



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:22 AM UTC

PDB ID : 6OVG / pdb_00006ovg
Title : L-Methionine Depletion with an Engineered Human Enzyme Disrupts Prostate Cancer Metabolism
Authors : Yan, W.; Irani, S.; Zhang, J.
Deposited on : 2019-05-07
Resolution : 2.72 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

<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:

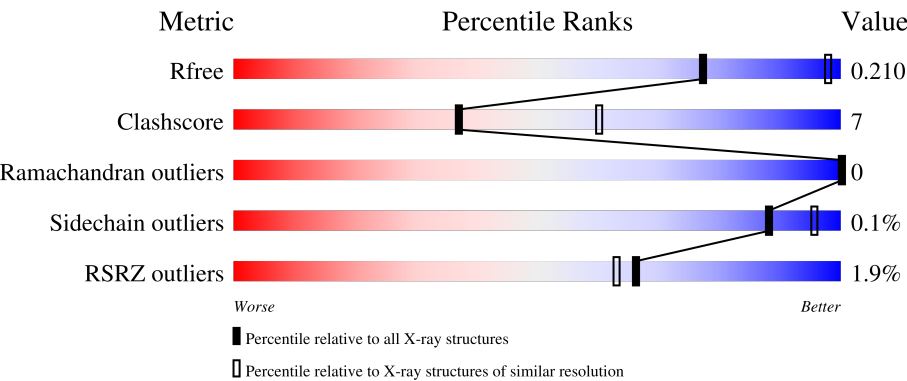
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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 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	415	80%12%7%
1	B	415	% 81%12%7%
1	C	415	% 80%12%7%
1	D	415	2% 78%14%7%
1	E	415	2% 78%16%7%

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Mol	Chain	Length	Quality of chain
1	F	415	% 78% 16% 7%
1	G	415	3% 76% 17% 7%
1	H	415	4% 73% 20% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24368 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 Cystathionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	P	S	0	0	0
			2982	1902	508	551	1	20			
1	B	386	Total	C	N	O	P	S	0	0	0
			2993	1908	510	554	1	20			
1	C	387	Total	C	N	O	P	S	0	0	0
			3000	1913	511	555	1	20			
1	D	386	Total	C	N	O	P	S	0	0	0
			2989	1903	510	555	1	20			
1	E	388	Total	C	N	O	P	S	0	0	0
			3004	1915	512	556	1	20			
1	F	387	Total	C	N	O	P	S	0	0	0
			3000	1913	511	555	1	20			
1	G	388	Total	C	N	O	P	S	0	0	0
			3007	1918	512	556	1	20			
1	H	387	Total	C	N	O	P	S	0	0	0
			2997	1910	511	555	1	20			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP P32929
A	-8	GLY	-	expression tag	UNP P32929
A	-7	GLY	-	expression tag	UNP P32929
A	-6	HIS	-	expression tag	UNP P32929
A	-5	HIS	-	expression tag	UNP P32929
A	-4	HIS	-	expression tag	UNP P32929
A	-3	HIS	-	expression tag	UNP P32929
A	-2	HIS	-	expression tag	UNP P32929
A	-1	HIS	-	expression tag	UNP P32929
A	0	GLY	-	expression tag	UNP P32929
A	1	GLY	-	expression tag	UNP P32929
A	59	ILE	GLU	conflict	UNP P32929
A	63	LEU	SER	conflict	UNP P32929

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Chain	Residue	Modelled	Actual	Comment	Reference
A	91	MET	LEU	conflict	UNP P32929
A	119	ALA	ARG	conflict	UNP P32929
A	268	ARG	LYS	conflict	UNP P32929
A	311	GLY	THR	conflict	UNP P32929
A	339	VAL	GLU	conflict	UNP P32929
A	353	SER	ILE	conflict	UNP P32929
B	-9	MET	-	initiating methionine	UNP P32929
B	-8	GLY	-	expression tag	UNP P32929
B	-7	GLY	-	expression tag	UNP P32929
B	-6	HIS	-	expression tag	UNP P32929
B	-5	HIS	-	expression tag	UNP P32929
B	-4	HIS	-	expression tag	UNP P32929
B	-3	HIS	-	expression tag	UNP P32929
B	-2	HIS	-	expression tag	UNP P32929
B	-1	HIS	-	expression tag	UNP P32929
B	0	GLY	-	expression tag	UNP P32929
B	1	GLY	-	expression tag	UNP P32929
B	59	ILE	GLU	conflict	UNP P32929
B	63	LEU	SER	conflict	UNP P32929
B	91	MET	LEU	conflict	UNP P32929
B	119	ALA	ARG	conflict	UNP P32929
B	268	ARG	LYS	conflict	UNP P32929
B	311	GLY	THR	conflict	UNP P32929
B	339	VAL	GLU	conflict	UNP P32929
B	353	SER	ILE	conflict	UNP P32929
C	-9	MET	-	initiating methionine	UNP P32929
C	-8	GLY	-	expression tag	UNP P32929
C	-7	GLY	-	expression tag	UNP P32929
C	-6	HIS	-	expression tag	UNP P32929
C	-5	HIS	-	expression tag	UNP P32929
C	-4	HIS	-	expression tag	UNP P32929
C	-3	HIS	-	expression tag	UNP P32929
C	-2	HIS	-	expression tag	UNP P32929
C	-1	HIS	-	expression tag	UNP P32929
C	0	GLY	-	expression tag	UNP P32929
C	1	GLY	-	expression tag	UNP P32929
C	59	ILE	GLU	conflict	UNP P32929
C	63	LEU	SER	conflict	UNP P32929
C	91	MET	LEU	conflict	UNP P32929
C	119	ALA	ARG	conflict	UNP P32929
C	268	ARG	LYS	conflict	UNP P32929
C	311	GLY	THR	conflict	UNP P32929

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Chain	Residue	Modelled	Actual	Comment	Reference
C	339	VAL	GLU	conflict	UNP P32929
C	353	SER	ILE	conflict	UNP P32929
D	-9	MET	-	initiating methionine	UNP P32929
D	-8	GLY	-	expression tag	UNP P32929
D	-7	GLY	-	expression tag	UNP P32929
D	-6	HIS	-	expression tag	UNP P32929
D	-5	HIS	-	expression tag	UNP P32929
D	-4	HIS	-	expression tag	UNP P32929
D	-3	HIS	-	expression tag	UNP P32929
D	-2	HIS	-	expression tag	UNP P32929
D	-1	HIS	-	expression tag	UNP P32929
D	0	GLY	-	expression tag	UNP P32929
D	1	GLY	-	expression tag	UNP P32929
D	59	ILE	GLU	conflict	UNP P32929
D	63	LEU	SER	conflict	UNP P32929
D	91	MET	LEU	conflict	UNP P32929
D	119	ALA	ARG	conflict	UNP P32929
D	268	ARG	LYS	conflict	UNP P32929
D	311	GLY	THR	conflict	UNP P32929
D	339	VAL	GLU	conflict	UNP P32929
D	353	SER	ILE	conflict	UNP P32929
E	-9	MET	-	initiating methionine	UNP P32929
E	-8	GLY	-	expression tag	UNP P32929
E	-7	GLY	-	expression tag	UNP P32929
E	-6	HIS	-	expression tag	UNP P32929
E	-5	HIS	-	expression tag	UNP P32929
E	-4	HIS	-	expression tag	UNP P32929
E	-3	HIS	-	expression tag	UNP P32929
E	-2	HIS	-	expression tag	UNP P32929
E	-1	HIS	-	expression tag	UNP P32929
E	0	GLY	-	expression tag	UNP P32929
E	1	GLY	-	expression tag	UNP P32929
E	59	ILE	GLU	conflict	UNP P32929
E	63	LEU	SER	conflict	UNP P32929
E	91	MET	LEU	conflict	UNP P32929
E	119	ALA	ARG	conflict	UNP P32929
E	268	ARG	LYS	conflict	UNP P32929
E	311	GLY	THR	conflict	UNP P32929
E	339	VAL	GLU	conflict	UNP P32929
E	353	SER	ILE	conflict	UNP P32929
F	-9	MET	-	initiating methionine	UNP P32929
F	-8	GLY	-	expression tag	UNP P32929

