



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:57 PM UTC

PDB ID : 7ZVY / pdb_00007zvy
Title : Thermococcus kadokarensis phosphomannose isomerase
Authors : Hoh, f.; Calio, A.
Deposited on : 2022-05-17
Resolution : 2.16 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

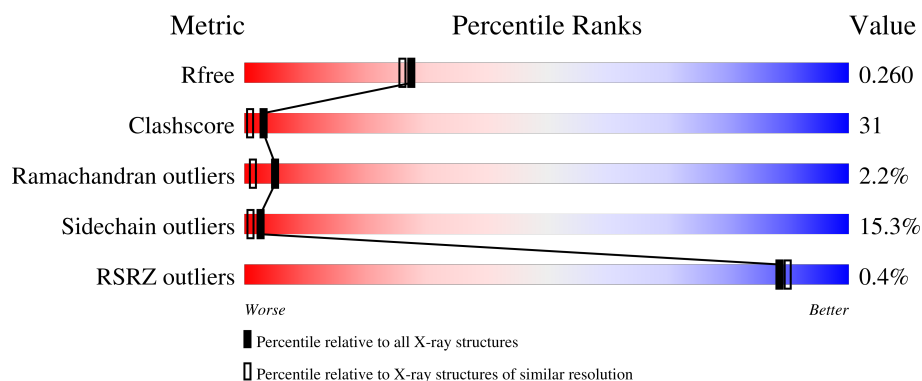
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	116	
1	C	116	
1	D	116	
1	F	116	
2	B	114	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	110	41%43%13%•
3	H	110	35%45%7%13%
4	G	105	39%40%16%••

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7172 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 Cupin_2 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	0	0
			931	607	156	167	1			
1	C	112	Total	C	N	O	S	0	0	0
			931	607	156	167	1			
1	D	112	Total	C	N	O	S	0	0	0
			931	607	156	167	1			
1	F	107	Total	C	N	O	S	0	0	0
			888	578	150	159	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	GLY	-	expression tag	UNP Q5JD98
A	115	SER	-	expression tag	UNP Q5JD98
A	116	PHE	-	expression tag	UNP Q5JD98
C	114	GLY	-	expression tag	UNP Q5JD98
C	115	SER	-	expression tag	UNP Q5JD98
C	116	PHE	-	expression tag	UNP Q5JD98
D	114	GLY	-	expression tag	UNP Q5JD98
D	115	SER	-	expression tag	UNP Q5JD98
D	116	PHE	-	expression tag	UNP Q5JD98
F	114	GLY	-	expression tag	UNP Q5JD98
F	115	SER	-	expression tag	UNP Q5JD98
F	116	PHE	-	expression tag	UNP Q5JD98

- Molecule 2 is a protein called Cupin_2 domain-containing protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	110	Total	C	N	O	0	0	0
			914	596	153	165			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	GLY	-	expression tag	UNP Q5JD98
B	115	SER	-	expression tag	UNP Q5JD98
B	116	PHE	-	expression tag	UNP Q5JD98

- Molecule 3 is a protein called Cupin_2 domain-containing protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	106	Total	C	N	O	0	0	0
			883	576	148	159			
3	H	96	Total	C	N	O	0	0	0
			800	524	136	140			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	GLY	-	expression tag	UNP Q5JD98
E	115	SER	-	expression tag	UNP Q5JD98
E	116	PHE	-	expression tag	UNP Q5JD98
H	114	GLY	-	expression tag	UNP Q5JD98
H	115	SER	-	expression tag	UNP Q5JD98
H	116	PHE	-	expression tag	UNP Q5JD98

- Molecule 4 is a protein called Cupin_2 domain-containing protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	101	Total	C	N	O	0	0	0
			840	550	139	151			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	114	GLY	-	expression tag	UNP Q5JD98
G	115	SER	-	expression tag	UNP Q5JD98
G	116	PHE	-	expression tag	UNP Q5JD98

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	F	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Zn	0	0
			1	1		

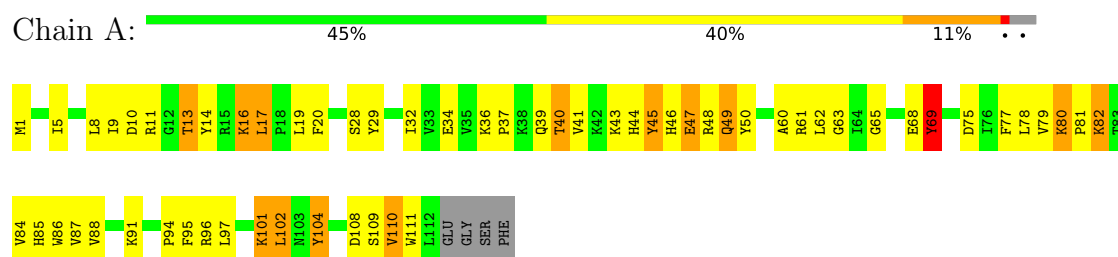
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		
6	B	6	Total	O	0	0
			6	6		
6	C	3	Total	O	0	0
			3	3		
6	D	5	Total	O	0	0
			5	5		
6	E	5	Total	O	0	0
			5	5		
6	F	13	Total	O	0	0
			13	13		
6	G	4	Total	O	0	0
			4	4		
6	H	3	Total	O	0	0
			3	3		

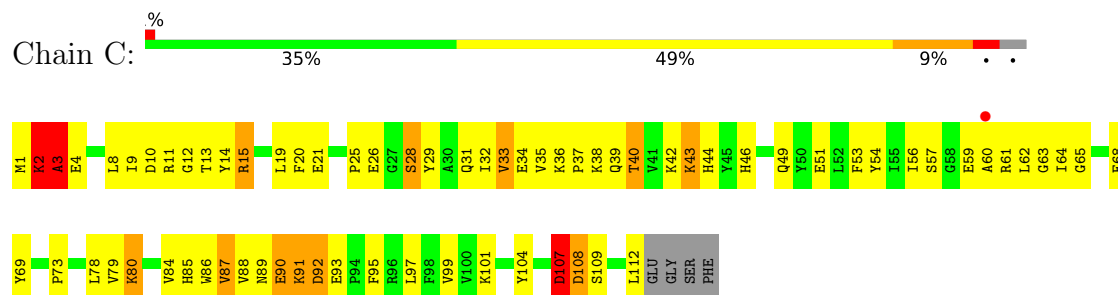
3 Residue-property plots [i](#)

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.

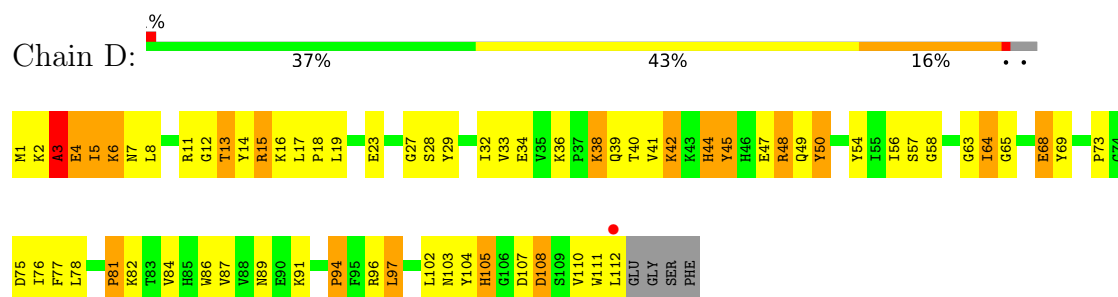
• Molecule 1: Cupin_2 domain-containing protein



