



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2025 – 01:57 pm BST

PDB ID : 9GV3 / pdb\_00009gv3  
Title : Crystal structure of the complex between Nb474 mutant R53A,D125A and Trypanosoma congolense fructose-1,6-bisphosphate aldolase  
Authors : McNae, I.W.; Dornan, J.; Walkinshaw, M.D.  
Deposited on : 2024-09-21  
Resolution : 1.75 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](mailto: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>.

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

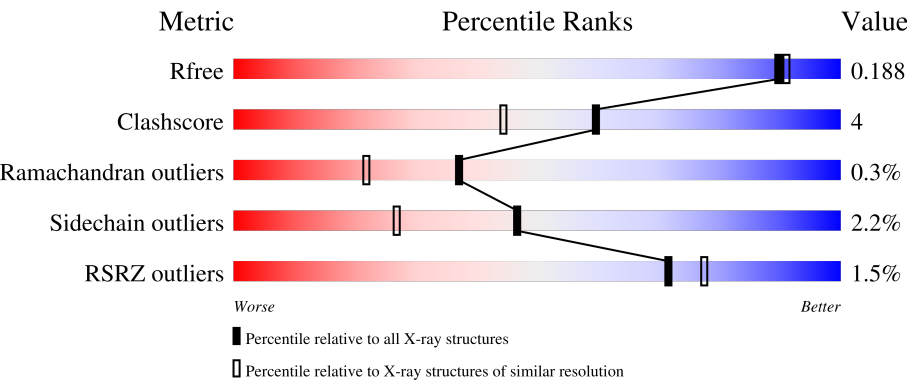
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

# 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 1.75 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.



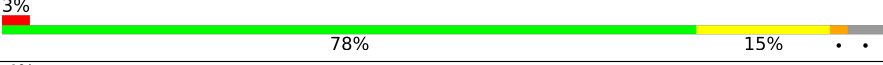

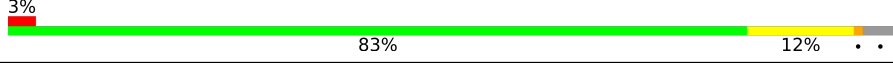
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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  $\geq 3$ , 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	387	
1	B	387	
1	C	387	
1	D	387	
2	E	143	

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Mol	Chain	Length	Quality of chain
2	F	143	
2	G	143	
2	H	143	

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	ACT	B	402	-	-	X	-
3	ACT	C	402	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16673 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 Fructose-bisphosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	3	0
			2803	1756	506	524	17			
1	B	358	Total	C	N	O	S	0	4	0
			2771	1740	499	515	17			
1	C	360	Total	C	N	O	S	0	4	0
			2786	1749	502	518	17			
1	D	358	Total	C	N	O	S	0	4	0
			2769	1739	499	514	17			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	373	GLU	-	expression tag	UNP G0UWE7
A	374	ASN	-	expression tag	UNP G0UWE7
A	375	LEU	-	expression tag	UNP G0UWE7
A	376	TYR	-	expression tag	UNP G0UWE7
A	377	PHE	-	expression tag	UNP G0UWE7
A	378	GLN	-	expression tag	UNP G0UWE7
A	379	SER	-	expression tag	UNP G0UWE7
A	380	GLY	-	expression tag	UNP G0UWE7
A	381	GLY	-	expression tag	UNP G0UWE7
A	382	HIS	-	expression tag	UNP G0UWE7
A	383	HIS	-	expression tag	UNP G0UWE7
A	384	HIS	-	expression tag	UNP G0UWE7
A	385	HIS	-	expression tag	UNP G0UWE7
A	386	HIS	-	expression tag	UNP G0UWE7
A	387	HIS	-	expression tag	UNP G0UWE7
B	373	GLU	-	expression tag	UNP G0UWE7
B	374	ASN	-	expression tag	UNP G0UWE7
B	375	LEU	-	expression tag	UNP G0UWE7
B	376	TYR	-	expression tag	UNP G0UWE7
B	377	PHE	-	expression tag	UNP G0UWE7
B	378	GLN	-	expression tag	UNP G0UWE7