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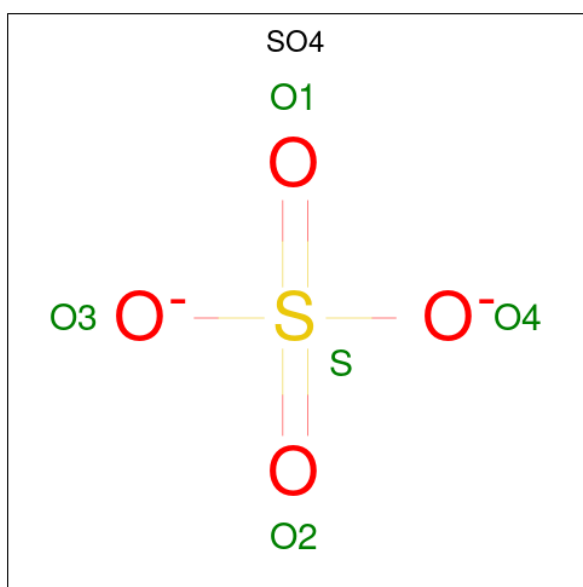
Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	GLY	-	expression tag	UNP P32929
F	-6	HIS	-	expression tag	UNP P32929
F	-5	HIS	-	expression tag	UNP P32929
F	-4	HIS	-	expression tag	UNP P32929
F	-3	HIS	-	expression tag	UNP P32929
F	-2	HIS	-	expression tag	UNP P32929
F	-1	HIS	-	expression tag	UNP P32929
F	0	GLY	-	expression tag	UNP P32929
F	1	GLY	-	expression tag	UNP P32929
F	59	ILE	GLU	conflict	UNP P32929
F	63	LEU	SER	conflict	UNP P32929
F	91	MET	LEU	conflict	UNP P32929
F	119	ALA	ARG	conflict	UNP P32929
F	268	ARG	LYS	conflict	UNP P32929
F	311	GLY	THR	conflict	UNP P32929
F	339	VAL	GLU	conflict	UNP P32929
F	353	SER	ILE	conflict	UNP P32929
G	-9	MET	-	initiating methionine	UNP P32929
G	-8	GLY	-	expression tag	UNP P32929
G	-7	GLY	-	expression tag	UNP P32929
G	-6	HIS	-	expression tag	UNP P32929
G	-5	HIS	-	expression tag	UNP P32929
G	-4	HIS	-	expression tag	UNP P32929
G	-3	HIS	-	expression tag	UNP P32929
G	-2	HIS	-	expression tag	UNP P32929
G	-1	HIS	-	expression tag	UNP P32929
G	0	GLY	-	expression tag	UNP P32929
G	1	GLY	-	expression tag	UNP P32929
G	59	ILE	GLU	conflict	UNP P32929
G	63	LEU	SER	conflict	UNP P32929
G	91	MET	LEU	conflict	UNP P32929
G	119	ALA	ARG	conflict	UNP P32929
G	268	ARG	LYS	conflict	UNP P32929
G	311	GLY	THR	conflict	UNP P32929
G	339	VAL	GLU	conflict	UNP P32929
G	353	SER	ILE	conflict	UNP P32929
H	-9	MET	-	initiating methionine	UNP P32929
H	-8	GLY	-	expression tag	UNP P32929
H	-7	GLY	-	expression tag	UNP P32929
H	-6	HIS	-	expression tag	UNP P32929
H	-5	HIS	-	expression tag	UNP P32929
H	-4	HIS	-	expression tag	UNP P32929

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	HIS	-	expression tag	UNP P32929
H	-2	HIS	-	expression tag	UNP P32929
H	-1	HIS	-	expression tag	UNP P32929
H	0	GLY	-	expression tag	UNP P32929
H	1	GLY	-	expression tag	UNP P32929
H	59	ILE	GLU	conflict	UNP P32929
H	63	LEU	SER	conflict	UNP P32929
H	91	MET	LEU	conflict	UNP P32929
H	119	ALA	ARG	conflict	UNP P32929
H	268	ARG	LYS	conflict	UNP P32929
H	311	GLY	THR	conflict	UNP P32929
H	339	VAL	GLU	conflict	UNP P32929
H	353	SER	ILE	conflict	UNP P32929

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		

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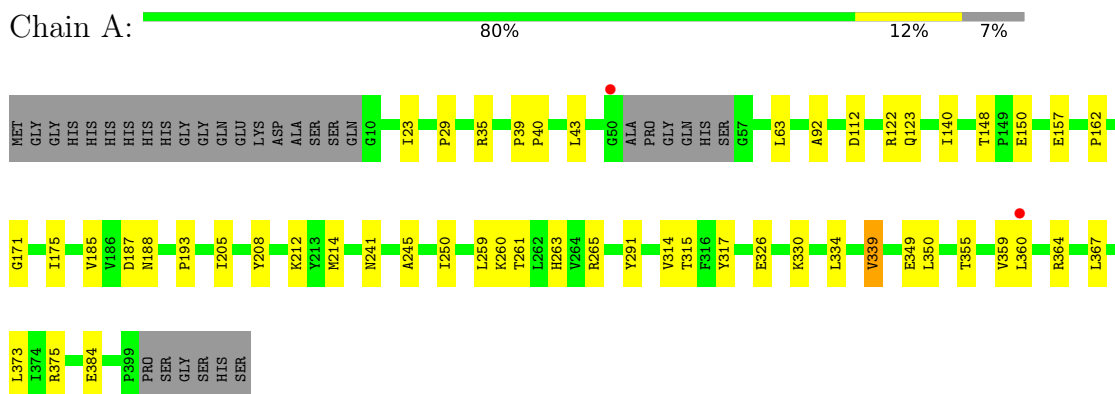
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	55	Total 55	O 55	0	0
3	C	66	Total 66	O 66	0	0
3	D	61	Total 61	O 61	0	0
3	E	44	Total 44	O 44	0	0
3	F	35	Total 35	O 35	0	0
3	G	39	Total 39	O 39	0	0
3	H	18	Total 18	O 18	0	0

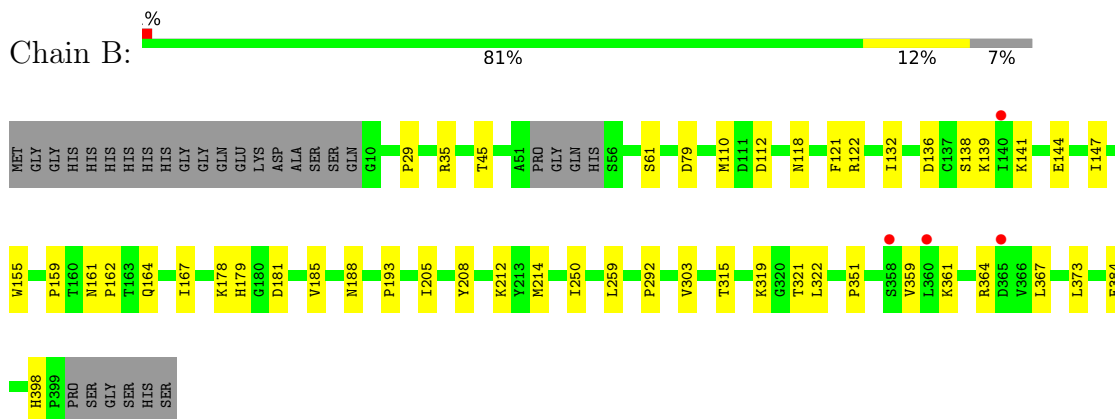
3 Residue-property plots [i](#)

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.

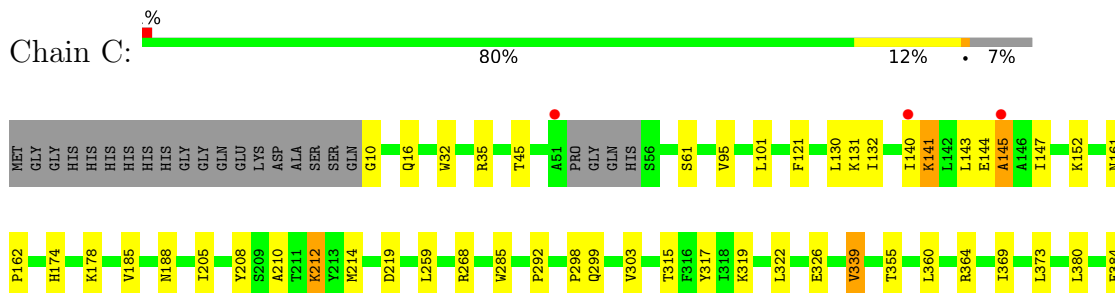
• Molecule 1: Cystathionine gamma-lyase

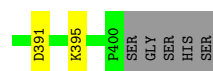


• Molecule 1: Cystathionine gamma-lyase

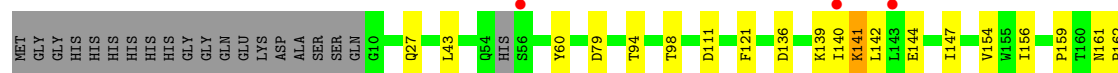
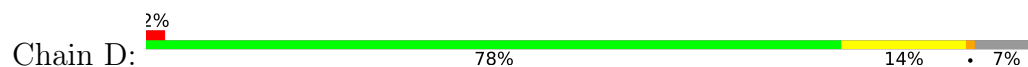