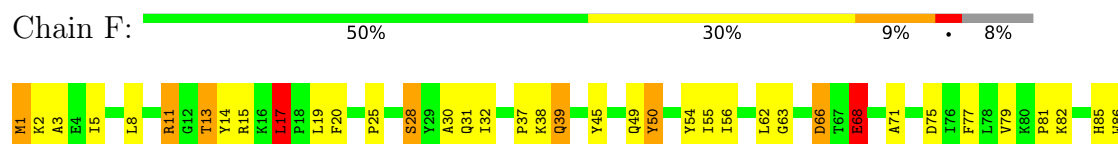
• Molecule 1: Cupin_2 domain-containing protein



• Molecule 1: Cupin_2 domain-containing protein

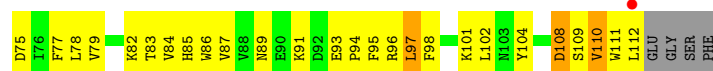
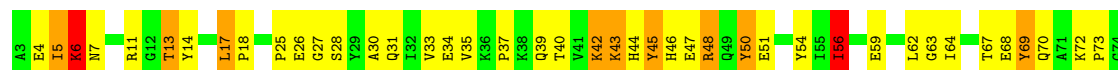


• Molecule 1: Cupin_2 domain-containing protein

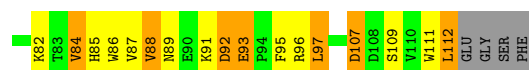




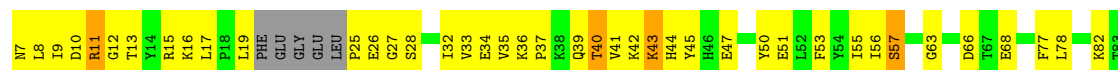
• Molecule 2: Cupin_2 domain-containing protein



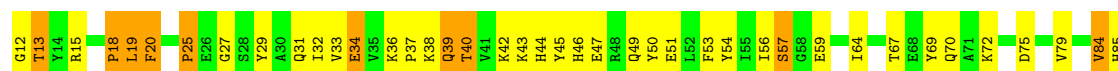
• Molecule 3: Cupin_2 domain-containing protein



• Molecule 3: Cupin_2 domain-containing protein



• Molecule 4: Cupin_2 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	91.16Å 91.16Å 113.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.79 – 2.16 64.79 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.1 (64.79-2.16) 98.3 (64.79-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.221 , 0.289 0.236 , 0.260	Depositor DCC
R_{free} test set	2731 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l 0.469 for h,-h-k,-l 0.470 for -k,-h,-l	Xtriage
Reported twinning fraction	0.288 for H, K, L 0.235 for K, H, -L 0.243 for -h,-k,l 0.233 for -K, -H, -L	Depositor
Outliers	0 of 55488 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7172	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.17	4/956 (0.4%)	1.60	11/1291 (0.9%)
1	C	1.48	6/956 (0.6%)	1.37	3/1291 (0.2%)
1	D	1.26	8/956 (0.8%)	1.52	8/1291 (0.6%)
1	F	1.12	2/911 (0.2%)	1.41	3/1228 (0.2%)
2	B	1.18	2/939 (0.2%)	1.42	4/1270 (0.3%)
3	E	1.12	2/908 (0.2%)	1.36	3/1229 (0.2%)
3	H	1.08	0/820	1.35	2/1106 (0.2%)
4	G	1.20	5/865 (0.6%)	1.48	5/1171 (0.4%)
All	All	1.21	29/7311 (0.4%)	1.44	39/9877 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
3	E	0	1
All	All	0	3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	107	ASP	CG-OD1	27.54	1.77	1.25
3	E	107	ASP	CG-OD2	10.26	1.44	1.25
1	D	64	ILE	C-O	8.53	1.32	1.24
1	C	107	ASP	CG-OD2	8.52	1.41	1.25
1	C	3	ALA	C-O	7.71	1.33	1.24
1	C	108	ASP	C-O	7.28	1.32	1.24
2	B	45	TYR	C-O	7.19	1.32	1.23
1	D	57	SER	C-O	7.13	1.32	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ARG	C-O	7.07	1.33	1.24
1	D	44	HIS	C-O	6.60	1.31	1.23
4	G	107	ASP	CG-OD2	6.57	1.37	1.25
1	D	94	PRO	C-O	-6.53	1.16	1.23
4	G	87	VAL	C-O	6.46	1.30	1.24
1	D	105	HIS	CE1-NE2	6.30	1.38	1.32
3	E	43	LYS	C-O	6.21	1.31	1.23
2	B	43	LYS	C-O	6.13	1.30	1.23
4	G	75	ASP	C-O	6.12	1.31	1.23
4	G	107	ASP	CG-OD1	6.01	1.36	1.25
1	D	45	TYR	C-O	5.86	1.30	1.23
1	C	108	ASP	C-N	5.78	1.41	1.33
1	A	82	LYS	C-O	5.61	1.31	1.23
1	D	68	GLU	C-O	-5.46	1.17	1.24
1	A	94	PRO	C-O	-5.37	1.17	1.23
1	A	43	LYS	C-O	5.37	1.30	1.23
4	G	109	SER	C-O	5.18	1.30	1.24
1	F	68	GLU	C-O	-5.15	1.17	1.24
1	F	66	ASP	CG-OD1	5.11	1.35	1.25
1	C	4	GLU	C-O	5.05	1.29	1.24
1	D	44	HIS	CE1-NE2	5.02	1.37	1.32

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	THR	CA-CB-OG1	-14.02	88.57	109.60
1	A	48	ARG	CB-CG-CD	-9.60	89.21	111.30
1	A	48	ARG	CB-CA-C	-8.69	94.80	109.75
1	D	81	PRO	N-CA-C	-7.12	101.25	111.22
1	A	40	THR	OG1-CB-CG2	7.08	123.47	109.30
1	A	17	LEU	O-C-N	-7.01	114.94	121.32
1	C	107	ASP	CB-CG-OD1	-6.98	102.35	118.40
4	G	18	PRO	CB-CA-C	-6.69	102.83	111.46
2	B	108	ASP	N-CA-C	-6.35	102.80	111.56
3	E	109	SER	CA-C-N	6.33	130.29	122.37
3	E	109	SER	C-N-CA	6.33	130.29	122.37
3	H	112	LEU	CA-C-O	-6.28	110.12	120.80
4	G	70	GLN	CA-C-O	-6.26	115.17	122.37
1	A	80	LYS	CB-CA-C	6.04	120.35	109.61
1	D	38	LYS	CB-CG-CD	-6.01	97.48	111.30
1	D	108	ASP	N-CA-C	-5.84	106.00	114.12
1	A	69	TYR	N-CA-C	-5.80	103.04	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	112	LEU	CA-C-O	-5.80	110.94	120.80
1	C	43	LYS	O-C-N	5.74	130.08	123.02
1	F	11	ARG	N-CA-C	-5.71	104.53	112.30
4	G	54	TYR	CA-C-O	-5.67	114.23	120.30
1	F	17	LEU	O-C-N	-5.59	116.24	121.32
1	A	20	PHE	CB-CA-C	-5.57	103.82	111.73
1	A	13	THR	N-CA-C	-5.53	106.38	113.01
1	D	3	ALA	CA-C-N	5.48	132.01	121.54
1	D	3	ALA	C-N-CA	5.48	132.01	121.54
1	A	48	ARG	CA-C-N	-5.41	112.41	121.39
1	A	48	ARG	C-N-CA	-5.41	112.41	121.39
2	B	95	PHE	CB-CA-C	5.38	118.91	110.19
4	G	112	LEU	CA-C-O	-5.37	111.66	120.80
1	F	90	GLU	N-CA-C	-5.33	106.82	113.38
1	D	56	ILE	N-CA-C	-5.33	106.61	111.67
2	B	89	ASN	CA-CB-CG	-5.25	107.35	112.60
4	G	108	ASP	CA-CB-CG	5.22	117.82	112.60
3	H	98	PHE	N-CA-C	-5.21	100.74	109.24
1	D	19	LEU	O-C-N	5.21	129.63	123.33
1	C	42	LYS	CB-CA-C	-5.18	102.11	112.99
2	B	56	ILE	N-CA-C	-5.17	106.76	111.67
1	D	29	TYR	CB-CA-C	5.10	118.20	109.99

