



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2021 – 04:07 PM EDT

PDB ID : 6U6Z  
Title : Human SAMHD1 bound to deoxyribo(TG\*TTCA)-oligonucleotide  
Authors : Taylor, A.B.; Yu, C.H.; Ivanov, D.N.  
Deposited on : 2019-08-30  
Resolution : 2.10 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:

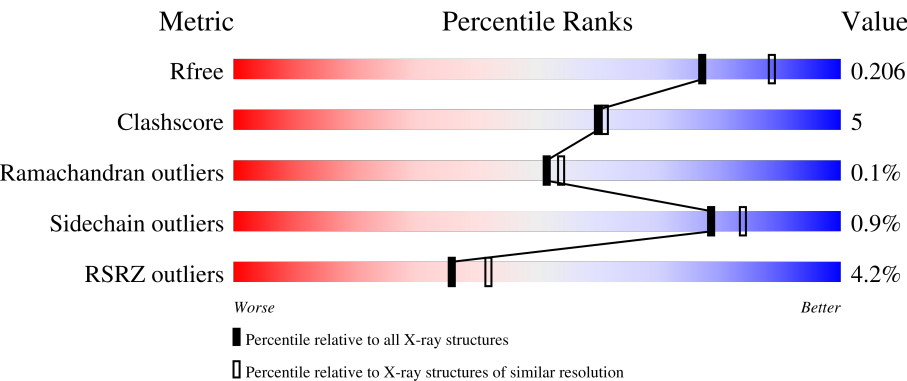
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

