



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:58 PM UTC

PDB ID : 7QNM / pdb_00007qnm
Title : Crystallization and structural analyses of ZgHAD, a L-2-haloacid dehalogenase from the marine Flavobacterium Zobellia galactanivorans
Authors : Grigorian, E.; Roret, T.; Leblanc, C.; Delage, L.; Czjzek, M.
Deposited on : 2021-12-21
Resolution : 2.73 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
Mogul : 2022.3.0, CSD as543be (2022)
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

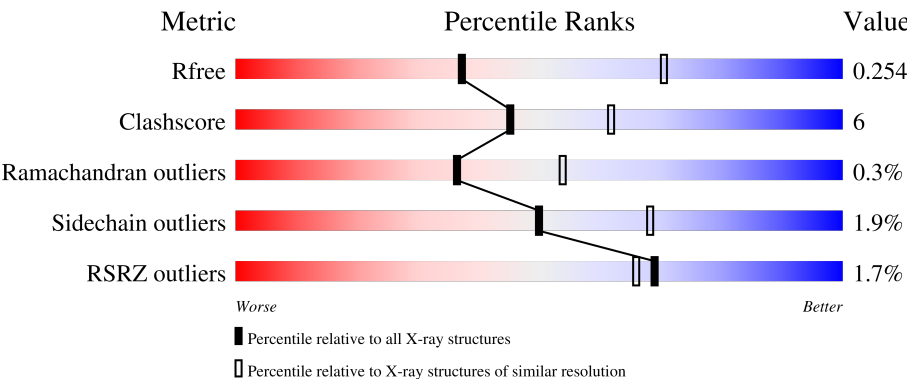
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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.



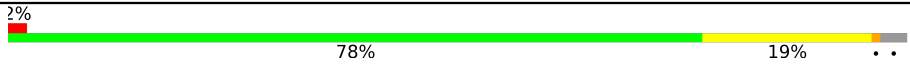
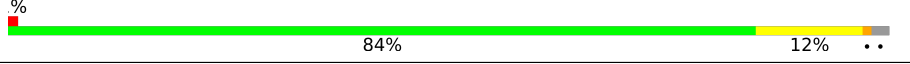
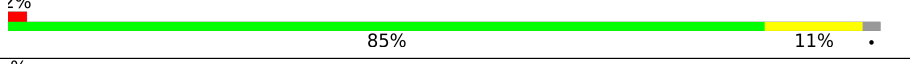
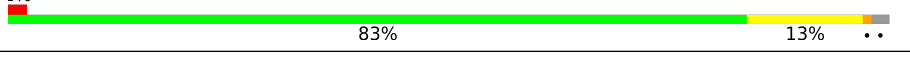
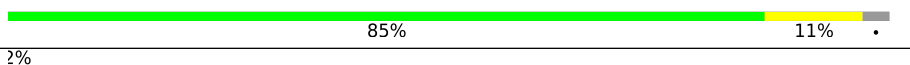
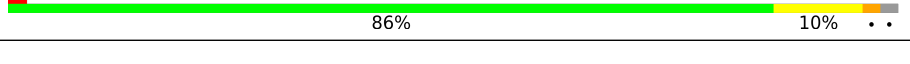
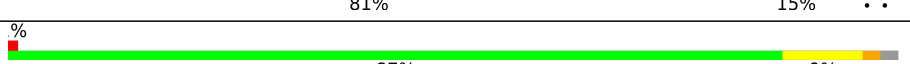
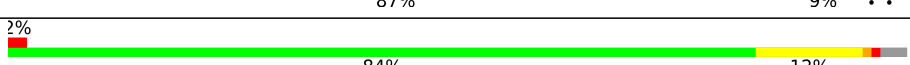
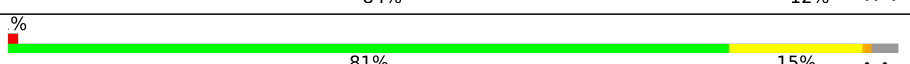
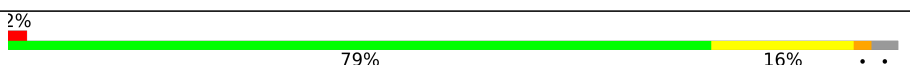
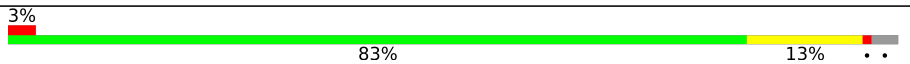
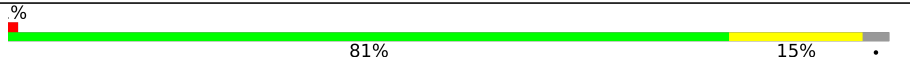
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	227	0% 87% 10% ..
1	B	227	2% 87% 8% ..
1	C	227	0% 80% 17% ..
1	D	227	4% 78% 17% ..
1	E	227	2% 82% 13% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	227	
1	G	227	
1	H	227	
1	I	227	
1	J	227	
1	K	227	
1	L	227	
1	M	227	
1	N	227	
1	O	227	
1	P	227	
1	Q	227	
1	R	227	
1	S	227	
1	T	227	
1	U	227	
1	V	227	
1	W	227	
1	X	227	
1	Y	227	
1	Z	227	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 45004 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 (S)-2-haloacid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	B	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	C	222	Total	C	N	O	S	0	0	0
			1729	1108	292	322	7			
1	D	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	E	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	F	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	G	222	Total	C	N	O	S	0	0	0
			1729	1108	292	322	7			
1	H	222	Total	C	N	O	S	0	0	0
			1729	1108	292	322	7			
1	I	222	Total	C	N	O	S	0	0	0
			1729	1108	292	322	7			
1	J	222	Total	C	N	O	S	0	0	0
			1729	1108	292	322	7			
1	K	222	Total	C	N	O	S	0	0	0
			1729	1108	292	322	7			
1	L	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	M	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	N	222	Total	C	N	O	S	0	0	0
			1729	1108	292	322	7			
1	O	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	P	222	Total	C	N	O	S	0	0	0
			1729	1108	292	322	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	222	Total	C	N	O	S	0	0	0
			1729	1108	292	322	7			
1	R	222	Total	C	N	O	S	0	0	0
			1729	1108	292	322	7			
1	S	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	T	222	Total	C	N	O	S	0	0	0
			1729	1108	292	322	7			
1	U	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	V	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	W	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	X	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	Y	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			
1	Z	221	Total	C	N	O	S	0	0	0
			1720	1102	290	321	7			

There are 26 discrepancies between the modelled and reference sequences:

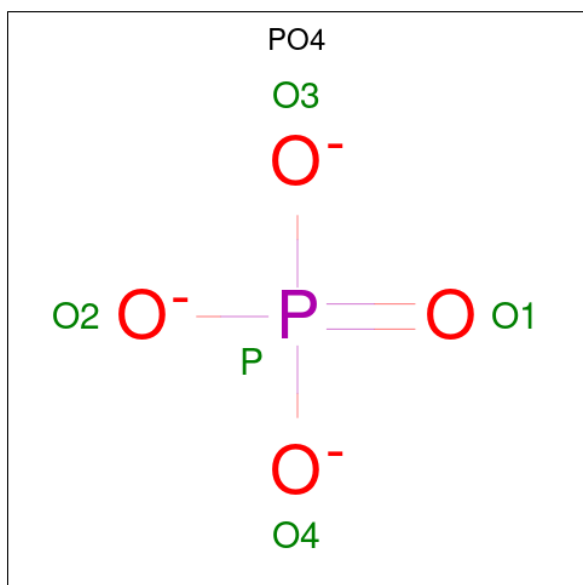
Chain	Residue	Modelled	Actual	Comment	Reference
A	179	ASN	HIS	engineered mutation	UNP G0L7V6
B	179	ASN	HIS	engineered mutation	UNP G0L7V6
C	179	ASN	HIS	engineered mutation	UNP G0L7V6
D	179	ASN	HIS	engineered mutation	UNP G0L7V6
E	179	ASN	HIS	engineered mutation	UNP G0L7V6
F	179	ASN	HIS	engineered mutation	UNP G0L7V6
G	179	ASN	HIS	engineered mutation	UNP G0L7V6
H	179	ASN	HIS	engineered mutation	UNP G0L7V6
I	179	ASN	HIS	engineered mutation	UNP G0L7V6
J	179	ASN	HIS	engineered mutation	UNP G0L7V6
K	179	ASN	HIS	engineered mutation	UNP G0L7V6
L	179	ASN	HIS	engineered mutation	UNP G0L7V6
M	179	ASN	HIS	engineered mutation	UNP G0L7V6
N	179	ASN	HIS	engineered mutation	UNP G0L7V6
O	179	ASN	HIS	engineered mutation	UNP G0L7V6
P	179	ASN	HIS	engineered mutation	UNP G0L7V6
Q	179	ASN	HIS	engineered mutation	UNP G0L7V6
R	179	ASN	HIS	engineered mutation	UNP G0L7V6
S	179	ASN	HIS	engineered mutation	UNP G0L7V6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
T	179	ASN	HIS	engineered mutation	UNP G0L7V6
U	179	ASN	HIS	engineered mutation	UNP G0L7V6
V	179	ASN	HIS	engineered mutation	UNP G0L7V6
W	179	ASN	HIS	engineered mutation	UNP G0L7V6
X	179	ASN	HIS	engineered mutation	UNP G0L7V6
Y	179	ASN	HIS	engineered mutation	UNP G0L7V6
Z	179	ASN	HIS	engineered mutation	UNP G0L7V6

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	M	1	Total	O	P	0	0
			5	4	1		
2	N	1	Total	O	P	0	0
			5	4	1		
2	O	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		
2	Q	1	Total	O	P	0	0
			5	4	1		
2	R	1	Total	O	P	0	0
			5	4	1		
2	S	1	Total	O	P	0	0
			5	4	1		
2	T	1	Total	O	P	0	0
			5	4	1		
2	U	1	Total	O	P	0	0
			5	4	1		
2	V	1	Total	O	P	0	0
			5	4	1		
2	W	1	Total	O	P	0	0
			5	4	1		
2	X	1	Total	O	P	0	0
			5	4	1		
2	Y	1	Total	O	P	0	0
			5	4	1		
2	Z	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		

Continued on next page...

