT	A	407	-	7,7,7	0.55	0	4,8,8	3.60	3 (75%)
6	FLC	D	403	-	12,12,12	1.13	1 (8%)	17,17,17	2.25	8 (47%)
3	GLY	D	402	-	4,4,4	1.05	0	3,4,4	1.37	0
5	DTT	C	407	-	7,7,7	0.68	0	4,8,8	2.61	1 (25%)
6	FLC	B	403	-	12,12,12	1.39	0	17,17,17	2.50	6 (35%)
4	BME	A	403	-	3,3,3	0.39	0	2,2,2	0.26	0
4	BME	A	406	-	3,3,3	0.20	0	2,2,2	0.49	0
4	BME	A	405	-	3,3,3	0.42	0	2,2,2	0.22	0
4	BME	C	406	-	3,3,3	0.27	0	2,2,2	0.17	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
4	BME	A	404	-	-	0/1/1/1	-
3	GLY	A	402	-	-	0/2/2/2	-
3	GLY	C	402	-	-	0/2/2/2	-
4	BME	C	404	-	-	1/1/1/1	-
3	GLY	B	402	-	-	2/2/2/2	-
4	BME	C	405	-	-	1/1/1/1	-
4	BME	B	404	-	-	1/1/1/1	-
4	BME	D	404	-	-	1/1/1/1	-
4	BME	C	403	-	-	0/1/1/1	-
5	DTT	A	407	-	-	2/8/8/8	-
6	FLC	D	403	-	-	8/16/16/16	-
3	GLY	D	402	-	-	2/2/2/2	-
5	DTT	C	407	-	-	4/8/8/8	-
6	FLC	B	403	-	-	9/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BME	A	403	-	-	0/1/1/1	-
4	BME	A	406	-	-	0/1/1/1	-
4	BME	A	405	-	-	1/1/1/1	-
4	BME	C	406	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	403	FLC	OA2-CAC	-2.44	1.22	1.30
3	C	402	GLY	OXT-C	-2.22	1.23	1.30

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	407	DTT	C3-C4-S4	-5.67	98.58	114.43
6	B	403	FLC	OB2-CBC-CB	5.49	123.68	113.14
5	C	407	DTT	O3-C3-C2	4.74	119.53	109.57
6	B	403	FLC	OHB-CB-CBC	-4.73	102.25	108.96
6	B	403	FLC	OB2-CBC-OB1	-3.66	112.15	123.86
6	B	403	FLC	CG-CB-CBC	3.60	118.00	110.03
6	D	403	FLC	OG1-CGC-CG	-3.59	112.77	122.95
6	D	403	FLC	CB-CG-CGC	-3.32	104.85	113.92
6	D	403	FLC	OB2-CBC-CB	3.25	119.37	113.14
6	D	403	FLC	OG2-CGC-CG	3.19	124.45	114.35
6	D	403	FLC	CB-CA-CAC	-3.18	105.22	113.92
5	A	407	DTT	C2-C1-S1	-3.08	105.84	114.43
5	A	407	DTT	O3-C3-C2	3.07	116.02	109.57
6	D	403	FLC	CA-CB-CBC	2.82	116.27	110.03
4	C	403	BME	O1-C1-C2	-2.72	100.22	110.82
4	D	404	BME	O1-C1-C2	-2.64	100.50	110.82
6	D	403	FLC	CG-CB-CBC	2.63	115.85	110.03
4	C	404	BME	O1-C1-C2	2.32	119.87	110.82
6	B	403	FLC	CG-CB-CA	-2.28	103.47	109.31
6	D	403	FLC	OHB-CB-CBC	-2.26	105.76	108.96
3	A	402	GLY	OXT-C-CA	2.16	121.98	113.38
6	B	403	FLC	CB-CG-CGC	2.12	119.72	113.92
3	B	402	GLY	OXT-C-CA	2.12	121.79	113.38
3	B	402	GLY	OXT-C-O	-2.10	117.93	123.33
4	A	404	BME	C1-C2-S2	-2.09	96.65	111.57

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	BME	O1-C1-C2-S2
4	C	404	BME	O1-C1-C2-S2
4	C	405	BME	O1-C1-C2-S2
5	A	407	DTT	C2-C3-C4-S4
5	A	407	DTT	O3-C3-C4-S4
6	B	403	FLC	CG-CB-CBC-OB1
6	B	403	FLC	CG-CB-CBC-OB2
6	B	403	FLC	OHB-CB-CBC-OB1
6	B	403	FLC	OHB-CB-CBC-OB2
6	B	403	FLC	OHB-CB-CG-CGC
6	D	403	FLC	CBC-CB-CG-CGC
6	D	403	FLC	OHB-CB-CG-CGC
6	B	403	FLC	CA-CB-CG-CGC
6	B	403	FLC	CBC-CB-CG-CGC
6	D	403	FLC	CA-CB-CG-CGC
3	D	402	GLY	OXT-C-CA-N
6	D	403	FLC	CAC-CA-CB-CBC
3	B	402	GLY	OXT-C-CA-N
3	D	402	GLY	O-C-CA-N
5	C	407	DTT	O3-C3-C4-S4
3	B	402	GLY	O-C-CA-N
6	D	403	FLC	CA-CB-CBC-OB1
6	D	403	FLC	CA-CB-CBC-OB2
5	C	407	DTT	O2-C2-C3-C4
4	B	404	BME	O1-C1-C2-S2
6	D	403	FLC	CG-CB-CBC-OB1
6	D	403	FLC	CG-CB-CBC-OB2
5	C	407	DTT	O2-C2-C3-O3
6	B	403	FLC	CB-CG-CGC-OG1
6	B	403	FLC	CB-CG-CGC-OG2
5	C	407	DTT	C1-C2-C3-C4
4	C	406	BME	O1-C1-C2-S2
4	D	404	BME	O1-C1-C2-S2

There are no ring outliers.

