



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 03:32 am BST

PDB ID : 3R0H  
Title : Structure of INAD PDZ45 in complex with NG2 peptide  
Authors : Wei, Z.; Liu, W.; Zhang, M.  
Deposited on : 2011-03-08  
Resolution : 2.60 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

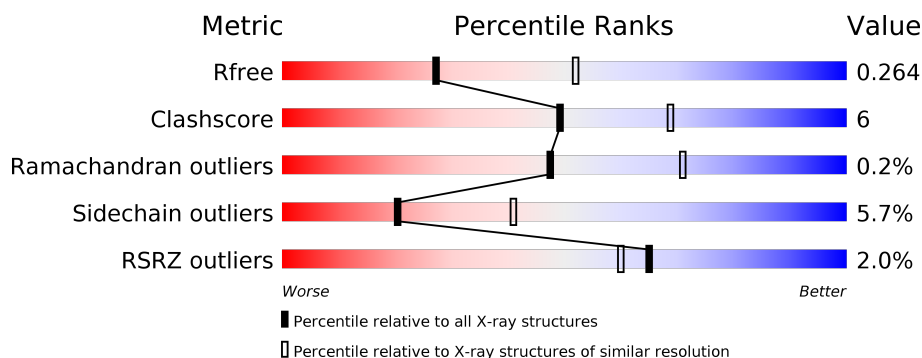
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.



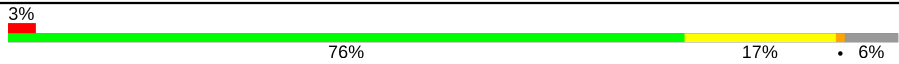


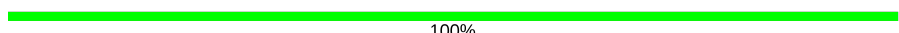


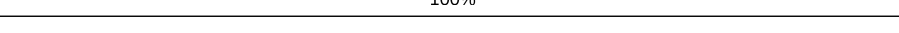
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	206	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	206	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	C	206	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>
1	D	206	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>• •</div> </div> </div>
1	E	206	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>•</div> </div> </div>
1	F	206	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	206	
1	H	206	
2	a	9	
2	b	9	
2	c	9	
2	d	9	
2	e	9	
2	f	9	
2	g	9	
2	h	9	

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	DTT	D	1	-	X	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12877 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 Inactivation-no-after-potential D protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1516	966	257	284	9			
1	B	196	Total	C	N	O	S	0	0	0
			1489	947	252	281	9			
1	C	198	Total	C	N	O	S	0	0	0
			1521	970	259	283	9			
1	D	199	Total	C	N	O	S	0	0	0
			1518	967	258	284	9			
1	E	199	Total	C	N	O	S	0	0	0
			1516	966	258	283	9			
1	F	198	Total	C	N	O	S	0	0	0
			1513	963	257	284	9			
1	G	193	Total	C	N	O	S	0	0	0
			1480	944	253	274	9			
1	H	193	Total	C	N	O	S	0	0	0
			1472	939	251	273	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	GLY	-	EXPRESSION TAG	UNP Q24008
A	470	PRO	-	EXPRESSION TAG	UNP Q24008
A	471	GLY	-	EXPRESSION TAG	UNP Q24008
A	472	SER	-	EXPRESSION TAG	UNP Q24008
B	469	GLY	-	EXPRESSION TAG	UNP Q24008
B	470	PRO	-	EXPRESSION TAG	UNP Q24008
B	471	GLY	-	EXPRESSION TAG	UNP Q24008
B	472	SER	-	EXPRESSION TAG	UNP Q24008
C	469	GLY	-	EXPRESSION TAG	UNP Q24008
C	470	PRO	-	EXPRESSION TAG	UNP Q24008
C	471	GLY	-	EXPRESSION TAG	UNP Q24008
C	472	SER	-	EXPRESSION TAG	UNP Q24008
D	469	GLY	-	EXPRESSION TAG	UNP Q24008

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Chain	Residue	Modelled	Actual	Comment	Reference
D	470	PRO	-	EXPRESSION TAG	UNP Q24008
D	471	GLY	-	EXPRESSION TAG	UNP Q24008
D	472	SER	-	EXPRESSION TAG	UNP Q24008
E	469	GLY	-	EXPRESSION TAG	UNP Q24008
E	470	PRO	-	EXPRESSION TAG	UNP Q24008
E	471	GLY	-	EXPRESSION TAG	UNP Q24008
E	472	SER	-	EXPRESSION TAG	UNP Q24008
F	469	GLY	-	EXPRESSION TAG	UNP Q24008
F	470	PRO	-	EXPRESSION TAG	UNP Q24008
F	471	GLY	-	EXPRESSION TAG	UNP Q24008
F	472	SER	-	EXPRESSION TAG	UNP Q24008
G	469	GLY	-	EXPRESSION TAG	UNP Q24008
G	470	PRO	-	EXPRESSION TAG	UNP Q24008
G	471	GLY	-	EXPRESSION TAG	UNP Q24008
G	472	SER	-	EXPRESSION TAG	UNP Q24008
H	469	GLY	-	EXPRESSION TAG	UNP Q24008
H	470	PRO	-	EXPRESSION TAG	UNP Q24008
H	471	GLY	-	EXPRESSION TAG	UNP Q24008
H	472	SER	-	EXPRESSION TAG	UNP Q24008

- Molecule 2 is a protein called NG2.