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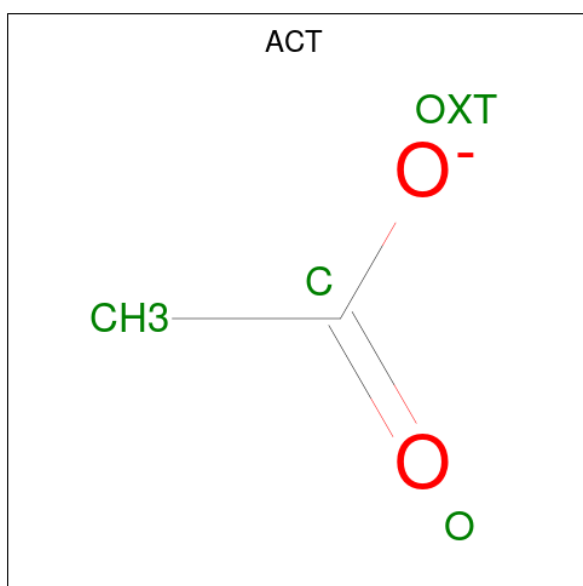
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Chain	Residue	Modelled	Actual	Comment	Reference
B	379	SER	-	expression tag	UNP G0UWE7
B	380	GLY	-	expression tag	UNP G0UWE7
B	381	GLY	-	expression tag	UNP G0UWE7
B	382	HIS	-	expression tag	UNP G0UWE7
B	383	HIS	-	expression tag	UNP G0UWE7
B	384	HIS	-	expression tag	UNP G0UWE7
B	385	HIS	-	expression tag	UNP G0UWE7
B	386	HIS	-	expression tag	UNP G0UWE7
B	387	HIS	-	expression tag	UNP G0UWE7
C	373	GLU	-	expression tag	UNP G0UWE7
C	374	ASN	-	expression tag	UNP G0UWE7
C	375	LEU	-	expression tag	UNP G0UWE7
C	376	TYR	-	expression tag	UNP G0UWE7
C	377	PHE	-	expression tag	UNP G0UWE7
C	378	GLN	-	expression tag	UNP G0UWE7
C	379	SER	-	expression tag	UNP G0UWE7
C	380	GLY	-	expression tag	UNP G0UWE7
C	381	GLY	-	expression tag	UNP G0UWE7
C	382	HIS	-	expression tag	UNP G0UWE7
C	383	HIS	-	expression tag	UNP G0UWE7
C	384	HIS	-	expression tag	UNP G0UWE7
C	385	HIS	-	expression tag	UNP G0UWE7
C	386	HIS	-	expression tag	UNP G0UWE7
C	387	HIS	-	expression tag	UNP G0UWE7
D	373	GLU	-	expression tag	UNP G0UWE7
D	374	ASN	-	expression tag	UNP G0UWE7
D	375	LEU	-	expression tag	UNP G0UWE7
D	376	TYR	-	expression tag	UNP G0UWE7
D	377	PHE	-	expression tag	UNP G0UWE7
D	378	GLN	-	expression tag	UNP G0UWE7
D	379	SER	-	expression tag	UNP G0UWE7
D	380	GLY	-	expression tag	UNP G0UWE7
D	381	GLY	-	expression tag	UNP G0UWE7
D	382	HIS	-	expression tag	UNP G0UWE7
D	383	HIS	-	expression tag	UNP G0UWE7
D	384	HIS	-	expression tag	UNP G0UWE7
D	385	HIS	-	expression tag	UNP G0UWE7
D	386	HIS	-	expression tag	UNP G0UWE7
D	387	HIS	-	expression tag	UNP G0UWE7

- Molecule 2 is a protein called Nb474 mutant R53A,D125A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	137	Total	C	N	O	S	0	1	0
			1046	642	182	217	5			
2	F	137	Total	C	N	O	S	0	1	0
			1046	642	182	217	5			
2	G	137	Total	C	N	O	S	0	0	0
			1041	637	182	217	5			
2	H	137	Total	C	N	O	S	0	1	0
			1046	640	182	219	5			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

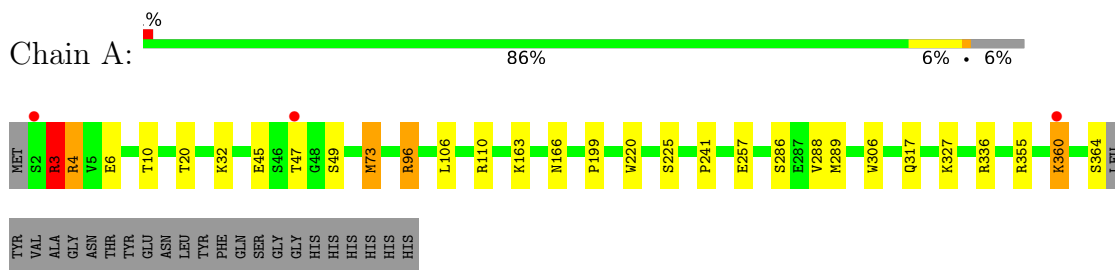
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total	O	0	0
			303	303		
5	B	261	Total	O	0	0
			261	261		
5	C	243	Total	O	0	0
			243	243		
5	D	278	Total	O	0	0
			278	278		
5	E	87	Total	O	0	0
			87	87		
5	F	53	Total	O	0	0
			53	53		
5	G	42	Total	O	0	0
			42	42		
5	H	76	Total	O	0	0
			76	76		

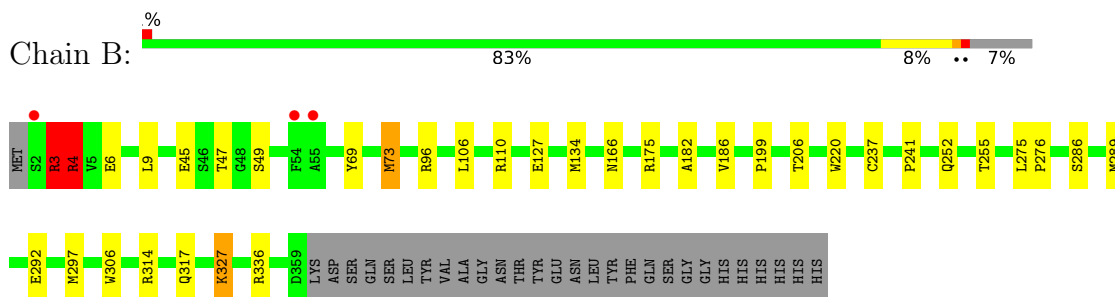
### 3 Residue-property plots [i](#)

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.