• Molecule 1: Cystathionine gamma-lyase

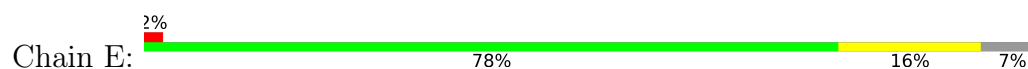




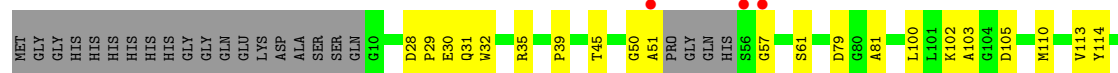
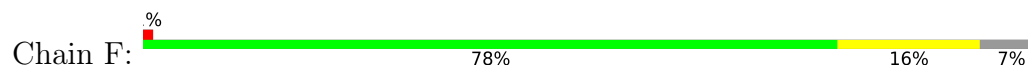
• Molecule 1: Cystathionine gamma-lyase



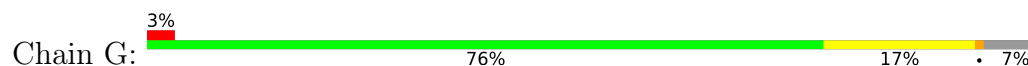
• Molecule 1: Cystathionine gamma-lyase

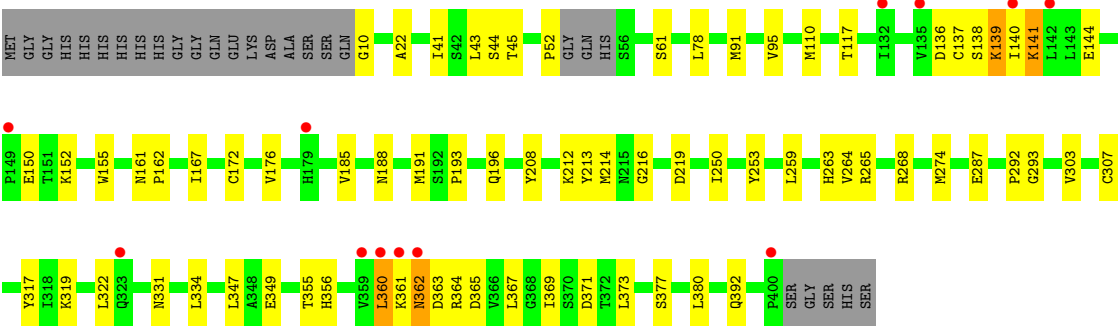


• Molecule 1: Cystathionine gamma-lyase



• Molecule 1: Cystathionine gamma-lyase





● Molecule 1: Cystathionine gamma-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	113.56Å 164.33Å 181.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 2.72 49.34 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.34-2.72) 99.1 (49.34-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.181 , 0.229 (Not available) , 0.210	Depositor DCC
R_{free} test set	4561 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24368	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.31% 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: SO4, LLP

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	0.18	0/3023	0.39	0/4100
1	B	0.16	0/3034	0.40	0/4115
1	C	0.17	0/3042	0.40	0/4127
1	D	0.19	0/3030	0.43	0/4109
1	E	0.17	0/3046	0.39	0/4132
1	F	0.15	0/3042	0.37	0/4127
1	G	0.17	0/3050	0.42	0/4139
1	H	0.20	1/3038 (0.0%)	0.38	0/4119
All	All	0.18	1/24305 (0.0%)	0.40	0/32968

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	3
1	D	0	2
1	G	0	4
1	H	0	1
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	320	GLY	C-O	-6.24	1.20	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	139	LYS	Peptide
1	C	140	ILE	Peptide
1	C	141	LYS	Peptide
1	C	145	ALA	Peptide
1	D	141	LYS	Peptide
1	D	321	THR	Peptide
1	G	139	LYS	Peptide
1	G	141	LYS	Peptide
1	G	360	LEU	Peptide
1	G	362	ASN	Peptide
1	H	139	LYS	Peptide