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	107	ASP	Sidechain
1	C	53	PHE	Peptide
3	E	107	ASP	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	931	0	934	54	0
1	C	931	0	934	66	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	931	0	934	88	0
1	F	888	0	895	47	2
2	B	914	0	909	54	2
3	E	883	0	874	48	0
3	H	800	0	811	72	0
4	G	840	0	829	56	0
5	A	2	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	A	11	0	0	0	0
6	B	6	0	0	2	0
6	C	3	0	0	0	0
6	D	5	0	0	1	0
6	E	5	0	0	1	0
6	F	13	0	0	1	0
6	G	4	0	0	1	0
6	H	3	0	0	0	0
All	All	7172	0	7120	444	2

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 31.

All (444) 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)
3:H:8:LEU:CD1	3:H:17:LEU:HD21	1.54	1.35
1:C:107:ASP:CG	1:C:107:ASP:OD1	1.77	1.23
1:D:4:GLU:O	1:D:5:ILE:HG12	1.41	1.20
3:H:8:LEU:HD11	3:H:17:LEU:HD21	1.15	1.10
1:F:102:LEU:HD13	3:H:28:SER:HB3	1.38	1.06
1:C:80:LYS:NZ	1:D:1:MET:HG2	1.77	0.99
3:H:8:LEU:CD1	3:H:17:LEU:CD2	2.40	0.98
4:G:29:TYR:HE2	4:G:31:GLN:HE21	1.08	0.94
1:F:79:VAL:HG11	1:F:85:HIS:ND1	1.83	0.93
1:D:4:GLU:OE2	1:D:6:LYS:HD2	1.69	0.93
1:A:47:GLU:HB2	1:A:108:ASP:HB2	1.52	0.91
1:C:8:LEU:HD11	1:C:15:ARG:HD3	1.51	0.91
4:G:29:TYR:HE2	4:G:31:GLN:NE2	1.66	0.91
2:B:13:THR:HG21	2:B:42:LYS:HZ2	1.40	0.86
2:B:44:HIS:O	2:B:84:VAL:HA	1.76	0.86
3:H:40:THR:HB	3:H:88:VAL:HG22	1.57	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:GLU:CD	1:D:6:LYS:HD2	2.02	0.84
2:B:4:GLU:HB3	2:B:6:LYS:HE3	1.60	0.83
1:C:80:LYS:HZ1	1:D:1:MET:HG2	1.39	0.82
1:D:4:GLU:O	1:D:5:ILE:CG1	2.26	0.81
2:B:37:PRO:O	2:B:39:GLN:NE2	2.13	0.81
3:E:8:LEU:HD11	3:E:15:ARG:HB3	1.61	0.81
4:G:29:TYR:CE2	4:G:31:GLN:NE2	2.45	0.80
2:B:44:HIS:HA	2:B:111:TRP:HA	1.62	0.80
3:H:8:LEU:HD12	3:H:17:LEU:HD21	1.60	0.79
1:D:42:LYS:CD	1:D:42:LYS:H	1.96	0.79
2:B:83:THR:HG23	6:B:205:HOH:O	1.82	0.79
1:D:42:LYS:H	1:D:42:LYS:HD2	1.48	0.78
4:G:43:LYS:HD3	4:G:86:TRP:CE3	2.19	0.78
3:H:9:ILE:HD12	3:H:16:LYS:HE3	1.66	0.77
1:D:4:GLU:CG	1:D:6:LYS:HD2	2.15	0.77
1:A:79:VAL:HG11	1:A:85:HIS:ND1	2.00	0.77
1:D:5:ILE:O	1:D:7:ASN:N	2.15	0.76
3:E:40:THR:HB	3:E:88:VAL:HG22	1.68	0.76
2:B:13:THR:HG21	2:B:42:LYS:NZ	2.01	0.76
1:D:4:GLU:HG3	1:D:6:LYS:HD2	1.69	0.75
3:H:8:LEU:HD12	3:H:17:LEU:CD2	2.13	0.75
1:D:63:GLY:HA3	1:D:86:TRP:CZ2	2.23	0.74
4:G:56:ILE:HG22	4:G:57:SER:OG	1.87	0.74
1:A:28:SER:OG	4:G:102:LEU:HD13	1.88	0.74
1:C:11:ARG:O	1:C:13:THR:N	2.20	0.73
1:F:79:VAL:HG11	1:F:85:HIS:HD1	1.54	0.72
2:B:109:SER:HB3	2:B:111:TRP:HE1	1.54	0.72
3:E:15:ARG:HG3	3:E:36:LYS:HE3	1.70	0.72
1:F:45:TYR:CD1	1:F:82:LYS:HA	2.23	0.72
3:H:8:LEU:HD11	3:H:17:LEU:CD2	2.07	0.72
3:H:8:LEU:CG	3:H:17:LEU:HD21	2.19	0.72
1:D:4:GLU:HG3	1:D:6:LYS:CD	2.20	0.72
3:E:19:LEU:HD21	3:E:32:ILE:HD13	1.71	0.72
1:F:13:THR:HG21	6:F:306:HOH:O	1.89	0.71
1:C:80:LYS:HZ1	1:D:1:MET:CG	2.03	0.70
1:C:9:ILE:HG22	1:C:11:ARG:HD3	1.74	0.70
2:B:45:TYR:CE2	2:B:110:VAL:HB	2.26	0.69
1:F:37:PRO:O	1:F:39:GLN:OE1	2.10	0.69
4:G:51:GLU:OE2	4:G:101:LYS:NZ	2.26	0.69
1:D:13:THR:HG21	1:D:42:LYS:HZ2	1.57	0.69
1:D:97:LEU:N	1:D:97:LEU:HD23	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:GLN:HE21	1:C:33:VAL:CG1	2.06	0.68
3:H:9:ILE:HD12	3:H:16:LYS:CE	2.24	0.68
4:G:27:GLY:O	4:G:104:TYR:HB3	1.93	0.68
1:F:5:ILE:HD12	1:F:5:ILE:O	1.95	0.67
3:H:37:PRO:HB3	3:H:92:ASP:O	1.93	0.67
1:D:4:GLU:C	1:D:5:ILE:HG12	2.19	0.67
2:B:84:VAL:HG23	2:B:112:LEU:HD13	1.77	0.66
1:D:75:ASP:HB3	1:D:77:PHE:CE1	2.30	0.66
3:H:9:ILE:CD1	3:H:16:LYS:HE3	2.26	0.65
1:D:34:GLU:HG2	1:D:96:ARG:HG2	1.79	0.65
1:F:97:LEU:N	1:F:97:LEU:HD23	2.12	0.65
1:C:40:THR:HB	1:C:88:VAL:HG22	1.79	0.65
1:F:75:ASP:HB3	1:F:77:PHE:CE2	2.32	0.65
3:H:9:ILE:CD1	3:H:16:LYS:CE	2.75	0.65
3:H:19:LEU:HD11	3:H:32:ILE:CD1	2.27	0.65
2:B:13:THR:CG2	2:B:14:TYR:HD1	2.10	0.64
3:H:43:LYS:HD2	3:H:84:VAL:HG11	1.79	0.64
4:G:46:HIS:NE2	4:G:51:GLU:OE1	2.26	0.64
1:F:1:MET:N	3:H:78:LEU:O	2.31	0.64
1:C:46:HIS:NE2	1:C:51:GLU:OE1	2.25	0.63
3:E:56:ILE:HG22	3:E:57:SER:OG	1.99	0.63
1:A:29:TYR:HB3	1:A:101:LYS:HG3	1.80	0.63
1:C:56:ILE:O	1:C:73:PRO:HB3	1.99	0.63
3:H:13:THR:HA	3:H:39:GLN:OE1	1.99	0.63
3:E:8:LEU:CD1	3:E:17:LEU:HG	2.28	0.62
3:H:90:GLU:HB2	3:H:91:LYS:HZ3	1.64	0.62
1:C:46:HIS:HE2	1:C:51:GLU:CD	2.07	0.62
2:B:44:HIS:HB3	2:B:111:TRP:CD2	2.33	0.62
1:C:44:HIS:O	1:C:84:VAL:HA	1.99	0.62
1:F:45:TYR:HD1	1:F:82:LYS:HA	1.62	0.62
1:D:4:GLU:OE2	1:D:6:LYS:CD	2.45	0.62
3:H:12:GLY:O	3:H:36:LYS:NZ	2.27	0.62
1:A:63:GLY:O	1:A:85:HIS:HA	2.00	0.62
3:H:97:LEU:HD12	3:H:99:VAL:HG22	1.81	0.62
1:C:10:ASP:C	1:C:11:ARG:HD2	2.25	0.61
3:H:7:ASN:O	3:H:17:LEU:HD23	2.00	0.61
3:E:44:HIS:HB3	3:E:111:TRP:CE3	2.36	0.61
2:B:34:GLU:HG2	2:B:96:ARG:HG2	1.81	0.61
1:F:28:SER:OG	3:H:102:LEU:HD13	2.01	0.61
1:A:5:ILE:HD11	1:A:32:ILE:HG13	1.81	0.60
4:G:18:PRO:HA	4:G:31:GLN:HB3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:GLN:HB3	1:F:104:TYR:HA	1.81	0.60