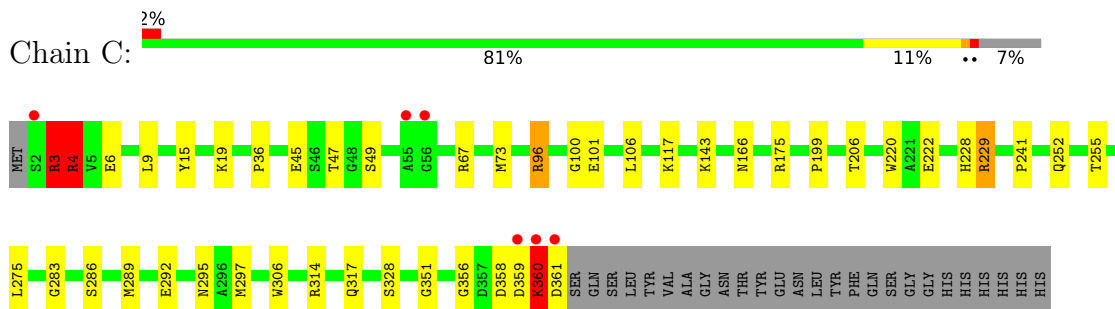
- Molecule 1: Fructose-bisphosphate aldolase



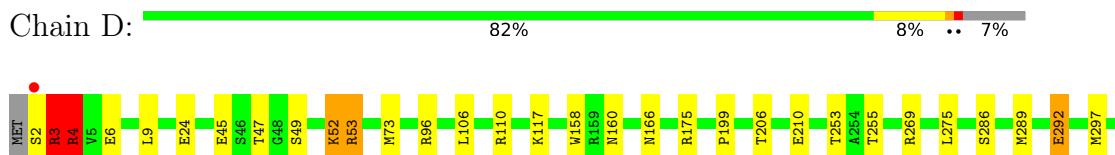
- Molecule 1: Fructose-bisphosphate aldolase



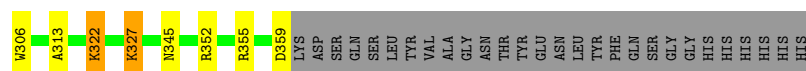
- Molecule 1: Fructose-bisphosphate aldolase



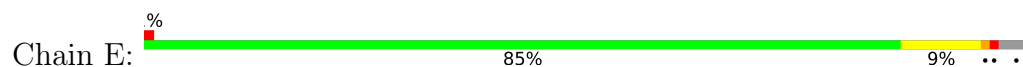
- Molecule 1: Fructose-bisphosphate aldolase



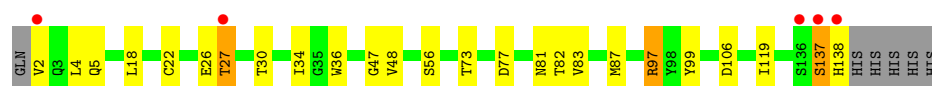
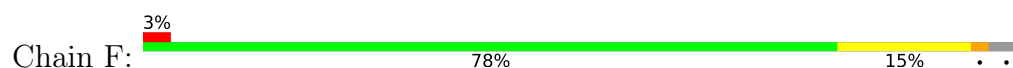




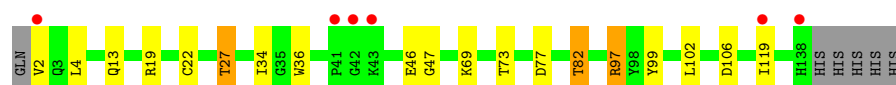
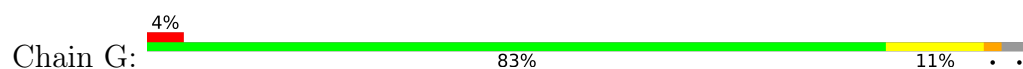
- Molecule 2: Nb474 mutant R53A,D125A



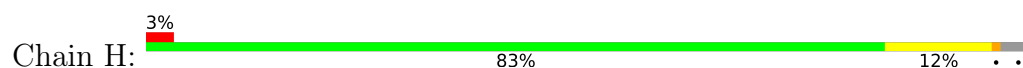
- Molecule 2: Nb474 mutant R53A,D125A



- Molecule 2: Nb474 mutant R53A,D125A



- Molecule 2: Nb474 mutant R53A,D125A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.50Å 111.17Å 123.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.56 – 1.75 97.56 – 1.75	Depositor EDS
% Data completeness (in resolution range)	70.5 (97.56-1.75) 70.5 (97.56-1.75)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.160 , 0.188 0.160 , 0.188	Depositor DCC
$R_{free}$ test set	9820 reflections (3.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ACT, GOL