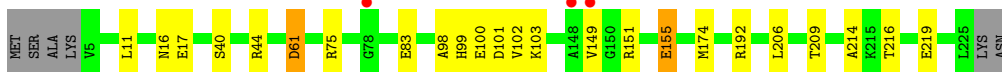
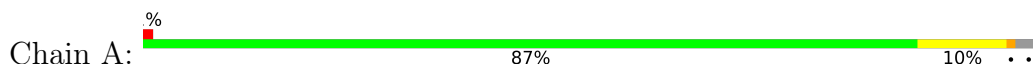
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O 1 1	0	0
3	D	2	Total O 2 2	0	0
3	F	1	Total O 1 1	0	0
3	G	3	Total O 3 3	0	0
3	H	4	Total O 4 4	0	0
3	I	3	Total O 3 3	0	0
3	J	2	Total O 2 2	0	0
3	K	6	Total O 6 6	0	0
3	L	1	Total O 1 1	0	0
3	M	1	Total O 1 1	0	0
3	N	2	Total O 2 2	0	0
3	O	4	Total O 4 4	0	0
3	P	7	Total O 7 7	0	0
3	Q	2	Total O 2 2	0	0
3	R	2	Total O 2 2	0	0
3	T	2	Total O 2 2	0	0
3	U	2	Total O 2 2	0	0
3	W	1	Total O 1 1	0	0
3	X	2	Total O 2 2	0	0
3	Y	1	Total O 1 1	0	0
3	Z	1	Total O 1 1	0	0

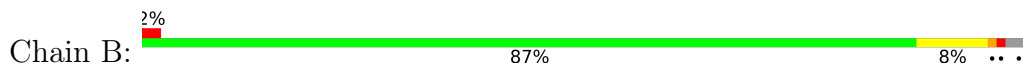
3 Residue-property plots

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.

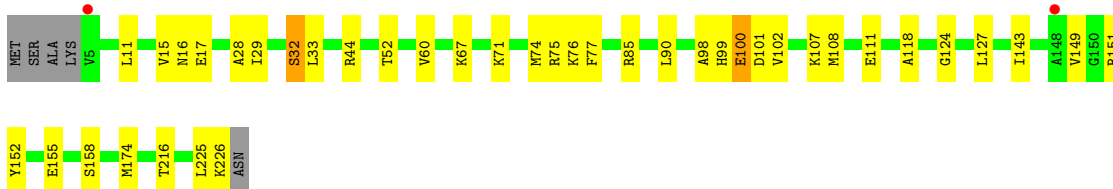
- Molecule 1: (S)-2-haloacid dehalogenase



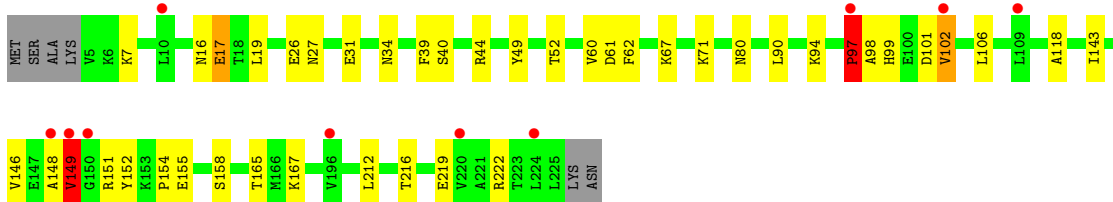
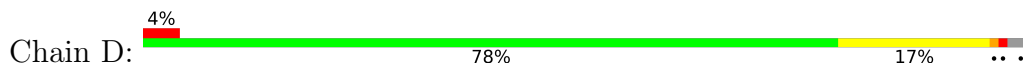
- Molecule 1: (S)-2-haloacid dehalogenase



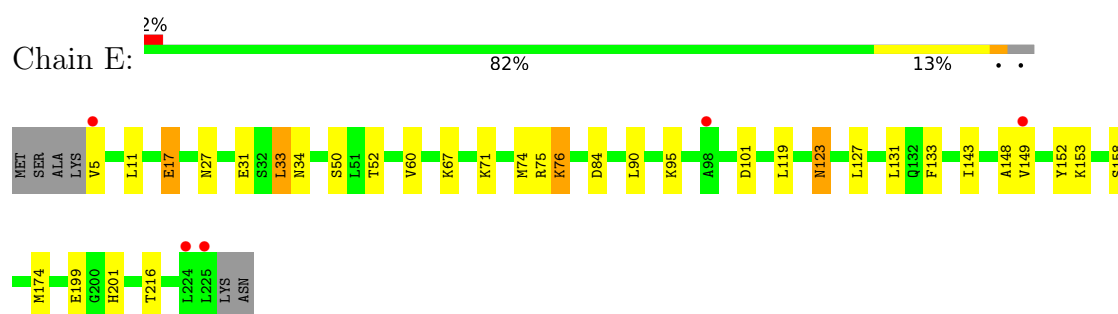
- Molecule 1: (S)-2-haloacid dehalogenase



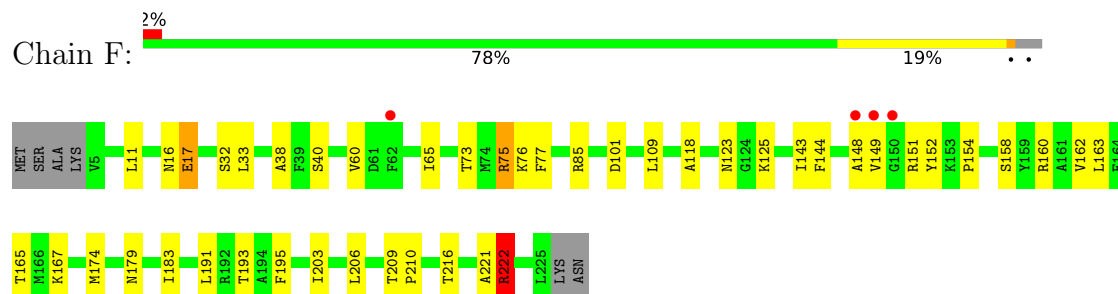
- Molecule 1: (S)-2-haloacid dehalogenase



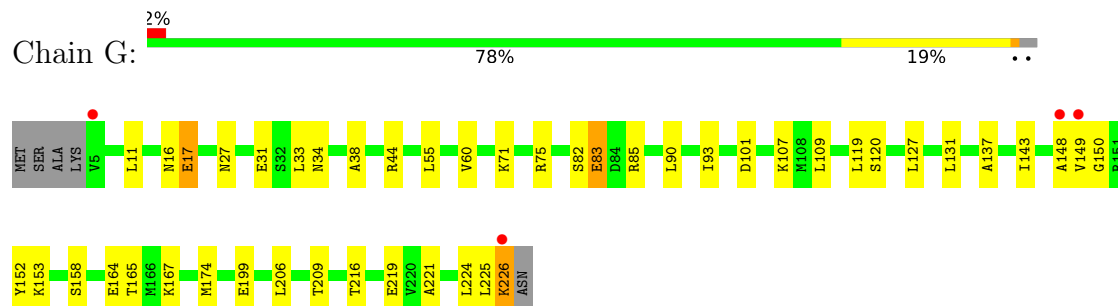
- Molecule 1: (S)-2-haloacid dehalogenase



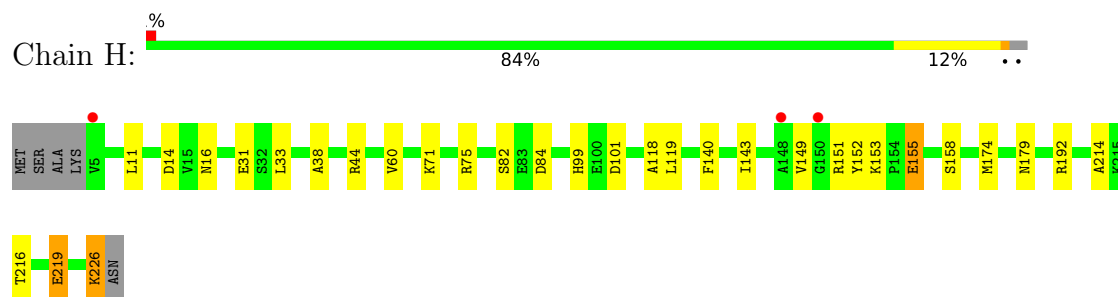
- Molecule 1: (S)-2-haloacid dehalogenase