# 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 2.10 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 <sub>free</sub>	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	535	<div><div>%</div><div><div></div><div>75%</div><div>8%</div><div>17%</div></div></div>
1	B	535	<div><div>7%</div><div><div></div><div>69%</div><div>10%</div><div>20%</div></div></div>
1	C	535	<div><div>%</div><div><div></div><div>72%</div><div>10%</div><div>18%</div></div></div>
1	D	535	<div><div>4%</div><div><div></div><div>71%</div><div>7%</div><div>21%</div></div></div>
2	E	6	<div><div></div><div><div>17%</div><div>33%</div><div>17%</div><div>33%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	6	<div><div></div><div></div><div></div><div></div></div> <div>17%33%17%33%</div>
2	G	6	<div><div></div><div></div><div></div><div></div></div> <div>17%33%17%33%</div>
2	H	6	<div><div></div><div></div><div></div><div></div></div> <div>17%50%33%</div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14600 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 Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3613	2315	629	651	18			
1	B	429	Total	C	N	O	S	0	0	0
			3499	2243	605	633	18			
1	C	438	Total	C	N	O	S	0	0	0
			3577	2290	624	645	18			
1	D	420	Total	C	N	O	S	0	0	0
			3429	2198	595	619	17			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	MET	-	initiating methionine	UNP Q9Y3Z3
A	93	TRP	-	expression tag	UNP Q9Y3Z3
A	94	SER	-	expression tag	UNP Q9Y3Z3
A	95	HIS	-	expression tag	UNP Q9Y3Z3
A	96	PRO	-	expression tag	UNP Q9Y3Z3
A	97	GLN	-	expression tag	UNP Q9Y3Z3
A	98	PHE	-	expression tag	UNP Q9Y3Z3
A	99	GLU	-	expression tag	UNP Q9Y3Z3
A	100	LYS	-	expression tag	UNP Q9Y3Z3
A	101	GLY	-	expression tag	UNP Q9Y3Z3
A	102	SER	-	expression tag	UNP Q9Y3Z3
A	103	GLY	-	expression tag	UNP Q9Y3Z3
A	104	SER	-	expression tag	UNP Q9Y3Z3
A	105	GLU	-	expression tag	UNP Q9Y3Z3
A	106	ASN	-	expression tag	UNP Q9Y3Z3
A	107	LEU	-	expression tag	UNP Q9Y3Z3
A	108	TYR	-	expression tag	UNP Q9Y3Z3
A	109	PHE	-	expression tag	UNP Q9Y3Z3
A	110	GLN	-	expression tag	UNP Q9Y3Z3
A	111	GLY	-	expression tag	UNP Q9Y3Z3
A	112	GLY	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLY	-	expression tag	UNP Q9Y3Z3
A	114	GLY	-	expression tag	UNP Q9Y3Z3
A	115	GLY	-	expression tag	UNP Q9Y3Z3
B	92	MET	-	initiating methionine	UNP Q9Y3Z3
B	93	TRP	-	expression tag	UNP Q9Y3Z3
B	94	SER	-	expression tag	UNP Q9Y3Z3
B	95	HIS	-	expression tag	UNP Q9Y3Z3
B	96	PRO	-	expression tag	UNP Q9Y3Z3
B	97	GLN	-	expression tag	UNP Q9Y3Z3