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	0.91	0/2862	1.30	16/3872 (0.4%)
1	B	0.88	0/2831	1.27	16/3832 (0.4%)
1	C	0.89	1/2848 (0.0%)	1.32	17/3854 (0.4%)
1	D	0.91	0/2831	1.33	20/3832 (0.5%)
2	E	0.79	0/1068	1.33	8/1449 (0.6%)
2	F	0.78	0/1068	1.34	6/1449 (0.4%)
2	G	0.75	0/1060	1.39	9/1438 (0.6%)
2	H	0.85	0/1068	1.34	5/1449 (0.3%)
All	All	0.87	1/15636 (0.0%)	1.32	97/21175 (0.5%)

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	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
2	E	0	2
2	F	0	1
2	G	0	1
2	H	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	36	PRO	CA-CB	5.40	1.60	1.53

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	82	THR	CA-CB-OG1	-11.77	91.95	109.60
1	D	322	LYS	CB-CG-CD	10.64	135.76	111.30
1	B	3	ARG	CB-CA-C	10.58	127.89	110.22
1	C	3	ARG	CA-CB-CG	10.57	135.25	114.10
1	D	3	ARG	CB-CA-C	10.51	127.04	109.80
1	A	3	ARG	CB-CA-C	10.46	127.69	110.22
1	C	3	ARG	CB-CA-C	10.35	126.78	109.80
1	A	3	ARG	CA-CB-CG	10.06	134.22	114.10
1	B	3	ARG	CA-CB-CG	9.90	133.90	114.10
1	C	297	MET	CA-CB-CG	-8.53	97.04	114.10
1	D	47	THR	CA-CB-OG1	-8.26	97.21	109.60
1	A	327	LYS	CB-CG-CD	7.98	129.65	111.30
1	D	297	MET	CA-CB-CG	-7.95	98.21	114.10
1	A	96	ARG	CG-CD-NE	-7.78	94.89	112.00
2	G	106	ASP	CA-CB-CG	7.75	120.35	112.60
2	F	4	LEU	N-CA-CB	-7.59	99.58	110.44
1	B	297	MET	CA-CB-CG	-7.37	99.36	114.10
2	F	73	THR	CA-CB-OG1	-7.29	98.66	109.60
2	F	106	ASP	CA-CB-CG	7.25	119.85	112.60
1	C	47	THR	CA-CB-OG1	-7.06	99.01	109.60
1	D	253	THR	CA-CB-OG1	-6.87	99.30	109.60
1	B	127	GLU	N-CA-CB	-6.71	101.12	110.25
2	G	73	THR	CA-CB-OG1	-6.71	99.53	109.60
1	B	47	THR	CA-CB-OG1	-6.68	99.59	109.60
2	E	27	THR	CA-CB-OG1	6.56	119.44	109.60
2	E	73	THR	CA-CB-OG1	-6.54	99.79	109.60
1	B	73	MET	CG-SD-CE	6.50	115.20	100.90
1	C	4	ARG	CB-CG-CD	6.45	126.12	111.30
1	C	96	ARG	CA-CB-CG	-6.43	101.23	114.10
1	C	229	ARG	NE-CZ-NH2	6.41	124.97	119.20
1	D	117	LYS	CD-CE-NZ	-6.41	91.40	111.90
1	C	117	LYS	CD-CE-NZ	-6.38	91.48	111.90
1	A	47	THR	CA-CB-OG1	-6.38	100.03	109.60
1	B	3	ARG	N-CA-CB	-6.37	99.46	110.17
1	D	4	ARG	CB-CG-CD	6.35	125.90	111.30
2	G	27	THR	OG1-CB-CG2	6.34	121.99	109.30
1	C	101	GLU	CG-CD-OE2	-6.34	103.82	118.40
2	E	106	ASP	CA-CB-CG	6.30	118.90	112.60
1	C	359	ASP	CB-CA-C	6.28	121.97	110.36
1	C	3	ARG	N-CA-CB	-6.27	99.81	110.16
1	D	327	LYS	CG-CD-CE	6.20	125.56	111.30
