



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2021 – 04:07 PM EDT

PDB ID : 6U6X
Title : Human SAMHD1 bound to deoxyribo(C*G*C*C*T)-oligonucleotide
Authors : Taylor, A.B.; Bhattacharya, A.; Wang, Z.; Ivanov, D.N.
Deposited on : 2019-08-30
Resolution : 2.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

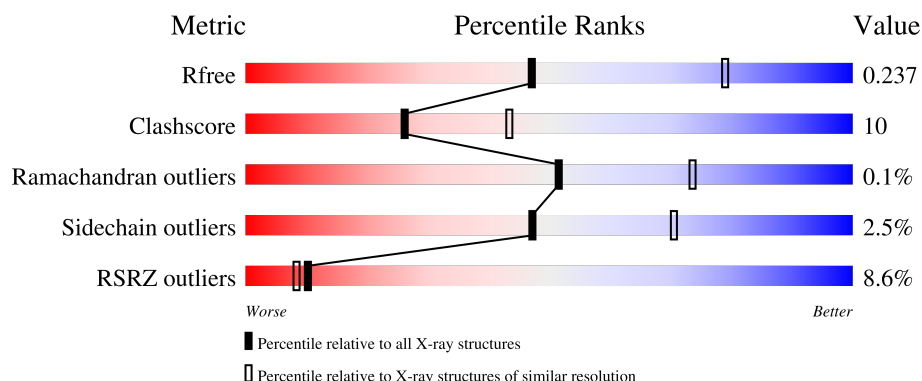
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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.



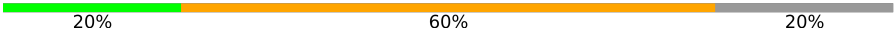


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	533	
1	B	533	
1	C	533	
1	D	533	
2	E	5	

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Mol	Chain	Length	Quality of chain
2	F	5	 20% 60% 20%
2	G	5	 60% 20% 20%
2	H	5	 60% 20% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13531 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	427	Total	C	N	O	S	0	1	0
			3497	2243	605	630	19			
1	B	383	Total	C	N	O	S	0	0	0
			3139	2019	547	556	17			
1	C	376	Total	C	N	O	S	0	0	0
			3075	1973	532	554	16			
1	D	430	Total	C	N	O	S	0	1	0
			3531	2265	613	634	19			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MET	-	initiating methionine	UNP Q9Y3Z3
A	95	TRP	-	expression tag	UNP Q9Y3Z3
A	96	SER	-	expression tag	UNP Q9Y3Z3
A	97	HIS	-	expression tag	UNP Q9Y3Z3
A	98	PRO	-	expression tag	UNP Q9Y3Z3
A	99	GLN	-	expression tag	UNP Q9Y3Z3
A	100	PHE	-	expression tag	UNP Q9Y3Z3
A	101	GLU	-	expression tag	UNP Q9Y3Z3
A	102	LYS	-	expression tag	UNP Q9Y3Z3
A	103	GLY	-	expression tag	UNP Q9Y3Z3
A	104	SER	-	expression tag	UNP Q9Y3Z3
A	105	GLY	-	expression tag	UNP Q9Y3Z3
A	106	SER	-	expression tag	UNP Q9Y3Z3
A	107	GLU	-	expression tag	UNP Q9Y3Z3
A	108	ASN	-	expression tag	UNP Q9Y3Z3
A	109	LEU	-	expression tag	UNP Q9Y3Z3
A	110	TYR	-	expression tag	UNP Q9Y3Z3
A	111	PHE	-	expression tag	UNP Q9Y3Z3
A	112	GLN	-	expression tag	UNP Q9Y3Z3
A	113	GLY	-	expression tag	UNP Q9Y3Z3
A	311	ALA	ASP	engineered mutation	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	94	MET	-	initiating methionine	UNP Q9Y3Z3
B	95	TRP	-	expression tag	UNP Q9Y3Z3
B	96	SER	-	expression tag	UNP Q9Y3Z3
B	97	HIS	-	expression tag	UNP Q9Y3Z3
B	98	PRO	-	expression tag	UNP Q9Y3Z3
B	99	GLN	-	expression tag	UNP Q9Y3Z3
B	100	PHE	-	expression tag	UNP Q9Y3Z3
B	101	GLU	-	expression tag	UNP Q9Y3Z3
B	102	LYS	-	expression tag	UNP Q9Y3Z3
B	103	GLY	-	expression tag	UNP Q9Y3Z3
B	104	SER	-	expression tag	UNP Q9Y3Z3
B	105	GLY	-	expression tag	UNP Q9Y3Z3
B	106	SER	-	expression tag	UNP Q9Y3Z3
B	107	GLU	-	expression tag	UNP Q9Y3Z3
B	108	ASN	-	expression tag	UNP Q9Y3Z3
B	109	LEU	-	expression tag	UNP Q9Y3Z3
B	110	TYR	-	expression tag	UNP Q9Y3Z3
B	111	PHE	-	expression tag	UNP Q9Y3Z3
B	112	GLN	-	expression tag	UNP Q9Y3Z3
B	113	GLY	-	expression tag	UNP Q9Y3Z3
B	311	ALA	ASP	engineered mutation	UNP Q9Y3Z3
C	94	MET	-	initiating methionine	UNP Q9Y3Z3
C	95	TRP	-	expression tag	UNP Q9Y3Z3
C	96	SER	-	expression tag	UNP Q9Y3Z3
C	97	HIS	-	expression tag	UNP Q9Y3Z3
C	98	PRO	-	expression tag	UNP Q9Y3Z3
C	99	GLN	-	expression tag	UNP Q9Y3Z3
C	100	PHE	-	expression tag	UNP Q9Y3Z3
C	101	GLU	-	expression tag	UNP Q9Y3Z3
C	102	LYS	-	expression tag	UNP Q9Y3Z3
C	103	GLY	-	expression tag	UNP Q9Y3Z3
C	104	SER	-	expression tag	UNP Q9Y3Z3
C	105	GLY	-	expression tag	UNP Q9Y3Z3
C	106	SER	-	expression tag	UNP Q9Y3Z3
C	107	GLU	-	expression tag	UNP Q9Y3Z3
C	108	ASN	-	expression tag	UNP Q9Y3Z3
C	109	LEU	-	expression tag	UNP Q9Y3Z3
C	110	TYR	-	expression tag	UNP Q9Y3Z3
C	111	PHE	-	expression tag	UNP Q9Y3Z3
C	112	GLN	-	expression tag	UNP Q9Y3Z3
C	113	GLY	-	expression tag	UNP Q9Y3Z3
C	311	ALA	ASP	engineered mutation	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	94	MET	-	initiating methionine	UNP Q9Y3Z3
D	95	TRP	-	expression tag	UNP Q9Y3Z3
D	96	SER	-	expression tag	UNP Q9Y3Z3
D	97	HIS	-	expression tag	UNP Q9Y3Z3
D	98	PRO	-	expression tag	UNP Q9Y3Z3
D	99	GLN	-	expression tag	UNP Q9Y3Z3
D	100	PHE	-	expression tag	UNP Q9Y3Z3
D	101	GLU	-	expression tag	UNP Q9Y3Z3
D	102	LYS	-	expression tag	UNP Q9Y3Z3
D	103	GLY	-	expression tag	UNP Q9Y3Z3
D	104	SER	-	expression tag	UNP Q9Y3Z3
D	105	GLY	-	expression tag	UNP Q9Y3Z3
D	106	SER	-	expression tag	UNP Q9Y3Z3
D	107	GLU	-	expression tag	UNP Q9Y3Z3
D	108	ASN	-	expression tag	UNP Q9Y3Z3
D	109	LEU	-	expression tag	UNP Q9Y3Z3
D	110	TYR	-	expression tag	UNP Q9Y3Z3
D	111	PHE	-	expression tag	UNP Q9Y3Z3
D	112	GLN	-	expression tag	UNP Q9Y3Z3
D	113	GLY	-	expression tag	UNP Q9Y3Z3
D	311	ALA	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is a DNA chain called DNA SC-GS-SC-SC-DT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	4	Total 76	C 37	N 14	O 19	P 3	S 3	0	0	0
2	G	4	Total 53	C 24	N 8	O 15	P 3	S 3	0	0	0
2	F	4	Total 68	C 33	N 11	O 18	P 3	S 3	0	0	0
2	H	4	Total 76	C 37	N 14	O 19	P 3	S 3	0	0	0