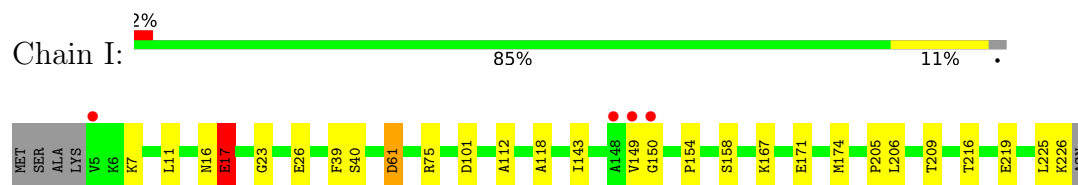
- Molecule 1: (S)-2-haloacid dehalogenase



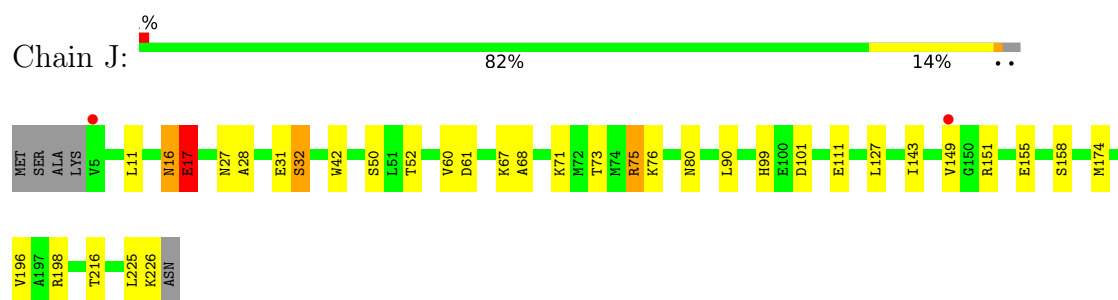
- Molecule 1: (S)-2-haloacid dehalogenase



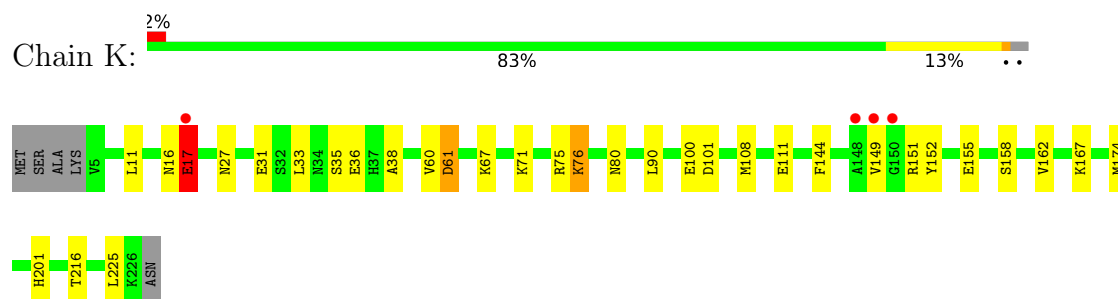
- Molecule 1: (S)-2-haloacid dehalogenase



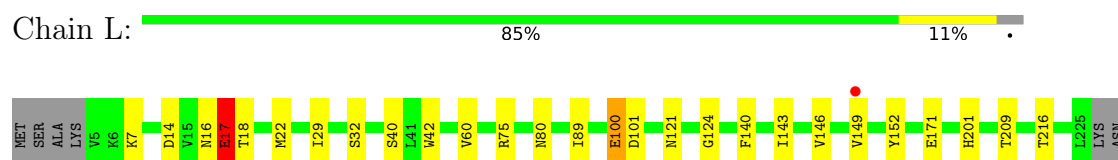
- Molecule 1: (S)-2-haloacid dehalogenase



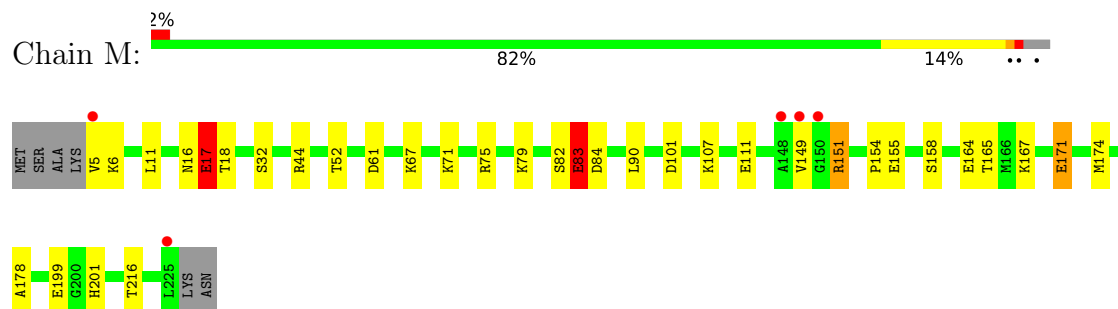
- Molecule 1: (S)-2-haloacid dehalogenase



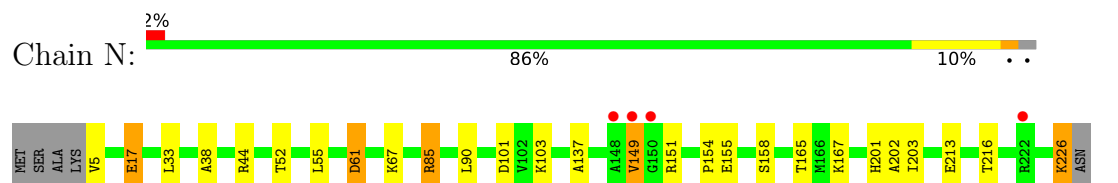
- Molecule 1: (S)-2-haloacid dehalogenase



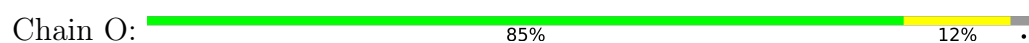
- Molecule 1: (S)-2-haloacid dehalogenase

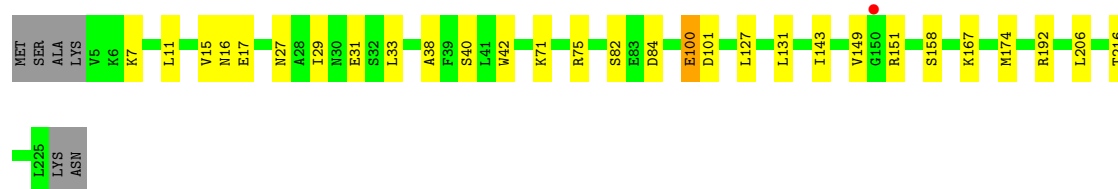


- Molecule 1: (S)-2-haloacid dehalogenase

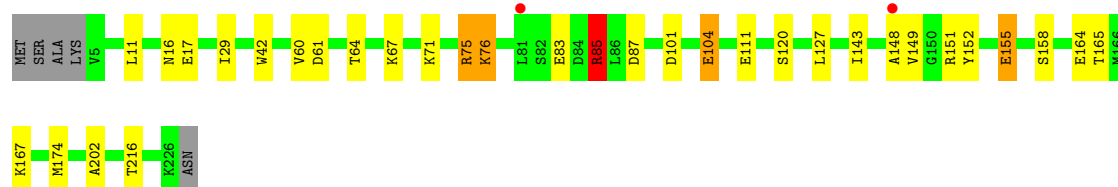
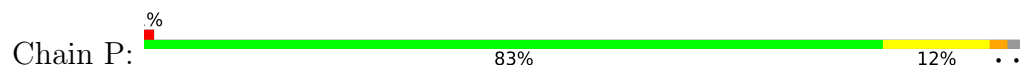


- Molecule 1: (S)-2-haloacid dehalogenase

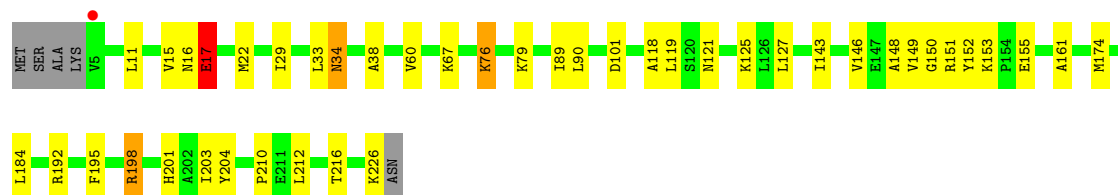
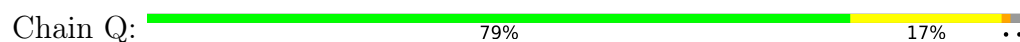