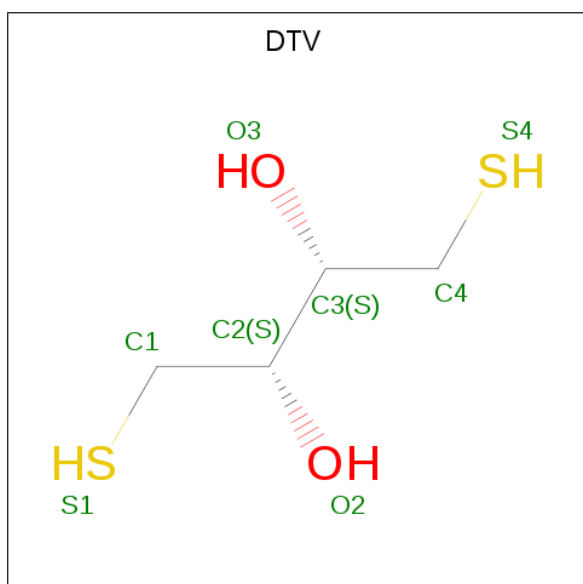
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	a	9	Total	C	N	O	0	0	0
			79	51	15	13			
2	b	9	Total	C	N	O	0	0	0
			79	51	15	13			
2	c	9	Total	C	N	O	0	0	0
			79	51	15	13			
2	d	9	Total	C	N	O	0	0	0
			79	51	15	13			
2	e	9	Total	C	N	O	0	0	0
			79	51	15	13			
2	f	9	Total	C	N	O	0	0	0
			79	51	15	13			
2	g	9	Total	C	N	O	0	0	0
			79	51	15	13			
2	h	9	Total	C	N	O	0	0	0
			79	51	15	13			

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



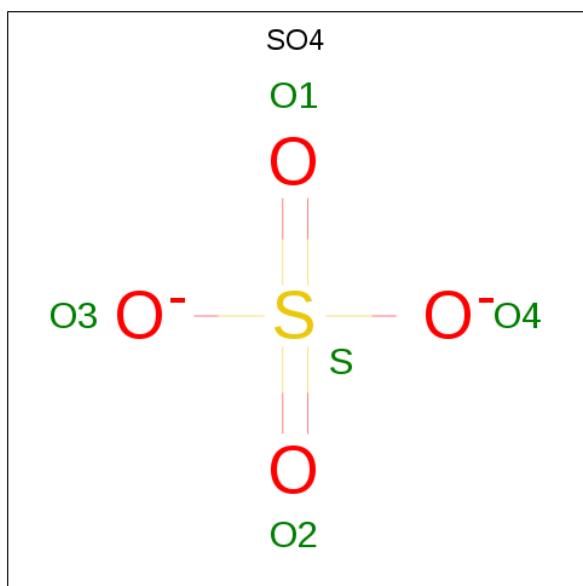
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		
3	B	1	Total	C	O	S	0	0
			8	4	2	2		
3	D	1	Total	C	O	S	0	0
			8	4	2	2		
3	D	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 4 is (2S,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTV) (formula:  $C_4H_{10}O_2S_2$ ).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		
6	a	1	Total	O	0	0
			1	1		
6	B	12	Total	O	0	0
			12	12		
6	b	1	Total	O	0	0
			1	1		

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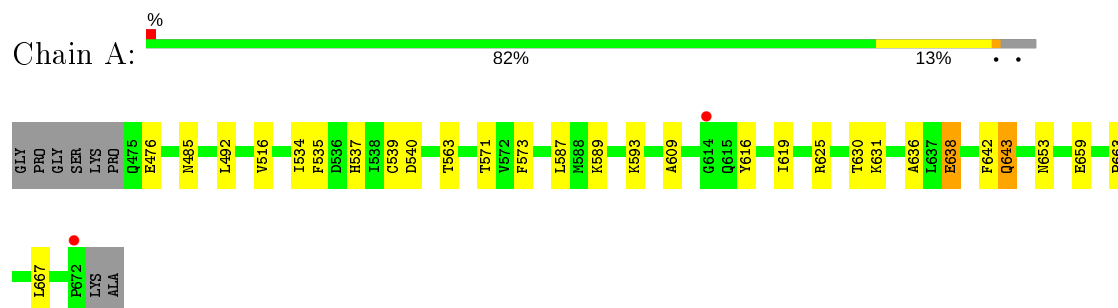
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	31	Total 31	O 31	0	0
6	c	1	Total 1	O 1	0	0
6	D	31	Total 31	O 31	0	0
6	d	2	Total 2	O 2	0	0
6	E	24	Total 24	O 24	0	0
6	e	1	Total 1	O 1	0	0
6	F	11	Total 11	O 11	0	0
6	G	15	Total 15	O 15	0	0
6	g	1	Total 1	O 1	0	0
6	H	13	Total 13	O 13	0	0
6	h	1	Total 1	O 1	0	0



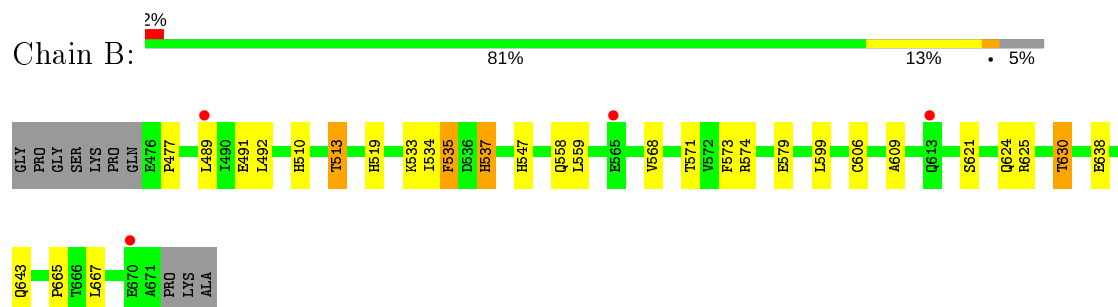
### 3 Residue-property plots [i](#)