- 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		

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

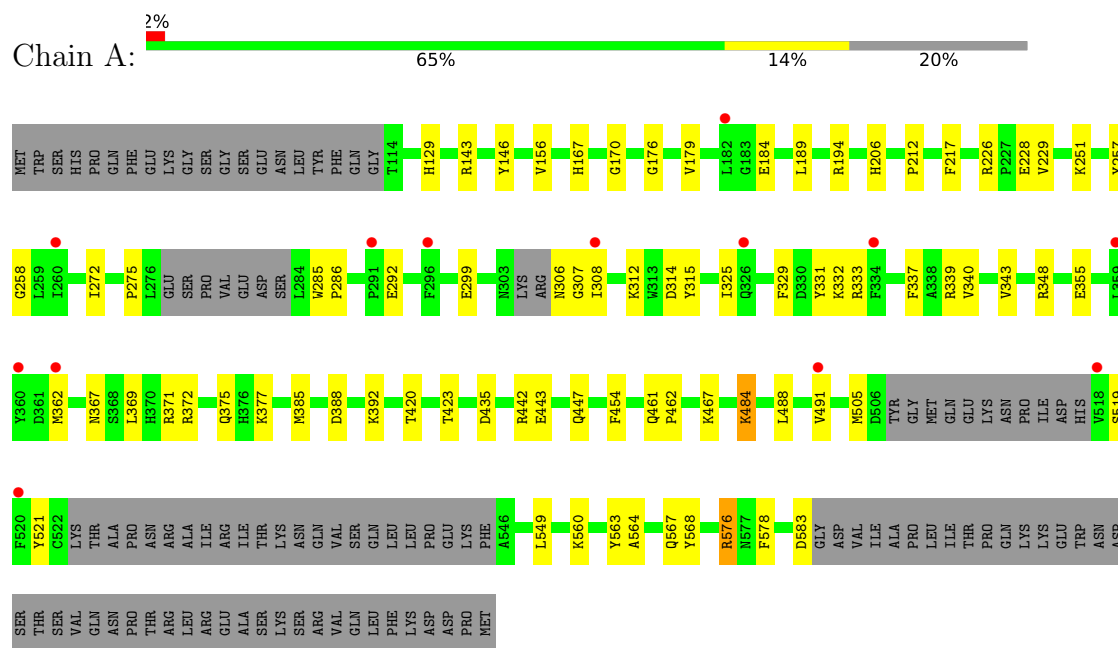
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total 4	O 4	0	0
4	D	8	Total 8	O 8	0	0

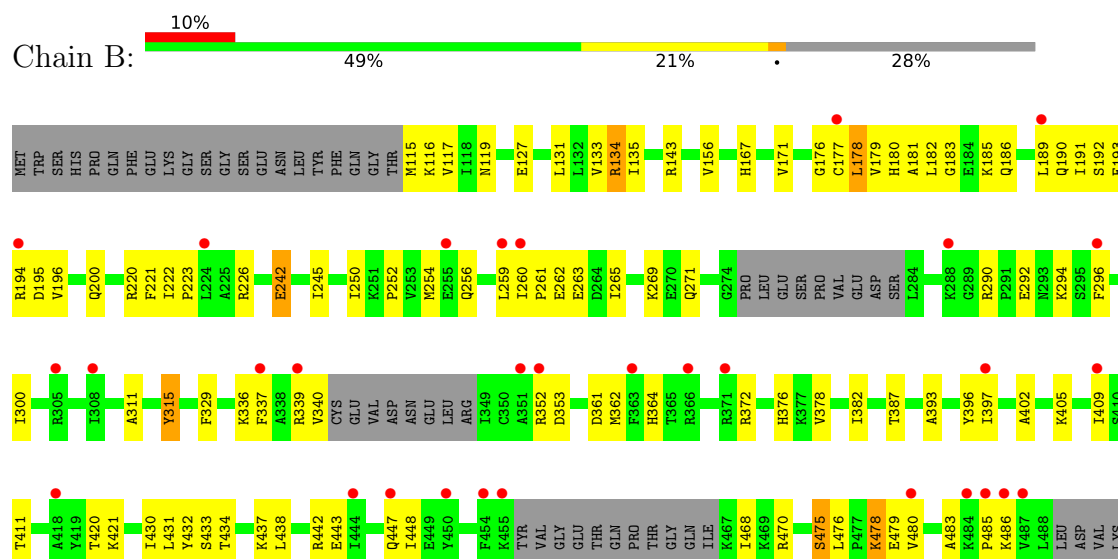
3 Residue-property plots

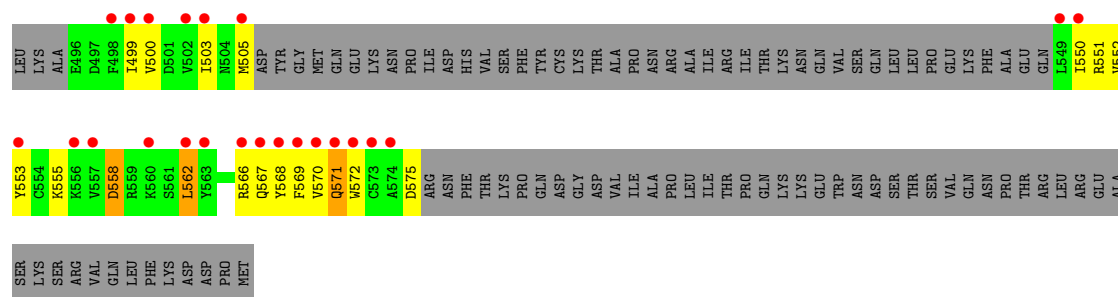
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