1:C:64:ILE:HG13	1:C:69:TYR:HE1	1.66	0.60
2:B:45:TYR:CZ	2:B:110:VAL:HB	2.36	0.60
4:G:51:GLU:HB2	4:G:79:VAL:HB	1.82	0.60
3:E:63:GLY:HA3	3:E:86:TRP:CZ2	2.37	0.60
1:A:45:TYR:CD1	1:A:82:LYS:HA	2.36	0.59
2:B:13:THR:HG23	2:B:14:TYR:HD1	1.67	0.59
1:C:80:LYS:HZ2	1:D:1:MET:HG2	1.67	0.59
1:F:79:VAL:HG11	1:F:85:HIS:CE1	2.36	0.59
1:C:36:LYS:HB2	1:C:39:GLN:HG3	1.84	0.59
3:H:15:ARG:NH1	3:H:34:GLU:OE1	2.26	0.59
2:B:42:LYS:HB2	2:B:111:TRP:HE3	1.67	0.59
2:B:50:TYR:HD2	2:B:78:LEU:HD11	1.67	0.59
1:C:80:LYS:NZ	1:D:1:MET:CG	2.60	0.59
1:D:42:LYS:HD2	1:D:42:LYS:N	2.17	0.58
1:F:105:HIS:O	1:F:106:GLY:C	2.45	0.58
4:G:37:PRO:HB3	4:G:92:ASP:O	2.02	0.58
3:H:47:GLU:O	3:H:82:LYS:HE3	2.02	0.57
3:E:20:PHE:O	3:E:23:GLU:HB2	2.03	0.57
1:F:79:VAL:CG1	1:F:85:HIS:HD1	2.18	0.57
2:B:4:GLU:HB3	2:B:6:LYS:CE	2.33	0.57
3:H:51:GLU:HB3	3:H:53:PHE:CE1	2.40	0.57
3:E:19:LEU:HD21	3:E:32:ILE:CD1	2.34	0.57
3:H:9:ILE:HD13	3:H:16:LYS:HE2	1.86	0.57
1:D:41:VAL:HG13	1:D:111:TRP:HH2	1.70	0.56
1:D:63:GLY:HA2	1:D:68:GLU:HA	1.86	0.56
2:B:31:GLN:HE22	2:B:101:LYS:HE3	1.70	0.56
1:F:11:ARG:O	1:F:13:THR:N	2.28	0.56
1:D:42:LYS:HD3	1:D:111:TRP:CZ3	2.40	0.56
4:G:44:HIS:CE1	4:G:85:HIS:CD2	2.93	0.56
3:H:68:GLU:HG3	3:H:86:TRP:CZ2	2.41	0.56
1:D:5:ILE:C	1:D:7:ASN:H	2.11	0.56
1:D:27:GLY:HA2	1:D:104:TYR:O	2.06	0.56
1:A:5:ILE:HG12	1:A:19:LEU:HD21	1.88	0.56
1:A:44:HIS:HB3	1:A:111:TRP:CD2	2.41	0.56
1:A:10:ASP:O	1:A:11:ARG:HD3	2.06	0.56
4:G:15:ARG:HD2	4:G:34:GLU:HB3	1.87	0.56
2:B:27:GLY:HA2	2:B:104:TYR:O	2.06	0.55
1:C:38:LYS:HG2	1:C:90:GLU:O	2.05	0.55
2:B:63:GLY:HA3	2:B:86:TRP:CE2	2.41	0.55
1:D:13:THR:HG21	1:D:42:LYS:NZ	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ARG:NH1	1:D:105:HIS:HD2	2.03	0.55
4:G:46:HIS:HB3	4:G:108:ASP:OD1	2.05	0.55
2:B:30:ALA:O	2:B:31:GLN:HB3	2.07	0.55
3:H:42:LYS:HE2	3:H:111:TRP:CZ3	2.41	0.55
4:G:12:GLY:N	6:G:301:HOH:O	2.38	0.55
1:A:9:ILE:HB	1:A:16:LYS:HG2	1.89	0.55
1:A:44:HIS:HA	1:A:111:TRP:HA	1.89	0.55
3:H:9:ILE:CD1	3:H:16:LYS:HE2	2.37	0.55
1:C:46:HIS:NE2	1:C:51:GLU:CD	2.65	0.54
3:E:89:ASN:ND2	3:E:93:GLU:O	2.39	0.54
1:D:48:ARG:NH1	1:D:48:ARG:HB2	2.23	0.54
1:D:13:THR:CG2	1:D:14:TYR:HD1	2.21	0.54
3:E:44:HIS:O	3:E:84:VAL:HA	2.08	0.54
1:D:4:GLU:CG	1:D:6:LYS:CD	2.84	0.54
1:F:103:ASN:O	1:F:103:ASN:ND2	2.32	0.54
2:B:7:ASN:O	2:B:18:PRO:HD2	2.08	0.54
4:G:38:LYS:HD3	4:G:90:GLU:C	2.32	0.54
1:D:44:HIS:O	1:D:84:VAL:HA	2.07	0.53
3:E:8:LEU:HD13	3:E:17:LEU:HG	1.90	0.53
1:D:65:GLY:N	1:D:84:VAL:O	2.38	0.53
1:D:63:GLY:HA3	1:D:86:TRP:CE2	2.43	0.53
4:G:19:LEU:HD21	4:G:32:ILE:HD13	1.90	0.53
4:G:20:PHE:CD1	4:G:20:PHE:N	2.76	0.53
1:A:37:PRO:O	1:A:39:GLN:HG2	2.09	0.53
1:F:5:ILE:O	1:F:5:ILE:CD1	2.56	0.53
2:B:79:VAL:HG11	2:B:85:HIS:CE1	2.44	0.53
3:E:19:LEU:HD22	3:E:31:GLN:HA	1.91	0.53
3:H:40:THR:CB	3:H:88:VAL:HG22	2.33	0.53
1:C:25:PRO:HD3	1:D:50:TYR:CD2	2.44	0.52
1:D:41:VAL:N	1:D:87:VAL:O	2.39	0.52
1:A:50:TYR:HD1	1:A:78:LEU:HD11	1.74	0.52
3:E:7:ASN:N	6:E:201:HOH:O	2.41	0.52
4:G:42:LYS:HE2	4:G:111:TRP:CZ3	2.43	0.52
1:A:1:MET:SD	4:G:64:ILE:HB	2.50	0.52
1:A:50:TYR:CE1	4:G:25:PRO:HD3	2.45	0.52
1:D:4:GLU:HG2	1:D:5:ILE:N	2.25	0.52
1:D:45:TYR:HD2	1:D:112:LEU:HD11	1.75	0.52
1:D:4:GLU:OE2	1:D:6:LYS:HB2	2.09	0.52
1:C:44:HIS:NE2	1:C:85:HIS:NE2	2.58	0.52
1:A:47:GLU:HG2	1:A:108:ASP:O	2.10	0.52
1:A:69:TYR:CD2	1:A:69:TYR:N	2.77	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LYS:HB2	1:C:112:LEU:HB2	1.91	0.52
1:D:42:LYS:CD	1:D:42:LYS:N	2.70	0.52
1:A:1:MET:SD	4:G:64:ILE:O	2.68	0.52
1:A:34:GLU:CG	1:A:96:ARG:HG2	2.40	0.52
4:G:20:PHE:N	4:G:20:PHE:HD1	2.08	0.52
2:B:45:TYR:HD2	2:B:112:LEU:HD11	1.75	0.51
3:H:27:GLY:O	3:H:102:LEU:HA	2.09	0.51
3:E:75:ASP:HB3	3:E:77:PHE:CE2	2.45	0.51
1:F:50:TYR:CE2	1:F:81:PRO:HG3	2.45	0.51
4:G:49:GLN:OE1	4:G:101:LYS:HD3	2.09	0.51
2:B:94:PRO:HG3	6:B:204:HOH:O	2.10	0.51
1:C:80:LYS:H	1:C:80:LYS:HZ3	1.59	0.51
4:G:13:THR:HG21	4:G:42:LYS:NZ	2.25	0.51
3:H:8:LEU:HG	3:H:17:LEU:CG	2.40	0.51
3:H:9:ILE:HB	3:H:16:LYS:HB3	1.91	0.51
1:C:29:TYR:HE1	1:C:31:GLN:OE1	1.93	0.51
1:D:103:ASN:O	1:D:105:HIS:CD2	2.64	0.51
3:E:70:GLN:O	3:E:72:LYS:HD2	2.11	0.51
3:H:15:ARG:HH11	3:H:34:GLU:CD	2.17	0.51
2:B:54:TYR:HB3	2:B:98:PHE:HB3	1.93	0.51
1:D:11:ARG:O	1:D:13:THR:N	2.43	0.51
3:E:8:LEU:HD13	3:E:17:LEU:CG	2.40	0.51
3:E:46:HIS:HD2	3:E:85:HIS:HE1	1.59	0.51
1:F:8:LEU:HA	1:F:17:LEU:HD23	1.93	0.51
1:C:29:TYR:HB2	1:C:104:TYR:CD1	2.46	0.51
4:G:43:LYS:HD2	4:G:84:VAL:HG11	1.93	0.51
1:A:34:GLU:HG2	1:A:96:ARG:HG2	1.93	0.51
3:H:8:LEU:HG	3:H:17:LEU:HG	1.93	0.51
2:B:11:ARG:HG2	2:B:14:TYR:CE1	2.47	0.50
1:C:8:LEU:C	1:C:9:ILE:HD12	2.36	0.50
3:H:10:ASP:C	3:H:12:GLY:H	2.19	0.50
1:A:14:TYR:HB2	1:A:34:GLU:O	2.10	0.50
1:C:1:MET:N	1:D:78:LEU:O	2.44	0.50
1:C:63:GLY:HA2	1:C:68:GLU:HA	1.93	0.50
4:G:47:GLU:HG3	4:G:108:ASP:HB2	1.92	0.50
1:C:35:VAL:HB	1:C:95:PHE:HB3	1.94	0.50