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

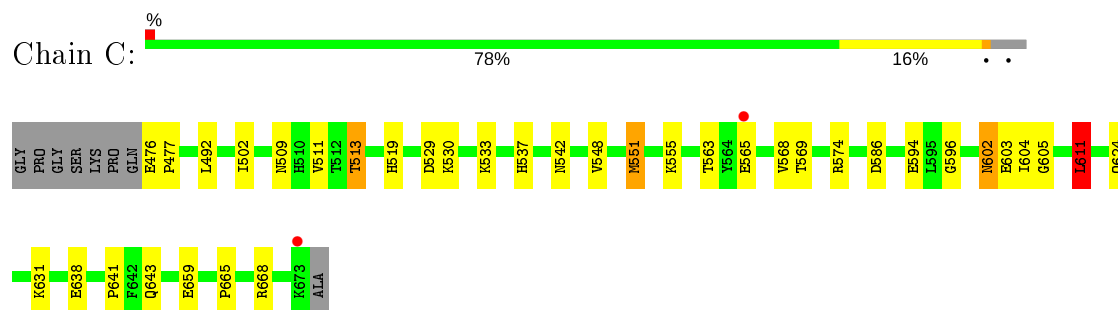
- Molecule 1: Inactivation-no-after-potential D protein



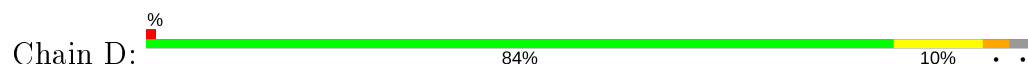
- Molecule 1: Inactivation-no-after-potential D protein

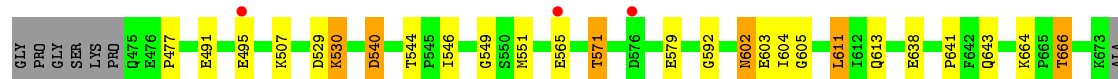


- Molecule 1: Inactivation-no-after-potential D protein

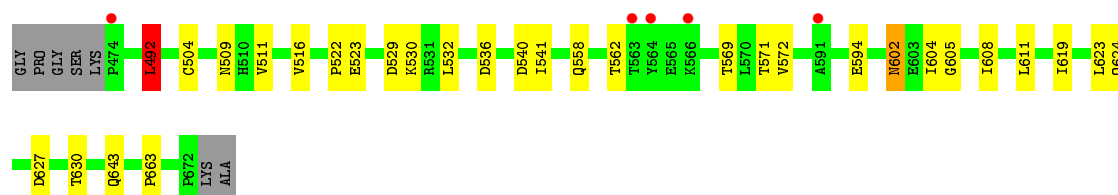
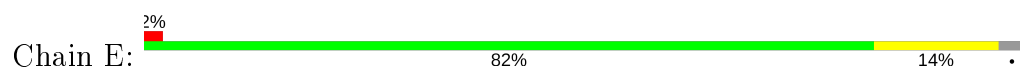


- Molecule 1: Inactivation-no-after-potential D protein

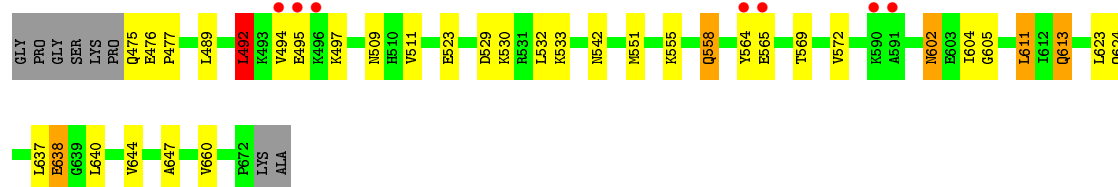
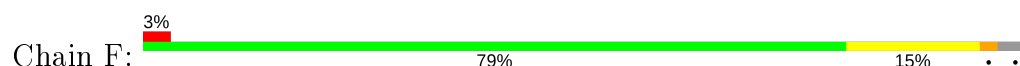




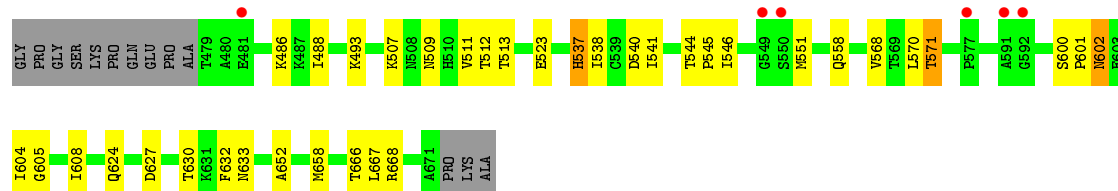
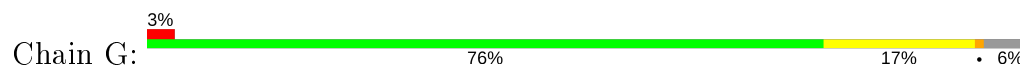
- Molecule 1: Inactivation-no-after-potential D protein



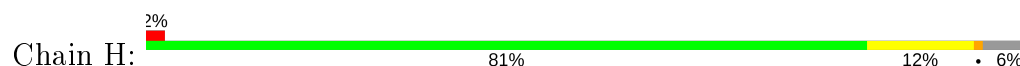
- Molecule 1: Inactivation-no-after-potential D protein



- Molecule 1: Inactivation-no-after-potential D protein



- Molecule 1: Inactivation-no-after-potential D protein



- Molecule 2: NG2



There are no outlier residues recorded for this chain.