B	98	PHE	-	expression tag	UNP Q9Y3Z3
B	99	GLU	-	expression tag	UNP Q9Y3Z3
B	100	LYS	-	expression tag	UNP Q9Y3Z3
B	101	GLY	-	expression tag	UNP Q9Y3Z3
B	102	SER	-	expression tag	UNP Q9Y3Z3
B	103	GLY	-	expression tag	UNP Q9Y3Z3
B	104	SER	-	expression tag	UNP Q9Y3Z3
B	105	GLU	-	expression tag	UNP Q9Y3Z3
B	106	ASN	-	expression tag	UNP Q9Y3Z3
B	107	LEU	-	expression tag	UNP Q9Y3Z3
B	108	TYR	-	expression tag	UNP Q9Y3Z3
B	109	PHE	-	expression tag	UNP Q9Y3Z3
B	110	GLN	-	expression tag	UNP Q9Y3Z3
B	111	GLY	-	expression tag	UNP Q9Y3Z3
B	112	GLY	-	expression tag	UNP Q9Y3Z3
B	113	GLY	-	expression tag	UNP Q9Y3Z3
B	114	GLY	-	expression tag	UNP Q9Y3Z3
B	115	GLY	-	expression tag	UNP Q9Y3Z3
C	92	MET	-	initiating methionine	UNP Q9Y3Z3
C	93	TRP	-	expression tag	UNP Q9Y3Z3
C	94	SER	-	expression tag	UNP Q9Y3Z3
C	95	HIS	-	expression tag	UNP Q9Y3Z3
C	96	PRO	-	expression tag	UNP Q9Y3Z3
C	97	GLN	-	expression tag	UNP Q9Y3Z3
C	98	PHE	-	expression tag	UNP Q9Y3Z3
C	99	GLU	-	expression tag	UNP Q9Y3Z3
C	100	LYS	-	expression tag	UNP Q9Y3Z3
C	101	GLY	-	expression tag	UNP Q9Y3Z3
C	102	SER	-	expression tag	UNP Q9Y3Z3
C	103	GLY	-	expression tag	UNP Q9Y3Z3
C	104	SER	-	expression tag	UNP Q9Y3Z3
C	105	GLU	-	expression tag	UNP Q9Y3Z3
C	106	ASN	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	107	LEU	-	expression tag	UNP Q9Y3Z3
C	108	TYR	-	expression tag	UNP Q9Y3Z3
C	109	PHE	-	expression tag	UNP Q9Y3Z3
C	110	GLN	-	expression tag	UNP Q9Y3Z3
C	111	GLY	-	expression tag	UNP Q9Y3Z3
C	112	GLY	-	expression tag	UNP Q9Y3Z3
C	113	GLY	-	expression tag	UNP Q9Y3Z3
C	114	GLY	-	expression tag	UNP Q9Y3Z3
C	115	GLY	-	expression tag	UNP Q9Y3Z3
D	92	MET	-	initiating methionine	UNP Q9Y3Z3
D	93	TRP	-	expression tag	UNP Q9Y3Z3
D	94	SER	-	expression tag	UNP Q9Y3Z3
D	95	HIS	-	expression tag	UNP Q9Y3Z3
D	96	PRO	-	expression tag	UNP Q9Y3Z3
D	97	GLN	-	expression tag	UNP Q9Y3Z3
D	98	PHE	-	expression tag	UNP Q9Y3Z3
D	99	GLU	-	expression tag	UNP Q9Y3Z3
D	100	LYS	-	expression tag	UNP Q9Y3Z3
D	101	GLY	-	expression tag	UNP Q9Y3Z3
D	102	SER	-	expression tag	UNP Q9Y3Z3
D	103	GLY	-	expression tag	UNP Q9Y3Z3
D	104	SER	-	expression tag	UNP Q9Y3Z3
D	105	GLU	-	expression tag	UNP Q9Y3Z3
D	106	ASN	-	expression tag	UNP Q9Y3Z3
D	107	LEU	-	expression tag	UNP Q9Y3Z3
D	108	TYR	-	expression tag	UNP Q9Y3Z3
D	109	PHE	-	expression tag	UNP Q9Y3Z3
D	110	GLN	-	expression tag	UNP Q9Y3Z3
D	111	GLY	-	expression tag	UNP Q9Y3Z3
D	112	GLY	-	expression tag	UNP Q9Y3Z3
D	113	GLY	-	expression tag	UNP Q9Y3Z3
D	114	GLY	-	expression tag	UNP Q9Y3Z3
D	115	GLY	-	expression tag	UNP Q9Y3Z3