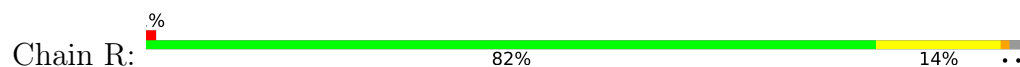
- Molecule 1: (S)-2-haloacid dehalogenase



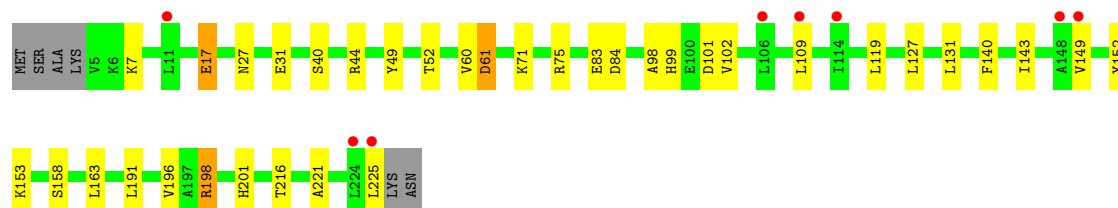
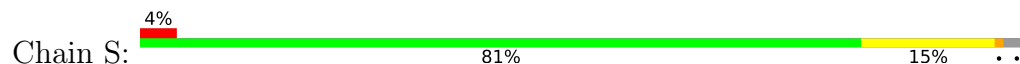
- Molecule 1: (S)-2-haloacid dehalogenase



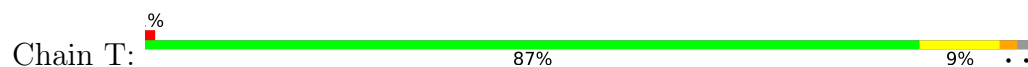
- Molecule 1: (S)-2-haloacid dehalogenase



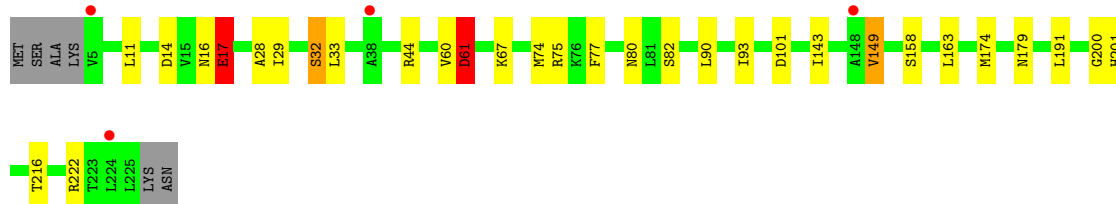
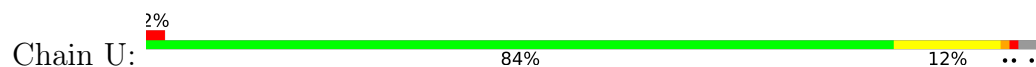
- Molecule 1: (S)-2-haloacid dehalogenase



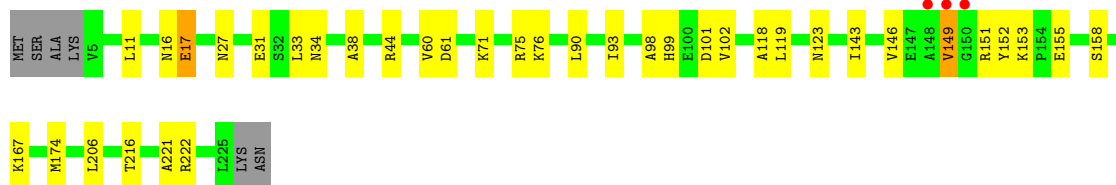
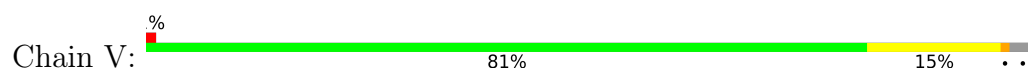
- Molecule 1: (S)-2-haloacid dehalogenase



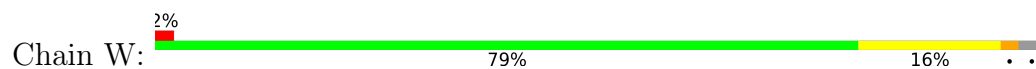
- Molecule 1: (S)-2-haloacid dehalogenase



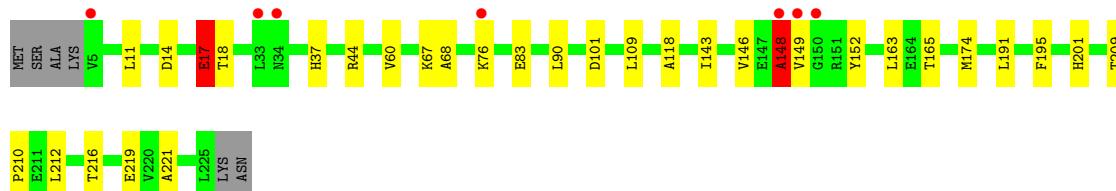
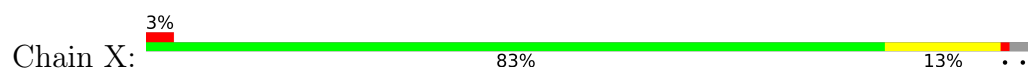
- Molecule 1: (S)-2-haloacid dehalogenase



- Molecule 1: (S)-2-haloacid dehalogenase



- Molecule 1: (S)-2-haloacid dehalogenase



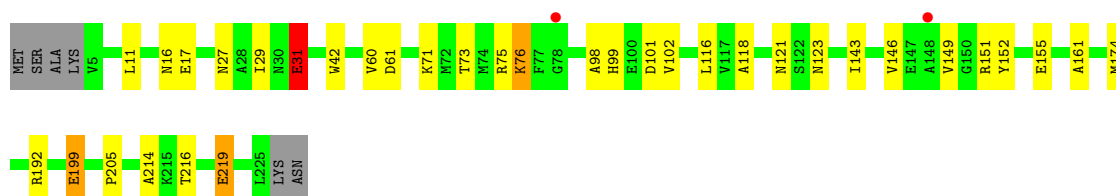
- Molecule 1: (S)-2-haloacid dehalogenase

Chain Y:  % 81% 15% .



- Molecule 1: (S)-2-haloacid dehalogenase

Chain Z:  % 82% 14% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.17Å 132.79Å 275.70Å 90.00° 92.31° 90.00°	Depositor
Resolution (Å)	49.51 – 2.73 49.51 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.51-2.73) 98.8 (49.51-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, REFMAC 5.8.0267	Depositor
R, R_{free}	0.206 , 0.254 0.210 , 0.254	Depositor DCC
R_{free} test set	7202 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	45004	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9379e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4

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	0.99	0/1749	1.45	1/2363 (0.0%)
1	B	1.06	2/1749 (0.1%)	1.50	3/2363 (0.1%)
1	C	1.05	1/1758 (0.1%)	1.50	2/2374 (0.1%)
1	D	0.98	0/1749	1.53	4/2363 (0.2%)
1	E	1.03	1/1749 (0.1%)	1.52	2/2363 (0.1%)
1	F	1.10	2/1749 (0.1%)	1.54	8/2363 (0.3%)
1	G	0.98	1/1758 (0.1%)	1.49	4/2374 (0.2%)
1	H	0.99	1/1758 (0.1%)	1.46	4/2374 (0.2%)
1	I	0.98	0/1758	1.44	1/2374 (0.0%)
1	J	0.98	0/1758	1.50	1/2374 (0.0%)
1	K	0.99	1/1758 (0.1%)	1.48	8/2374 (0.3%)
1	L	0.99	1/1749 (0.1%)	1.47	2/2363 (0.1%)
1	M	1.11	5/1749 (0.3%)	1.49	4/2363 (0.2%)
1	N	1.06	1/1758 (0.1%)	1.55	3/2374 (0.1%)
1	O	1.03	1/1749 (0.1%)	1.43	3/2363 (0.1%)
1	P	1.00	1/1758 (0.1%)	1.49	3/2374 (0.1%)
1	Q	1.02	1/1758 (0.1%)	1.54	6/2374 (0.3%)
1	R	1.02	2/1758 (0.1%)	1.49	4/2374 (0.2%)
1	S	0.98	0/1749	1.49	0/2363
1	T	0.98	0/1758	1.46	1/2374 (0.0%)
1	U	0.98	0/1749	1.47	1/2363 (0.0%)
1	V	0.98	0/1749	1.51	3/2363 (0.1%)
1	W	1.11	5/1749 (0.3%)	1.52	5/2363 (0.2%)
1	X	1.05	2/1749 (0.1%)	1.47	3/2363 (0.1%)
1	Y	1.18	5/1749 (0.3%)	1.51	4/2363 (0.2%)
1	Z	1.08	1/1749 (0.1%)	1.50	2/2363 (0.1%)
All	All	1.03	34/45573 (0.1%)	1.49	82/61559 (0.1%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	F	0	1
1	K	0	1
1	L	0	1
1	M	0	2
1	N	0	1
1	O	0	1
1	P	0	3
1	Q	0	1
1	R	0	1
1	W	0	1
1	X	0	1
1	Z	0	1
All	All	0	18