- Molecule 2: NG2

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: NG2

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: NG2

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: NG2

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: NG2

Chain f:  100%


There are no outlier residues recorded for this chain.

- Molecule 2: NG2

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: NG2

Chain h:  89% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.08Å 134.99Å 215.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.53 – 2.60 29.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.53-2.60) 99.2 (29.53-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.198 , 0.263 0.203 , 0.264	Depositor DCC
$R_{free}$ test set	3349 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12877	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.93 % 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 7.3967e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DTT, DTV, SO4

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	0.47	0/1545	0.62	0/2092
1	B	0.47	0/1517	0.63	0/2058
1	C	0.51	0/1550	0.67	1/2097 (0.0%)
1	D	0.52	0/1547	0.67	1/2096 (0.0%)
1	E	0.50	0/1546	0.65	2/2096 (0.1%)
1	F	0.47	0/1542	0.63	1/2090 (0.0%)
1	G	0.49	0/1507	0.63	0/2038
1	H	0.47	0/1499	0.63	0/2029
2	a	0.58	0/81	0.68	0/108
2	b	0.51	0/81	0.64	0/108
2	c	0.57	0/81	0.65	0/108
2	d	0.55	0/81	0.62	0/108
2	e	0.56	0/81	0.59	0/108
2	f	0.48	0/81	0.65	0/108
2	g	0.47	0/81	0.59	0/108
2	h	0.48	0/81	0.71	0/108
All	All	0.49	0/12901	0.64	5/17460 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	611	LEU	CA-CB-CG	7.51	132.57	115.30
1	F	492	LEU	CA-CB-CG	6.32	129.83	115.30
1	E	492	LEU	CA-CB-CG	6.12	129.39	115.30
1	C	611	LEU	CA-CB-CG	6.02	129.15	115.30
1	E	611	LEU	CA-CB-CG	5.34	127.58	115.30

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	1516	0	1550	17	0
1	B	1489	0	1503	17	0
1	C	1521	0	1567	26	0
1	D	1518	0	1547	19	0
1	E	1516	0	1544	15	0
1	F	1513	0	1540	21	0
1	G	1480	0	1525	20	0
1	H	1472	0	1508	15	0
2	a	79	0	76	0	0
2	b	79	0	76	0	0
2	c	79	0	76	0	0
2	d	79	0	76	0	0
2	e	79	0	76	0	0
2	f	79	0	76	0	0
2	g	79	0	76	0	0
2	h	79	0	76	0	0
3	A	8	0	10	0	0
3	B	8	0	10	0	0
3	D	16	0	20	6	0
4	B	8	0	10	3	0
5	C	5	0	0	0	0
5	G	10	0	0	0	0
5	H	10	0	0	0	0
6	A	10	0	0	0	0
6	B	12	0	0	1	0
6	C	31	0	0	1	0
6	D	31	0	0	0	0
6	E	24	0	0	0	0
6	F	11	0	0	0	0
6	G	15	0	0	0	0
6	H	13	0	0	1	0
6	a	1	0	0	0	0
6	b	1	0	0	0	0
6	c	1	0	0	0	0
6	d	2	0	0	0	0
6	e	1	0	0	0	0
6	g	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	h	1	0	0	0	0
All	All	12877	0	12942	145	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 6.