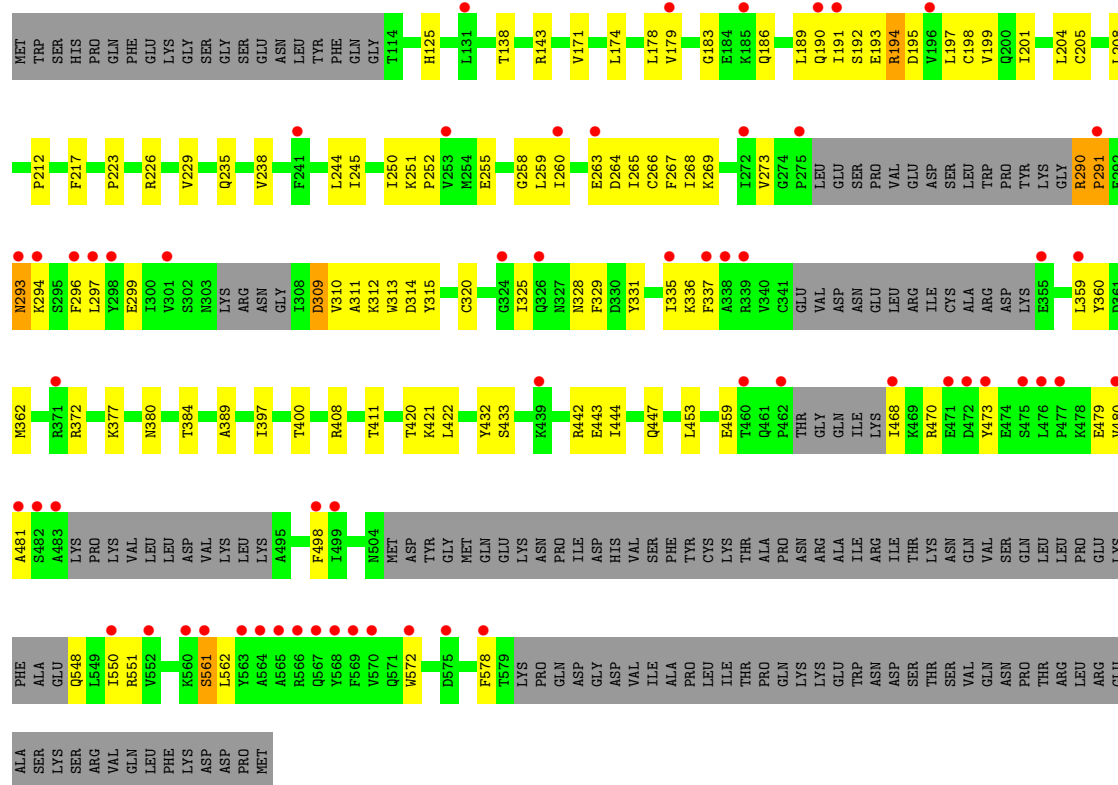


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

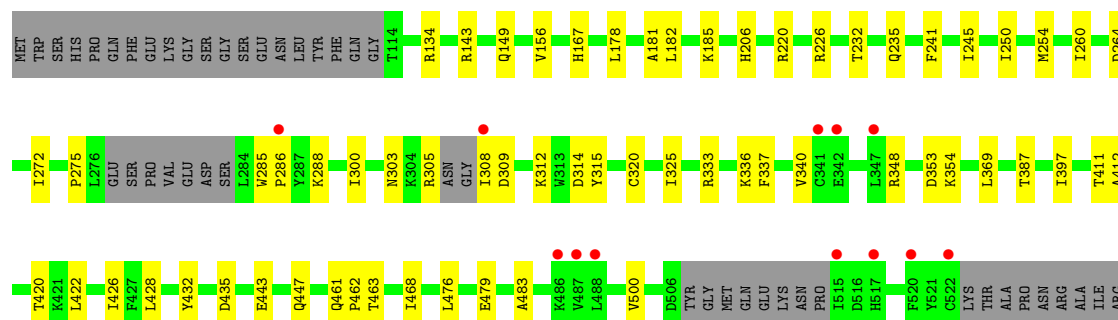


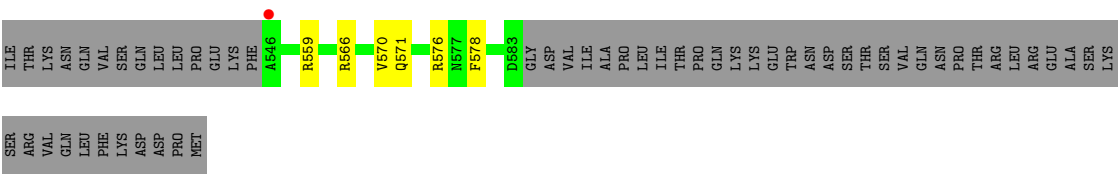


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





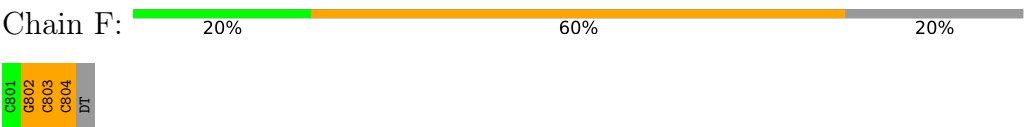
● Molecule 2: DNA SC-GS-SC-SC-DT



● Molecule 2: DNA SC-GS-SC-SC-DT



● Molecule 2: DNA SC-GS-SC-SC-DT



● Molecule 2: DNA SC-GS-SC-SC-DT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.36Å 81.87Å 106.00Å 69.72° 76.30° 82.77°	Depositor
Resolution (Å)	61.66 – 2.58 61.66 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.8 (61.66-2.58) 97.8 (61.66-2.58)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.196 , 0.236 0.196 , 0.237	Depositor DCC
R_{free} test set	2263 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13531	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GS, SC, ZN

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	0.44	0/3578	0.58	0/4825
1	B	0.43	0/3211	0.63	0/4322
1	C	0.40	0/3145	0.60	0/4239
1	D	0.39	0/3613	0.56	0/4871
All	All	0.42	0/13547	0.59	0/18257

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3497	0	3461	51	0
1	B	3139	0	3126	102	0
1	C	3075	0	3027	86	0
1	D	3531	0	3500	45	0
2	E	76	0	46	4	0
2	F	68	0	41	4	0
2	G	53	0	29	3	0
2	H	76	0	46	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	0	0	0
4	D	8	0	0	1	0
All	All	13531	0	13276	279	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 10.