1	A	360	LYS	CA-CB-CG	6.18	126.45	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	110	ARG	CA-CB-CG	-6.17	101.77	114.10
1	D	53	ARG	CD-NE-CZ	-6.10	115.86	124.40
1	D	345	ASN	CA-CB-CG	-6.10	106.50	112.60
2	E	69	LYS	CB-CA-C	-6.08	100.42	109.90
1	D	352	ARG	CD-NE-CZ	6.06	132.88	124.40
1	C	360	LYS	CG-CD-CE	6.03	125.17	111.30
2	G	27	THR	CA-CB-OG1	6.01	118.61	109.60
1	C	143	LYS	CG-CD-CE	6.00	125.10	111.30
2	F	48	VAL	N-CA-CB	-5.97	104.84	111.41
1	D	52	LYS	CG-CD-CE	5.95	124.99	111.30
1	B	255	THR	CA-CB-OG1	-5.93	100.70	109.60
1	A	360	LYS	CB-CG-CD	5.91	124.90	111.30
2	G	27	THR	CB-CA-C	5.89	119.25	109.53
2	H	30	THR	CA-CB-OG1	-5.88	100.78	109.60
2	G	46	GLU	CB-CG-CD	5.86	122.56	112.60
1	A	73	MET	CG-SD-CE	5.83	113.73	100.90
1	C	292	GLU	CB-CA-C	-5.71	101.31	110.79
1	B	110	ARG	CA-CB-CG	-5.70	102.70	114.10
1	B	206	THR	CA-CB-OG1	-5.67	101.09	109.60
1	A	73	MET	CB-CG-SD	-5.66	95.72	112.70
1	D	255	THR	CA-CB-OG1	-5.63	101.16	109.60
2	H	2	VAL	N-CA-CB	5.62	121.06	111.50
1	A	10	THR	CA-CB-OG1	-5.61	101.19	109.60
1	C	255	THR	CA-CB-OG1	-5.58	101.24	109.60
1	A	3	ARG	N-CA-CB	-5.57	100.81	110.17
2	E	27	THR	CB-CA-C	5.56	118.70	109.53
1	B	327	LYS	CG-CD-CE	5.55	124.08	111.30
1	B	134	MET	CG-SD-CE	5.55	113.11	100.90
1	A	110	ARG	CA-CB-CG	-5.53	103.04	114.10
2	E	19	ARG	CG-CD-NE	-5.53	99.84	112.00
1	D	73	MET	CB-CG-SD	-5.52	96.14	112.70
1	D	206	THR	CA-CB-OG1	-5.51	101.33	109.60
2	F	81	ASN	CB-CA-C	5.47	118.83	111.82
1	C	101	GLU	CB-CA-C	5.47	119.41	109.83
2	H	73	THR	CA-CB-OG1	-5.47	101.39	109.60
2	G	4	LEU	N-CA-CB	-5.42	102.60	110.36
1	A	257	GLU	CB-CG-CD	5.42	121.81	112.60
2	H	93	GLU	CB-CG-CD	5.41	121.80	112.60
1	B	4	ARG	CB-CG-CD	5.37	123.66	111.30
1	B	292	GLU	CB-CA-C	-5.37	101.87	110.79
2	E	4	LEU	N-CA-CB	-5.34	103.06	110.38
1	A	32	LYS	N-CA-CB	5.30	117.91	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	69	LYS	CB-CA-C	-5.29	101.64	109.90
1	D	3	ARG	CG-CD-NE	-5.23	100.50	112.00
1	D	292	GLU	CB-CA-C	-5.20	102.16	110.79
1	B	96	ARG	CA-CB-CG	-5.19	103.72	114.10
1	D	96	ARG	CD-NE-CZ	5.18	131.66	124.40
2	E	97	ARG	CG-CD-NE	-5.17	100.62	112.00
1	D	96	ARG	CA-CB-CG	-5.14	103.81	114.10
1	C	206	THR	CA-CB-OG1	-5.12	101.91	109.60
2	G	69	LYS	N-CA-CB	5.09	117.48	109.69
1	B	69	TYR	N-CA-CB	-5.07	102.66	110.16
1	A	360	LYS	CG-CD-CE	5.04	122.89	111.30
2	F	30	THR	CA-CB-OG1	-5.01	102.09	109.60
1	A	163	LYS	CD-CE-NZ	-5.00	95.89	111.90