- Molecule 2 is a DNA chain called DNA polymer TG(PST)TCA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	P	S	0	0	1
			47	20	7	16	3	1			
2	F	4	Total	C	N	O	P	S	0	0	1
			47	20	7	16	3	1			
2	H	4	Total	C	N	O	P	S	0	0	1
			38	15	5	14	3	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	P	S	0	0	0
			52	24	7	17	3	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

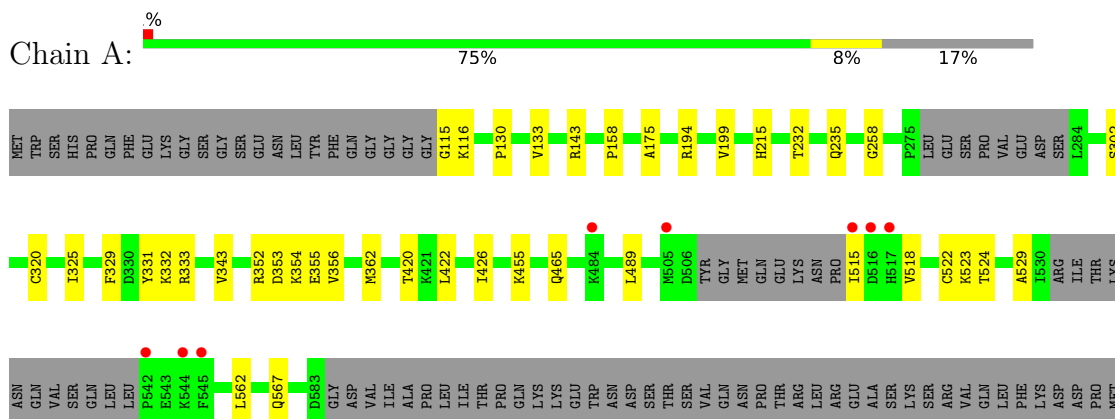
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total	O	0	0
			89	89		
4	B	52	Total	O	0	0
			52	52		
4	C	93	Total	O	0	0
			93	93		
4	D	56	Total	O	0	0
			56	56		
4	E	1	Total	O	0	0
			1	1		
4	F	1	Total	O	0	0
			1	1		
4	H	1	Total	O	0	0
			1	1		
4	G	1	Total	O	0	0
			1	1		

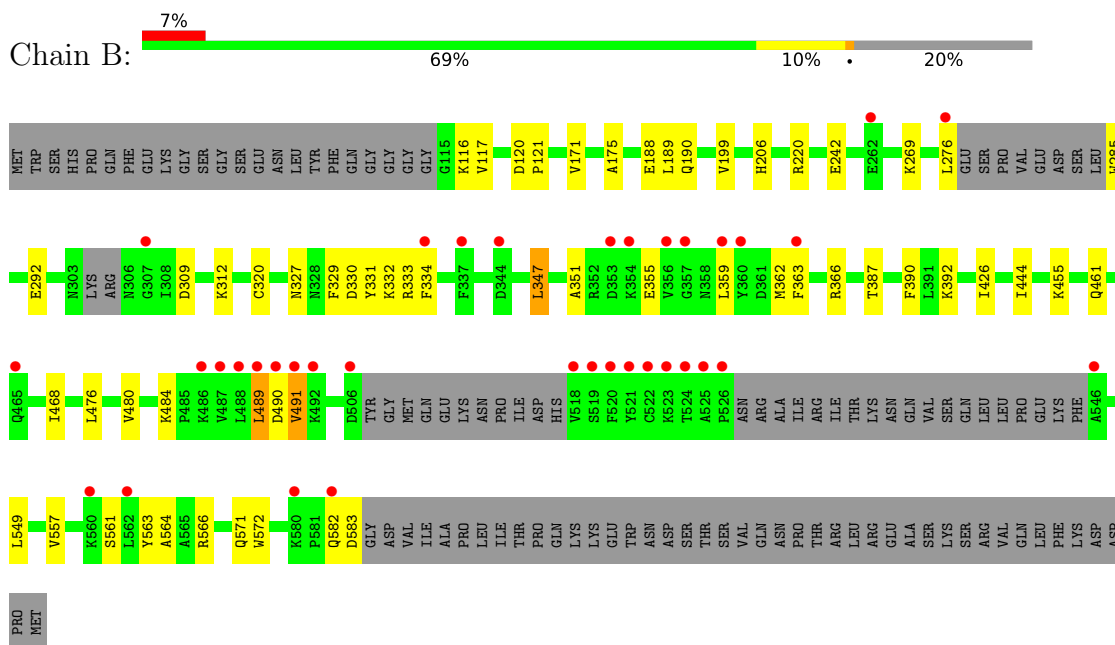
### 3 Residue-property plots [i](#)