All (145) 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:H:537:HIS:HD2	1:H:668:ARG:HH11	1.14	0.91
1:E:602:ASN:HD22	1:E:604:ILE:H	1.18	0.91
1:C:509:ASN:HD21	1:C:624:GLN:HE22	1.21	0.88
1:G:537:HIS:HD2	1:G:668:ARG:HH11	1.21	0.88
1:F:602:ASN:HD22	1:F:604:ILE:H	1.21	0.85
1:C:602:ASN:HD22	1:C:604:ILE:H	1.26	0.82
1:G:509:ASN:HD22	1:G:511:VAL:H	1.31	0.78
1:C:509:ASN:HD22	1:C:511:VAL:H	1.33	0.76
1:H:537:HIS:CD2	1:H:668:ARG:HH11	2.02	0.76
1:H:537:HIS:HD2	1:H:668:ARG:NH1	1.85	0.75
1:G:602:ASN:HD22	1:G:604:ILE:H	1.38	0.71
1:F:602:ASN:ND2	1:F:604:ILE:H	1.89	0.71
1:C:509:ASN:ND2	1:C:624:GLN:HE22	1.87	0.70
1:D:540:ASP:HB3	1:D:571:THR:HG23	1.73	0.69
1:E:492:LEU:HD13	1:E:529:ASP:HB2	1.75	0.69
1:B:510:HIS:H	1:B:624:GLN:HE22	1.40	0.68
1:D:602:ASN:ND2	1:D:605:GLY:H	1.92	0.67
1:G:540:ASP:HB2	1:G:571:THR:HG23	1.77	0.66
1:B:489:LEU:HD23	1:B:571:THR:HG22	1.78	0.65
1:D:540:ASP:HB3	1:D:571:THR:CG2	2.27	0.65
1:D:546:ILE:HG23	1:D:551:MET:CE	2.27	0.65
1:D:643:GLN:HB2	3:D:1:DTT:S1	2.37	0.65
1:D:641:PRO:HB3	3:D:1:DTT:H2	1.78	0.65
1:E:602:ASN:ND2	1:E:604:ILE:H	1.90	0.64
1:E:509:ASN:HD22	1:E:511:VAL:H	1.45	0.64
1:B:513:THR:OG1	1:B:665:PRO:O	2.10	0.64
1:H:579:GLU:OE2	1:H:666:THR:HG23	1.98	0.64
1:H:631:LYS:HB3	1:H:659:GLU:HB2	1.79	0.63
1:F:489:LEU:HD11	1:F:569:THR:HG23	1.80	0.62
1:A:643:GLN:OE1	1:D:643:GLN:HG3	2.01	0.61
1:B:643:GLN:N	4:B:2:DTV:S4	2.72	0.61
1:D:602:ASN:HD22	1:D:604:ILE:H	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:THR:H	1:E:643:GLN:HE22	1.49	0.60
1:F:623:LEU:HD21	1:F:660:VAL:HG21	1.82	0.60
1:C:602:ASN:ND2	1:C:604:ILE:H	1.98	0.60
1:D:602:ASN:HD21	1:D:605:GLY:H	1.49	0.60
1:A:563:THR:H	1:E:643:GLN:NE2	2.00	0.60
1:C:602:ASN:HD22	1:C:604:ILE:N	1.99	0.59
1:C:641:PRO:HB3	3:D:1:DTT:H3	1.84	0.59
1:H:563:THR:HG23	1:H:564:TYR:H	1.68	0.59
1:C:537:HIS:HD2	1:C:668:ARG:HH11	1.50	0.59
1:A:609:ALA:O	1:A:625:ARG:NH1	2.36	0.57
1:H:513:THR:OG1	1:H:665:PRO:O	2.22	0.57
1:G:509:ASN:ND2	1:G:511:VAL:H	2.02	0.57
1:D:546:ILE:HG23	1:D:551:MET:HE3	1.88	0.56
1:D:529:ASP:O	1:D:530:LYS:HB2	2.04	0.56
1:H:538:ILE:HG22	1:H:546:ILE:HD12	1.87	0.56
1:D:507:LYS:HG2	1:D:549:GLY:O	2.06	0.56
1:F:542:ASN:HA	1:F:569:THR:HB	1.87	0.55
1:C:513:THR:OG1	1:C:665:PRO:O	2.18	0.55
1:A:631:LYS:HB3	1:A:659:GLU:HB2	1.89	0.55
1:A:616:TYR:HB2	1:A:619:ILE:HD12	1.88	0.54
1:C:603:GLU:O	1:C:638:GLU:HB2	2.06	0.54
1:E:509:ASN:HD21	1:E:624:GLN:HE22	1.55	0.54
1:A:642:PHE:HB3	4:B:2:DTV:H1C1	1.89	0.54
1:C:602:ASN:ND2	1:C:605:GLY:H	2.06	0.53
1:B:547:HIS:CE1	1:B:667:LEU:HD11	2.43	0.53
1:H:631:LYS:CB	1:H:659:GLU:HB2	2.38	0.53
1:C:537:HIS:CD2	1:C:668:ARG:HH11	2.26	0.52
1:C:509:ASN:ND2	1:C:511:VAL:H	2.03	0.52
1:D:546:ILE:HA	1:D:551:MET:HE1	1.92	0.52
1:G:486:LYS:O	1:G:488:ILE:HG12	2.09	0.52
1:E:504:CYS:SG	1:E:663:PRO:HG2	2.50	0.52
1:E:540:ASP:HB3	1:E:571:THR:HB	1.91	0.51
1:F:494:VAL:HG11	1:F:564:TYR:HB2	1.93	0.51
1:B:579:GLU:OE1	1:B:665:PRO:HA	2.11	0.51
1:A:516:VAL:HG11	1:A:663:PRO:HB3	1.93	0.51
1:D:643:GLN:N	3:D:1:DTT:S1	2.75	0.51
1:G:608:ILE:HD12	1:G:627:ASP:HB2	1.93	0.51
1:D:603:GLU:O	1:D:638:GLU:HB2	2.11	0.51
1:B:534:ILE:O	1:B:535:PHE:HB2	2.11	0.50
1:E:532:LEU:HD21	1:E:572:VAL:HG21	1.92	0.50
1:F:558:GLN:HA	1:F:558:GLN:NE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:537:HIS:HD2	1:G:668:ARG:NH1	2.01	0.50
1:A:485:ASN:HA	1:A:573:PHE:CE2	2.47	0.50
1:C:537:HIS:HD2	1:C:668:ARG:HD2	1.77	0.49
1:C:643:GLN:HB2	3:D:1:DTT:S4	2.53	0.49
1:D:579:GLU:OE2	1:D:666:THR:HG23	2.13	0.49
1:B:533:LYS:HG2	1:B:574:ARG:NH2	2.28	0.48
1:D:477:PRO:HB2	1:D:491:GLU:HB2	1.96	0.48
1:G:568:VAL:HG12	1:G:570:LEU:HG	1.95	0.48
1:E:516:VAL:HG13	1:E:536:ASP:O	2.14	0.48
1:E:619:ILE:HG12	1:E:623:LEU:HD12	1.96	0.48
1:A:643:GLN:HB2	4:B:2:DTV:S1	2.53	0.48
1:F:509:ASN:ND2	1:F:624:GLN:OE1	2.46	0.48
1:C:631:LYS:HB3	1:C:659:GLU:HB2	1.96	0.47
1:B:491:GLU:HA	1:B:568:VAL:O	2.15	0.47
1:F:602:ASN:ND2	1:F:605:GLY:H	2.13	0.47
1:B:559:LEU:HD23	1:F:644:VAL:HG21	1.97	0.47
1:B:558:GLN:HG2	1:F:647:ALA:HB3	1.98	0.46
1:F:611:LEU:HD21	1:F:613:GLN:HE21	1.80	0.46