3:H:19:LEU:HD11	3:H:32:ILE:HD12	1.92	0.50
3:H:45:TYR:CD2	3:H:82:LYS:HA	2.47	0.50
1:A:5:ILE:O	1:A:5:ILE:HG22	2.10	0.50
1:D:64:ILE:HD12	1:D:69:TYR:CE1	2.47	0.50
1:C:25:PRO:HD3	1:D:50:TYR:CE2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LYS:CE	1:D:1:MET:HG2	2.42	0.50
3:E:15:ARG:CZ	3:E:36:LYS:HD3	2.42	0.50
2:B:51:GLU:OE1	2:B:85:HIS:NE2	2.45	0.50
2:B:79:VAL:HG11	2:B:85:HIS:ND1	2.27	0.50
1:D:50:TYR:CE1	1:D:81:PRO:HD3	2.46	0.50
4:G:50:TYR:HB2	4:G:102:LEU:HB2	1.93	0.50
3:E:48:ARG:HB3	3:E:48:ARG:CZ	2.42	0.50
3:H:63:GLY:HA3	3:H:86:TRP:CZ2	2.47	0.49
2:B:42:LYS:HD2	2:B:111:TRP:CZ3	2.47	0.49
4:G:34:GLU:HG3	4:G:96:ARG:HG2	1.94	0.49
1:C:54:TYR:CE1	1:D:54:TYR:CE1	3.00	0.49
1:A:49:GLN:NE2	1:A:104:TYR:HD2	2.09	0.49
1:C:19:LEU:HD22	1:C:31:GLN:HA	1.94	0.49
3:H:7:ASN:O	3:H:8:LEU:HD12	2.12	0.49
1:F:3:ALA:HB1	1:F:19:LEU:HD22	1.94	0.49
1:A:91:LYS:HZ3	2:B:91:LYS:HE3	1.78	0.49
2:B:35:VAL:HG21	2:B:87:VAL:HG11	1.95	0.49
2:B:84:VAL:HG22	2:B:86:TRP:HZ3	1.77	0.49
1:C:46:HIS:HB3	1:C:49:GLN:HG2	1.95	0.49
1:F:8:LEU:HD11	1:F:15:ARG:HD2	1.95	0.49
1:C:19:LEU:HB3	1:C:20:PHE:CD2	2.48	0.49
1:D:8:LEU:HA	1:D:17:LEU:HD23	1.94	0.49
3:E:97:LEU:HD23	3:E:97:LEU:N	2.28	0.49
3:E:29:TYR:HE2	3:E:31:GLN:NE2	2.09	0.49
4:G:97:LEU:N	4:G:97:LEU:HD23	2.28	0.49
3:H:63:GLY:O	3:H:85:HIS:HA	2.12	0.48
1:F:55:ILE:HG13	1:F:71:ALA:HB1	1.95	0.48
2:B:44:HIS:HB3	2:B:111:TRP:CE3	2.49	0.48
2:B:75:ASP:HB3	2:B:77:PHE:CE2	2.48	0.48
3:E:8:LEU:HD12	3:E:17:LEU:HG	1.94	0.48
3:H:37:PRO:HB3	3:H:92:ASP:C	2.38	0.48
1:A:50:TYR:CZ	1:A:81:PRO:HD3	2.49	0.48
3:E:60:ALA:HB1	3:E:87:VAL:HG12	1.96	0.48
1:D:45:TYR:CD2	1:D:112:LEU:HD11	2.49	0.48
1:A:84:VAL:HG12	1:A:86:TRP:HZ3	1.79	0.48
1:D:69:TYR:N	1:D:69:TYR:CD1	2.82	0.48
1:D:91:LYS:HE3	1:F:91:LYS:NZ	2.29	0.48
4:G:49:GLN:HA	4:G:103:ASN:O	2.14	0.48
4:G:38:LYS:HA	4:G:89:ASN:O	2.14	0.48
4:G:44:HIS:O	4:G:84:VAL:HA	2.14	0.48
1:D:13:THR:HG22	1:D:14:TYR:HD1	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASP:C	1:A:11:ARG:HD3	2.39	0.47
1:C:19:LEU:CD2	1:C:31:GLN:HA	2.44	0.47
3:H:8:LEU:HD12	3:H:17:LEU:HD23	1.91	0.47
1:F:38:LYS:HA	1:F:89:ASN:O	2.13	0.47
1:D:13:THR:HA	1:D:39:GLN:NE2	2.29	0.47
1:D:47:GLU:C	1:D:48:ARG:HG3	2.39	0.47
1:F:3:ALA:HB2	1:F:20:PHE:CZ	2.49	0.47
1:F:66:ASP:OD1	1:F:66:ASP:C	2.58	0.47
3:H:56:ILE:HG22	3:H:57:SER:OG	2.15	0.47
1:C:1:MET:N	1:D:64:ILE:HD13	2.30	0.47
1:F:63:GLY:HA3	1:F:86:TRP:CE2	2.49	0.47
1:D:34:GLU:OE1	1:D:96:ARG:NE	2.43	0.47
1:D:48:ARG:HB2	1:D:48:ARG:HH11	1.79	0.47
3:E:8:LEU:HD12	3:E:16:LYS:O	2.14	0.47
1:F:63:GLY:O	1:F:85:HIS:HA	2.15	0.47
3:E:11:ARG:O	3:E:13:THR:N	2.47	0.47
1:F:8:LEU:HG	1:F:15:ARG:HG2	1.96	0.47
1:A:19:LEU:HD11	1:A:32:ILE:HG12	1.97	0.46
1:C:97:LEU:HD12	1:C:99:VAL:HG22	1.96	0.46
1:F:11:ARG:C	1:F:13:THR:H	2.19	0.46
3:E:13:THR:HA	3:E:39:GLN:OE1	2.15	0.46
3:E:18:PRO:O	3:E:19:LEU:HD13	2.15	0.46
2:B:84:VAL:HG22	2:B:86:TRP:CZ3	2.50	0.46
1:C:51:GLU:HB2	1:C:79:VAL:HB	1.96	0.46
1:C:20:PHE:CD1	1:D:78:LEU:HB3	2.50	0.46
1:D:94:PRO:HG3	6:D:204:HOH:O	2.14	0.46
3:H:19:LEU:HD11	3:H:32:ILE:HD11	1.98	0.46
1:C:37:PRO:HB3	1:C:92:ASP:C	2.40	0.46
3:E:54:TYR:HD1	3:E:76:ILE:HG12	1.81	0.46
2:B:7:ASN:O	2:B:17:LEU:HA	2.16	0.46
3:E:21:GLU:C	3:E:23:GLU:H	2.23	0.46
1:A:60:ALA:HB3	1:A:95:PHE:CD2	2.50	0.46
2:B:46:HIS:HB3	2:B:108:ASP:OD2	2.16	0.46
1:C:60:ALA:O	1:C:61:ARG:C	2.59	0.46
3:E:34:GLU:HG2	3:E:96:ARG:HG2	1.98	0.45
3:E:37:PRO:HB3	3:E:93:GLU:N	2.31	0.45
4:G:19:LEU:HD21	4:G:32:ILE:CD1	2.45	0.45
1:C:64:ILE:HG13	1:C:69:TYR:CE1	2.51	0.45
3:E:54:TYR:HD1	3:E:76:ILE:CG1	2.29	0.45
1:F:13:THR:CG2	1:F:14:TYR:HD1	2.29	0.45
3:E:63:GLY:HA3	3:E:86:TRP:CH2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:LEU:HD22	3:E:28:SER:OG	2.17	0.45
1:C:13:THR:HG23	1:C:14:TYR:CD2	2.52	0.45
1:D:38:LYS:HA	1:D:89:ASN:O	2.17	0.45
1:D:44:HIS:HB3	1:D:111:TRP:HA	1.99	0.45
3:H:7:ASN:C	3:H:8:LEU:HD12	2.41	0.45
2:B:47:GLU:HB3	2:B:48:ARG:NH1	2.31	0.45
1:C:31:GLN:HE21	1:C:33:VAL:HG12	1.79	0.45
3:E:38:LYS:HA	3:E:89:ASN:O	2.17	0.45
4:G:37:PRO:HA	4:G:89:ASN:ND2	2.32	0.45
3:H:8:LEU:HG	3:H:17:LEU:HD21	1.98	0.45
1:F:25:PRO:HG3	3:H:50:TYR:CD1	2.52	0.44
1:F:50:TYR:CD2	3:H:25:PRO:HD3	2.53	0.44
2:B:109:SER:HB3	2:B:111:TRP:NE1	2.27	0.44
1:C:51:GLU:O	1:C:78:LEU:HD12	2.17	0.44
1:F:25:PRO:HD3	3:H:50:TYR:CE2	2.52	0.44
1:F:63:GLY:HA2	1:F:68:GLU:HA	1.98	0.44
1:F:102:LEU:CD1	3:H:28:SER:HB3	2.27	0.44
1:A:86:TRP:CD1	1:A:86:TRP:C	2.95	0.44
3:H:90:GLU:HB2	3:H:91:LYS:NZ	2.30	0.44
1:C:37:PRO:HB2	1:C:92:ASP:HA	1.99	0.44
3:E:23:GLU:OE1	3:E:23:GLU:HA	2.18	0.44
3:H:15:ARG:HG3	3:H:36:LYS:HE2	2.00	0.44
2:B:97:LEU:N	2:B:97:LEU:HD23	2.32	0.44
4:G:13:THR:HG21	4:G:42:LYS:HZ3	1.82	0.44
4:G:38:LYS:HD3	4:G:91:LYS:N	2.32	0.44
1:C:1:MET:O	1:C:2:LYS:HB2	2.17	0.44
1:C:107:ASP:OD2	1:C:109:SER:N	2.46	0.44
3:E:63:GLY:HA3	3:E:86:TRP:CE2	2.53	0.44