All (279) 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:552:VAL:HG21	1:B:569:PHE:CE1	2.00	0.96
1:B:552:VAL:HG21	1:B:569:PHE:CD1	2.00	0.96
1:B:393:ALA:HB1	1:B:397:ILE:CD1	1.95	0.95
1:C:191:ILE:HG23	1:C:191:ILE:O	1.67	0.92
1:B:372:ARG:NH2	2:G:804:SC:S2P	2.45	0.90
1:A:484:LYS:HE3	1:A:488:LEU:HA	1.55	0.89
1:C:190:GLN:HB3	1:C:294:LYS:NZ	1.88	0.88
1:B:479:GLU:HG2	1:B:572:TRP:HE1	1.36	0.87
1:B:485:PRO:HG3	1:B:567:GLN:O	1.74	0.86
1:A:129:HIS:HE1	1:A:257:TYR:CD2	1.94	0.85
1:D:566:ARG:O	1:D:570:VAL:HG23	1.75	0.85
1:A:325:ILE:HG12	1:A:372:ARG:HH21	1.40	0.84
1:B:393:ALA:HB1	1:B:397:ILE:HD12	1.56	0.84
1:B:485:PRO:HB3	1:B:571:GLN:HG2	1.58	0.84
1:C:468:ILE:HG13	1:C:550:ILE:HD11	1.60	0.83
1:B:572:TRP:O	1:B:575:ASP:HB2	1.80	0.82
1:B:222:ILE:HG13	1:B:223:PRO:HD3	1.61	0.81
1:B:245:ILE:HG23	1:B:250:ILE:HB	1.62	0.81
1:B:566:ARG:O	1:B:570:VAL:HG23	1.82	0.80
1:A:129:HIS:CE1	1:A:257:TYR:CD2	2.71	0.78
1:B:479:GLU:CG	1:B:572:TRP:HE1	1.97	0.78
1:B:503:ILE:HD12	1:B:551:ARG:HD2	1.66	0.77
1:A:337:PHE:HD2	1:A:355:GLU:OE2	1.67	0.77
1:B:562:LEU:HD12	1:B:562:LEU:O	1.86	0.74
1:B:552:VAL:CG2	1:B:569:PHE:CE1	2.70	0.74
1:B:393:ALA:HB1	1:B:397:ILE:HD11	1.70	0.74
1:C:480:VAL:HG11	1:C:498:PHE:CG	2.23	0.73
1:C:179:VAL:HG22	1:C:191:ILE:HD11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:THR:HG21	1:C:244:LEU:HD21	1.73	0.71
1:B:178:LEU:O	1:B:178:LEU:HD12	1.91	0.71
1:B:186:GLN:HE22	1:B:340:VAL:HG12	1.58	0.69
1:B:562:LEU:HD12	1:B:562:LEU:C	2.13	0.69
1:A:372:ARG:HG2	2:E:804:SC:H3'	1.73	0.68
1:B:178:LEU:HD12	1:B:178:LEU:C	2.13	0.68
1:B:186:GLN:HE21	1:B:339:ARG:NH1	1.91	0.68
1:B:176:GLY:HA3	1:B:200:GLN:HE21	1.58	0.68
1:A:306:ASN:OD1	1:A:307:GLY:N	2.27	0.68
1:C:255:GLU:HB3	1:C:259:LEU:O	1.94	0.67
1:C:191:ILE:O	1:C:191:ILE:CG2	2.41	0.67
1:A:377:LYS:H	2:E:804:SC:HN42	1.41	0.66
1:B:134:ARG:HH11	1:B:134:ARG:CG	2.07	0.66
1:B:192:SER:HB2	1:B:194:ARG:HG2	1.78	0.65
1:C:290:ARG:HB3	1:C:291:PRO:HD2	1.78	0.65
1:D:462:PRO:HA	1:D:578:PHE:CD1	2.32	0.65
1:C:190:GLN:HB3	1:C:294:LYS:HZ1	1.61	0.64
1:B:181:ALA:O	1:B:185:LYS:HG2	1.97	0.64
1:B:402:ALA:O	1:B:405:LYS:HG2	1.98	0.63
1:C:195:ASP:O	1:C:199:VAL:HG23	1.97	0.63
1:C:186:GLN:HB2	1:C:189:LEU:HD12	1.79	0.63
1:C:238:VAL:HG11	1:C:273:VAL:HB	1.81	0.63
1:C:258:GLY:C	1:C:259:LEU:HD12	2.19	0.63
1:C:193:GLU:OE2	1:C:193:GLU:HA	1.97	0.62
1:A:461:GLN:HG2	1:A:549:LEU:HD23	1.81	0.62
1:C:459:GLU:HB2	1:C:551:ARG:HG2	1.82	0.61
1:D:167:HIS:ND1	1:D:314:ASP:OD2	2.25	0.61
1:C:480:VAL:HG11	1:C:498:PHE:CD2	2.35	0.60
1:B:260:ILE:CG2	1:B:263:GLU:HG2	2.30	0.60
1:B:499:ILE:HG12	1:B:555:LYS:HE2	1.84	0.60
1:B:433:SER:O	1:B:442:ARG:NH1	2.34	0.60
1:B:393:ALA:CB	1:B:397:ILE:HD12	2.29	0.60
1:C:190:GLN:HB3	1:C:294:LYS:HZ3	1.65	0.59
1:D:320:CYS:HB3	1:D:325:ILE:O	2.01	0.59
1:B:254:MET:O	1:B:259:LEU:HB2	2.02	0.59
1:C:325:ILE:HD11	1:C:372:ARG:NH1	2.17	0.59
1:D:566:ARG:O	1:D:570:VAL:CG2	2.49	0.59
1:B:265:ILE:HG22	1:B:269:LYS:HE3	1.82	0.59
1:C:183:GLY:HA3	1:C:191:ILE:HG21	1.84	0.59
1:B:143:ARG:HD2	1:B:420:THR:HA	1.84	0.59
1:B:340:VAL:HG13	1:B:340:VAL:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:GLU:O	1:B:447:GLN:HG2	2.02	0.58
1:B:220:ARG:HG2	1:B:387:THR:HG21	1.85	0.58
1:D:397:ILE:HG21	1:D:426:ILE:HD11	1.87	0.57
1:C:453:LEU:HD12	2:F:802:GS:S2P	2.44	0.57
1:D:275:PRO:HB3	1:D:286:PRO:HB2	1.86	0.57
1:C:212:PRO:HD2	1:C:217:PHE:CD1	2.40	0.57
1:B:117:VAL:HG22	1:B:127:GLU:HG2	1.88	0.56
1:B:432:TYR:CE1	1:C:421:LYS:HG2	2.40	0.56
1:A:337:PHE:CD2	1:A:355:GLU:OE2	2.55	0.56
1:A:462:PRO:HB3	1:A:578:PHE:CE1	2.41	0.55
1:B:421:LYS:HG2	1:C:432:TYR:CD1	2.41	0.55
1:B:353:ASP:OD1	1:B:353:ASP:N	2.38	0.55
1:A:189:LEU:HD21	1:A:340:VAL:HG11	1.87	0.55
1:C:255:GLU:HA	1:C:259:LEU:H	1.72	0.55
1:C:372:ARG:HH11	1:C:372:ARG:HB3	1.72	0.55
1:D:336:LYS:HE3	1:D:337:PHE:CZ	2.41	0.54
1:B:221:PHE:CE2	1:B:409:ILE:HG22	2.42	0.54
1:A:143:ARG:HD2	1:A:420:THR:HA	1.88	0.54
1:C:179:VAL:HG22	1:C:191:ILE:CD1	2.36	0.54
1:B:117:VAL:O	2:F:803:SC:H5"	2.07	0.54
1:B:500:VAL:HG12	1:B:552:VAL:HG13	1.88	0.54
1:D:206[B]:HIS:HA	1:D:272:ILE:HG12	1.90	0.53
1:D:134:ARG:HG3	1:D:134:ARG:HH11	1.72	0.53
1:C:433:SER:O	1:C:442:ARG:NH1	2.41	0.53
1:D:303:ASN:H	1:D:309:ASP:HB3	1.73	0.53