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	17	GLU	CD-OE2	20.85	1.65	1.25
1	Z	199	GLU	CD-OE2	18.40	1.60	1.25
1	W	5	VAL	C-O	-17.59	0.88	1.23
1	C	100	GLU	CD-OE2	16.43	1.56	1.25
1	N	85	ARG	CZ-NH2	15.92	1.54	1.33
1	O	100	GLU	CD-OE2	14.80	1.53	1.25
1	F	75	ARG	CZ-NH2	14.25	1.51	1.33
1	X	17	GLU	CD-OE2	13.72	1.51	1.25
1	B	100	GLU	CD-OE1	13.46	1.50	1.25
1	M	17	GLU	CD-OE2	13.21	1.50	1.25
1	M	83	GLU	CD-OE2	10.33	1.45	1.25
1	Y	17	GLU	CD-OE1	-10.33	1.05	1.25
1	F	160	ARG	CZ-NH1	9.80	1.46	1.32
1	Y	100	GLU	CD-OE2	9.77	1.44	1.25
1	Q	17	GLU	CD-OE1	-8.80	1.08	1.25
1	Y	36	GLU	CD-OE2	8.52	1.41	1.25
1	M	199	GLU	CD-OE2	8.51	1.41	1.25
1	P	104	GLU	CD-OE2	7.49	1.39	1.25
1	E	199	GLU	CD-OE1	7.39	1.39	1.25
1	M	17	GLU	CD-OE1	-7.34	1.11	1.25
1	R	31	GLU	CD-OE2	7.19	1.39	1.25
1	R	17	GLU	CD-OE1	6.96	1.38	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	5	VAL	C-N	-6.68	1.24	1.33
1	L	17	GLU	CD-OE2	6.60	1.37	1.25
1	Y	199	GLU	CD-OE2	6.55	1.37	1.25
1	G	85	ARG	CZ-NH2	6.17	1.41	1.33
1	W	5	VAL	N-CA	-6.15	1.34	1.46
1	X	148	ALA	C-O	6.14	1.32	1.24
1	M	171	GLU	CD-OE2	6.05	1.36	1.25
1	W	5	VAL	CA-C	5.33	1.64	1.52
1	K	16	ASN	C-O	-5.32	1.17	1.24
1	W	100	GLU	CD-OE2	5.31	1.35	1.25
1	B	100	GLU	CD-OE2	-5.11	1.15	1.25
1	H	16	ASN	C-O	-5.03	1.18	1.24

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	85	ARG	NE-CZ-NH2	20.33	137.50	119.20
1	Q	17	GLU	OE1-CD-OE2	-17.08	81.91	122.90
1	N	85	ARG	NH1-CZ-NH2	-12.07	103.61	119.30
1	M	83	GLU	OE1-CD-OE2	-11.97	94.17	122.90
1	Q	17	GLU	CG-CD-OE1	9.75	140.83	118.40
1	W	5	VAL	O-C-N	-8.81	108.90	123.00
1	F	222	ARG	NE-CZ-NH2	8.69	127.02	119.20
1	Q	226	LYS	CA-C-O	-8.29	106.70	120.80
1	G	226	LYS	CA-C-O	-8.10	107.03	120.80
1	Q	34	ASN	CB-CA-C	-8.07	101.04	111.86
1	D	97	PRO	CB-CA-C	7.98	121.62	110.60
1	W	5	VAL	CA-C-O	7.72	133.92	120.80
1	P	85	ARG	CG-CD-NE	-7.56	95.37	112.00
1	G	85	ARG	NE-CZ-NH2	7.51	125.96	119.20
1	M	83	GLU	CG-CD-OE2	7.50	135.65	118.40
1	D	97	PRO	N-CA-CB	-7.34	94.93	103.23
1	X	17	GLU	CG-CD-OE2	-6.82	102.73	118.40
1	Y	17	GLU	CG-CD-OE2	-6.67	103.06	118.40
1	O	100	GLU	N-CA-CB	-6.63	99.39	110.39
1	H	226	LYS	CA-C-O	-6.50	109.75	120.80
1	R	209	THR	CB-CA-C	6.46	119.85	109.51
1	Y	100	GLU	CG-CD-OE2	6.39	133.10	118.40
1	J	75	ARG	CB-CG-CD	-6.36	96.67	111.30
1	W	5	VAL	CA-CB-CG1	6.31	121.13	110.40
1	A	75	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	R	17	GLU	OE1-CD-OE2	-6.27	107.84	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	226	LYS	CB-CA-C	-6.24	98.24	110.10
1	W	7	LYS	CB-CA-C	6.07	117.12	108.68
1	C	100	GLU	N-CA-CB	-6.06	100.22	110.41
1	N	226	LYS	CA-C-O	-6.05	110.51	120.80
1	X	17	GLU	OE1-CD-OE2	6.03	137.38	122.90
1	T	226	LYS	CA-C-O	-6.02	110.56	120.80
1	K	36	GLU	N-CA-CB	-5.96	101.04	110.22
1	V	34	ASN	CB-CA-C	-5.95	103.45	111.89
1	Q	76	LYS	N-CA-CB	-5.82	100.64	110.41
1	L	100	GLU	N-CA-CB	-5.76	101.34	110.28
1	Y	17	GLU	OE1-CD-OE2	5.71	136.61	122.90
1	F	75	ARG	CB-CG-CD	-5.68	98.23	111.30
1	K	100	GLU	N-CA-CB	-5.64	101.53	110.22
1	R	6	LYS	CB-CA-C	-5.64	99.52	109.62
1	E	34	ASN	CB-CA-C	-5.55	104.00	112.11
1	M	171	GLU	OE1-CD-OE2	-5.45	109.82	122.90
1	F	222	ARG	NH1-CZ-NH2	-5.45	112.22	119.30
1	X	148	ALA	O-C-N	-5.42	114.37	122.39
1	K	76	LYS	N-CA-CB	-5.40	101.42	110.39
1	B	100	GLU	OE1-CD-OE2	-5.37	110.00	122.90
1	B	225	LEU	CA-C-O	5.37	129.93	120.80
1	K	17	GLU	CA-C-N	5.37	127.47	120.28
1	K	17	GLU	C-N-CA	5.37	127.47	120.28
1	Y	100	GLU	OE1-CD-OE2	-5.37	110.02	122.90
1	M	151	ARG	CG-CD-NE	-5.30	100.34	112.00
1	U	61	ASP	CB-CA-C	5.29	118.51	109.72
1	C	100	GLU	CB-CA-C	5.23	120.36	109.95
1	F	123	ASN	CA-C-N	5.23	125.75	120.00
1	F	123	ASN	C-N-CA	5.23	125.75	120.00
1	P	76	LYS	N-CA-CB	-5.22	101.73	110.39
1	H	99	HIS	CA-C-N	5.21	127.27	120.28
1	H	99	HIS	C-N-CA	5.21	127.27	120.28
1	Z	76	LYS	N-CA-CB	-5.21	101.66	110.41
1	K	17	GLU	CG-CD-OE1	-5.18	106.50	118.40
1	K	35	SER	CA-C-N	5.16	127.71	120.28
1	K	35	SER	C-N-CA	5.16	127.71	120.28
1	F	151	ARG	CG-CD-NE	-5.16	100.66	112.00
1	L	17	GLU	CG-CD-OE2	-5.14	106.57	118.40
1	D	62	PHE	CA-C-N	5.13	125.67	119.98
1	D	62	PHE	C-N-CA	5.13	125.67	119.98
1	Q	198	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	H	31	GLU	N-CA-CB	-5.11	102.58	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	85	ARG	CB-CA-C	-5.11	102.83	110.90
1	Z	31	GLU	N-CA-CB	-5.11	102.65	110.26
1	W	5	VAL	N-CA-CB	5.09	120.15	111.50
1	B	76	LYS	N-CA-CB	-5.09	101.86	110.41
1	G	107	LYS	CA-C-N	5.08	127.33	120.38
1	G	107	LYS	C-N-CA	5.08	127.33	120.38
1	O	100	GLU	CG-CD-OE2	-5.08	106.73	118.40
1	F	65	ILE	CA-C-N	5.06	125.71	119.99
1	F	65	ILE	C-N-CA	5.06	125.71	119.99
1	O	7	LYS	CB-CA-C	-5.04	101.85	109.26
1	E	76	LYS	N-CA-CB	-5.02	102.22	110.40
1	V	221	ALA	CA-C-N	5.02	127.00	120.28
1	V	221	ALA	C-N-CA	5.02	127.00	120.28
1	I	75	ARG	CG-CD-NE	-5.01	100.97	112.00