1:G:509:ASN:HD21	1:G:624:GLN:HE22	1.62	0.46
1:B:537:HIS:HB3	1:B:573:PHE:HB3	1.97	0.46
1:H:611:LEU:HD21	1:H:624:GLN:HA	1.96	0.46
1:A:485:ASN:HA	1:A:573:PHE:CZ	2.51	0.46
1:C:596:GLY:O	1:C:611:LEU:HA	2.15	0.46
1:E:602:ASN:ND2	1:E:605:GLY:H	2.14	0.45
1:G:537:HIS:CD2	1:G:668:ARG:HH11	2.13	0.45
1:E:608:ILE:HD12	1:E:627:ASP:HB2	1.97	0.45
1:E:529:ASP:O	1:E:530:LYS:HB2	2.16	0.45
1:F:492:LEU:HD13	1:F:529:ASP:HB2	1.98	0.45
1:A:636:ALA:HB1	1:A:638:GLU:OE2	2.15	0.45
1:B:510:HIS:H	1:B:624:GLN:NE2	2.10	0.45
1:H:581:GLU:HB2	1:H:664:LYS:HD2	1.98	0.45
1:A:653:ASN:HD22	1:D:592:GLY:HA2	1.82	0.45
3:D:1:DTT:H12	3:D:1:DTT:H41	1.34	0.45
1:C:533:LYS:HB2	1:C:574:ARG:HH21	1.82	0.44
1:C:542:ASN:HA	1:C:569:THR:CG2	2.47	0.44
1:G:540:ASP:OD1	1:G:545:PRO:HA	2.18	0.44
1:H:534:ILE:HD11	6:H:69:HOH:O	2.18	0.44
1:F:602:ASN:C	1:F:602:ASN:HD22	2.20	0.44
1:B:519:HIS:HA	1:B:534:ILE:HD11	1.99	0.43
1:H:565:GLU:N	1:H:565:GLU:OE1	2.38	0.43
1:F:509:ASN:HD22	1:F:511:VAL:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:602:ASN:ND2	1:G:605:GLY:H	2.16	0.43
1:C:529:ASP:O	1:C:530:LYS:HB2	2.18	0.43
1:B:609:ALA:O	1:B:625:ARG:NH1	2.52	0.43
1:B:599:LEU:HB3	1:B:606:CYS:HB3	2.01	0.43
1:H:534:ILE:O	1:H:535:PHE:HB2	2.19	0.43
1:G:509:ASN:HD22	1:G:511:VAL:N	2.07	0.42
1:A:539:CYS:HB2	1:A:571:THR:OG1	2.19	0.42
1:A:534:ILE:O	1:A:535:PHE:HB2	2.19	0.42
1:D:495:GLU:HA	1:D:565:GLU:O	2.19	0.42
1:A:540:ASP:HB3	1:A:571:THR:HG23	2.01	0.42
1:F:476:GLU:HA	1:F:477:PRO:HD2	1.89	0.42
1:G:632:PHE:HD1	1:G:658:MET:HG2	1.85	0.41
1:G:633:ASN:ND2	1:G:652:ALA:HB1	2.35	0.41
1:B:630:THR:O	6:B:65:HOH:O	2.22	0.41
1:C:509:ASN:HD22	1:C:511:VAL:N	2.11	0.41
1:F:638:GLU:HG3	1:F:638:GLU:H	1.66	0.41
1:G:540:ASP:HB2	1:G:571:THR:CG2	2.47	0.41
1:C:551:MET:HB3	1:C:555:LYS:HD3	2.03	0.41
1:C:542:ASN:HA	1:C:569:THR:HG23	2.01	0.41
1:F:495:GLU:O	1:F:497:LYS:HG3	2.20	0.41
1:A:589:LYS:HE3	1:A:593:LYS:O	2.20	0.41
1:F:532:LEU:HD21	1:F:572:VAL:HG21	2.02	0.41
1:C:502:ILE:HD12	1:C:519:HIS:HB3	2.02	0.41
1:F:637:LEU:HA	1:F:640:LEU:HD12	2.02	0.40
1:G:602:ASN:ND2	1:G:604:ILE:H	2.12	0.40
1:C:594:GLU:HG2	6:C:29:HOH:O	2.20	0.40
1:G:538:ILE:HG22	1:G:546:ILE:HD12	2.02	0.40
1:G:600:SER:HA	1:G:601:PRO:HD2	2.00	0.40
1:C:476:GLU:N	1:C:477:PRO:HD2	2.37	0.40
1:H:638:GLU:H	1:H:638:GLU:HG3	1.53	0.40
1:F:529:ASP:O	1:F:530:LYS:HB2	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	196/206 (95%)	191 (97%)	5 (3%)	0	100	100
1	B	194/206 (94%)	186 (96%)	6 (3%)	2 (1%)	15	32
1	C	196/206 (95%)	186 (95%)	10 (5%)	0	100	100
1	D	197/206 (96%)	190 (96%)	7 (4%)	0	100	100
1	E	197/206 (96%)	185 (94%)	11 (6%)	1 (0%)	29	52
1	F	196/206 (95%)	187 (95%)	8 (4%)	1 (0%)	29	52
1	G	191/206 (93%)	182 (95%)	9 (5%)	0	100	100
1	H	191/206 (93%)	186 (97%)	5 (3%)	0	100	100
2	a	7/9 (78%)	7 (100%)	0	0	100	100
2	b	7/9 (78%)	7 (100%)	0	0	100	100
2	c	7/9 (78%)	7 (100%)	0	0	100	100
2	d	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	e	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	f	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	g	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	h	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1614/1720 (94%)	1544 (96%)	66 (4%)	4 (0%)	47	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	565	GLU
1	B	535	PHE
1	B	477	PRO
1	E	522	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	167/175 (95%)	159 (95%)	8 (5%)	25	49
1	B	163/175 (93%)	157 (96%)	6 (4%)	34	60
1	C	169/175 (97%)	159 (94%)	10 (6%)	19	39
1	D	167/175 (95%)	158 (95%)	9 (5%)	22	44
1	E	167/175 (95%)	158 (95%)	9 (5%)	22	44
1	F	167/175 (95%)	156 (93%)	11 (7%)	16	33
1	G	164/175 (94%)	149 (91%)	15 (9%)	9	18
1	H	162/175 (93%)	152 (94%)	10 (6%)	18	37
2	a	7/7 (100%)	7 (100%)	0	100	100
2	b	7/7 (100%)	7 (100%)	0	100	100
2	c	7/7 (100%)	7 (100%)	0	100	100
2	d	7/7 (100%)	7 (100%)	0	100	100
2	e	7/7 (100%)	7 (100%)	0	100	100
2	f	7/7 (100%)	7 (100%)	0	100	100
2	g	7/7 (100%)	7 (100%)	0	100	100
2	h	7/7 (100%)	6 (86%)	1 (14%)	3	5
All	All	1382/1456 (95%)	1303 (94%)	79 (6%)	20	41