1:B:434:THR:HG21	1:C:400:THR:HG21	1.90	0.53
1:C:372:ARG:NH1	1:C:372:ARG:HB3	2.23	0.53
1:A:226:ARG:HH21	1:A:229:VAL:HG11	1.74	0.53
1:B:468:ILE:HD12	1:B:468:ILE:H	1.73	0.53
1:B:483:ALA:HB2	1:B:572:TRP:HD1	1.74	0.53
1:C:245:ILE:HG23	1:C:250:ILE:HB	1.91	0.53
1:C:259:LEU:HD12	1:C:259:LEU:N	2.24	0.53
1:A:275:PRO:HB2	1:A:286:PRO:HB2	1.91	0.52
1:B:131:LEU:O	1:B:135:ILE:HG13	2.09	0.52
1:C:174:LEU:HD12	1:C:314:ASP:HB2	1.92	0.52
1:C:229:VAL:O	1:C:229:VAL:HG23	2.10	0.52
1:A:367:ASN:O	1:A:371:ARG:HG2	2.09	0.52
1:B:134:ARG:HH11	1:B:134:ARG:HG3	1.75	0.51
1:C:397:ILE:O	1:C:408:ARG:HG2	2.09	0.51
1:D:185:LYS:NZ	1:D:336:LYS:HA	2.26	0.51
1:D:206[A]:HIS:HA	1:D:272:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:HIS:CD2	1:D:354:LYS:HA	2.46	0.51
1:B:397:ILE:HG22	1:B:397:ILE:O	2.10	0.51
1:A:372:ARG:HD2	2:E:804:SC:H5"	1.91	0.51
1:C:226:ARG:NH1	1:C:411:THR:HA	2.26	0.51
1:C:293:ASN:ND2	1:C:293:ASN:H	2.08	0.51
1:C:480:VAL:HG12	1:C:481:ALA:N	2.26	0.51
1:D:308:ILE:N	1:D:312:LYS:HZ1	2.09	0.51
1:B:193:GLU:O	1:B:196:VAL:HG12	2.10	0.51
1:B:156:VAL:O	2:G:802:GS:H8	2.10	0.50
1:B:476:LEU:O	1:B:480:VAL:HG23	2.11	0.50
1:C:459:GLU:OE1	1:C:551:ARG:NE	2.45	0.50
1:D:178:LEU:HD23	1:D:300:ILE:HG23	1.92	0.50
1:C:459:GLU:CB	1:C:551:ARG:HG2	2.42	0.50
1:C:194:ARG:HB2	1:C:259:LEU:HG	1.93	0.50
1:D:143:ARG:HD2	1:D:420:THR:HA	1.93	0.50
1:A:435:ASP:O	1:A:442:ARG:NH2	2.44	0.50
1:B:186:GLN:NE2	1:B:339:ARG:NH1	2.59	0.50
1:D:435:ASP:N	4:D:801:HOH:O	2.33	0.50
1:B:475:SER:O	1:B:478:LYS:HB3	2.12	0.49
1:D:220:ARG:HG2	1:D:387:THR:HG21	1.93	0.49
1:B:503:ILE:CD1	1:B:551:ARG:HD2	2.41	0.49
1:C:223:PRO:HB3	1:C:470:ARG:HB3	1.95	0.49
1:C:336:LYS:HD3	1:C:337:PHE:HE1	1.78	0.49
1:C:325:ILE:HD11	1:C:372:ARG:HH11	1.76	0.49
1:B:485:PRO:HD2	1:B:568:TYR:CE2	2.47	0.49
1:B:226:ARG:HD2	1:B:411:THR:HG22	1.94	0.49
1:A:333:ARG:HH12	1:A:355:GLU:HG2	1.78	0.49
1:D:428:LEU:HD22	1:D:432:TYR:CZ	2.48	0.48
1:D:167:HIS:CE1	1:D:315:TYR:HB3	2.48	0.48
1:B:171:VAL:HG22	1:B:311:ALA:HA	1.96	0.48
1:B:479:GLU:HG2	1:B:572:TRP:NE1	2.17	0.48
1:C:251:LYS:HG3	1:C:252:PRO:HD3	1.95	0.48
1:D:320:CYS:SG	1:D:369:LEU:HD21	2.53	0.48
1:A:257:TYR:CD1	1:A:257:TYR:N	2.81	0.48
1:C:226:ARG:HH12	1:C:411:THR:HA	1.79	0.48
1:C:479:GLU:HB2	1:C:572:TRP:HE1	1.77	0.48
1:C:329:PHE:CD1	1:C:362:MET:HB2	2.49	0.48
1:B:252:PRO:O	1:B:256:GLN:HG3	2.14	0.48
1:B:468:ILE:HD11	1:B:550:ILE:HD11	1.96	0.48
1:A:206[B]:HIS:HA	1:A:272:ILE:HG12	1.96	0.47
1:B:167:HIS:CE1	1:B:315:TYR:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:VAL:HG22	1:B:300:ILE:HD13	1.95	0.47
1:B:500:VAL:HB	1:B:552:VAL:HG22	1.96	0.47
1:B:259:LEU:O	1:B:261:PRO:HD3	2.13	0.47
1:A:375:GLN:NE2	1:A:505:MET:SD	2.88	0.47
1:C:309:ASP:OD2	1:C:311:ALA:HB3	2.15	0.47
1:B:179:VAL:O	1:B:182:LEU:N	2.48	0.47
1:A:491:VAL:HG21	1:A:560:LYS:HB3	1.96	0.46
1:C:190:GLN:CB	1:C:294:LYS:HG2	2.45	0.46
1:C:255:GLU:CB	1:C:259:LEU:O	2.61	0.46
1:B:337:PHE:HB3	1:B:352:ARG:HD2	1.97	0.46
1:B:361:ASP:OD1	1:D:333:ARG:NH2	2.44	0.46
1:C:251:LYS:CG	1:C:252:PRO:HD3	2.46	0.46
1:A:156:VAL:O	2:E:802:GS:H8	2.15	0.46
1:B:133:VAL:O	1:B:133:VAL:HG12	2.15	0.46
1:C:143:ARG:HD2	1:C:420:THR:HA	1.98	0.46
1:B:134:ARG:CG	1:B:134:ARG:NH1	2.72	0.46
1:B:250:ILE:HG22	1:B:254:MET:HG3	1.98	0.46
1:B:468:ILE:CD1	1:B:550:ILE:HD11	2.45	0.46
1:C:290:ARG:HB3	1:C:291:PRO:CD	2.44	0.46
1:C:443:GLU:OE2	1:C:447:GLN:NE2	2.42	0.46
1:C:561:SER:O	1:C:562:LEU:C	2.52	0.46
1:A:343:VAL:HG21	1:A:519:SER:HB3	1.97	0.46
1:B:189:LEU:HB3	1:B:296:PHE:CZ	2.51	0.46
1:C:468:ILE:N	1:C:548:GLN:HE22	2.13	0.46
1:A:325:ILE:HD12	1:A:369:LEU:HD23	1.97	0.46
1:B:156:VAL:HG11	1:B:376:HIS:CE1	2.51	0.46
1:B:242:GLU:HG2	1:B:269:LYS:HE2	1.99	0.45
1:A:285:TRP:CE3	1:A:292:GLU:HG2	2.51	0.45
1:A:443:GLU:O	1:A:447:GLN:HG3	2.16	0.45
1:B:119:ASN:ND2	2:F:804:SC:S2P	2.89	0.45
1:C:377:LYS:HG2	1:C:551:ARG:NH1	2.31	0.45
1:B:178:LEU:O	1:B:181:ALA:HB3	2.16	0.45
1:C:171:VAL:HG12	1:C:314:ASP:HB3	1.99	0.45
1:A:146:TYR:O	1:A:423:THR:HB	2.17	0.45
1:A:306:ASN:OD1	1:A:308:ILE:N	2.35	0.45
1:C:190:GLN:HB3	1:C:294:LYS:HG2	1.99	0.45
1:C:296:PHE:O	1:C:299:GLU:HB2	2.17	0.45
1:D:185:LYS:HZ3	1:D:336:LYS:HA	1.81	0.45
1:D:479:GLU:OE1	1:D:576:ARG:NH1	2.48	0.45
1:B:382:ILE:HG23	1:B:448:ILE:HD12	1.99	0.44