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLU	Sidechain
1	B	100	GLU	Sidechain
1	C	100	GLU	Sidechain
1	F	75	ARG	Sidechain
1	K	17	GLU	Sidechain
1	L	100	GLU	Sidechain
1	M	171	GLU	Sidechain
1	M	83	GLU	Sidechain
1	N	85	ARG	Sidechain
1	O	100	GLU	Sidechain
1	P	104	GLU	Sidechain
1	P	111	GLU	Sidechain
1	P	75	ARG	Sidechain
1	Q	17	GLU	Sidechain
1	R	17	GLU	Sidechain
1	W	5	VAL	Peptide
1	X	148	ALA	Mainchain
1	Z	199	GLU	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	1720	0	1763	19	4
1	B	1720	0	1763	18	4
1	C	1729	0	1776	25	4
1	D	1720	0	1763	25	5
1	E	1720	0	1763	22	0
1	F	1720	0	1763	25	4
1	G	1729	0	1776	29	2
1	H	1729	0	1776	21	0
1	I	1729	0	1776	16	2
1	J	1729	0	1775	32	2
1	K	1729	0	1776	20	1
1	L	1720	0	1763	20	1
1	M	1720	0	1763	30	0
1	N	1729	0	1776	21	1
1	O	1720	0	1763	26	0
1	P	1729	0	1776	36	2
1	Q	1729	0	1776	37	1
1	R	1729	0	1776	33	0
1	S	1720	0	1763	35	1
1	T	1729	0	1776	14	1
1	U	1720	0	1763	25	0
1	V	1720	0	1763	23	3
1	W	1720	0	1763	38	0
1	X	1720	0	1763	18	3
1	Y	1720	0	1763	30	0
1	Z	1720	0	1763	25	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	1	0
2	O	5	0	0	0	0
2	P	5	0	0	1	0
2	Q	5	0	0	0	0
2	R	5	0	0	0	0
2	S	5	0	0	0	0
2	T	5	0	0	0	0
2	U	5	0	0	0	0
2	V	5	0	0	0	0
2	W	5	0	0	1	0
2	X	5	0	0	0	0
2	Y	5	0	0	0	0
2	Z	5	0	0	0	0
3	A	5	0	0	3	0
3	B	1	0	0	0	0
3	D	2	0	0	0	0
3	F	1	0	0	0	0
3	G	3	0	0	1	0
3	H	4	0	0	0	0
3	I	3	0	0	1	0
3	J	2	0	0	0	0
3	K	6	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	2	0	0	0	0
3	O	4	0	0	0	0
3	P	7	0	0	0	0
3	Q	2	0	0	0	0
3	R	2	0	0	0	0
3	T	2	0	0	0	0
3	U	2	0	0	0	0
3	W	1	0	0	0	0
3	X	2	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
All	All	45004	0	45980	536	21