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	2982	0	2973	31	0
1	B	2993	0	2983	33	0
1	C	3000	0	2990	36	0
1	D	2989	0	2967	54	0
1	E	3004	0	2992	55	0
1	F	3000	0	2990	39	0
1	G	3007	0	2997	46	0
1	H	2997	0	2982	61	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	A	68	0	0	0	0
3	B	55	0	0	0	0
3	C	66	0	0	2	0
3	D	61	0	0	2	0
3	E	44	0	0	1	0
3	F	35	0	0	1	0
3	G	39	0	0	1	0
3	H	18	0	0	1	0
All	All	24368	0	23874	338	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 (338) 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:141:LYS:NZ	1:D:144:GLU:HB2	1.49	1.24
1:E:284:PRO:O	1:E:319:LYS:NZ	1.66	1.23
1:E:171:GLY:O	1:E:175:ILE:HD12	1.47	1.12
1:F:141:LYS:HE2	1:F:144:GLU:OE2	1.48	1.10
1:D:141:LYS:HZ2	1:D:144:GLU:HB2	1.28	0.94
1:D:141:LYS:HZ1	1:D:144:GLU:HB2	1.23	0.91
1:H:157:GLU:HG3	1:H:187:ASP:HB3	1.56	0.85
1:A:157:GLU:HG3	1:A:187:ASP:HB3	1.59	0.85
1:D:322:LEU:H	1:D:322:LEU:HD22	1.42	0.84
1:E:171:GLY:O	1:E:175:ILE:CD1	2.24	0.84
1:A:63:LEU:HA	1:A:241:ASN:OD1	1.78	0.83
1:A:148:THR:HG22	1:A:150:GLU:H	1.49	0.78
1:D:321:THR:OG1	1:D:322:LEU:HD22	1.84	0.78
1:E:361:LYS:HE3	1:E:364:ARG:NH1	1.99	0.78
1:D:141:LYS:HE2	1:D:141:LYS:HA	1.67	0.77
1:D:363:ASP:OD1	1:D:367:LEU:HD13	1.85	0.75
1:D:284:PRO:O	1:D:319:LYS:NZ	2.20	0.75
1:E:364:ARG:NH2	1:E:371:ASP:OD2	2.20	0.75
1:E:285:TRP:C	1:E:319:LYS:HD2	2.13	0.73
1:E:284:PRO:C	1:E:319:LYS:NZ	2.48	0.71
1:D:327:ILE:CD1	1:D:397:ALA:HA	2.22	0.70
1:H:355:THR:HG23	1:H:356:HIS:ND1	2.07	0.70
1:C:141:LYS:HA	1:C:143:LEU:H	1.57	0.69
1:F:57:GLY:O	3:F:501:HOH:O	2.10	0.69
1:D:327:ILE:HD11	1:D:397:ALA:HA	1.74	0.69
1:G:355:THR:HG23	1:G:356:HIS:ND1	2.08	0.68
1:G:287:GLU:OE1	1:G:319:LYS:NZ	2.23	0.68
1:E:110:MET:HE2	1:E:167:ILE:HD11	1.75	0.68
1:C:384:GLU:OE2	3:C:601:HOH:O	2.11	0.68
1:D:141:LYS:NZ	1:D:144:GLU:CB	2.44	0.68
1:E:321:THR:HG23	1:E:323:GLN:H	1.57	0.68
1:F:363:ASP:O	1:F:367:LEU:HG	1.94	0.67
1:E:140:ILE:HG23	1:E:141:LYS:HD3	1.75	0.67
1:F:100:LEU:O	1:F:235:ARG:NH2	2.28	0.66
1:E:172:CYS:HA	1:E:175:ILE:HD13	1.78	0.66
1:G:363:ASP:O	1:G:367:LEU:HG	1.96	0.65
1:H:140:ILE:HG21	1:H:175:ILE:HD13	1.79	0.64
1:D:329:LEU:O	3:D:501:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:VAL:HG22	1:D:205:ILE:HB	1.79	0.64
1:E:185:VAL:HG22	1:E:205:ILE:HB	1.78	0.64
1:G:10:GLY:N	3:G:502:HOH:O	2.28	0.64
1:A:185:VAL:HG22	1:A:205:ILE:HB	1.80	0.63
1:D:139:LYS:HG2	1:D:142:LEU:HD13	1.80	0.63
1:C:141:LYS:O	1:C:141:LYS:HG3	2.00	0.62
1:E:361:LYS:O	1:E:364:ARG:HG2	1.99	0.62
1:B:292:PRO:HB3	1:B:303:VAL:HG21	1.81	0.62
1:H:63:LEU:HD13	1:H:241:ASN:HD22	1.65	0.62
1:A:359:VAL:O	1:A:364:ARG:NH2	2.33	0.62
1:C:364:ARG:HB3	1:C:369:ILE:HB	1.81	0.61
1:D:287:GLU:HB2	1:D:319:LYS:HG2	1.82	0.61
1:D:214:MET:HE3	1:D:259:LEU:HD11	1.81	0.61
1:H:349:GLU:OE2	1:H:375:ARG:NH2	2.34	0.60
1:E:284:PRO:C	1:E:319:LYS:HZ2	2.08	0.60
1:E:144:GLU:HG3	1:E:175:ILE:HG21	1.83	0.60
1:G:250:ILE:HD12	1:H:250:ILE:HG21	1.84	0.60
1:D:292:PRO:HB3	1:D:303:VAL:HG21	1.82	0.60
1:E:386:LEU:O	1:E:390:LEU:HD12	2.02	0.59
1:F:141:LYS:HE2	1:F:144:GLU:CD	2.27	0.59
1:F:151:THR:C	1:F:152:LYS:HD2	2.28	0.59
1:E:361:LYS:HA	1:E:364:ARG:HB3	1.83	0.59
1:D:79:ASP:OD1	1:D:208:TYR:OH	2.12	0.59
1:E:211:THR:HB	1:E:212:LLP:HD3	1.84	0.59
1:C:317:TYR:CZ	1:C:373:LEU:HD13	2.38	0.59
1:E:175:ILE:HD12	1:E:175:ILE:H	1.67	0.58
1:F:30:GLU:OE2	1:H:48:LYS:NZ	2.36	0.58
1:B:147:ILE:HG21	1:B:179:HIS:CD2	2.38	0.58
1:H:212:LLP:HG3	1:H:341:LEU:HG	1.84	0.58
1:B:141:LYS:HG2	1:B:144:GLU:HB3	1.86	0.58
1:B:147:ILE:HG21	1:B:179:HIS:HD2	1.69	0.58
1:A:162:PRO:O	1:A:315:THR:HG21	2.04	0.58
1:F:156:ILE:HD11	1:F:186:VAL:HG22	1.86	0.58
1:D:322:LEU:HD22	1:D:322:LEU:N	2.15	0.57
1:F:171:GLY:O	1:F:175:ILE:HD12	2.04	0.57
1:H:136:ASP:OD1	1:H:138:SER:OG	2.17	0.57
1:H:110:MET:SD	1:H:167:ILE:HD11	2.45	0.57
1:B:118:ASN:ND2	1:B:122:ARG:NH1	2.51	0.57
1:G:213:TYR:O	1:G:265:ARG:NH2	2.37	0.57
1:F:185:VAL:HG22	1:F:205:ILE:HB	1.87	0.56
1:C:339:VAL:HG22	1:C:355:THR:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:ASP:OD1	1:D:366:VAL:HB	2.05	0.56
1:C:45:THR:HA	1:C:61:SER:HB2	1.88	0.56
1:E:361:LYS:CE	1:E:364:ARG:NH1	2.67	0.56
1:E:141:LYS:HA	1:E:144:GLU:OE1	2.06	0.55
1:E:159:PRO:HB2	1:E:164:GLN:HG2	1.88	0.55
1:G:141:LYS:HG3	1:G:144:GLU:HB2	1.88	0.55
1:D:141:LYS:HZ2	1:D:144:GLU:CB	2.12	0.55
1:G:136:ASP:OD1	1:G:138:SER:OG	2.23	0.55
1:E:253:TYR:OH	1:H:219:ASP:OD1	2.23	0.55
1:F:322:LEU:HB2	1:F:371:ASP:HB3	1.88	0.55
1:D:322:LEU:H	1:D:322:LEU:CD2	2.15	0.55
1:D:27:GLN:HE22	1:D:256:ASN:HD21	1.53	0.55
1:H:271:LYS:NZ	1:H:272:ASN:OD1	2.40	0.54
1:H:349:GLU:HG2	1:H:350:LEU:N	2.21	0.54
1:D:140:ILE:HG12	1:D:141:LYS:HG2	1.89	0.54
1:H:287:GLU:OE2	1:H:319:LYS:HD3	2.08	0.54
1:F:28:ASP:O	1:F:31:GLN:HG3	2.08	0.54
1:H:184:LEU:HD23	1:H:203:ALA:HA	1.90	0.54
1:A:261:THR:O	1:A:265:ARG:HG3	2.08	0.54
1:B:214:MET:HE3	1:B:259:LEU:HD21	1.90	0.54
1:H:172:CYS:O	1:H:176:VAL:HG23	2.08	0.54
1:B:112:ASP:HB2	1:B:367:LEU:HD22	1.90	0.54
1:E:388:GLU:OE1	3:E:501:HOH:O	2.18	0.53
1:E:184:LEU:HD23	1:E:203:ALA:HA	1.89	0.53
1:D:94:THR:O	1:D:98:THR:HG23	2.08	0.53
1:C:141:LYS:HB2	1:C:144:GLU:HB2	1.90	0.53
1:H:319:LYS:HE2	1:H:320:GLY:H	1.74	0.52
1:H:30:GLU:OE1	1:H:35:ARG:NH2	2.42	0.52
1:E:79:ASP:OD1	1:E:208:TYR:OH	2.15	0.52
1:B:321:THR:OG1	1:B:322:LEU:N	2.43	0.52
1:G:331:ASN:O	1:G:392:GLN:NE2	2.41	0.51
1:E:280:LEU:HD11	1:E:390:LEU:HD22	1.91	0.51
1:H:321:THR:HG23	1:H:323:GLN:HB2	1.91	0.51
1:C:144:GLU:O	1:C:147:ILE:HB	2.10	0.51
1:E:326:GLU:O	1:E:330:LYS:HG2	2.09	0.51
1:G:139:LYS:N	1:G:139:LYS:HD2	2.26	0.51
1:H:322:LEU:HD13	1:H:371:ASP:HB3	1.93	0.51
1:C:391:ASP:O	1:C:395:LYS:HG3	2.10	0.51
1:E:327:ILE:O	1:E:331:ASN:ND2	2.40	0.51
1:F:110:MET:SD	1:F:167:ILE:HD11	2.50	0.51
1:C:131:LYS:HD2	1:C:131:LYS:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:PHE:HB3	1:H:132:ILE:HG21	1.92	0.51
1:A:317:TYR:CZ	1:A:373:LEU:HD12	2.46	0.50
1:A:349:GLU:HG2	1:A:350:LEU:N	2.25	0.50
1:B:136:ASP:OD1	1:B:138:SER:OG	2.22	0.50
1:A:384:GLU:CD	1:A:384:GLU:H	2.18	0.50
1:H:302:LEU:HA	1:H:305:ARG:HG2	1.93	0.50
1:D:193:PRO:HD3	1:D:208:TYR:CE1	2.46	0.50
1:F:32:TRP:CZ2	1:F:39:PRO:HB3	2.47	0.50
1:A:214:MET:HE3	1:A:259:LEU:HD11	1.94	0.50
1:B:118:ASN:CG	1:B:122:ARG:HH11	2.19	0.50
1:F:231:SER:O	1:F:235:ARG:HG3	2.12	0.50
1:G:41:ILE:HG21	1:G:250:ILE:HG12	1.94	0.50
1:E:364:ARG:HG3	1:E:365:ASP:N	2.26	0.50
1:E:144:GLU:HG2	1:E:175:ILE:HG23	1.94	0.49
1:F:131:LYS:HD3	1:F:132:ILE:N	2.26	0.49
1:D:349:GLU:OE1	1:D:355:THR:HG23	2.12	0.49
1:D:363:ASP:CG	1:D:367:LEU:HD13	2.37	0.49
1:B:118:ASN:ND2	1:B:122:ARG:HH11	2.10	0.49
1:B:319:LYS:O	1:B:398:HIS:NE2	2.32	0.49
1:D:188:ASN:HB3	1:D:208:TYR:CE1	2.48	0.49
1:G:216:GLY:HA3	1:G:265:ARG:NH2	2.28	0.49
1:H:156:ILE:HD11	1:H:186:VAL:HG22	1.95	0.49
1:C:268:ARG:HB3	1:C:380:LEU:HD22	1.94	0.49
1:D:111:ASP:OD2	1:D:136:ASP:HA	2.13	0.49
1:E:281:GLU:HG3	1:E:289:VAL:HB	1.93	0.49
1:F:253:TYR:OH	1:G:219:ASP:OD1	2.28	0.49
1:B:159:PRO:HB2	1:B:164:GLN:HG2	1.94	0.49
1:G:95:VAL:HG21	1:H:243:LEU:HA	1.93	0.49
1:H:12:LEU:HD11	1:H:305:ARG:C	2.38	0.49
1:E:150:GLU:HG3	1:E:150:GLU:O	2.13	0.48
1:E:385:ASP:OD2	1:H:17:HIS:ND1	2.45	0.48
1:C:101:LEU:HD22	1:C:152:LYS:HB3	1.94	0.48
1:G:369:ILE:HA	1:G:373:LEU:HD13	1.96	0.48
1:D:141:LYS:CE	1:D:144:GLU:HB2	2.37	0.48
1:G:263:HIS:CD2	1:G:264:VAL:HG13	2.48	0.48
1:C:322:LEU:O	1:C:326:GLU:HG3	2.13	0.48
1:D:98:THR:HG21	1:D:121:PHE:HE1	1.78	0.48
1:E:144:GLU:HG3	1:E:175:ILE:CG2	2.44	0.48
1:E:214:MET:HE3	1:E:259:LEU:HD21	1.96	0.48
1:G:362:ASN:ND2	1:G:365:ASP:HB2	2.29	0.48
1:B:181:ASP:O	1:B:181:ASP:OD1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LYS:HD3	1:C:145:ALA:H	1.78	0.48
1:C:219:ASP:HB2	1:D:43:LEU:HB3	1.95	0.48
1:D:154:VAL:HG23	1:D:182:ILE:HD11	1.95	0.47
1:E:381:GLU:HB2	1:E:386:LEU:HD21	1.95	0.47
1:C:292:PRO:HB3	1:C:303:VAL:HG21	1.95	0.47
1:D:141:LYS:NZ	1:D:144:GLU:OE2	2.39	0.47
1:C:174:HIS:CE1	1:C:178:LYS:HE2	2.50	0.47
1:G:317:TYR:CZ	1:G:373:LEU:HD12	2.49	0.47
1:B:29:PRO:O	1:B:35:ARG:HA	2.13	0.47
1:C:10:GLY:N	3:C:604:HOH:O	2.46	0.47
1:G:193:PRO:HD3	1:G:208:TYR:CE2	2.50	0.47
1:A:188:ASN:HB3	1:A:208:TYR:CE1	2.49	0.47
1:A:23:ILE:HA	1:A:260:LYS:HD3	1.97	0.47
1:E:102:LYS:HG2	1:E:105:ASP:OD2	2.15	0.47
1:E:188:ASN:HB3	1:E:208:TYR:CE2	2.50	0.47