4:G:59:GLU:HB3	4:G:91:LYS:HD2	1.98	0.44
1:F:30:ALA:O	1:F:31:GLN:HB3	2.18	0.44
1:A:8:LEU:HA	1:A:17:LEU:HD23	2.00	0.44
1:A:78:LEU:HB3	4:G:20:PHE:CE2	2.53	0.44
1:D:48:ARG:C	1:D:81:PRO:HB3	2.43	0.44
3:E:8:LEU:HD22	3:H:8:LEU:HD13	2.00	0.44
1:F:56:ILE:HD11	1:F:98:PHE:HB2	2.00	0.44
1:F:102:LEU:C	1:F:104:TYR:N	2.74	0.44
1:A:1:MET:HE1	4:G:67:THR:OG1	2.18	0.43
1:C:62:LEU:HD12	1:C:87:VAL:HG23	2.00	0.43
3:H:15:ARG:HD2	3:H:34:GLU:OE1	2.17	0.43
3:H:41:VAL:N	3:H:87:VAL:O	2.50	0.43
1:A:50:TYR:CE2	1:A:81:PRO:HG3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ALA:HB3	1:A:95:PHE:CE2	2.53	0.43
1:D:8:LEU:HG	1:D:15:ARG:HG2	2.00	0.43
3:E:55:ILE:HD12	3:E:95:PHE:CZ	2.53	0.43
1:F:63:GLY:HA3	1:F:86:TRP:CZ2	2.52	0.43
1:C:89:ASN:OD1	1:C:91:LYS:HG2	2.19	0.43
2:B:69:TYR:CD1	2:B:69:TYR:N	2.86	0.43
1:C:28:SER:OG	1:D:102:LEU:HD22	2.18	0.43
1:C:80:LYS:HE3	1:D:1:MET:CG	2.48	0.43
4:G:42:LYS:HE2	4:G:42:LYS:H	1.83	0.43
1:C:107:ASP:OD1	1:C:107:ASP:CB	2.62	0.43
1:A:78:LEU:HD21	1:A:80:LYS:HG3	2.00	0.43
1:D:49:GLN:HA	1:D:102:LEU:O	2.19	0.43
1:A:61:ARG:O	1:A:87:VAL:HA	2.19	0.43
1:D:45:TYR:CD1	1:D:82:LYS:HA	2.53	0.43
3:E:61:ARG:O	3:E:87:VAL:HA	2.18	0.43
3:H:37:PRO:CB	3:H:92:ASP:O	2.66	0.43
1:C:91:LYS:HB3	1:C:91:LYS:HE3	1.59	0.43
1:D:58:GLY:O	1:D:73:PRO:HD3	2.19	0.43
2:B:45:TYR:CD2	2:B:112:LEU:HD11	2.52	0.42
1:C:63:GLY:HA3	1:C:86:TRP:CZ2	2.54	0.42
1:D:50:TYR:CD1	1:D:50:TYR:N	2.86	0.42
1:F:54:TYR:HB3	1:F:98:PHE:HB3	2.02	0.42
4:G:38:LYS:HD2	4:G:90:GLU:HA	2.00	0.42
1:A:1:MET:HB2	4:G:69:TYR:OH	2.19	0.42
3:H:43:LYS:HD2	3:H:84:VAL:CG1	2.47	0.42
3:H:44:HIS:HB3	3:H:111:TRP:CE3	2.55	0.42
1:A:5:ILE:HG23	1:A:17:LEU:HB3	2.00	0.42
1:A:50:TYR:CD2	4:G:25:PRO:HG3	2.55	0.42
2:B:31:GLN:NE2	2:B:101:LYS:HE3	2.35	0.42
1:F:55:ILE:HD12	1:F:95:PHE:CZ	2.54	0.42
1:D:4:GLU:CG	1:D:6:LYS:CG	2.96	0.42
1:D:44:HIS:HA	1:D:112:LEU:HD13	2.02	0.42
4:G:43:LYS:HD3	4:G:86:TRP:HE3	1.78	0.42
1:A:62:LEU:O	1:A:68:GLU:HA	2.20	0.42
1:C:3:ALA:HB2	1:D:76:ILE:O	2.20	0.42
1:C:107:ASP:OD2	1:C:108:ASP:N	2.53	0.42
1:F:13:THR:HG23	1:F:14:TYR:HD1	1.85	0.42
3:H:43:LYS:HB3	3:H:112:LEU:HD22	2.02	0.42
2:B:72:LYS:O	2:B:73:PRO:C	2.59	0.42
1:C:2:LYS:HE3	1:D:69:TYR:HE2	1.84	0.42
3:E:33:VAL:HG22	3:E:97:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:HB2	1:A:102:LEU:HB2	2.02	0.42
4:G:13:THR:HG22	4:G:39:GLN:OE1	2.20	0.42
1:C:28:SER:OG	1:D:102:LEU:HD13	2.20	0.41
1:D:50:TYR:CE1	1:D:81:PRO:HG3	2.55	0.41
1:D:23:GLU:OE2	1:D:23:GLU:HA	2.20	0.41
3:E:13:THR:HG23	3:E:14:TYR:CD1	2.54	0.41
1:A:36:LYS:O	1:A:39:GLN:HB2	2.20	0.41
1:A:50:TYR:O	1:A:101:LYS:HA	2.19	0.41
1:A:60:ALA:HB1	1:A:87:VAL:HG13	2.02	0.41
1:C:31:GLN:HG3	1:C:32:ILE:O	2.20	0.41
4:G:46:HIS:HB3	4:G:49:GLN:HG2	2.01	0.41
3:H:11:ARG:NH1	3:H:42:LYS:HZ1	2.17	0.41
2:B:54:TYR:CD1	2:B:54:TYR:C	2.98	0.41
4:G:36:LYS:O	4:G:39:GLN:HB2	2.20	0.41
1:A:44:HIS:HB2	1:A:110:VAL:O	2.21	0.41
3:E:13:THR:HG21	3:E:42:LYS:CE	2.50	0.41
4:G:40:THR:HB	4:G:88:VAL:HG22	2.02	0.41
4:G:45:TYR:O	4:G:109:SER:HA	2.20	0.41
3:H:13:THR:OG1	3:H:42:LYS:NZ	2.52	0.41
3:H:35:VAL:HB	3:H:95:PHE:HB3	2.02	0.41
3:H:90:GLU:CD	3:H:90:GLU:H	2.27	0.41
1:D:4:GLU:O	1:D:5:ILE:CB	2.69	0.41
4:G:27:GLY:HA2	4:G:104:TYR:O	2.20	0.41
3:H:11:ARG:NH1	3:H:11:ARG:HB3	2.36	0.41
1:C:91:LYS:C	1:C:93:GLU:H	2.28	0.41
1:D:7:ASN:O	1:D:18:PRO:HD2	2.20	0.41
4:G:51:GLU:HB3	4:G:53:PHE:CE1	2.55	0.41
3:E:92:ASP:N	3:E:92:ASP:OD1	2.53	0.41
1:A:41:VAL:N	1:A:87:VAL:O	2.51	0.41
1:A:75:ASP:HB3	1:A:77:PHE:CE2	2.56	0.41
1:A:78:LEU:HB2	4:G:20:PHE:CD2	2.55	0.41
2:B:6:LYS:HE2	2:B:6:LYS:HB3	1.64	0.41
1:D:47:GLU:HB2	1:D:108:ASP:HB2	2.03	0.41
3:E:13:THR:HG23	3:E:14:TYR:HD1	1.86	0.41
3:E:13:THR:HG21	3:E:42:LYS:HE2	2.02	0.41
3:H:8:LEU:HG	3:H:17:LEU:CD2	2.51	0.41
3:H:11:ARG:HB3	3:H:11:ARG:HH11	1.86	0.41
1:C:97:LEU:CD1	1:C:99:VAL:HG22	2.51	0.41
1:A:45:TYR:CE1	1:A:82:LYS:HA	2.57	0.40
1:A:46:HIS:ND1	1:A:109:SER:HA	2.35	0.40
2:B:56:ILE:HG13	2:B:97:LEU:HA	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ILE:HG12	1:D:54:TYR:OH	2.20	0.40
1:D:13:THR:OG1	1:D:40:THR:O	2.38	0.40
1:A:78:LEU:CB	4:G:20:PHE:CE2	3.05	0.40
2:B:44:HIS:HB3	2:B:111:TRP:CG	2.56	0.40
2:B:64:ILE:HG22	2:B:83:THR:HG21	2.02	0.40
1:D:2:LYS:HD2	1:D:3:ALA:N	2.36	0.40
1:D:4:GLU:HG3	1:D:6:LYS:CG	2.51	0.40
1:F:2:LYS:HG3	3:H:77:PHE:CE1	2.56	0.40
3:H:34:GLU:HG2	3:H:96:ARG:HD3	2.03	0.40
3:H:55:ILE:N	3:H:55:ILE:HD13	2.36	0.40
2:B:25:PRO:O	2:B:28:SER:HB2	2.21	0.40
1:D:110:VAL:O	1:D:112:LEU:HD12	2.20	0.40
3:H:63:GLY:HA3	3:H:86:TRP:CE2	2.56	0.40
1:A:1:MET:HG2	4:G:64:ILE:HG21	2.03	0.40
2:B:13:THR:OG1	2:B:40:THR:O	2.38	0.40
1:D:50:TYR:N	1:D:50:TYR:HD1	2.20	0.40
1:C:29:TYR:HB3	1:C:101:LYS:HB2	2.04	0.40
1:F:25:PRO:O	1:F:28:SER:HB2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:GLU:OE1	1:F:105:HIS:NE2[2_655]	1.62	0.58
2:B:26:GLU:OE1	1:F:105:HIS:CD2[2_655]	1.82	0.38