1:C:260:ILE:CG2	1:C:263:GLU:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:GLN:HE22	1:D:167:HIS:CD2	2.35	0.44
1:D:226:ARG:NH1	1:D:411:THR:HA	2.31	0.44
1:A:329:PHE:CD1	1:A:362:MET:HB2	2.51	0.44
1:C:329:PHE:CE2	1:C:331:TYR:HB3	2.53	0.44
1:B:179:VAL:O	1:B:180:HIS:C	2.56	0.44
1:D:288:LYS:HA	1:D:288:LYS:HD3	1.84	0.44
1:B:499:ILE:CG1	1:B:555:LYS:HE2	2.48	0.44
1:C:264:ASP:OD2	1:C:290:ARG:NH2	2.51	0.44
1:D:462:PRO:HA	1:D:578:PHE:CE1	2.52	0.44
1:A:385:MET:HG2	1:A:454:PHE:CE2	2.53	0.44
1:B:431:LEU:HD23	1:B:432:TYR:HE1	1.82	0.44
1:B:562:LEU:C	1:B:562:LEU:CD1	2.86	0.44
1:C:235:GLN:O	1:C:238:VAL:HG22	2.17	0.44
1:D:181:ALA:HB1	1:D:185:LYS:HZ2	1.84	0.43
1:D:260:ILE:O	1:D:264:ASP:HB2	2.19	0.43
1:A:312:LYS:HG2	1:A:315:TYR:OH	2.19	0.43
1:B:486:LYS:HE2	1:B:486:LYS:HB2	1.86	0.43
1:B:195:ASP:OD1	1:B:290:ARG:NE	2.45	0.43
1:C:468:ILE:HG12	1:C:548:GLN:NE2	2.34	0.43
1:D:250:ILE:O	1:D:254:MET:HG3	2.19	0.43
1:B:183:GLY:HA2	1:B:191:ILE:HD12	1.99	0.43
1:B:186:GLN:NE2	1:B:339:ARG:CZ	2.81	0.43
1:C:320:CYS:HB3	1:C:325:ILE:O	2.18	0.43
1:D:443:GLU:O	1:D:447:GLN:HG3	2.18	0.43
1:A:388:ASP:O	1:A:392:LYS:HG3	2.19	0.43
1:C:470:ARG:HA	1:C:473:TYR:CD1	2.54	0.43
1:D:156:VAL:O	2:H:802:GS:H8	2.18	0.43
1:D:576:ARG:HH11	1:D:576:ARG:HD3	1.72	0.43
1:C:204:LEU:HD23	1:C:204:LEU:HA	1.69	0.43
1:C:310:VAL:HG12	1:C:313:TRP:CZ3	2.54	0.43
1:A:564:ALA:O	1:A:568:TYR:HD1	2.02	0.42
1:B:195:ASP:OD1	1:B:290:ARG:NH2	2.51	0.42
1:D:232:THR:OG1	1:D:235:GLN:HG3	2.19	0.42
1:A:333:ARG:NH1	1:A:355:GLU:OE2	2.52	0.42
1:A:226:ARG:NH2	1:A:229:VAL:HG11	2.33	0.42
1:C:205:CYS:HB3	1:C:208:LEU:HD12	2.01	0.42
1:D:285:TRP:CE3	1:D:286:PRO:HD2	2.54	0.42
1:B:437:LYS:HA	1:B:437:LYS:HD2	1.91	0.42
1:D:353:ASP:N	1:D:353:ASP:OD1	2.52	0.42
1:B:329:PHE:CD1	1:B:362:MET:HB2	2.54	0.42
1:B:397:ILE:HD11	1:B:430:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:PRO:HD2	1:B:568:TYR:CD2	2.54	0.42
1:B:336:LYS:HE3	1:B:337:PHE:CE1	2.55	0.42
1:C:198:CYS:O	1:C:268:ILE:HG12	2.20	0.42
1:C:372:ARG:NH2	2:F:804:SC:S2P	2.92	0.42
1:D:305:ARG:HE	1:D:305:ARG:HB2	1.69	0.42
1:A:576:ARG:HE	1:A:576:ARG:HB3	1.57	0.42
1:B:223:PRO:HB3	1:B:470:ARG:HB3	2.02	0.42
1:C:380:ASN:O	1:C:384:THR:HG23	2.20	0.42
1:A:299:GLU:OE1	1:A:348:ARG:HD2	2.20	0.42
1:B:190:GLN:O	1:B:294:LYS:NZ	2.51	0.42
1:C:143:ARG:NH2	1:C:422:LEU:O	2.52	0.42
1:A:563:TYR:O	1:A:567:GLN:HG2	2.19	0.41
1:B:396:TYR:CG	1:B:437:LYS:HB3	2.55	0.41
1:C:178:LEU:HD12	1:C:335:ILE:HG23	2.02	0.41
1:A:170:GLY:HA3	1:A:314:ASP:OD2	2.19	0.41
1:A:176:GLY:HA2	1:A:179:VAL:HG12	2.02	0.41
1:A:194:ARG:HD3	1:A:258:GLY:O	2.20	0.41
1:B:397:ILE:HG13	1:B:438:LEU:HD21	2.02	0.41
1:A:331:TYR:CE1	1:A:332:LYS:HG3	2.55	0.41
1:B:483:ALA:HB2	1:B:572:TRP:CD1	2.55	0.41
1:C:267:PHE:HZ	1:C:297:LEU:HB3	1.85	0.41
1:D:483:ALA:HB1	1:D:571:GLN:CG	2.50	0.41
1:C:190:GLN:HB3	1:C:294:LYS:CE	2.50	0.41
1:C:263:GLU:O	1:C:264:ASP:OD1	2.39	0.41
1:A:212:PRO:HD2	1:A:217:PHE:CD1	2.56	0.41
1:B:260:ILE:HG21	1:B:263:GLU:HG2	1.99	0.41
1:C:197:LEU:O	1:C:201:ILE:HG13	2.20	0.41
1:D:178:LEU:O	1:D:182:LEU:HG	2.20	0.41
1:D:241:PHE:O	1:D:245:ILE:HG12	2.21	0.41
1:A:251:LYS:HE3	1:A:251:LYS:HB2	1.85	0.41
1:B:376:HIS:CE1	1:B:378:VAL:HB	2.55	0.41
1:C:190:GLN:O	1:C:192:SER:N	2.54	0.41
1:C:312:LYS:HA	1:C:315:TYR:CE2	2.56	0.41
1:C:468:ILE:HD11	1:C:578:PHE:HZ	1.86	0.41
1:A:339:ARG:HD3	1:A:521:TYR:CZ	2.56	0.41
1:C:269:LYS:O	1:C:273:VAL:HG12	2.20	0.41
1:A:312:LYS:HA	1:A:315:TYR:CE2	2.57	0.40
1:B:431:LEU:HD23	1:B:432:TYR:CE1	2.55	0.40
1:C:125:HIS:NE2	2:G:804:SC:OP1	2.54	0.40
1:C:389:ALA:HB2	1:C:444:ILE:HB	2.03	0.40
1:A:167:HIS:CE1	1:A:315:TYR:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLU:HG3	1:A:229:VAL:H	1.85	0.40
1:D:340:VAL:HA	1:D:348:ARG:O	2.20	0.40
1:D:476:LEU:HB3	1:D:500:VAL:HG11	2.03	0.40
1:A:228:GLU:H	1:A:228:GLU:HG2	1.33	0.40
1:D:412:ALA:HB3	1:D:422:LEU:HD22	2.03	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	418/533 (78%)	405 (97%)	13 (3%)	0	100	100
1	B	371/533 (70%)	353 (95%)	17 (5%)	1 (0%)	41	62
1	C	362/533 (68%)	349 (96%)	12 (3%)	1 (0%)	41	62
1	D	421/533 (79%)	413 (98%)	8 (2%)	0	100	100
All	All	1572/2132 (74%)	1520 (97%)	50 (3%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	558	ASP
1	C	291	PRO