1:F:50:GLY:HA3	1:F:51:ALA:HA	1.60	0.47
1:A:193:PRO:HD3	1:A:208:TYR:CE1	2.50	0.47
1:B:188:ASN:HB3	1:B:208:TYR:CE2	2.50	0.47
1:A:140:ILE:HG13	1:A:175:ILE:CD1	2.45	0.47
1:F:193:PRO:HD3	1:F:208:TYR:CE2	2.50	0.47
1:B:45:THR:HA	1:B:61:SER:HB2	1.97	0.47
1:B:121:PHE:O	1:B:132:ILE:HD13	2.15	0.47
1:E:222:MET:HE1	1:E:252:CYS:HA	1.97	0.47
1:H:326:GLU:O	1:H:330:LYS:HD3	2.15	0.47
1:A:315:THR:HG22	1:A:375:ARG:HG3	1.97	0.46
1:B:79:ASP:OD1	1:B:208:TYR:OH	2.25	0.46
1:G:161:ASN:HA	1:G:162:PRO:HA	1.66	0.46
1:D:384:GLU:H	1:D:384:GLU:CD	2.23	0.46
1:E:46:THR:OG1	1:F:339:VAL:HG12	2.15	0.46
1:B:384:GLU:OE2	1:C:16:GLN:NE2	2.48	0.46
1:C:210:ALA:HA	1:C:214:MET:HB2	1.98	0.46
1:F:211:THR:HG23	1:F:221:VAL:HA	1.98	0.46
1:G:172:CYS:O	1:G:176:VAL:HG22	2.15	0.46
1:B:361:LYS:HA	1:B:364:ARG:HB2	1.98	0.46
1:G:45:THR:HA	1:G:61:SER:HB2	1.97	0.46
1:G:188:ASN:HB3	1:G:208:TYR:CE2	2.50	0.46
1:G:292:PRO:HB3	1:G:303:VAL:HG21	1.97	0.46
1:H:106:GLN:N	1:H:150:GLU:O	2.45	0.46
1:G:347:LEU:HB2	1:G:377:SER:HB3	1.98	0.46
1:H:357:ALA:O	3:H:501:HOH:O	2.21	0.46
1:G:322:LEU:HB2	1:G:371:ASP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:349:GLU:OE1	1:H:355:THR:HG22	2.15	0.46
1:H:369:ILE:HA	1:H:373:LEU:HD13	1.97	0.46
1:B:185:VAL:HG22	1:B:205:ILE:HB	1.97	0.46
1:H:69:ASN:O	1:H:73:LYS:HD3	2.16	0.46
1:H:162:PRO:O	1:H:315:THR:HG21	2.16	0.46
1:C:285:TRP:HA	1:C:319:LYS:HD2	1.98	0.46
1:H:92:ALA:HB1	1:H:245:ALA:HB1	1.98	0.46
1:H:321:THR:OG1	1:H:322:LEU:N	2.48	0.46
1:A:29:PRO:O	1:A:35:ARG:HA	2.16	0.46
1:D:268:ARG:HB3	1:D:380:LEU:HD22	1.97	0.46
1:H:63:LEU:O	1:H:68:ARG:NH2	2.48	0.46
1:D:365:ASP:HA	1:D:368:GLY:H	1.81	0.45
1:B:178:LYS:N	1:B:178:LYS:HD3	2.30	0.45
1:B:110:MET:HE2	1:B:167:ILE:HD11	1.99	0.45
1:E:229:CYS:SG	1:E:231:SER:OG	2.75	0.45
1:D:218:SER:OG	1:D:345:GLU:OE1	2.34	0.45
1:D:321:THR:OG1	1:D:322:LEU:N	2.49	0.45
1:E:128:PHE:HA	1:F:103:ALA:HB2	1.99	0.45
1:H:299:GLN:O	1:H:303:VAL:HG23	2.17	0.45
1:A:334:LEU:HD23	1:A:334:LEU:HA	1.72	0.45
1:C:174:HIS:O	1:C:178:LYS:HD3	2.16	0.45
1:F:102:LYS:HG2	1:F:105:ASP:OD2	2.16	0.45
1:G:91:MET:HE1	1:G:117:THR:HA	1.97	0.45
1:H:319:LYS:HA	1:H:319:LYS:HD2	1.75	0.45
1:D:144:GLU:HA	1:D:147:ILE:HB	1.99	0.45
1:G:361:LYS:O	1:G:364:ARG:HB2	2.16	0.45
1:C:161:ASN:HA	1:C:162:PRO:HA	1.78	0.45
1:F:45:THR:HA	1:F:61:SER:HB2	1.98	0.45
1:F:141:LYS:CE	1:F:144:GLU:OE2	2.40	0.45
1:F:219:ASP:OD2	1:G:253:TYR:OH	2.31	0.45
1:E:361:LYS:HE3	1:E:364:ARG:HH12	1.77	0.45
1:A:43:LEU:HD21	1:A:250:ILE:HG13	1.99	0.45
1:D:321:THR:HA	1:D:372:THR:HG22	1.98	0.45
1:A:112:ASP:HB2	1:A:367:LEU:HD22	1.99	0.44
1:F:79:ASP:OD1	1:F:208:TYR:OH	2.23	0.44
1:G:360:LEU:O	1:G:364:ARG:HG3	2.16	0.44
1:H:317:TYR:CZ	1:H:373:LEU:HD12	2.52	0.44
1:C:130:LEU:C	1:C:131:LYS:HD2	2.43	0.44
1:C:188:ASN:HB3	1:C:208:TYR:CE2	2.52	0.44
1:D:322:LEU:HD13	1:D:322:LEU:HA	1.77	0.44
1:C:121:PHE:HB3	1:C:132:ILE:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:VAL:HG13	1:F:114:TYR:O	2.18	0.44
1:D:326:GLU:O	1:D:330:LYS:HG3	2.17	0.44
1:E:161:ASN:HA	1:E:162:PRO:HA	1.77	0.44
1:G:191:MET:HE2	1:G:307:CYS:SG	2.58	0.44
1:B:155:TRP:CZ3	1:B:185:VAL:HG11	2.53	0.44
1:E:193:PRO:HD3	1:E:208:TYR:CE2	2.53	0.44
1:G:150:GLU:HA	1:G:152:LYS:HZ1	1.81	0.44
1:G:349:GLU:OE1	1:G:355:THR:HG22	2.18	0.44
1:H:193:PRO:HD3	1:H:208:TYR:CE1	2.53	0.44
1:A:360:LEU:O	1:A:364:ARG:HG3	2.17	0.44
1:B:161:ASN:HA	1:B:162:PRO:HA	1.79	0.43
1:C:360:LEU:O	1:C:364:ARG:HG3	2.18	0.43
1:H:322:LEU:HD11	1:H:350:LEU:HD21	1.98	0.43
1:H:361:LYS:HD3	1:H:364:ARG:CZ	2.48	0.43
1:B:193:PRO:HD3	1:B:208:TYR:CE2	2.54	0.43
1:C:214:MET:HE3	1:C:259:LEU:HD21	1.99	0.43
1:D:332:LEU:O	3:D:501:HOH:O	2.21	0.43
1:D:140:ILE:HG12	1:D:141:LYS:HD2	1.99	0.43
1:F:238:PHE:O	1:F:242:SER:OG	2.36	0.43
1:F:361:LYS:O	1:F:364:ARG:HB2	2.18	0.43
1:G:268:ARG:HB3	1:G:380:LEU:HD22	2.01	0.43
1:G:334:LEU:HD23	1:G:334:LEU:HA	1.79	0.43
1:C:32:TRP:O	1:C:35:ARG:NH1	2.51	0.43
1:C:95:VAL:HG21	1:D:243:LEU:HA	2.00	0.43
1:H:108:ILE:HB	1:H:154:VAL:HG22	2.00	0.43
1:H:291:TYR:CD1	1:H:314:VAL:HG22	2.54	0.43
1:E:171:GLY:C	1:E:175:ILE:CD1	2.91	0.43
1:H:79:ASP:OD1	1:H:208:TYR:OH	2.32	0.43
1:H:131:LYS:HD3	1:H:131:LYS:N	2.32	0.43
1:H:140:ILE:O	1:H:143:LEU:HB3	2.18	0.43
1:H:315:THR:HG22	1:H:375:ARG:HG3	2.01	0.43
1:G:155:TRP:CZ3	1:G:185:VAL:HG11	2.54	0.43
1:G:188:ASN:OD1	1:G:196:GLN:NE2	2.47	0.43
1:H:141:LYS:HE3	1:H:141:LYS:HB3	1.71	0.43
1:H:214:MET:HE3	1:H:259:LEU:HD21	1.99	0.43
1:B:121:PHE:HB3	1:B:132:ILE:HG21	2.01	0.42
1:A:92:ALA:HB1	1:A:245:ALA:HB1	2.01	0.42
1:F:143:LEU:O	1:F:147:ILE:HG13	2.18	0.42
1:F:188:ASN:HB3	1:F:208:TYR:CE2	2.54	0.42
1:G:110:MET:HE2	1:G:167:ILE:HD11	2.00	0.42
1:G:137:CYS:O	1:G:140:ILE:HD13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:ALA:HB2	1:F:199:LEU:HD12	2.02	0.42
1:C:315:THR:HG22	1:C:373:LEU:HD11	2.01	0.42
1:A:260:LYS:O	1:A:263:HIS:HE1	2.03	0.42
1:D:156:ILE:HD11	1:D:186:VAL:HG22	2.01	0.42
1:E:176:VAL:HG13	1:E:182:ILE:HD13	2.02	0.42
1:E:322:LEU:O	1:E:326:GLU:HG3	2.19	0.42
1:H:321:THR:HG23	1:H:323:GLN:H	1.85	0.42
1:A:291:TYR:CD1	1:A:314:VAL:HG22	2.55	0.42
1:A:326:GLU:O	1:A:330:LYS:HD3	2.20	0.41
1:D:283:ASN:HB3	1:D:286:VAL:HG23	2.02	0.41
1:E:112:ASP:HB2	1:E:367:LEU:HD22	2.02	0.41
1:G:22:ALA:HB2	1:G:78:LEU:HD21	2.01	0.41
1:H:16:GLN:HE21	1:H:17:HIS:CD2	2.38	0.41
1:H:155:TRP:CZ3	1:H:185:VAL:HG11	2.55	0.41
1:H:171:GLY:O	1:H:175:ILE:HD12	2.20	0.41
1:G:43:LEU:HD21	1:G:250:ILE:HG13	2.02	0.41
1:G:367:LEU:HB2	1:G:369:ILE:HG13	2.02	0.41
1:E:103:ALA:HB2	1:F:128:PHE:HA	2.02	0.41
1:F:268:ARG:HB3	1:F:380:LEU:HD22	2.02	0.41
1:G:52:PRO:HD2	1:H:330:LYS:HE3	2.02	0.41
1:G:214:MET:HE3	1:G:259:LEU:HD21	2.01	0.41
1:H:297:HIS:HB3	1:H:300:HIS:HB2	2.01	0.41
1:C:212:LLP:OP3	1:D:60:TYR:OH	2.29	0.41
1:D:212:LLP:HG2	1:D:341:LEU:O	2.21	0.41
1:A:122:ARG:HG2	1:A:123:GLN:HG3	2.02	0.41
1:E:113:VAL:HG23	1:E:118:ASN:HB2	2.02	0.41
1:E:144:GLU:CG	1:E:175:ILE:CG2	2.98	0.41
1:E:29:PRO:O	1:E:35:ARG:HA	2.20	0.41
1:B:259:LEU:HD23	1:B:259:LEU:HA	1.90	0.41
1:C:339:VAL:HG22	1:C:355:THR:CG2	2.50	0.41
1:D:159:PRO:HD2	1:D:191:MET:HG2	2.02	0.41
1:A:140:ILE:HG13	1:A:175:ILE:HD13	2.03	0.41
1:A:250:ILE:HD13	1:B:250:ILE:HG21	2.02	0.41
1:A:339:VAL:HG22	1:A:355:THR:CG2	2.51	0.41
1:B:315:THR:HG22	1:B:373:LEU:HD21	2.02	0.41
1:C:185:VAL:HG22	1:C:205:ILE:HB	2.01	0.41
1:F:210:ALA:HA	1:F:214:MET:HB2	2.01	0.41
1:A:171:GLY:O	1:A:175:ILE:HD12	2.21	0.41
1:B:118:ASN:ND2	1:B:359:VAL:HG22	2.36	0.41
1:F:29:PRO:O	1:F:35:ARG:HA	2.21	0.41
1:H:140:ILE:O	1:H:143:LEU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:285:TRP:HB3	1:H:398:HIS:HD2	1.86	0.41
1:H:319:LYS:HE2	1:H:320:GLY:N	2.36	0.41
1:E:36:ALA:HB1	1:G:44:SER:CB	2.51	0.41
1:G:274:MET:HE1	1:G:293:GLY:O	2.22	0.40
1:C:298:PRO:HB2	1:C:299:GLN:NE2	2.36	0.40
1:D:319:LYS:HB3	1:D:319:LYS:HE2	1.85	0.40
1:H:334:LEU:HD23	1:H:334:LEU:HA	1.83	0.40
1:A:39:PRO:HA	1:A:40:PRO:HD3	1.97	0.40
1:D:161:ASN:HA	1:D:162:PRO:HA	1.82	0.40
1:F:222:MET:HE1	1:F:252:CYS:HA	2.04	0.40
1:F:349:GLU:HG2	1:F:350:LEU:N	2.36	0.40
1:H:35:ARG:HD2	1:H:35:ARG:HA	1.81	0.40
1:B:351:PRO:HD2	1:B:373:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	379/415 (91%)	367 (97%)	12 (3%)	0	100	100
1	B	381/415 (92%)	371 (97%)	10 (3%)	0	100	100
1	C	382/415 (92%)	370 (97%)	12 (3%)	0	100	100
1	D	379/415 (91%)	363 (96%)	16 (4%)	0	100	100
1	E	383/415 (92%)	369 (96%)	14 (4%)	0	100	100
1	F	382/415 (92%)	371 (97%)	11 (3%)	0	100	100
1	G	383/415 (92%)	369 (96%)	14 (4%)	0	100	100
1	H	380/415 (92%)	365 (96%)	15 (4%)	0	100	100
All	All	3049/3320 (92%)	2945 (97%)	104 (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	324/347 (93%)	323 (100%)	1 (0%)	86	93
1	B	325/347 (94%)	325 (100%)	0	100	100
1	C	326/347 (94%)	325 (100%)	1 (0%)	86	93
1	D	324/347 (93%)	324 (100%)	0	100	100
1	E	326/347 (94%)	326 (100%)	0	100	100
1	F	326/347 (94%)	326 (100%)	0	100	100
1	G	327/347 (94%)	327 (100%)	0	100	100
1	H	325/347 (94%)	325 (100%)	0	100	100
All	All	2603/2776 (94%)	2601 (100%)	2 (0%)	88	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	339	VAL
1	C	339	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	323	GLN
1	B	118	ASN
1	B	123	GLN
1	B	174	HIS
1	B	241	ASN
1	C	174	HIS
1	C	179	HIS
1	C	256	ASN