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: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



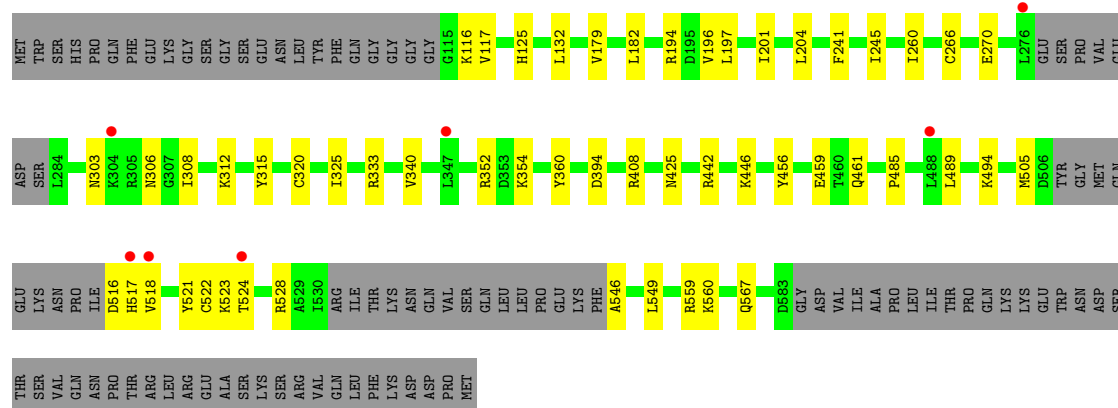
#### • Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



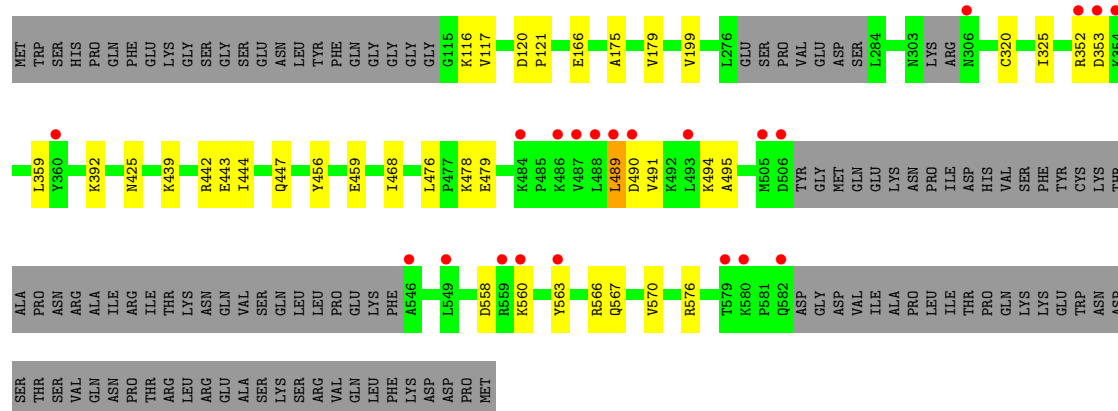
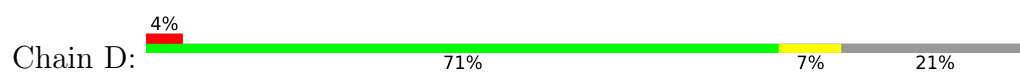
#### • Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1







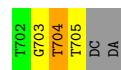
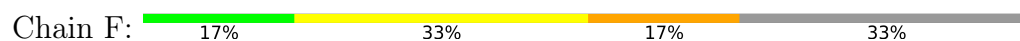
● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



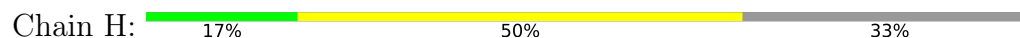
● Molecule 2: DNA polymer TG(PST)TCA



● Molecule 2: DNA polymer TG(PST)TCA

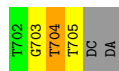


● Molecule 2: DNA polymer TG(PST)TCA



- Molecule 2: DNA polymer TG(PST)TCA

Chain G:  17% 33% 17% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.61Å 94.67Å 96.32Å 72.90° 70.95° 64.96°	Depositor
Resolution (Å)	68.27 – 2.10 68.27 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.0 (68.27-2.10) 93.0 (68.27-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.174 , 0.206 0.174 , 0.206	Depositor DCC
$R_{free}$ test set	6455 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.3	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	14600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: ZN, PST

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	0.45	0/3698	0.58	0/4986
1	B	0.39	0/3580	0.54	0/4828
1	C	0.47	0/3660	0.57	0/4936
1	D	0.42	0/3508	0.54	0/4731
2	E	0.89	0/28	1.10	0/41
2	F	0.94	0/28	1.01	0/41
2	G	1.00	0/34	1.06	0/49
2	H	0.78	0/28	0.90	0/41
All	All	0.44	0/14564	0.56	0/19653

There are no bond length outliers.