5.3.2 Protein sidechains [i](#)

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	378/474 (80%)	373 (99%)	5 (1%)	69	85
1	B	337/474 (71%)	320 (95%)	17 (5%)	24	45
1	C	331/474 (70%)	321 (97%)	10 (3%)	41	65
1	D	382/474 (81%)	378 (99%)	4 (1%)	76	89
All	All	1428/1896 (75%)	1392 (98%)	36 (2%)	47	70

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	467	LYS
1	A	484	LYS
1	A	576	ARG
1	A	583	ASP
1	B	115	MET
1	B	116	LYS
1	B	134	ARG
1	B	177	CYS
1	B	178	LEU
1	B	242	GLU
1	B	262	GLU
1	B	271	GLN
1	B	292	GLU
1	B	315	TYR
1	B	475	SER
1	B	478	LYS
1	B	505	MET
1	B	553	TYR
1	B	558	ASP
1	B	562	LEU
1	B	571	GLN
1	C	194	ARG
1	C	265	ILE
1	C	266	CYS
1	C	290	ARG
1	C	293	ASN
1	C	309	ASP
1	C	328	ASN
1	C	359	LEU
1	C	360	TYR

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Mol	Chain	Res	Type
1	C	561	SER
1	D	461	GLN
1	D	463	THR
1	D	468	ILE
1	D	559	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	B	186	GLN
1	B	200	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 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	GS	G	802	2	18,24,25	1.20	2 (11%)	19,35,38	2.56	4 (21%)
2	GS	F	802	2	18,24,25	1.26	2 (11%)	19,35,38	2.62	4 (21%)
2	SC	E	801	2	15,17,21	0.83	0	17,24,31	0.99	1 (5%)
2	SC	F	803	2	15,20,21	0.80	0	17,28,31	0.98	1 (5%)
2	SC	F	801	2	8,8,21	0.40	0	9,10,31	0.63	0
2	SC	H	804	2	15,20,21	0.68	0	17,28,31	1.03	1 (5%)
2	SC	E	804	2	15,20,21	0.73	0	17,28,31	0.96	1 (5%)
2	SC	G	803	2	15,20,21	0.72	0	17,28,31	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SC	F	804	2	15,20,21	0.79	0	17,28,31	0.96	1 (5%)
2	GS	H	802	2	18,24,25	1.21	2 (11%)	19,35,38	2.52	4 (21%)
2	GS	E	802	2	18,24,25	1.11	2 (11%)	19,35,38	2.66	4 (21%)
2	SC	E	803	2	15,20,21	0.86	0	17,28,31	1.03	1 (5%)
2	SC	H	803	2	15,20,21	0.82	0	17,28,31	1.00	1 (5%)
2	SC	G	801	2	8,8,21	0.43	0	9,10,31	0.88	1 (11%)
2	SC	G	804	2	0,3,21	0.00	-	0,3,31	0.00	-
2	SC	H	801	2	15,17,21	0.78	0	17,24,31	0.99	1 (5%)

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	GS	G	802	2	-	0/2/21/22	0/3/3/3
2	GS	F	802	2	-	0/2/21/22	0/3/3/3
2	SC	E	801	2	-	3/3/18/22	0/2/2/2
2	SC	F	803	2	-	0/4/21/22	0/2/2/2
2	SC	F	801	2	-	0/2/12/22	0/1/1/2
2	SC	H	804	2	-	2/4/21/22	0/2/2/2
2	SC	E	804	2	-	1/4/21/22	0/2/2/2
2	SC	G	803	2	-	1/4/21/22	0/2/2/2
2	SC	F	804	2	-	1/4/21/22	0/2/2/2
2	GS	H	802	2	-	0/2/21/22	0/3/3/3
2	GS	E	802	2	-	0/2/21/22	0/3/3/3
2	SC	E	803	2	-	1/4/21/22	0/2/2/2
2	SC	H	803	2	-	1/4/21/22	0/2/2/2
2	SC	G	801	2	-	2/2/12/22	0/1/1/2
2	SC	H	801	2	-	1/3/18/22	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	802	GS	C6-N1	4.13	1.40	1.33
2	H	802	GS	C6-N1	3.80	1.39	1.33
2	G	802	GS	C6-N1	3.76	1.39	1.33
2	E	802	GS	C6-N1	3.19	1.38	1.33
2	H	802	GS	C8-N7	-2.46	1.30	1.34
2	E	802	GS	C8-N7	-2.34	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	802	GS	C8-N7	-2.30	1.30	1.34
2	F	802	GS	C8-N7	-2.12	1.30	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	802	GS	C5-C6-N1	-8.88	111.28	123.43
2	E	802	GS	C5-C6-N1	-8.66	111.59	123.43
2	G	802	GS	C5-C6-N1	-8.56	111.72	123.43
2	H	802	GS	C5-C6-N1	-8.53	111.76	123.43
2	E	802	GS	C6-N1-C2	5.95	125.39	115.93
2	F	802	GS	C6-N1-C2	5.63	124.88	115.93
2	G	802	GS	C6-N1-C2	5.55	124.75	115.93
2	H	802	GS	C6-N1-C2	5.41	124.52	115.93
2	H	804	SC	C2-N3-C4	3.87	120.26	116.34
2	E	803	SC	C2-N3-C4	3.79	120.18	116.34
2	F	803	SC	C2-N3-C4	3.76	120.15	116.34
2	H	803	SC	C2-N3-C4	3.72	120.11	116.34
2	G	803	SC	C2-N3-C4	3.68	120.07	116.34
2	F	804	SC	C2-N3-C4	3.65	120.04	116.34
2	E	804	SC	C2-N3-C4	3.63	120.02	116.34
2	H	801	SC	C2-N3-C4	3.60	119.99	116.34
2	E	801	SC	C2-N3-C4	3.51	119.90	116.34
2	E	802	GS	C2-N3-C4	-3.12	111.79	115.36
2	F	802	GS	C2-N3-C4	-3.06	111.86	115.36
2	G	802	GS	C2-N3-C4	-2.97	111.96	115.36
2	H	802	GS	C2-N3-C4	-2.82	112.14	115.36
2	E	802	GS	N3-C2-N1	-2.53	123.85	127.22
2	G	802	GS	N3-C2-N1	-2.33	124.12	127.22
2	G	801	SC	C1'-C2'-C3'	-2.29	100.63	103.20
2	F	802	GS	N3-C2-N1	-2.23	124.25	127.22
2	H	802	GS	N3-C2-N1	-2.15	124.36	127.22