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Mol	Chain	Res	Type
1	C	299	GLN
1	D	49	GLN
1	D	118	ASN
1	D	174	HIS
1	D	241	ASN
1	D	256	ASN
1	D	392	GLN
1	E	27	GLN
1	E	123	GLN
1	E	241	ASN
1	E	256	ASN
1	E	306	GLN
1	F	123	GLN
1	G	123	GLN
1	G	299	GLN
1	G	362	ASN
1	H	14	HIS
1	H	16	GLN
1	H	106	GLN
1	H	179	HIS
1	H	241	ASN
1	H	256	ASN
1	H	323	GLN
1	H	398	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
1	LLP	D	212	1	23,24,25	2.58	5 (21%)	25,32,34	1.39	4 (16%)
1	LLP	E	212	1	23,24,25	2.58	7 (30%)	25,32,34	1.50	6 (24%)
1	LLP	F	212	1	23,24,25	2.58	6 (26%)	25,32,34	1.30	4 (16%)
1	LLP	G	212	1	23,24,25	2.61	6 (26%)	25,32,34	1.39	4 (16%)
1	LLP	B	212	1	23,24,25	2.58	6 (26%)	25,32,34	1.29	4 (16%)
1	LLP	C	212	1	23,24,25	2.61	6 (26%)	25,32,34	1.42	5 (20%)
1	LLP	A	212	1	23,24,25	2.58	6 (26%)	25,32,34	1.38	3 (12%)
1	LLP	H	212	1	23,24,25	2.58	7 (30%)	25,32,34	1.24	4 (16%)