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	ARG	Sidechain
1	B	314	ARG	Sidechain
1	C	314	ARG	Sidechain
1	C	67	ARG	Sidechain
1	D	53	ARG	Sidechain
2	E	19	ARG	Sidechain
2	E	97	ARG	Sidechain
2	F	97	ARG	Sidechain
2	G	97	ARG	Sidechain
2	H	97	ARG	Sidechain

## 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	2803	0	2809	15	0
1	B	2771	0	2782	20	0
1	C	2786	0	2800	26	0
1	D	2769	0	2783	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1046	0	983	9	0
2	F	1046	0	983	15	0
2	G	1041	0	972	13	0
2	H	1046	0	978	9	0
3	B	8	0	6	3	0
3	C	8	0	6	4	0
4	D	6	0	8	2	0
5	A	303	0	0	1	0
5	B	261	0	0	5	0
5	C	243	0	0	8	0
5	D	278	0	0	5	0
5	E	87	0	0	2	0
5	F	53	0	0	1	0
5	G	42	0	0	5	0
5	H	76	0	0	2	0
All	All	16673	0	15110	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 4.

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:B:252:GLN:HB2	5:B:712:HOH:O	1.32	1.27
1:C:96:ARG:HD3	5:C:673:HOH:O	1.34	1.24
3:B:402:ACT:H2	5:B:591:HOH:O	1.31	1.22
2:G:2:VAL:N	5:G:201:HOH:O	1.86	1.06
2:H:2:VAL:HG22	2:H:26:GLU:OE1	1.60	1.02
2:F:2:VAL:HG11	2:F:27:THR:HG21	1.50	0.89
1:C:286:SER:H	1:C:289:MET:HE3	1.37	0.89
1:B:286:SER:H	1:B:289:MET:HE3	1.36	0.88
1:D:286:SER:H	1:D:289:MET:HE3	1.41	0.84
1:D:175:ARG:HD3	5:D:504:HOH:O	1.80	0.82
2:E:2:VAL:N	5:E:201:HOH:O	2.12	0.82
1:D:4:ARG:NH2	5:D:501:HOH:O	2.10	0.81
1:D:3:ARG:HG2	1:D:3:ARG:HH11	1.47	0.78
2:G:82:THR:HG21	5:G:241:HOH:O	1.83	0.76
2:H:45:ARG:HD2	5:H:214:HOH:O	1.90	0.72
1:A:286:SER:H	1:A:289:MET:HE2	1.56	0.71
2:H:22:CYS:HB3	2:H:83:VAL:CG1	2.21	0.70
1:A:336:ARG:NH2	5:A:401:HOH:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:TYR:OH	5:C:501:HOH:O	2.12	0.68
1:D:210:GLU:OE1	5:D:502:HOH:O	2.11	0.68
1:B:175:ARG:HD3	5:B:520:HOH:O	1.97	0.64
1:D:3:ARG:NH1	1:D:3:ARG:CG	2.61	0.63
1:B:336:ARG:NH1	5:B:503:HOH:O	2.30	0.62
1:D:313:ALA:HB3	4:D:401:GOL:H32	1.80	0.62
1:C:3:ARG:HH21	1:C:4:ARG:H	1.46	0.62
2:E:27:THR:HG23	5:E:253:HOH:O	1.99	0.62
1:A:3:ARG:HH21	1:A:4:ARG:H	1.48	0.61
1:B:327:LYS:HA	1:B:327:LYS:HE2	1.82	0.61
2:G:77:ASP:HB3	2:G:82:THR:HG22	1.82	0.61
1:C:175:ARG:HD3	5:C:505:HOH:O	2.00	0.60
1:D:286:SER:H	1:D:289:MET:CE	2.14	0.60
1:B:3:ARG:HH21	1:B:4:ARG:H	1.49	0.60
2:G:82:THR:HG23	5:G:221:HOH:O	2.01	0.60
2:H:22:CYS:HB3	2:H:83:VAL:HG13	1.83	0.59
2:F:77:ASP:HB3	2:F:82:THR:HG22	1.85	0.59
1:C:286:SER:H	1:C:289:MET:CE	2.15	0.58
1:C:19:LYS:HE3	5:C:727:HOH:O	2.04	0.58
1:D:3:ARG:HH11	1:D:3:ARG:CG	2.12	0.58
2:F:2:VAL:CG1	2:F:27:THR:HG21	2.28	0.58
3:B:402:ACT:CH3	5:B:591:HOH:O	2.13	0.58
2:H:137:SER:O	2:H:138:HIS:C	2.47	0.57
1:C:229:ARG:HG3	3:C:401:ACT:H2	1.86	0.57
1:C:45:GLU:HB3	1:C:49:SER:HB2	1.85	0.57
1:D:158:TRP:HE1	1:D:160:ASN:HD21	1.52	0.56
2:G:34:ILE:CD1	2:G:102:LEU:CD2	2.83	0.56
1:C:286:SER:N	1:C:289:MET:HE3	2.16	0.56
1:A:45:GLU:HB3	1:A:49:SER:HB2	1.88	0.55
2:H:22:CYS:HB3	2:H:83:VAL:HG12	1.88	0.54
2:F:137:SER:O	2:F:138:HIS:C	2.50	0.54
2:E:47:GLY:HA3	2:E:119[A]:ILE:HG23	1.91	0.53
1:A:166:ASN:HB3	1:C:6:GLU:O	2.09	0.53
1:A:3:ARG:HG3	1:D:9:LEU:HD12	1.91	0.53
2:G:13:GLN:HG3	5:G:223:HOH:O	2.08	0.53
1:B:45:GLU:HB3	1:B:49:SER:HB2	1.91	0.52
2:F:2:VAL:HG22	2:F:26:GLU:OE2	2.09	0.52
1:D:45:GLU:HB3	1:D:49:SER:HB2	1.90	0.52
1:B:166:ASN:HB3	1:D:6:GLU:O	2.09	0.52
1:D:2:SER:N	5:D:506:HOH:O	2.43	0.52
2:E:34:ILE:CD1	2:E:102:LEU:CD2	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:LEU:H	2:H:81:ASN:ND2	2.07	0.51