There are no bond angle outliers.

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	3613	0	3584	29	0
1	B	3499	0	3464	38	0
1	C	3577	0	3548	31	0
1	D	3429	0	3403	28	0
2	E	47	0	23	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	47	0	23	6	0
2	G	52	0	26	3	0
2	H	38	0	17	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	89	0	0	3	0
4	B	52	0	0	0	0
4	C	93	0	0	1	0
4	D	56	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
All	All	14600	0	14088	131	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 5.

All (131) 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:489:LEU:HD22	1:B:564:ALA:HB2	1.50	0.94
1:A:515:ILE:HA	1:A:518:VAL:HG12	1.67	0.75
1:B:347:LEU:HD12	1:B:347:LEU:H	1.50	0.74
1:D:439:LYS:HE3	1:D:442:ARG:HH21	1.54	0.72
1:D:116:LYS:HE3	2:E:703:DG:OP1	1.89	0.71
1:B:489:LEU:CD2	1:B:564:ALA:HB2	2.23	0.69
1:A:422:LEU:HD12	1:A:426:ILE:HG13	1.76	0.68
1:B:347:LEU:HD12	1:B:347:LEU:N	2.11	0.66
1:A:352:ARG:NH1	1:A:353:ASP:OD1	2.28	0.66
1:A:352:ARG:HG2	1:A:354:LYS:HG2	1.79	0.64
1:A:465:GLN:NE2	4:A:802:HOH:O	2.30	0.64
1:C:442:ARG:HG2	1:C:446:LYS:HE2	1.80	0.64
1:B:489:LEU:HD11	1:B:563:TYR:CE2	2.33	0.63
1:A:116:LYS:HE2	2:H:703:DG:OP1	1.99	0.62
1:D:491:VAL:HG21	1:D:560:LYS:HB2	1.82	0.62
1:B:566:ARG:NH2	1:B:582:GLN:O	2.32	0.59
1:C:522:CYS:SG	1:C:524:THR:HG22	2.42	0.59
1:B:489:LEU:HD22	1:B:564:ALA:CB	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LEU:HD13	1:B:276:LEU:O	2.03	0.58
1:C:182:LEU:HD22	1:C:340:VAL:HG23	1.86	0.58
1:C:116:LYS:HE2	2:F:703:DG:OP1	2.05	0.57
1:B:489:LEU:HD11	1:B:563:TYR:CD2	2.40	0.56
1:C:505:MET:HG3	1:C:546:ALA:O	2.03	0.56
1:B:363:PHE:HD2	1:B:366:ARG:NH2	2.03	0.56
1:C:485:PRO:HG2	1:C:489:LEU:HD11	1.87	0.56
1:C:408:ARG:NH2	4:C:804:HOH:O	2.39	0.55
1:B:468:ILE:HG21	1:B:476:LEU:HD11	1.89	0.55
1:A:522:CYS:SG	1:A:524:THR:HG22	2.47	0.54
1:D:439:LYS:HE3	1:D:442:ARG:NH2	2.23	0.54
1:A:194:ARG:HD2	1:A:258:GLY:O	2.08	0.54
1:B:582:GLN:CD	1:B:583:ASP:H	2.10	0.54
1:C:303:ASN:CG	1:C:306:ASN:HB2	2.28	0.54
1:B:390:PHE:CZ	1:B:426:ILE:CG2	2.91	0.53
1:C:132:LEU:HD22	1:C:204:LEU:HD12	1.91	0.52
1:A:215:HIS:HE1	4:A:884:HOH:O	1.91	0.51
1:B:309:ASP:OD1	1:B:312:LYS:HG2	2.10	0.51
1:A:422:LEU:CD1	1:A:426:ILE:HG13	2.39	0.51
1:C:266:CYS:O	1:C:270:GLU:HG3	2.10	0.51
2:F:704:PST:SP	2:F:704:PST:H71	2.51	0.51
1:B:285:TRP:CE3	1:B:292:GLU:HG3	2.45	0.51
1:A:331:TYR:CE1	1:A:332:LYS:HG3	2.46	0.51
1:B:392:LYS:HD2	1:B:444:ILE:HD11	1.92	0.51
1:D:566:ARG:O	1:D:570:VAL:HG23	2.11	0.51
1:A:333:ARG:NE	1:A:355:GLU:OE2	2.37	0.51
1:B:334:PHE:CE2	1:B:351:ALA:HB2	2.47	0.50
1:D:489:LEU:HD12	1:D:490:ASP:H	1.76	0.50
1:A:232:THR:OG1	1:A:235:GLN:HG3	2.12	0.50
1:C:194:ARG:NH1	1:C:260:ILE:HD12	2.27	0.50
1:A:356:VAL:HG12	1:C:360:TYR:CZ	2.48	0.49
1:A:455:LYS:HG3	1:A:562:LEU:HD11	1.93	0.49
1:D:175:ALA:HB1	1:D:199:VAL:HG12	1.95	0.49
1:D:443:GLU:O	1:D:447:GLN:HG3	2.13	0.49
1:B:242:GLU:OE1	1:B:269:LYS:NZ	2.36	0.48
1:C:197:LEU:O	1:C:201:ILE:HG13	2.14	0.48
1:B:329:PHE:CD1	1:B:362:MET:HB2	2.49	0.48
1:A:320:CYS:HB3	1:A:325:ILE:O	2.15	0.47
1:B:491:VAL:HG21	1:B:561:SER:HA	1.97	0.47
1:D:352:ARG:HG2	1:D:353:ASP:N	2.29	0.47
1:D:489:LEU:HD21	1:D:563:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:TYR:OH	1:C:459:GLU:HB2	2.13	0.47
1:B:320:CYS:SG	1:B:327:ASN:HB2	2.55	0.47
1:B:117:VAL:O	2:G:704:PST:H5'	2.15	0.47
1:D:392:LYS:HD2	1:D:444:ILE:HD11	1.95	0.47