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
1	LLP	D	212	1	-	8/16/17/19	0/1/1/1
1	LLP	E	212	1	-	8/16/17/19	0/1/1/1
1	LLP	F	212	1	-	8/16/17/19	0/1/1/1
1	LLP	G	212	1	-	8/16/17/19	0/1/1/1
1	LLP	B	212	1	-	7/16/17/19	0/1/1/1
1	LLP	C	212	1	-	9/16/17/19	0/1/1/1
1	LLP	A	212	1	-	8/16/17/19	0/1/1/1
1	LLP	H	212	1	-	9/16/17/19	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	212	LLP	C4-C4'	7.58	1.62	1.46
1	C	212	LLP	C4-C4'	7.58	1.62	1.46
1	B	212	LLP	C4-C4'	7.56	1.62	1.46
1	F	212	LLP	C4-C4'	7.54	1.62	1.46
1	G	212	LLP	C4-C4'	7.50	1.62	1.46
1	A	212	LLP	C4-C4'	7.37	1.62	1.46
1	D	212	LLP	C4-C4'	7.36	1.62	1.46
1	E	212	LLP	C4-C4'	7.29	1.62	1.46
1	A	212	LLP	C4'-NZ	5.07	1.44	1.27
1	G	212	LLP	C4'-NZ	5.07	1.44	1.27
1	C	212	LLP	C4'-NZ	5.06	1.44	1.27
1	D	212	LLP	C4'-NZ	4.95	1.43	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	212	LLP	C4'-NZ	4.94	1.43	1.27
1	H	212	LLP	C4'-NZ	4.90	1.43	1.27
1	B	212	LLP	C4'-NZ	4.88	1.43	1.27
1	E	212	LLP	C4'-NZ	4.83	1.43	1.27
1	D	212	LLP	C4-C5	-4.45	1.35	1.42
1	E	212	LLP	C4-C5	-4.38	1.35	1.42
1	G	212	LLP	C4-C5	-4.24	1.36	1.42
1	F	212	LLP	C4-C5	-4.19	1.36	1.42
1	A	212	LLP	C4-C5	-4.13	1.36	1.42
1	C	212	LLP	C4-C5	-4.07	1.36	1.42
1	B	212	LLP	C4-C5	-4.06	1.36	1.42
1	H	212	LLP	C4-C5	-4.06	1.36	1.42
1	C	212	LLP	C2'-C2	3.83	1.56	1.50
1	B	212	LLP	C2'-C2	3.79	1.56	1.50
1	H	212	LLP	C2'-C2	3.78	1.56	1.50
1	E	212	LLP	C2'-C2	3.74	1.56	1.50
1	F	212	LLP	C2'-C2	3.71	1.56	1.50
1	G	212	LLP	C2'-C2	3.71	1.56	1.50
1	A	212	LLP	C2'-C2	3.69	1.56	1.50
1	D	212	LLP	C2'-C2	3.68	1.56	1.50
1	G	212	LLP	C6-N1	3.34	1.41	1.34
1	E	212	LLP	C6-N1	3.31	1.41	1.34
1	C	212	LLP	C6-N1	3.29	1.41	1.34
1	A	212	LLP	C6-N1	3.27	1.41	1.34
1	D	212	LLP	C6-N1	3.23	1.41	1.34
1	H	212	LLP	C6-N1	3.18	1.40	1.34
1	B	212	LLP	C6-N1	3.11	1.40	1.34
1	F	212	LLP	C6-N1	3.07	1.40	1.34
1	C	212	LLP	C5'-C5	2.24	1.56	1.50
1	A	212	LLP	C5'-C5	2.13	1.56	1.50
1	G	212	LLP	C5'-C5	2.13	1.56	1.50
1	H	212	LLP	C5'-C5	2.13	1.56	1.50
1	B	212	LLP	C5'-C5	2.11	1.56	1.50
1	E	212	LLP	C5'-C5	2.11	1.56	1.50
1	E	212	LLP	C4-C3	-2.08	1.37	1.41
1	F	212	LLP	C5'-C5	2.05	1.56	1.50
1	H	212	LLP	C3-C2	2.02	1.43	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	LLP	C4-C4'-NZ	-4.11	105.08	124.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	212	LLP	C4-C4'-NZ	-3.65	107.22	124.04
1	G	212	LLP	C4-C4'-NZ	-3.64	107.24	124.04
1	B	212	LLP	C4-C4'-NZ	-3.59	107.46	124.04
1	D	212	LLP	C4-C4'-NZ	-3.58	107.51	124.04
1	F	212	LLP	C4-C4'-NZ	-3.45	108.14	124.04
1	E	212	LLP	C4-C4'-NZ	-3.37	108.48	124.04
1	H	212	LLP	C4-C4'-NZ	-3.11	109.68	124.04
1	E	212	LLP	CE-NZ-C4'	-2.99	109.15	118.72
1	H	212	LLP	CE-NZ-C4'	-2.82	109.70	118.72
1	E	212	LLP	C2'-C2-C3	-2.76	117.56	120.80
1	D	212	LLP	C5-C6-N1	-2.66	119.50	123.83
1	F	212	LLP	C5-C6-N1	-2.65	119.53	123.83
1	C	212	LLP	C5-C6-N1	-2.60	119.60	123.83
1	E	212	LLP	C5-C6-N1	-2.60	119.60	123.83
1	A	212	LLP	C5-C6-N1	-2.57	119.66	123.83
1	D	212	LLP	C3-C4-C5	2.55	120.32	118.28
1	D	212	LLP	CE-NZ-C4'	-2.50	110.72	118.72
1	G	212	LLP	C5-C6-N1	-2.48	119.79	123.83
1	B	212	LLP	C5-C6-N1	-2.48	119.80	123.83
1	C	212	LLP	C3-C4-C5	2.46	120.25	118.28
1	H	212	LLP	C5-C6-N1	-2.43	119.88	123.83
1	E	212	LLP	C2'-C2-N1	2.41	122.18	117.64
1	E	212	LLP	C3-C4-C5	2.41	120.21	118.28
1	C	212	LLP	OP4-C5'-C5	2.40	113.84	109.36
1	A	212	LLP	C3-C4-C5	2.37	120.18	118.28
1	F	212	LLP	CE-NZ-C4'	-2.34	111.23	118.72
1	G	212	LLP	C3-C4-C5	2.29	120.11	118.28
1	B	212	LLP	CE-NZ-C4'	-2.24	111.54	118.72
1	G	212	LLP	CE-NZ-C4'	-2.23	111.56	118.72
1	B	212	LLP	C3-C4-C5	2.20	120.05	118.28
1	C	212	LLP	CE-NZ-C4'	-2.13	111.89	118.72
1	F	212	LLP	C3-C4-C5	2.12	119.98	118.28
1	H	212	LLP	C3-C4-C5	2.01	119.89	118.28