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	110/116 (95%)	97 (88%)	12 (11%)	1 (1%)	14 9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	110/116 (95%)	97 (88%)	9 (8%)	4 (4%)	2	0
1	D	110/116 (95%)	101 (92%)	4 (4%)	5 (4%)	2	0
1	F	105/116 (90%)	96 (91%)	7 (7%)	2 (2%)	6	2
2	B	108/114 (95%)	94 (87%)	12 (11%)	2 (2%)	6	2
3	E	104/110 (94%)	94 (90%)	8 (8%)	2 (2%)	6	2
3	H	90/110 (82%)	82 (91%)	8 (9%)	0	100	100
4	G	99/105 (94%)	92 (93%)	5 (5%)	2 (2%)	6	2
All	All	836/903 (93%)	753 (90%)	65 (8%)	18 (2%)	5	1

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3	ALA
1	D	4	GLU
1	D	5	ILE
1	D	6	LYS
1	F	106	GLY
1	C	12	GLY
1	D	12	GLY
3	E	12	GLY
1	F	103	ASN
4	G	25	PRO
2	B	5	ILE
2	B	6	LYS
1	C	2	LYS
3	E	25	PRO
1	C	65	GLY
1	A	65	GLY
1	C	3	ALA
4	G	109	SER

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	100/103 (97%)	87 (87%)	13 (13%)	4	1
1	C	100/103 (97%)	85 (85%)	15 (15%)	3	1
1	D	100/103 (97%)	88 (88%)	12 (12%)	5	2
1	F	95/103 (92%)	82 (86%)	13 (14%)	3	1
2	B	98/101 (97%)	78 (80%)	20 (20%)	1	0
3	E	95/98 (97%)	79 (83%)	16 (17%)	2	0
3	H	87/98 (89%)	76 (87%)	11 (13%)	4	2
4	G	90/93 (97%)	73 (81%)	17 (19%)	1	0
All	All	765/802 (95%)	648 (85%)	117 (15%)	3	1