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	476	GLU
1	A	492	LEU
1	A	537	HIS
1	A	587	LEU
1	A	630	THR
1	A	638	GLU
1	A	643	GLN
1	A	667	LEU
1	B	492	LEU
1	B	513	THR
1	B	537	HIS
1	B	621	SER
1	B	630	THR
1	B	638	GLU
1	C	492	LEU
1	C	513	THR

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Mol	Chain	Res	Type
1	C	548	VAL
1	C	551	MET
1	C	563	THR
1	C	565	GLU
1	C	568	VAL
1	C	586	ASP
1	C	602	ASN
1	C	611	LEU
1	D	530	LYS
1	D	540	ASP
1	D	544	THR
1	D	571	THR
1	D	602	ASN
1	D	611	LEU
1	D	613	GLN
1	D	664	LYS
1	D	666	THR
1	E	492	LEU
1	E	523	GLU
1	E	541	ILE
1	E	558	GLN
1	E	562	THR
1	E	569	THR
1	E	594	GLU
1	E	602	ASN
1	E	630	THR
1	F	475	GLN
1	F	492	LEU
1	F	523	GLU
1	F	533	LYS
1	F	551	MET
1	F	555	LYS
1	F	558	GLN
1	F	602	ASN
1	F	611	LEU
1	F	613	GLN
1	F	638	GLU
1	G	493	LYS
1	G	507	LYS
1	G	512	THR
1	G	513	THR
1	G	523	GLU

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Mol	Chain	Res	Type
1	G	537	HIS
1	G	541	ILE
1	G	544	THR
1	G	551	MET
1	G	558	GLN
1	G	571	THR
1	G	602	ASN
1	G	630	THR
1	G	666	THR
1	G	667	LEU
1	H	486	LYS
1	H	499	MET
1	H	513	THR
1	H	533	LYS
1	H	537	HIS
1	H	544	THR
1	H	550	SER
1	H	589	LYS
1	H	638	GLU
1	H	667	LEU
2	h	4	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	557	HIS
1	A	561	HIS
1	B	509	ASN
1	B	561	HIS
1	B	624	GLN
1	B	643	GLN
1	C	509	ASN
1	C	537	HIS
1	C	602	ASN
1	C	613	GLN
1	C	653	ASN
1	D	602	ASN
1	E	509	ASN
1	E	519	HIS
1	E	557	HIS
1	E	558	GLN
1	E	561	HIS

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Mol	Chain	Res	Type
1	E	602	ASN
1	E	643	GLN
1	E	653	ASN
1	F	509	ASN
1	F	558	GLN
1	F	602	ASN
1	F	613	GLN
1	F	624	GLN
1	G	509	ASN
1	G	519	HIS
1	G	537	HIS
1	G	558	GLN
1	G	584	ASN
1	G	602	ASN
1	G	613	GLN
1	H	525	GLN
1	H	537	HIS
1	H	558	GLN
1	H	643	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 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	DTT	B	3	-	7,7,7	0.60	0	4,8,8	1.88	1 (25%)
5	SO4	G	3	-	4,4,4	0.28	0	6,6,6	0.46	0
3	DTT	D	4	-	7,7,7	0.79	0	4,8,8	1.37	1 (25%)
4	DTV	B	2	-	7,7,7	0.48	0	4,8,8	1.79	1 (25%)
3	DTT	D	1	-	7,7,7	0.40	0	4,8,8	2.35	2 (50%)
5	SO4	C	5	-	4,4,4	0.48	0	6,6,6	0.41	0
5	SO4	H	4	-	4,4,4	0.19	0	6,6,6	0.47	0
5	SO4	G	2	-	4,4,4	0.31	0	6,6,6	0.51	0
3	DTT	A	5	-	7,7,7	0.79	0	4,8,8	1.23	1 (25%)
5	SO4	H	1	-	4,4,4	0.36	0	6,6,6	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTT	B	3	-	-	4/8/8/8	-
3	DTT	D	4	-	-	2/8/8/8	-
4	DTV	B	2	-	-	7/8/8/8	-
3	DTT	D	1	-	-	8/8/8/8	-
3	DTT	A	5	-	-	2/8/8/8	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	DTT	C3-C4-S4	-3.25	105.03	114.47
3	B	3	DTT	C3-C4-S4	-3.07	105.53	114.47
4	B	2	DTV	C3-C4-S4	-2.49	107.22	114.47
3	D	1	DTT	C2-C1-S1	-2.22	108.00	114.47
3	A	5	DTT	C2-C1-S1	-2.17	108.16	114.47
3	D	4	DTT	C2-C1-S1	-2.01	108.64	114.47

There are no chirality outliers.