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	801	SC	O4'-C1'-N1-C6
2	H	801	SC	O4'-C1'-N1-C6
2	E	803	SC	O4'-C1'-N1-C6
2	G	803	SC	O4'-C1'-N1-C6
2	H	803	SC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
2	E	804	SC	O4'-C1'-N1-C6
2	F	804	SC	O4'-C1'-N1-C6
2	H	804	SC	O4'-C1'-N1-C6
2	G	801	SC	C3'-C4'-C5'-O5'
2	G	801	SC	O4'-C4'-C5'-O5'
2	E	801	SC	C3'-C4'-C5'-O5'
2	E	801	SC	O4'-C4'-C5'-O5'
2	H	804	SC	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	802	GS	1	0
2	F	802	GS	1	0
2	F	803	SC	1	0
2	E	804	SC	3	0
2	F	804	SC	2	0
2	H	802	GS	1	0
2	E	802	GS	1	0
2	G	804	SC	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/533 (80%)	0.26	13 (3%) 50 46	46, 74, 133, 181	0
1	B	383/533 (71%)	0.75	54 (14%) 2 2	70, 112, 166, 192	0
1	C	376/533 (70%)	0.91	59 (15%) 2 1	65, 116, 166, 201	0
1	D	430/533 (80%)	0.36	13 (3%) 50 46	46, 79, 138, 175	0
2	E	0/5	-	-	-	-
2	F	0/5	-	-	-	-
2	G	0/5	-	-	-	-
2	H	0/5	-	-	-	-
All	All	1616/2152 (75%)	0.56	139 (8%) 10 8	46, 93, 159, 201	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	476	LEU	6.4
1	D	486	LYS	6.4
1	B	569	PHE	6.3
1	D	520	PHE	6.2
1	C	483	ALA	6.1
1	C	572	TRP	6.1
1	C	567	GLN	5.9
1	B	189	LEU	5.9
1	C	297	LEU	5.8
1	B	487	VAL	5.7
1	C	569	PHE	5.7
1	D	341	CYS	5.6
1	B	557	VAL	5.5
1	C	301	VAL	5.4
1	C	568	TYR	5.3
1	C	472	ASP	5.2
1	C	339	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	565	ALA	5.2
1	B	455	LYS	5.2
1	B	498	PHE	5.1
1	C	481	ALA	5.0
1	C	371	ARG	4.9
1	C	480	VAL	4.9
1	B	500	VAL	4.8
1	C	564	ALA	4.7
1	A	518	VAL	4.7
1	B	567	GLN	4.6
1	B	499	ILE	4.5
1	D	517	HIS	4.5
1	D	488	LEU	4.4
1	C	462	PRO	4.3
1	B	571	GLN	4.3
1	B	486	LYS	4.2
1	C	190	GLN	4.2
1	C	560	LYS	4.1
1	C	338	ALA	4.0
1	B	568	TYR	4.0
1	C	275	PRO	3.9
1	B	566	ARG	3.9
1	C	298	TYR	3.9
1	B	397	ILE	3.9
1	C	563	TYR	3.8
1	B	352	ARG	3.8
1	B	556	LYS	3.7
1	B	562	LEU	3.7
1	C	468	ILE	3.6
1	C	550	ILE	3.6
1	B	563	TYR	3.6
1	D	522	CYS	3.6
1	B	447	GLN	3.5
1	B	550	ILE	3.5
1	C	241	PHE	3.3
1	D	347	LEU	3.3
1	C	477	PRO	3.2
1	A	334	PHE	3.2
1	B	255	GLU	3.2
1	A	359	LEU	3.1
1	A	308	ILE	3.1
1	A	360	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	259	LEU	3.1
1	B	553	TYR	3.1
1	C	552	VAL	3.1
1	B	337	PHE	2.9
1	B	371	ARG	2.9
1	B	194	ARG	2.9
1	C	475	SER	2.9
1	B	485	PRO	2.8
1	B	549	LEU	2.8
1	C	566	ARG	2.8
1	B	444	ILE	2.8
1	C	272	ILE	2.8
1	C	185	LYS	2.8
1	B	502	VAL	2.8
1	C	498	PHE	2.8
1	C	294	LYS	2.7
1	B	351	ALA	2.7
1	B	363	PHE	2.7
1	B	454	PHE	2.7
1	B	503	ILE	2.7
1	B	574	ALA	2.6
1	A	260	ILE	2.6
1	C	191	ILE	2.6
1	C	296	PHE	2.6
1	B	505	MET	2.6
1	B	572	TRP	2.6
1	A	291	PRO	2.6
1	C	293	ASN	2.5
1	A	520	PHE	2.5
1	A	491	VAL	2.5
1	C	482	SER	2.5
1	C	575	ASP	2.5
1	B	573	CYS	2.5
1	B	305	ARG	2.5
1	B	484	LYS	2.5
1	A	182	LEU	2.5
1	B	570	VAL	2.4
1	C	578	PHE	2.4
1	B	308	ILE	2.4
1	B	409	ILE	2.4
1	B	366	ARG	2.4
1	C	359	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	196	VAL	2.4
1	B	450	TYR	2.4
1	C	355	GLU	2.4
1	B	224	LEU	2.4
1	B	296	PHE	2.3
1	B	418	ALA	2.3
1	B	339	ARG	2.3
1	C	471	GLU	2.3
1	B	288	LYS	2.3
1	C	473	TYR	2.3
1	C	263	GLU	2.3
1	C	570	VAL	2.3
1	D	308	ILE	2.3
1	C	460	THR	2.3
1	C	335	ILE	2.3
1	B	560	LYS	2.3
1	C	324	GLY	2.2
1	C	326	GLN	2.2
1	C	561	SER	2.2
1	B	260	ILE	2.2
1	A	362	MET	2.2
1	B	480	VAL	2.1
1	C	337	PHE	2.1
1	D	286	PRO	2.1
1	C	131	LEU	2.1
1	C	179	VAL	2.1
1	D	515	ILE	2.1
1	B	177	CYS	2.1
1	A	326	GLN	2.1
1	C	260	ILE	2.1
1	C	253	VAL	2.1
1	C	291	PRO	2.1
1	C	439	LYS	2.1
1	D	342	GLU	2.1
1	D	546	ALA	2.0
1	D	487	VAL	2.0
1	C	499	ILE	2.0
1	A	296	PHE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SC	F	804	19/20	0.71	0.25	149,166,176,185	0
2	SC	E	804	19/20	0.84	0.22	105,135,150,155	0
2	SC	H	804	19/20	0.88	0.15	127,146,157,158	0
2	SC	G	801	8/20	0.92	0.10	133,141,145,146	0
2	SC	G	804	4/20	0.93	0.12	157,157,158,160	0
2	SC	G	803	19/20	0.93	0.17	115,152,173,175	0
2	SC	E	801	16/20	0.93	0.19	80,122,143,144	0
2	SC	H	801	16/20	0.94	0.21	85,118,149,149	0
2	GS	G	802	22/23	0.95	0.11	105,113,125,146	0
2	SC	F	801	8/20	0.95	0.18	106,122,127,131	0
2	SC	F	803	19/20	0.95	0.14	105,122,134,154	0
2	SC	H	803	19/20	0.95	0.14	72,113,130,133	0
2	GS	F	802	22/23	0.96	0.17	81,94,101,123	0
2	SC	E	803	19/20	0.97	0.16	74,112,125,128	1
2	GS	H	802	22/23	0.97	0.14	54,62,72,82	0
2	GS	E	802	22/23	0.98	0.19	58,70,75,94	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	D	701	1/1	0.87	0.12	106,106,106,106	1
3	ZN	A	701	1/1	0.89	0.11	89,89,89,89	1
3	ZN	C	701	1/1	0.92	0.10	146,146,146,146	0
3	ZN	B	701	1/1	0.92	0.14	99,99,99,99	1

6.5 Other polymers [i](#)

There are no such residues in this entry.