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	212	LLP	C5'-OP4-P-OP2
1	A	212	LLP	C5'-OP4-P-OP3
1	A	212	LLP	O-C-CA-CB
1	B	212	LLP	C5'-OP4-P-OP1

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Mol	Chain	Res	Type	Atoms
1	B	212	LLP	C5'-OP4-P-OP2
1	B	212	LLP	C5'-OP4-P-OP3
1	B	212	LLP	O-C-CA-CB
1	C	212	LLP	C3-C4-C4'-NZ
1	C	212	LLP	C5'-OP4-P-OP1
1	C	212	LLP	C5'-OP4-P-OP2
1	C	212	LLP	C5'-OP4-P-OP3
1	C	212	LLP	O-C-CA-CB
1	D	212	LLP	C5'-OP4-P-OP1
1	D	212	LLP	C5'-OP4-P-OP2
1	D	212	LLP	C5'-OP4-P-OP3
1	D	212	LLP	O-C-CA-CB
1	E	212	LLP	C4-C4'-NZ-CE
1	E	212	LLP	C5'-OP4-P-OP1
1	E	212	LLP	C5'-OP4-P-OP2
1	E	212	LLP	C5'-OP4-P-OP3
1	E	212	LLP	O-C-CA-CB
1	F	212	LLP	C5'-OP4-P-OP1
1	F	212	LLP	C5'-OP4-P-OP2
1	F	212	LLP	C5'-OP4-P-OP3
1	F	212	LLP	O-C-CA-CB
1	G	212	LLP	C3-C4-C4'-NZ
1	G	212	LLP	C5'-OP4-P-OP1
1	G	212	LLP	C5'-OP4-P-OP2
1	G	212	LLP	C5'-OP4-P-OP3
1	G	212	LLP	O-C-CA-CB
1	H	212	LLP	C4-C4'-NZ-CE
1	H	212	LLP	C5'-OP4-P-OP1
1	H	212	LLP	C5'-OP4-P-OP2
1	H	212	LLP	C5'-OP4-P-OP3
1	H	212	LLP	O-C-CA-CB
1	D	212	LLP	C4-C4'-NZ-CE
1	G	212	LLP	CA-CB-CG-CD
1	A	212	LLP	C3-C4-C4'-NZ
1	B	212	LLP	C3-C4-C4'-NZ
1	F	212	LLP	C3-C4-C4'-NZ
1	C	212	LLP	C4-C4'-NZ-CE
1	A	212	LLP	CG-CD-CE-NZ
1	B	212	LLP	CG-CD-CE-NZ
1	C	212	LLP	CG-CD-CE-NZ
1	F	212	LLP	CG-CD-CE-NZ
1	G	212	LLP	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	E	212	LLP	C3-C4-C4'-NZ
1	A	212	LLP	C5'-OP4-P-OP1
1	E	212	LLP	C5-C4-C4'-NZ
1	H	212	LLP	CA-CB-CG-CD
1	D	212	LLP	C3-C4-C4'-NZ
1	H	212	LLP	C3-C4-C4'-NZ
1	A	212	LLP	CA-CB-CG-CD
1	D	212	LLP	C-CA-CB-CG
1	E	212	LLP	C-CA-CB-CG
1	A	212	LLP	CD-CE-NZ-C4'
1	C	212	LLP	CD-CE-NZ-C4'
1	F	212	LLP	CD-CE-NZ-C4'
1	B	212	LLP	CD-CE-NZ-C4'
1	G	212	LLP	CD-CE-NZ-C4'
1	D	212	LLP	C5-C4-C4'-NZ
1	H	212	LLP	C5-C4-C4'-NZ
1	C	212	LLP	C6-C5-C5'-OP4
1	H	212	LLP	CG-CD-CE-NZ
1	F	212	LLP	CA-CB-CG-CD

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	212	LLP	1	0
1	E	212	LLP	1	0
1	C	212	LLP	1	0
1	H	212	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	A	501	-	4,4,4	0.21	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	383/415 (92%)	-0.40	2 (0%) 87 86	17, 28, 56, 77	0
1	B	385/415 (92%)	-0.16	4 (1%) 79 78	17, 35, 71, 98	0
1	C	386/415 (93%)	-0.37	3 (0%) 82 81	17, 29, 58, 76	0
1	D	385/415 (92%)	-0.03	9 (2%) 61 58	17, 37, 78, 106	0
1	E	387/415 (93%)	0.19	8 (2%) 63 60	22, 47, 87, 105	0
1	F	386/415 (93%)	-0.08	6 (1%) 70 68	24, 40, 75, 94	0
1	G	387/415 (93%)	0.17	12 (3%) 51 48	25, 46, 85, 112	0
1	H	386/415 (93%)	0.44	16 (4%) 41 38	27, 52, 90, 118	0
All	All	3085/3320 (92%)	-0.03	60 (1%) 66 63	17, 39, 78, 118	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	51	ALA	5.2
1	F	57	GLY	5.0
1	G	140	ILE	4.5
1	E	359	VAL	4.1
1	C	51	ALA	3.7
1	C	145	ALA	3.7
1	E	358	SER	3.4
1	H	310	CYS	3.4
1	B	140	ILE	3.3
1	E	360	LEU	3.2
1	H	56	SER	3.2
1	F	56	SER	3.2
1	C	140	ILE	3.1
1	B	358	SER	3.1
1	H	53	GLY	2.9
1	H	52	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	360	LEU	2.8
1	B	360	LEU	2.8
1	H	19	ALA	2.8
1	H	140	ILE	2.7
1	D	369	ILE	2.7
1	H	360	LEU	2.7
1	A	360	LEU	2.7
1	G	179	HIS	2.6
1	G	361	LYS	2.6
1	H	34	SER	2.5
1	D	56	SER	2.5
1	H	367	LEU	2.5
1	D	356	HIS	2.5
1	D	366	VAL	2.4
1	D	140	ILE	2.4
1	H	361	LYS	2.4
1	G	359	VAL	2.4
1	H	142	LEU	2.4
1	G	362	ASN	2.4
1	D	318	ILE	2.3
1	F	140	ILE	2.3
1	E	361	LYS	2.3
1	E	399	PRO	2.3
1	H	137	CYS	2.3
1	H	366	VAL	2.3
1	D	370	SER	2.3
1	G	400	PRO	2.3
1	H	149	PRO	2.2
1	A	50	GLY	2.2
1	E	180	GLY	2.2
1	H	57	GLY	2.2
1	G	135	VAL	2.2
1	H	139	LYS	2.2
1	G	323	GLN	2.2
1	G	132	ILE	2.2
1	F	141	LYS	2.2
1	D	355	THR	2.1
1	E	321	THR	2.1
1	F	360	LEU	2.1
1	E	397	ALA	2.1
1	G	149	PRO	2.1
1	D	143	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	142	LEU	2.0
1	B	365	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	G	212	24/25	0.93	0.11	30,44,56,62	0
1	LLP	H	212	24/25	0.94	0.11	33,52,66,69	0
1	LLP	E	212	24/25	0.95	0.10	30,41,53,56	0
1	LLP	F	212	24/25	0.95	0.09	25,37,52,52	0
1	LLP	B	212	24/25	0.95	0.10	19,36,46,50	0
1	LLP	C	212	24/25	0.95	0.10	21,31,45,46	0
1	LLP	A	212	24/25	0.96	0.08	19,32,42,52	0
1	LLP	D	212	24/25	0.96	0.09	19,37,49,63	0

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
2	SO4	C	501	5/5	0.81	0.25	83,86,89,91	0
2	SO4	A	501	5/5	0.83	0.23	79,82,85,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.