1:B:286:SER:H	1:B:289:MET:CE	2.17	0.51
1:B:106:LEU:C	1:B:106:LEU:HD23	2.36	0.50
1:B:286:SER:N	1:B:289:MET:HE3	2.16	0.50
2:F:34:ILE:CD1	2:F:83:VAL:HG21	2.41	0.50
2:G:119:ILE:HG22	2:G:119:ILE:O	2.11	0.50
1:A:225[A]:SER:OG	3:B:402:ACT:OXT	2.30	0.50
2:G:47:GLY:HA3	2:G:119:ILE:CG2	2.42	0.50
1:A:106:LEU:C	1:A:106:LEU:HD23	2.38	0.49
1:C:106:LEU:HD23	1:C:106:LEU:C	2.37	0.49
1:D:286:SER:N	1:D:289:MET:HE3	2.19	0.49
1:C:295:ASN:HD21	1:C:351:GLY:C	2.21	0.49
1:B:6:GLU:O	1:D:166:ASN:HB3	2.12	0.48
1:A:286:SER:H	1:A:289:MET:CE	2.25	0.48
1:D:106:LEU:C	1:D:106:LEU:HD23	2.38	0.48
2:F:2:VAL:HG11	2:F:27:THR:CG2	2.35	0.48
1:C:73:MET:SD	1:C:317:GLN:HG2	2.53	0.48
1:C:96:ARG:NH1	1:C:100:GLY:O	2.47	0.48
2:G:34:ILE:CD1	2:G:102:LEU:HD22	2.43	0.48
2:F:82:THR:HG23	5:F:206:HOH:O	2.12	0.47
1:C:222:GLU:HA	3:C:402:ACT:H2	1.97	0.47
1:D:313:ALA:HB3	4:D:401:GOL:C3	2.45	0.47
1:B:182:ALA:O	1:B:186[B]:VAL:HG12	2.15	0.47
2:F:77:ASP:HB3	2:F:82:THR:CG2	2.44	0.47
1:C:252:GLN:HB2	5:C:713:HOH:O	2.14	0.46
1:C:358:ASP:C	1:C:360:LYS:H	2.22	0.46
1:A:6:GLU:O	1:C:166:ASN:HB3	2.16	0.46
2:G:47:GLY:HA3	2:G:119:ILE:HG23	1.98	0.45
2:F:47:GLY:HA3	2:F:119[A]:ILE:HG23	1.99	0.45
1:B:9:LEU:HD12	1:C:3:ARG:HG3	1.98	0.45
1:B:73:MET:SD	1:B:317:GLN:HG2	2.57	0.45
1:C:96:ARG:CD	5:C:673:HOH:O	2.20	0.45
1:A:73:MET:SD	1:A:317:GLN:HG2	2.57	0.45
2:H:18:LEU:HB2	2:H:87:MET:HE3	1.99	0.45
1:D:24:GLU:HG2	5:D:654:HOH:O	2.18	0.44
2:G:19:ARG:NH2	5:G:206:HOH:O	2.49	0.44
2:G:97:ARG:HD2	2:G:99:TYR:OH	2.18	0.44
1:B:3:ARG:NE	1:B:3:ARG:HA	2.33	0.44
1:C:356:GLY:O	1:C:360:LYS:HD3	2.18	0.44
2:E:47:GLY:HA3	2:E:119[A]:ILE:CG2	2.48	0.43
1:A:3:ARG:HG3	1:D:9:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:402:ACT:OXT	5:C:502:HOH:O	2.21	0.43
2:G:22:CYS:HB2	2:G:36:TRP:CZ2	2.53	0.43
2:H:3:GLN:HG2	5:H:238:HOH:O	2.18	0.43
2:E:22:CYS:HB2	2:E:36:TRP:CZ2	2.55	0.42
1:B:9:LEU:CD1	1:C:3:ARG:HG3	2.49	0.42
1:B:3:ARG:HG3	1:C:9:LEU:HD12	2.01	0.42
1:A:3:ARG:NE	1:A:3:ARG:HA	2.34	0.42
2:F:97:ARG:HD2	2:F:99:TYR:OH	2.19	0.42
1:A:220:TRP:CZ2	1:A:241:PRO:HB2	2.55	0.42
2:F:18:LEU:HB2	2:F:87:MET:HE3	2.02	0.41
1:C:220:TRP:CZ2	1:C:241:PRO:HB2	2.55	0.41
3:C:402:ACT:CH3	5:C:590:HOH:O	2.68	0.41
2:F:47:GLY:HA3	2:F:119[A]:ILE:CG2	2.50	0.41
1:A:288:VAL:HG11	1:A:355:ARG:CZ	2.50	0.41
1:C:228:HIS:HE1	1:D:269:ARG:O	2.04	0.41
2:E:97:ARG:HD2	2:E:99:TYR:OH	2.21	0.41
2:F:22:CYS:HB2	2:F:36:TRP:CZ2	2.56	0.41
1:D:292:GLU:OE2	1:D:355:ARG:HD3	2.21	0.40
1:B:220:TRP:CZ2	1:B:241:PRO:HB2	2.56	0.40
1:B:237:CYS:O	1:B:276:PRO:HD2	2.21	0.40
2:E:34:ILE:CD1	2:E:102:LEU:HD22	2.52	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	364/387 (94%)	358 (98%)	5 (1%)	1 (0%)	37	22
1	B	360/387 (93%)	352 (98%)	7 (2%)	1 (0%)	37	22
1	C	362/387 (94%)	353 (98%)	6 (2%)	3 (1%)	16	5
1	D	360/387 (93%)	353 (98%)	6 (2%)	1 (0%)	37	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	136/143 (95%)	133 (98%)	3 (2%)	0	100	100
2	F	136/143 (95%)	132 (97%)	4 (3%)	0	100	100
2	G	135/143 (94%)	131 (97%)	4 (3%)	0	100	100
2	H	136/143 (95%)	132 (97%)	2 (2%)	2 (2%)	8	1
All	All	1989/2120 (94%)	1944 (98%)	37 (2%)	8 (0%)	37	16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	283[A]	GLY
1	C	283[B]	GLY
1	B	199	PRO
1	C	199	PRO
2	H	106[A]	ASP
2	H	106[B]	ASP
1	A	199	PRO
1	D	199	PRO