14 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	BME	2	0
3	A	402	GLY	1	0
3	C	402	GLY	1	0
3	B	402	GLY	1	0
4	C	405	BME	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	BME	1	0
6	D	403	FLC	3	0
3	D	402	GLY	1	0
5	C	407	DTT	2	0
6	B	403	FLC	2	0
4	A	403	BME	3	0
4	A	406	BME	11	0
4	A	405	BME	4	0
4	C	406	BME	6	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, 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	296/327 (90%)	-0.06	11 (3%) 45 40	8, 22, 55, 77	3 (1%)
1	B	296/327 (90%)	0.14	14 (4%) 36 32	8, 25, 54, 86	3 (1%)
1	C	296/327 (90%)	0.08	15 (5%) 33 29	9, 23, 54, 83	3 (1%)
1	D	296/327 (90%)	0.04	12 (4%) 41 37	8, 25, 56, 86	3 (1%)
All	All	1184/1308 (90%)	0.05	52 (4%) 39 34	8, 24, 55, 86	12 (1%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	GLY	5.2
1	B	1	GLY	4.7
1	C	17	LYS	4.5
1	B	153	HIS	4.1
1	C	153	HIS	4.0
1	A	1	GLY	3.8
1	D	153	HIS	3.5
1	D	154	GLU	3.3
1	C	18	ASP	3.3
1	B	154	GLU	3.2
1	C	1	GLY	3.2
1	A	153	HIS	3.2
1	A	16	SER	3.1
1	A	17	LYS	3.0
1	B	149	GLU	3.0
1	B	17	LYS	2.9
1	C	16	SER	2.9
1	C	12	ALA	2.9
1	B	16	SER	2.8
1	B	309	GLY	2.8
1	D	17	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	149	GLU	2.8
1	B	19	ARG	2.8
1	B	18	ASP	2.8
1	A	236[A]	PHE	2.8
1	A	12	ALA	2.7
1	A	309	GLY	2.7
1	D	21	GLU	2.7
1	C	154	GLU	2.6
1	D	19	ARG	2.6
1	C	2	ASN	2.6
1	A	18	ASP	2.5
1	D	309	GLY	2.5
1	A	154	GLU	2.5
1	C	149	GLU	2.5
1	B	21	GLU	2.4
1	C	309	GLY	2.4
1	D	2	ASN	2.4
1	C	236[A]	PHE	2.4
1	A	14	PRO	2.3
1	D	16	SER	2.3
1	A	15	ILE	2.3
1	C	13	GLY	2.2
1	B	15	ILE	2.2
1	C	15	ILE	2.2
1	B	143	ARG	2.2
1	B	300	ASP	2.2
1	B	308	PRO	2.2
1	C	147	ARG	2.1
1	D	14	PRO	2.1
1	C	14	PRO	2.0
1	D	308	PRO	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 oligosaccharides 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. 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	DTT	A	407	8/8	0.72	0.20	50,55,64,74	0
6	FLC	D	403	13/13	0.76	0.18	49,59,65,69	0
4	BME	A	403	4/4	0.81	0.19	61,63,66,68	0
4	BME	A	404	4/4	0.81	0.19	47,47,51,56	0
6	FLC	B	403	13/13	0.82	0.17	48,57,65,68	0
5	DTT	C	407	8/8	0.83	0.16	43,51,57,63	0
4	BME	C	403	4/4	0.84	0.18	46,46,47,52	0
4	BME	D	404	4/4	0.84	0.20	40,42,46,48	0
4	BME	C	406	4/4	0.85	0.44	73,74,77,87	0
2	NA	C	408	1/1	0.85	0.20	52,52,52,52	0
4	BME	C	405	4/4	0.85	0.33	33,47,52,65	0
4	BME	A	406	4/4	0.86	0.37	57,63,69,86	0
4	BME	C	404	4/4	0.88	0.13	31,38,41,53	0
4	BME	A	405	4/4	0.89	0.13	34,36,40,45	0
4	BME	B	404	4/4	0.91	0.14	38,42,46,46	0
2	NA	A	408	1/1	0.93	0.11	33,33,33,33	0
3	GLY	D	402	5/5	0.94	0.07	23,26,28,29	0
3	GLY	B	402	5/5	0.95	0.08	22,22,23,25	0
2	NA	B	401	1/1	0.95	0.05	28,28,28,28	0
2	NA	D	401	1/1	0.95	0.08	30,30,30,30	0
3	GLY	A	402	5/5	0.95	0.07	22,25,27,27	0
3	GLY	C	402	5/5	0.97	0.07	23,24,27,28	0
2	NA	C	409	1/1	0.98	0.08	33,33,33,33	0
2	NA	C	401	1/1	0.98	0.03	21,21,21,21	0
2	NA	A	401	1/1	0.99	0.03	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.