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (536) 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:Y:17:GLU:CD	1:Y:17:GLU:OE2	1.65	1.36
1:J:75:ARG:NH2	1:M:84:ASP:OD1	1.57	1.34
1:H:84:ASP:OD2	1:K:75:ARG:NH2	1.68	1.27
1:W:5:VAL:HG13	1:W:6:LYS:CG	1.70	1.21
1:W:5:VAL:HG12	1:W:6:LYS:HB2	1.26	1.13
1:J:75:ARG:NH2	1:M:84:ASP:CG	2.12	1.07
1:J:71:LYS:NZ	1:M:83:GLU:OE2	1.85	1.07
1:P:83:GLU:CD	1:S:83:GLU:OE2	1.97	1.07
1:P:83:GLU:OE2	1:S:83:GLU:OE2	1.74	1.04
1:J:71:LYS:HD3	1:M:83:GLU:OE1	1.61	1.01
1:W:5:VAL:CG1	1:W:6:LYS:HB2	1.91	1.00
1:C:149:VAL:HG11	1:C:158:SER:HA	1.44	1.00
1:O:149:VAL:HG11	1:O:158:SER:HA	1.44	0.98
1:R:17:GLU:OE1	1:R:201:HIS:NE2	1.96	0.98
1:T:149:VAL:HG11	1:T:158:SER:HA	1.46	0.96
1:E:149:VAL:HG11	1:E:158:SER:HA	1.46	0.95
1:R:149:VAL:HG11	1:R:158:SER:HA	1.44	0.95
1:W:5:VAL:HG13	1:W:6:LYS:HG3	1.45	0.95
1:R:84:ASP:OD2	1:U:75:ARG:NH2	2.00	0.94
1:H:149:VAL:HG11	1:H:158:SER:HA	1.51	0.93
1:I:149:VAL:HG11	1:I:158:SER:HA	1.49	0.92
1:G:149:VAL:HG11	1:G:158:SER:HA	1.50	0.92
1:R:82:SER:HB2	1:U:80:ASN:HD21	1.35	0.90
1:A:151:ARG:HD3	1:A:155:GLU:OE1	1.72	0.88
1:W:5:VAL:HG13	1:W:6:LYS:HG2	1.54	0.88
1:H:151:ARG:HD3	1:H:155:GLU:OE1	1.73	0.87
1:S:149:VAL:HG11	1:S:158:SER:HA	1.55	0.86
1:U:33:LEU:HD11	1:U:74:MET:HA	1.59	0.85
1:W:5:VAL:CG1	1:W:6:LYS:CG	2.55	0.85
1:F:149:VAL:HG11	1:F:158:SER:HA	1.57	0.85
1:K:76:LYS:NZ	1:L:40:SER:OG	2.11	0.84
1:A:40:SER:OG	1:B:76:LYS:NZ	2.10	0.83
1:H:84:ASP:CG	1:K:75:ARG:NH2	2.38	0.81
1:P:75:ARG:HH21	1:S:84:ASP:CG	1.87	0.81
1:C:33:LEU:HD11	1:C:74:MET:HA	1.61	0.80
1:W:5:VAL:CG1	1:W:6:LYS:CB	2.59	0.80
1:E:17:GLU:HG2	1:E:201:HIS:CE1	2.18	0.79
1:J:149:VAL:HG11	1:J:158:SER:HA	1.65	0.78
1:X:148:ALA:O	1:Y:148:ALA:O	2.01	0.78
1:S:17:GLU:HG2	1:S:201:HIS:NE2	1.99	0.78
1:P:148:ALA:O	1:Q:148:ALA:O	2.01	0.77
1:A:149:VAL:HG13	3:A:403:HOH:O	1.83	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:71:LYS:CE	1:M:83:GLU:OE2	2.33	0.77
1:L:75:ARG:HH22	1:O:84:ASP:CG	1.93	0.76
1:K:149:VAL:HG11	1:K:158:SER:HA	1.66	0.76
1:J:71:LYS:CD	1:M:83:GLU:OE1	2.34	0.76
1:P:75:ARG:NH2	1:S:84:ASP:OD1	2.19	0.75
1:B:16:ASN:O	1:B:17:GLU:HB2	1.85	0.75
1:N:17:GLU:HG2	1:N:201:HIS:NE2	2.02	0.75
1:P:83:GLU:CG	1:S:83:GLU:OE2	2.35	0.75
1:A:155:GLU:HG3	1:B:55:LEU:HD22	1.68	0.74
1:E:27:ASN:O	1:E:31:GLU:HG2	1.88	0.73
1:J:16:ASN:O	1:J:17:GLU:HB2	1.89	0.73
1:R:17:GLU:OE2	1:R:22:MET:HG3	1.90	0.72
1:P:83:GLU:HG2	1:S:83:GLU:OE2	1.90	0.72
1:F:203:ILE:HD12	1:F:210:PRO:HD3	1.72	0.71
1:E:33:LEU:HD11	1:E:74:MET:HA	1.72	0.70
1:R:118:ALA:HB3	1:R:143:ILE:HG22	1.73	0.69
1:R:17:GLU:OE1	1:R:201:HIS:CE1	2.45	0.69
1:W:5:VAL:HG13	1:W:6:LYS:CB	2.23	0.69
1:W:60:VAL:O	1:W:152:TYR:OH	2.09	0.69
1:O:40:SER:CB	1:P:76:LYS:HZ1	2.05	0.69
1:S:99:HIS:O	1:S:102:VAL:HG22	1.94	0.68
1:U:16:ASN:O	1:U:17:GLU:HB2	1.93	0.68
1:H:151:ARG:CD	1:H:155:GLU:OE1	2.42	0.68
1:Z:151:ARG:HD3	1:Z:155:GLU:OE1	1.94	0.68
1:Q:151:ARG:HD3	1:Q:155:GLU:CD	2.19	0.67
1:A:99:HIS:O	1:A:102:VAL:HG22	1.94	0.67
1:M:5:VAL:HG12	1:M:6:LYS:N	2.10	0.67
1:U:28:ALA:O	1:U:32:SER:OG	2.12	0.67
1:Q:76:LYS:NZ	1:R:40:SER:OG	2.27	0.66
1:W:28:ALA:O	1:W:32:SER:OG	2.13	0.66
1:P:67:LYS:NZ	1:P:87:ASP:OD1	2.28	0.66
1:W:99:HIS:O	1:W:102:VAL:HG22	1.96	0.65
1:B:27:ASN:O	1:B:31:GLU:HG3	1.97	0.65
1:C:33:LEU:CD1	1:C:74:MET:HA	2.26	0.65
1:R:82:SER:HB2	1:U:80:ASN:ND2	2.11	0.65
1:D:99:HIS:O	1:D:102:VAL:HG22	1.97	0.65
1:F:73:THR:O	1:F:76:LYS:HB3	1.97	0.65
1:I:171:GLU:HG3	1:L:171:GLU:OE2	1.98	0.64
1:Z:60:VAL:O	1:Z:152:TYR:OH	2.15	0.64
1:W:44:ARG:HG3	1:X:44:ARG:HG3	1.80	0.64
1:P:83:GLU:HG2	1:S:83:GLU:HG2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:148:ALA:O	1:Q:148:ALA:C	2.41	0.64
1:I:61:ASP:OD1	1:I:61:ASP:C	2.40	0.63
1:C:118:ALA:HB3	1:C:143:ILE:HG22	1.81	0.63
1:F:167:LYS:NZ	1:G:137:ALA:O	2.23	0.63
1:H:226:LYS:O	1:H:226:LYS:HG2	1.99	0.63
1:M:149:VAL:HG11	1:M:158:SER:HA	1.81	0.63
1:C:99:HIS:O	1:C:102:VAL:HG22	1.98	0.62
1:Y:118:ALA:HB3	1:Y:143:ILE:HG22	1.80	0.62
1:E:33:LEU:CD1	1:E:74:MET:HA	2.29	0.62
1:Y:60:VAL:O	1:Y:152:TYR:OH	2.17	0.62
1:D:118:ALA:HB3	1:D:143:ILE:HG22	1.80	0.62
1:T:127:LEU:HD21	1:T:143:ILE:HG22	1.81	0.62
1:J:75:ARG:NH2	1:M:84:ASP:OD2	2.32	0.61
1:G:60:VAL:O	1:G:152:TYR:OH	2.17	0.61
1:Q:76:LYS:NZ	1:R:40:SER:CB	2.63	0.61
1:P:83:GLU:HG2	1:S:83:GLU:CG	2.31	0.61
1:C:28:ALA:O	1:C:32:SER:OG	2.19	0.60
1:Z:61:ASP:OD1	1:Z:123:ASN:ND2	2.33	0.60
1:F:167:LYS:HG2	1:G:143:ILE:HD12	1.82	0.60
1:F:143:ILE:HD11	1:G:167:LYS:HG2	1.83	0.60
1:K:76:LYS:NZ	1:L:40:SER:CB	2.65	0.60
1:K:76:LYS:HZ1	1:L:40:SER:CB	2.15	0.60
1:S:196:VAL:HG11	1:S:198:ARG:NH1	2.17	0.59
1:R:16:ASN:O	1:R:17:GLU:CB	2.50	0.59
1:X:60:VAL:O	1:X:152:TYR:OH	2.19	0.59
1:A:40:SER:HG	1:B:76:LYS:HZ1	1.46	0.59
1:O:27:ASN:O	1:O:31:GLU:HB2	2.03	0.59
1:D:16:ASN:O	1:D:17:GLU:HG3	2.02	0.59
1:U:14:ASP:OD2	1:U:179:ASN:ND2	2.36	0.59
1:C:151:ARG:HD3	1:C:155:GLU:CD	2.28	0.59
1:L:80:ASN:HD21	1:O:82:SER:HA	1.67	0.59
1:Z:151:ARG:HD3	1:Z:155:GLU:CD	2.27	0.58
1:K:27:ASN:O	1:K:31:GLU:HG3	2.04	0.58
1:W:5:VAL:O	1:W:6:LYS:O	2.21	0.58
1:A:149:VAL:HG22	3:A:403:HOH:O	2.02	0.58
1:E:52:THR:HG23	1:F:154:PRO:HG3	1.85	0.58
1:W:146:VAL:HA	1:W:149:VAL:HG22	1.85	0.58
1:Q:60:VAL:HG11	1:R:206:LEU:HD13	1.85	0.58
1:R:80:ASN:HD21	1:U:82:SER:HB3	1.68	0.58
1:V:149:VAL:HG21	1:V:158:SER:HA	1.85	0.57
1:H:60:VAL:O	1:H:152:TYR:OH	2.21	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:118:ALA:HB3	1:V:143:ILE:HG22	1.86	0.57
1:U:149:VAL:HG21	1:U:158:SER:HA	1.86	0.57
1:I:40:SER:CB	1:J:76:LYS:HZ1	2.15	0.57
1:Y:17:GLU:OE2	1:Y:17:GLU:CG	2.49	0.57
1:B:75:ARG:HH12	1:E:84:ASP:CG	2.11	0.56
1:R:82:SER:CB	1:U:80:ASN:HD21	2.14	0.56
1:W:73:THR:O	1:W:76:LYS:HB3	2.05	0.56
1:I:16:ASN:O	1:I:17:GLU:HB2	2.06	0.56
1:X:118:ALA:HB3	1:X:143:ILE:HG22	1.85	0.56
1:W:200:GLY:O	1:X:76:LYS:HE2	2.05	0.56
1:K:11:LEU:HD23	1:K:174:MET:HB3	1.87	0.56
1:I:206:LEU:HD13	1:J:60:VAL:HG11	1.88	0.56
1:V:99:HIS:O	1:V:102:VAL:HG22	2.05	0.56
1:Z:11:LEU:HD23	1:Z:174:MET:HB3	1.88	0.56
1:G:44:ARG:HG3	1:H:44:ARG:HG3	1.88	0.55
1:L:124:GLY:HA3	1:M:164:GLU:OE2	2.06	0.55
1:W:192:ARG:NE	1:W:211:GLU:OE1	2.31	0.55
1:C:151:ARG:HD3	1:C:155:GLU:OE1	2.06	0.55
1:U:67:LYS:HA	1:U:90:LEU:HD11	1.87	0.55
1:X:17:GLU:HG2	1:X:201:HIS:NE2	2.21	0.55
1:Z:118:ALA:HB3	1:Z:143:ILE:HG22	1.88	0.55