### 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	295/314 (94%)	288 (98%)	7 (2%)	44	24
1	B	291/314 (93%)	287 (99%)	4 (1%)	62	49
1	C	293/314 (93%)	286 (98%)	7 (2%)	44	24
1	D	291/314 (93%)	283 (97%)	8 (3%)	40	19
2	E	111/116 (96%)	109 (98%)	2 (2%)	54	37
2	F	111/116 (96%)	107 (96%)	4 (4%)	30	11
2	G	110/116 (95%)	109 (99%)	1 (1%)	75	65
2	H	111/116 (96%)	109 (98%)	2 (2%)	54	37
All	All	1613/1720 (94%)	1578 (98%)	35 (2%)	47	27

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	ARG
1	A	20	THR
1	A	96	ARG
1	A	306	TRP
1	A	360	LYS
1	A	364	SER
1	B	3	ARG
1	B	4	ARG
1	B	275	LEU
1	B	306	TRP
1	C	3	ARG
1	C	4	ARG
1	C	275	LEU
1	C	306	TRP
1	C	328	SER
1	C	360	LYS
1	C	361	ASP
1	D	3	ARG
1	D	4	ARG
1	D	52	LYS
1	D	275	LEU
1	D	306	TRP
1	D	322	LYS
1	D	327	LYS
1	D	359	ASP
2	E	27	THR
2	E	137	SER
2	F	5	GLN
2	F	27	THR
2	F	56	SER
2	F	137	SER
2	G	27	THR
2	H	27	THR
2	H	137	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
1	B	133	GLN

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Mol	Chain	Res	Type
1	B	213	GLN
1	C	295	ASN
1	D	160	ASN
2	E	86	GLN
2	E	88	ASN
2	F	3	GLN
2	F	129	GLN
2	G	86	GLN
2	G	88	ASN
2	G	132	GLN
2	H	81	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

5 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	$\# Z  > 2$
3	ACT	C	402	-	3,3,3	1.10	0	3,3,3	0.54	0
3	ACT	B	402	-	3,3,3	1.73	1 (33%)	3,3,3	0.76	0
4	GOL	D	401	-	5,5,5	0.27	0	5,5,5	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ACT	C	401	-	3,3,3	1.41	0	3,3,3	0.86	0
3	ACT	B	401	-	3,3,3	1.42	0	3,3,3	1.14	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	GOL	D	401	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	ACT	O-C	2.29	1.32	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	401	GOL	O1-C1-C2-C3
4	D	401	GOL	C1-C2-C3-O3
4	D	401	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	ACT	3	0
3	B	402	ACT	3	0
4	D	401	GOL	2	0
3	C	401	ACT	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	363/387 (93%)	-0.61	3 (0%) 82 86	13, 23, 47, 93	3 (0%)
1	B	358/387 (92%)	-0.43	3 (0%) 82 86	14, 27, 55, 92	4 (1%)
1	C	360/387 (93%)	-0.40	6 (1%) 69 74	13, 26, 58, 103	4 (1%)
1	D	358/387 (92%)	-0.60	1 (0%) 90 93	13, 25, 45, 100	4 (1%)
2	E	137/143 (95%)	-0.26	2 (1%) 71 77	18, 31, 55, 130	1 (0%)
2	F	137/143 (95%)	0.20	5 (3%) 46 53	19, 38, 71, 115	1 (0%)
2	G	137/143 (95%)	0.24	6 (4%) 39 44	29, 39, 73, 114	0
2	H	137/143 (95%)	-0.29	4 (2%) 54 60	16, 29, 58, 135	1 (0%)
All	All	1987/2120 (93%)	-0.38	30 (1%) 71 77	13, 28, 57, 135	18 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	138	HIS	5.3
2	H	2	VAL	4.8
2	E	138	HIS	4.6
2	F	138	HIS	4.4
2	F	2	VAL	4.0
1	C	359	ASP	3.8
2	G	41	PRO	3.4
1	C	55	ALA	3.4
1	B	2	SER	3.3
2	G	138	HIS	3.3
1	D	2	SER	3.1
2	F	27	THR	3.0
2	G	43	LYS	2.7
2	G	2	VAL	2.7
2	E	2	VAL	2.6
1	C	361	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	360	LYS	2.6
2	G	42	GLY	2.6
1	C	2	SER	2.3
2	F	137	SER	2.3
2	G	119	ILE	2.3
2	H	57	GLY	2.3
1	B	55	ALA	2.3
1	A	360	LYS	2.2
1	A	47	THR	2.2
1	B	54	PHE	2.2
2	F	136	SER	2.2
1	A	2	SER	2.1
1	C	56	GLY	2.0
2	H	137	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	ACT	C	401	4/4	0.81	0.18	52,53,54,72	0
3	ACT	B	402	4/4	0.85	0.14	39,47,59,64	0
3	ACT	B	401	4/4	0.85	0.18	46,49,70,71	0
4	GOL	D	401	6/6	0.88	0.13	34,47,60,61	0
3	ACT	C	402	4/4	0.89	0.13	43,54,61,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.