All (23) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	B	3	DTT	C1-C2-C3-O3
3	B	3	DTT	C1-C2-C3-C4
3	B	3	DTT	O2-C2-C3-C4
3	D	4	DTT	C1-C2-C3-C4
3	D	4	DTT	O2-C2-C3-O3
4	B	2	DTV	S1-C1-C2-C3
4	B	2	DTV	C1-C2-C3-O3
4	B	2	DTV	C1-C2-C3-C4
4	B	2	DTV	O2-C2-C3-O3
4	B	2	DTV	O2-C2-C3-C4
4	B	2	DTV	C2-C3-C4-S4
4	B	2	DTV	O3-C3-C4-S4
3	D	1	DTT	S1-C1-C2-O2
3	D	1	DTT	S1-C1-C2-C3
3	D	1	DTT	C1-C2-C3-O3
3	D	1	DTT	C1-C2-C3-C4
3	D	1	DTT	O2-C2-C3-O3
3	D	1	DTT	O2-C2-C3-C4
3	D	1	DTT	C2-C3-C4-S4
3	D	1	DTT	O3-C3-C4-S4
3	A	5	DTT	C1-C2-C3-C4
3	B	3	DTT	O2-C2-C3-O3
3	A	5	DTT	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2	DTV	3	0
3	D	1	DTT	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, 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	198/206 (96%)	-0.14	2 (1%) 82 80	30, 55, 83, 92	0
1	B	196/206 (95%)	-0.17	4 (2%) 65 60	30, 54, 75, 88	0
1	C	198/206 (96%)	-0.25	2 (1%) 82 80	20, 41, 72, 93	0
1	D	199/206 (96%)	-0.22	3 (1%) 73 70	21, 40, 74, 94	0
1	E	199/206 (96%)	-0.17	5 (2%) 57 51	30, 45, 78, 93	0
1	F	198/206 (96%)	-0.14	7 (3%) 44 36	32, 51, 81, 97	0
1	G	193/206 (93%)	0.04	6 (3%) 49 42	25, 50, 72, 84	0
1	H	193/206 (93%)	-0.09	4 (2%) 63 58	30, 49, 74, 84	0
2	a	9/9 (100%)	-0.34	0 100 100	36, 42, 51, 54	0
2	b	9/9 (100%)	-0.24	0 100 100	35, 43, 49, 51	0
2	c	9/9 (100%)	-0.39	0 100 100	32, 38, 46, 50	0
2	d	9/9 (100%)	-0.35	0 100 100	36, 41, 50, 56	0
2	e	9/9 (100%)	-0.40	0 100 100	35, 40, 50, 51	0
2	f	9/9 (100%)	-0.34	0 100 100	36, 42, 48, 51	0
2	g	9/9 (100%)	-0.34	0 100 100	33, 38, 49, 64	0
2	h	9/9 (100%)	-0.08	0 100 100	38, 43, 55, 65	0
All	All	1646/1720 (95%)	-0.15	33 (2%) 65 60	20, 48, 77, 97	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	591	ALA	4.5
1	A	672	PRO	3.6
1	F	565	GLU	3.5
1	H	591	ALA	3.4
1	E	564	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	591	ALA	3.1
1	F	564	TYR	3.0
1	H	481	GLU	2.9
1	G	577	PRO	2.7
1	F	495	GLU	2.7
1	H	550	SER	2.7
1	E	474	PRO	2.6
1	F	494	VAL	2.5
1	F	590	LYS	2.5
1	D	565	GLU	2.4
1	F	496	LYS	2.4
1	C	673	LYS	2.4
1	G	481	GLU	2.4
1	A	614	GLY	2.3
1	C	565	GLU	2.3
1	H	592	GLY	2.3
1	E	566	LYS	2.3
1	G	549	GLY	2.2
1	B	489	LEU	2.2
1	E	591	ALA	2.2
1	E	563	THR	2.2
1	B	613	GLN	2.2
1	G	550	SER	2.1
1	G	592	GLY	2.1
1	B	670	GLU	2.1
1	D	495	GLU	2.0
1	B	565	GLU	2.0
1	D	576	ASP	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 carbohydrates 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(Å <sup>2</sup> )	Q<0.9
5	SO4	C	5	5/5	0.82	0.30	46,51,54,72	0
3	DTT	B	3	8/8	0.87	0.27	47,48,51,56	0
3	DTT	D	4	8/8	0.89	0.25	53,57,58,60	0
4	DTV	B	2	8/8	0.90	0.30	36,43,53,62	0
3	DTT	A	5	8/8	0.92	0.18	48,51,56,62	0
3	DTT	D	1	8/8	0.93	0.22	32,42,48,51	0
5	SO4	H	1	5/5	0.93	0.21	36,42,51,55	0
5	SO4	G	2	5/5	0.95	0.15	50,51,61,62	0
5	SO4	H	4	5/5	0.97	0.12	38,39,45,47	0
5	SO4	G	3	5/5	0.97	0.09	28,33,38,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.