2:E:704:PST:H2'	2:E:705:DT:OP1	2.14	0.47
1:C:352:ARG:HH11	1:C:354:LYS:HZ2	1.61	0.47
1:D:494:LYS:HD2	1:D:494:LYS:N	2.29	0.47
1:B:334:PHE:CE2	1:B:359:LEU:HD13	2.50	0.46
1:A:343:VAL:HG22	1:A:529:ALA:HB2	1.97	0.46
1:C:117:VAL:O	2:F:704:PST:H5'	2.15	0.46
1:C:489:LEU:HD21	1:C:567:GLN:HG3	1.98	0.46
1:D:468:ILE:HG21	1:D:476:LEU:HD11	1.98	0.46
1:C:394:ASP:O	1:C:408:ARG:HD2	2.16	0.46
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.16	0.45
1:C:352:ARG:HD3	1:C:354:LYS:NZ	2.31	0.45
1:A:158:PRO:HB2	1:D:166:GLU:HB3	1.99	0.45
1:A:515:ILE:HA	1:A:518:VAL:CG1	2.43	0.45
1:A:329:PHE:CD1	1:A:362:MET:HB2	2.51	0.45
1:A:116:LYS:HB2	1:A:133:VAL:HG21	1.97	0.45
1:C:494:LYS:HB2	1:C:494:LYS:HE2	1.70	0.45
1:D:558:ASP:OD2	1:D:560:LYS:HG3	2.16	0.45
1:C:179:VAL:HG13	1:C:196:VAL:HG22	1.99	0.45
1:C:241:PHE:O	1:C:245:ILE:HG12	2.17	0.45
2:F:704:PST:H2'	2:F:705:DT:OP1	2.17	0.45
1:B:484:LYS:O	1:B:571:GLN:HG2	2.17	0.45
1:A:115:GLY:N	1:A:130:PRO:HG3	2.32	0.44
2:H:704:PST:H2'	2:H:705:DT:OP1	2.15	0.44
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.99	0.44
1:D:359:LEU:HD12	1:D:359:LEU:HA	1.86	0.44
1:B:171:VAL:HG21	1:B:206:HIS:CE1	2.52	0.44
1:B:333:ARG:CZ	1:B:355:GLU:HG3	2.47	0.44
1:B:188:GLU:HG2	1:B:189:LEU:N	2.33	0.44
1:B:330:ASP:OD1	1:B:332:LYS:NZ	2.34	0.43
1:C:352:ARG:HH11	1:C:354:LYS:NZ	2.15	0.43
1:D:489:LEU:HD13	1:D:489:LEU:HA	1.67	0.43
1:A:352:ARG:CZ	1:A:523:LYS:HB3	2.48	0.43
1:D:478:LYS:HD3	1:D:495:ALA:CB	2.48	0.43
1:D:175:ALA:O	1:D:179:VAL:HG12	2.19	0.43
1:A:143:ARG:HD2	1:A:420:THR:HA	2.01	0.43
1:B:220:ARG:HG2	1:B:387:THR:HG21	1.99	0.43
1:A:332:LYS:HE2	1:A:332:LYS:HB2	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ALA:HB1	1:A:199:VAL:HG12	2.00	0.42
1:D:320:CYS:HB3	1:D:325:ILE:O	2.18	0.42
2:G:704:PST:H2'	2:G:705:DT:OP1	2.18	0.42
1:B:455:LYS:HD3	1:B:557:VAL:HG13	2.01	0.42
2:G:703:DG:H5''	2:G:703:DG:N3	2.34	0.42
1:A:489:LEU:HD21	1:A:567:GLN:HG3	2.00	0.42
1:A:116:LYS:HB2	1:A:133:VAL:CG2	2.50	0.42
1:C:116:LYS:HE2	2:F:703:DG:P	2.60	0.42
1:B:480:VAL:HG22	1:B:572:TRP:CD2	2.55	0.42
1:C:306:ASN:HB3	1:C:308:ILE:H	1.84	0.42
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.20	0.42
1:D:489:LEU:HD23	1:D:567:GLN:CG	2.49	0.42
1:D:489:LEU:CD2	1:D:567:GLN:HG3	2.50	0.42
1:C:516:ASP:O	1:C:518:VAL:N	2.53	0.41
1:D:558:ASP:HB2	1:D:560:LYS:HG3	2.02	0.41
1:D:117:VAL:O	2:E:704:PST:H5'	2.20	0.41
1:B:331:TYR:CE1	1:B:332:LYS:HG3	2.56	0.41
1:C:320:CYS:HB3	1:C:325:ILE:O	2.21	0.41
1:B:188:GLU:O	1:B:190:GLN:HG3	2.21	0.41
1:C:352:ARG:NE	1:C:521:TYR:OH	2.53	0.41
1:C:354:LYS:HZ1	1:C:523:LYS:HD3	1.86	0.41
1:D:479:GLU:OE1	1:D:576:ARG:HD2	2.21	0.41
1:A:302:SER:O	4:A:801:HOH:O	2.22	0.41
1:C:461:GLN:HG2	1:C:549:LEU:HD23	2.02	0.41
1:D:456:TYR:OH	1:D:459:GLU:HB2	2.20	0.41
1:C:312:LYS:HA	1:C:315:TYR:CE2	2.56	0.41
1:B:461:GLN:HG2	1:B:549:LEU:HD23	2.03	0.40
2:F:704:PST:O5'	2:F:704:PST:H6	2.20	0.40
1:B:333:ARG:NH2	1:B:355:GLU:HG3	2.37	0.40
1:D:352:ARG:CG	1:D:353:ASP:N	2.84	0.40
1:B:426:ILE:HD12	1:B:426:ILE:HA	1.94	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	434/535 (81%)	427 (98%)	7 (2%)	0	100	100
1	B	419/535 (78%)	412 (98%)	7 (2%)	0	100	100
1	C	430/535 (80%)	419 (97%)	10 (2%)	1 (0%)	47	49
1	D	412/535 (77%)	406 (98%)	6 (2%)	0	100	100
All	All	1695/2140 (79%)	1664 (98%)	30 (2%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	517	HIS