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	16	LYS
1	A	40	THR
1	A	45	TYR
1	A	47	GLU
1	A	49	GLN
1	A	69	TYR
1	A	88	VAL
1	A	97	LEU
1	A	101	LYS
1	A	102	LEU
1	A	104	TYR
1	A	110	VAL
2	B	5	ILE
2	B	6	LYS
2	B	13	THR
2	B	17	LEU
2	B	33	VAL
2	B	42	LYS
2	B	43	LYS
2	B	48	ARG
2	B	50	TYR
2	B	56	ILE
2	B	59	GLU
2	B	62	LEU
2	B	67	THR
2	B	68	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	69	TYR
2	B	70	GLN
2	B	82	LYS
2	B	93	GLU
2	B	97	LEU
2	B	110	VAL
1	C	2	LYS
1	C	15	ARG
1	C	21	GLU
1	C	26	GLU
1	C	28	SER
1	C	33	VAL
1	C	34	GLU
1	C	40	THR
1	C	57	SER
1	C	59	GLU
1	C	80	LYS
1	C	87	VAL
1	C	90	GLU
1	C	91	LYS
1	C	92	ASP
1	D	13	THR
1	D	15	ARG
1	D	16	LYS
1	D	28	SER
1	D	32	ILE
1	D	33	VAL
1	D	36	LYS
1	D	42	LYS
1	D	48	ARG
1	D	50	TYR
1	D	97	LEU
1	D	107	ASP
3	E	21	GLU
3	E	33	VAL
3	E	38	LYS
3	E	40	THR
3	E	42	LYS
3	E	48	ARG
3	E	57	SER
3	E	68	GLU
3	E	82	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	84	VAL
3	E	88	VAL
3	E	91	LYS
3	E	92	ASP
3	E	93	GLU
3	E	97	LEU
3	E	112	LEU
1	F	1	MET
1	F	13	THR
1	F	17	LEU
1	F	28	SER
1	F	32	ILE
1	F	39	GLN
1	F	50	TYR
1	F	62	LEU
1	F	68	GLU
1	F	90	GLU
1	F	91	LYS
1	F	97	LEU
1	F	103	ASN
4	G	13	THR
4	G	19	LEU
4	G	20	PHE
4	G	33	VAL
4	G	34	GLU
4	G	39	GLN
4	G	40	THR
4	G	57	SER
4	G	72	LYS
4	G	84	VAL
4	G	87	VAL
4	G	88	VAL
4	G	90	GLU
4	G	91	LYS
4	G	93	GLU
4	G	97	LEU
4	G	112	LEU
3	H	11	ARG
3	H	26	GLU
3	H	33	VAL
3	H	40	THR
3	H	43	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	57	SER
3	H	66	ASP
3	H	90	GLU
3	H	91	LYS
3	H	93	GLU
3	H	97	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	49	GLN
1	A	105	HIS
2	B	7	ASN
2	B	31	GLN
1	D	39	GLN
3	E	46	HIS
1	F	46	HIS
1	F	105	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	112/116 (96%)	-0.15	0 100 100	41, 62, 101, 135	0
1	C	112/116 (96%)	-0.15	1 (0%) 81 83	42, 70, 104, 130	0
1	D	112/116 (96%)	-0.14	1 (0%) 81 83	38, 60, 100, 124	0
1	F	107/116 (92%)	-0.22	0 100 100	41, 60, 94, 128	0
2	B	110/114 (96%)	-0.17	1 (0%) 81 83	42, 63, 100, 119	0
3	E	106/110 (96%)	-0.17	0 100 100	42, 70, 102, 123	0
3	H	96/110 (87%)	-0.12	0 100 100	40, 64, 90, 105	0
4	G	101/105 (96%)	-0.20	0 100 100	44, 66, 99, 119	0
All	All	856/903 (94%)	-0.16	3 (0%) 88 90	38, 64, 100, 135	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	112	LEU	3.3
1	C	60	ALA	3.2
2	B	112	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
5	ZN	A	201	1/1	0.99	0.10	50,50,50,50	0
5	ZN	A	202	1/1	0.99	0.07	50,50,50,50	0
5	ZN	G	201	1/1	0.99	0.09	50,50,50,50	0
5	ZN	F	201	1/1	1.00	0.09	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.