### 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	390/473 (82%)	390 (100%)	0	100	100
1	B	378/473 (80%)	373 (99%)	5 (1%)	69	75
1	C	386/473 (82%)	380 (98%)	6 (2%)	62	69
1	D	370/473 (78%)	368 (100%)	2 (0%)	88	92
All	All	1524/1892 (80%)	1511 (99%)	13 (1%)	78	84

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	116	LYS
1	B	347	LEU
1	B	489	LEU
1	B	490	ASP
1	B	491	VAL
1	C	125	HIS
1	C	333	ARG

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Mol	Chain	Res	Type
1	C	425	ASN
1	C	528	ARG
1	C	559	ARG
1	C	560	LYS
1	D	425	ASN
1	D	489	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
2	PST	E	704	2	15,21,22	1.39	2 (13%)	16,30,33	1.75	2 (12%)
2	PST	F	704	2	15,21,22	1.16	1 (6%)	16,30,33	2.12	4 (25%)
2	PST	H	704	2	8,11,22	0.71	0	9,14,33	0.82	0
2	PST	G	704	2	15,21,22	1.28	2 (13%)	16,30,33	1.98	2 (12%)

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
2	PST	E	704	2	-	0/4/21/22	0/2/2/2
2	PST	F	704	2	-	0/4/21/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PST	H	704	2	-	0/3/15/22	0/1/1/2
2	PST	G	704	2	-	0/4/21/22	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	704	PST	C4-C5	4.18	1.50	1.41
2	G	704	PST	C4-C5	3.69	1.49	1.41
2	F	704	PST	C4-C5	3.19	1.48	1.41
2	E	704	PST	C2-N3	-2.16	1.33	1.38
2	G	704	PST	O3'-C3'	2.00	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	704	PST	C4-N3-C2	7.14	121.17	115.14
2	F	704	PST	C4-N3-C2	6.97	121.03	115.14
2	E	704	PST	C5-C6-N1	-4.83	116.99	122.19
2	E	704	PST	C4-N3-C2	4.61	119.03	115.14
2	G	704	PST	C5-C6-N1	-2.70	119.28	122.19
2	F	704	PST	C5M-C5-C6	2.40	123.75	118.68
2	F	704	PST	C2'-C1'-N1	-2.13	109.36	114.27
2	F	704	PST	C5-C6-N1	-2.08	119.95	122.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	704	PST	2	0
2	F	704	PST	4	0
2	H	704	PST	1	0
2	G	704	PST	2	0

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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

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	442/535 (82%)	0.15	8 (1%) 68 72	35, 55, 103, 147	0
1	B	429/535 (80%)	0.39	36 (8%) 11 14	38, 65, 124, 175	0
1	C	438/535 (81%)	0.09	7 (1%) 72 75	34, 55, 104, 153	0
1	D	420/535 (78%)	0.34	22 (5%) 27 32	37, 61, 120, 162	0
2	E	3/6 (50%)	-0.10	0 100 100	59, 59, 106, 126	0
2	F	3/6 (50%)	-0.34	0 100 100	73, 73, 101, 133	0
2	G	3/6 (50%)	-0.02	0 100 100	66, 66, 118, 132	0
2	H	3/6 (50%)	0.33	0 100 100	74, 74, 129, 137	0
All	All	1741/2164 (80%)	0.24	73 (4%) 36 42	34, 59, 114, 175	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	488	LEU	6.8
1	B	520	PHE	5.9
1	B	522	CYS	5.8
1	B	523	LYS	5.8
1	B	360	TYR	5.8
1	B	521	TYR	5.6
1	A	516	ASP	5.5
1	B	356	VAL	5.3
1	B	524	THR	4.8
1	D	353	ASP	4.5
1	B	486	LYS	4.4
1	B	525	ALA	4.3
1	D	486	LYS	4.3
1	D	360	TYR	4.0
1	D	490	ASP	3.9
1	B	353	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	519	SER	3.7
1	D	582	GLN	3.5
1	A	544	LYS	3.3
1	A	542	PRO	3.2
1	D	580	LYS	3.2
1	B	526	PRO	3.2
1	C	518	VAL	3.2
1	B	546	ALA	3.1
1	B	562	LEU	3.1
1	A	515	ILE	3.1
1	A	517	HIS	3.1
1	D	560	LYS	3.1
1	B	518	VAL	3.0
1	D	487	VAL	3.0
1	D	354	LYS	3.0
1	C	517	HIS	2.9
1	D	505	MET	2.9
1	B	488	LEU	2.9
1	B	354	LYS	2.9
1	B	357	GLY	2.9
1	D	563	TYR	2.9
1	B	490	ASP	2.8
1	D	489	LEU	2.8
1	D	546	ALA	2.8
1	B	262	GLU	2.7
1	D	484	LYS	2.7
1	C	304	LYS	2.6
1	B	492	LYS	2.6
1	C	276	LEU	2.6
1	B	344	ASP	2.6
1	B	276	LEU	2.6
1	A	545	PHE	2.5
1	D	352	ARG	2.5
1	D	493	LEU	2.4
1	B	465	GLN	2.4
1	D	549	LEU	2.4
1	D	579	THR	2.4
1	B	580	LYS	2.4
1	B	363	PHE	2.3
1	D	306	ASN	2.3
1	B	506	ASP	2.3
1	B	582	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	359	LEU	2.3
1	B	334	PHE	2.3
1	C	488	LEU	2.2
1	C	524	THR	2.2
1	B	337	PHE	2.2
1	B	489	LEU	2.2
1	B	487	VAL	2.2
1	A	484	LYS	2.2
1	B	560	LYS	2.2
1	B	491	VAL	2.1
1	A	505	MET	2.1
1	C	347	LEU	2.1
1	D	559	ARG	2.1
1	D	506	ASP	2.1
1	B	307	GLY	2.1

## 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, 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
2	PST	H	704	11/21	0.94	0.13	74,89,105,120	0
2	PST	G	704	20/21	0.94	0.18	67,120,136,139	0
2	PST	E	704	20/21	0.95	0.18	64,109,121,124	0
2	PST	F	704	20/21	0.96	0.17	73,119,136,138	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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	ZN	A	701	1/1	0.99	0.16	42,42,42,42	0
3	ZN	C	701	1/1	0.99	0.19	44,44,44,44	0
3	ZN	D	701	1/1	0.99	0.19	46,46,46,46	0
3	ZN	B	701	1/1	1.00	0.14	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.