1:L:17:GLU:HG2	1:L:201:HIS:NE2	2.21	0.55
1:Q:146:VAL:HA	1:Q:149:VAL:HG22	1.88	0.55
1:Z:214:ALA:HB1	1:Z:219:GLU:HB3	1.88	0.55
1:B:118:ALA:HB3	1:B:143:ILE:HG22	1.88	0.55
1:E:95:LYS:HA	1:E:133:PHE:CD2	2.42	0.55
1:I:150:GLY:O	3:I:401:HOH:O	2.18	0.55
1:K:61:ASP:OD1	1:K:61:ASP:C	2.49	0.55
1:S:71:LYS:O	1:S:75:ARG:HG2	2.07	0.55
1:V:167:LYS:HG2	1:W:143:ILE:HD11	1.88	0.55
1:Y:71:LYS:O	1:Y:75:ARG:HG2	2.06	0.55
1:P:148:ALA:O	1:Q:149:VAL:HA	2.07	0.54
1:Z:27:ASN:O	1:Z:31:GLU:HB2	2.07	0.54
1:E:60:VAL:HG11	1:F:206:LEU:HD13	1.90	0.54
1:I:225:LEU:O	1:I:226:LYS:HB3	2.07	0.54
1:W:71:LYS:O	1:W:75:ARG:HG2	2.07	0.54
1:C:71:LYS:O	1:C:75:ARG:HG2	2.08	0.54
1:T:28:ALA:O	1:T:32:SER:OG	2.25	0.54
1:A:40:SER:CB	1:B:76:LYS:NZ	2.71	0.54
1:B:71:LYS:O	1:B:75:ARG:HG3	2.08	0.54
1:P:149:VAL:HG11	1:P:158:SER:HA	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:118:ALA:HB3	1:Q:143:ILE:HG22	1.90	0.54
1:L:80:ASN:ND2	1:O:82:SER:HA	2.23	0.54
1:P:164:GLU:OE2	1:Q:125:LYS:HG3	2.08	0.54
1:V:71:LYS:O	1:V:75:ARG:HG2	2.08	0.54
1:Y:40:SER:CB	1:Z:76:LYS:NZ	2.71	0.54
1:Q:16:ASN:O	1:Q:17:GLU:CB	2.56	0.54
1:C:76:LYS:HZ1	1:D:40:SER:CB	2.20	0.53
1:H:14:ASP:OD2	1:H:179:ASN:ND2	2.41	0.53
1:N:167:LYS:HD2	1:O:143:ILE:HG13	1.90	0.53
1:L:140:PHE:O	1:M:167:LYS:NZ	2.33	0.53
1:W:118:ALA:HB3	1:W:143:ILE:HG22	1.91	0.53
1:Y:16:ASN:O	1:Y:17:GLU:CB	2.57	0.53
1:V:16:ASN:O	1:V:17:GLU:HB2	2.09	0.53
1:I:154:PRO:HG3	1:J:52:THR:HG23	1.90	0.53
1:R:17:GLU:CD	1:R:201:HIS:HE2	2.14	0.53
1:Z:71:LYS:O	1:Z:75:ARG:HG3	2.09	0.53
1:G:119:LEU:HG	1:G:153:LYS:HD3	1.91	0.53
1:Q:76:LYS:HZ2	1:R:40:SER:CB	2.22	0.53
1:J:28:ALA:O	1:J:32:SER:HB2	2.08	0.53
1:A:98:ALA:HB1	1:A:102:VAL:CG2	2.38	0.53
1:V:11:LEU:HD23	1:V:174:MET:HB3	1.91	0.53
1:P:83:GLU:OE2	1:S:83:GLU:CD	2.49	0.53
1:E:60:VAL:O	1:E:152:TYR:OH	2.27	0.52
1:N:101:ASP:CG	1:N:216:THR:HB	2.34	0.52
1:A:40:SER:CB	1:B:76:LYS:HZ1	2.19	0.52
1:M:107:LYS:O	1:M:111:GLU:HG3	2.09	0.52
1:Z:146:VAL:HA	1:Z:149:VAL:HG22	1.92	0.52
1:B:164:GLU:OE2	1:C:124:GLY:HA3	2.09	0.52
1:I:118:ALA:HB3	1:I:143:ILE:HG22	1.91	0.52
1:L:75:ARG:NH2	1:O:84:ASP:OD2	2.35	0.52
1:Y:16:ASN:O	1:Y:17:GLU:HB2	2.09	0.52
1:N:17:GLU:CG	1:N:201:HIS:NE2	2.73	0.51
1:S:98:ALA:HB1	1:S:102:VAL:HG21	1.91	0.51
1:T:118:ALA:HB3	1:T:143:ILE:HG23	1.92	0.51
1:J:67:LYS:HG2	1:J:71:LYS:HE3	1.93	0.51
1:I:40:SER:OG	1:J:76:LYS:NZ	2.19	0.51
1:S:27:ASN:O	1:S:31:GLU:HG3	2.09	0.51
1:O:11:LEU:HD23	1:O:174:MET:HB3	1.92	0.51
1:G:101:ASP:CG	1:G:216:THR:HB	2.35	0.51
1:W:11:LEU:HD23	1:W:174:MET:HB3	1.92	0.51
1:X:148:ALA:O	1:Y:148:ALA:C	2.53	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:99:HIS:O	1:Y:102:VAL:HG22	2.10	0.51
1:L:143:ILE:O	1:M:165:THR:HA	2.11	0.51
1:L:146:VAL:HA	1:L:149:VAL:HG22	1.91	0.51
1:O:127:LEU:HD23	1:O:143:ILE:HG22	1.92	0.51
1:Q:151:ARG:HD3	1:Q:155:GLU:OE1	2.11	0.51
1:V:98:ALA:HB1	1:V:102:VAL:CG2	2.40	0.51
1:M:61:ASP:OD1	1:M:61:ASP:C	2.54	0.50
1:A:16:ASN:O	1:A:17:GLU:HB2	2.11	0.50
1:N:149:VAL:HG21	1:N:158:SER:HA	1.93	0.50
1:L:14:ASP:O	1:L:18:THR:HB	2.12	0.50
1:P:75:ARG:NH2	1:S:84:ASP:CG	2.63	0.50
1:Z:98:ALA:HB1	1:Z:102:VAL:CG2	2.41	0.50
1:H:119:LEU:HG	1:H:153:LYS:HD3	1.93	0.50
1:R:101:ASP:CG	1:R:216:THR:HB	2.37	0.50
1:F:109:LEU:HD21	1:F:221:ALA:HA	1.94	0.50
1:G:131:LEU:HD12	1:G:143:ILE:HD13	1.94	0.50
1:Q:119:LEU:HG	1:Q:153:LYS:HD3	1.93	0.50
1:C:67:LYS:HA	1:C:90:LEU:HD11	1.93	0.50
1:C:98:ALA:HB1	1:C:102:VAL:CG2	2.42	0.50
1:D:167:LYS:HD3	1:E:143:ILE:HG13	1.93	0.50
1:N:61:ASP:OD1	1:N:61:ASP:C	2.54	0.50
1:Y:40:SER:OG	1:Z:76:LYS:NZ	2.41	0.50
1:I:205:PRO:HD2	1:J:68:ALA:HB1	1.94	0.49
1:S:98:ALA:HB1	1:S:102:VAL:CG2	2.41	0.49
1:E:11:LEU:HD23	1:E:174:MET:HB3	1.93	0.49
1:M:32:SER:O	1:M:79:LYS:HD3	2.11	0.49
1:Q:76:LYS:HZ2	1:R:40:SER:HB3	1.77	0.49
1:S:127:LEU:CD2	1:S:143:ILE:HG22	2.42	0.49
1:Y:174:MET:HA	1:Y:192:ARG:O	2.12	0.49
1:F:125:LYS:HE2	1:G:164:GLU:OE1	2.12	0.49
1:S:44:ARG:HG3	1:T:44:ARG:HG3	1.94	0.49
1:T:61:ASP:C	1:T:61:ASP:OD1	2.55	0.49
1:L:29:ILE:HD13	1:L:42:TRP:CE3	2.47	0.49
1:Q:203:ILE:HD12	1:Q:210:PRO:HD3	1.94	0.49
1:A:151:ARG:NH1	3:A:402:HOH:O	2.30	0.49
1:K:101:ASP:CG	1:K:216:THR:HB	2.38	0.49
1:L:60:VAL:O	1:L:152:TYR:OH	2.26	0.49
1:R:82:SER:CB	1:U:80:ASN:ND2	2.76	0.49
1:S:40:SER:OG	1:T:76:LYS:NZ	2.34	0.49
1:J:225:LEU:O	1:J:226:LYS:HB2	2.12	0.49
1:P:101:ASP:CG	1:P:216:THR:HB	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:152:TYR:O	1:P:155:GLU:HB3	2.12	0.49
1:C:225:LEU:O	1:C:226:LYS:HB2	2.12	0.49
1:O:16:ASN:O	1:O:17:GLU:HB2	2.12	0.49
1:W:205:PRO:HG2	1:X:68:ALA:HB1	1.93	0.49
1:D:149:VAL:HG21	1:D:158:SER:HA	1.95	0.49
1:G:71:LYS:O	1:G:75:ARG:HG3	2.12	0.49
1:Q:11:LEU:HD23	1:Q:174:MET:HB3	1.93	0.49
1:J:80:ASN:OD1	1:M:82:SER:HB2	2.12	0.49
1:M:52:THR:HG23	1:N:154:PRO:HG3	1.94	0.49
1:O:15:VAL:HG21	1:O:127:LEU:HD11	1.95	0.49
1:O:101:ASP:CG	1:O:216:THR:HB	2.38	0.49
1:P:16:ASN:O	1:P:17:GLU:HB2	2.12	0.48
1:J:11:LEU:HD23	1:J:174:MET:HB3	1.94	0.48
1:S:221:ALA:O	1:S:225:LEU:HG	2.13	0.48
1:H:11:LEU:HD23	1:H:174:MET:HB3	1.95	0.48
1:H:140:PHE:O	1:I:167:LYS:NZ	2.43	0.48
1:A:214:ALA:HB1	1:A:219:GLU:HB3	1.95	0.48
1:V:119:LEU:HG	1:V:153:LYS:HD3	1.95	0.48
1:P:60:VAL:O	1:P:152:TYR:OH	2.30	0.48
1:F:16:ASN:O	1:F:17:GLU:HB2	2.13	0.48
1:R:27:ASN:O	1:R:31:GLU:HB2	2.14	0.48
1:U:61:ASP:OD1	1:U:61:ASP:C	2.56	0.48
1:Z:99:HIS:O	1:Z:102:VAL:HG22	2.14	0.48
1:M:71:LYS:O	1:M:75:ARG:HG3	2.13	0.48
1:C:101:ASP:CG	1:C:216:THR:HB	2.39	0.48
1:U:11:LEU:HD23	1:U:174:MET:HB3	1.96	0.48
1:X:11:LEU:HD23	1:X:174:MET:HB3	1.94	0.48
1:V:143:ILE:HD11	1:W:167:LYS:HG2	1.96	0.47
1:W:17:GLU:HG2	1:W:201:HIS:CE1	2.49	0.47
1:E:101:ASP:CG	1:E:216:THR:HB	2.39	0.47
1:A:98:ALA:HB1	1:A:102:VAL:HG21	1.96	0.47
1:D:80:ASN:HD21	1:G:82:SER:HB3	1.79	0.47
1:O:29:ILE:HD13	1:O:42:TRP:CE3	2.50	0.47
1:S:109:LEU:HD21	1:S:221:ALA:HA	1.96	0.47
1:U:90:LEU:O	1:U:93:ILE:HG22	2.14	0.47
1:W:35:SER:OG	1:X:37:HIS:CD2	2.67	0.47
1:M:101:ASP:CG	1:M:216:THR:HB	2.40	0.47
1:P:71:LYS:HD3	1:S:83:GLU:OE1	2.15	0.47
1:W:101:ASP:CG	1:W:216:THR:HB	2.39	0.47
1:X:146:VAL:HA	1:X:149:VAL:HG12	1.95	0.47
1:Y:146:VAL:HA	1:Y:149:VAL:HG22	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:THR:HA	1:G:143:ILE:O	2.14	0.47
1:P:11:LEU:HD23	1:P:174:MET:HB3	1.95	0.47
1:E:67:LYS:HA	1:E:90:LEU:HD11	1.95	0.47
1:R:5:VAL:HG12	1:R:6:LYS:O	2.14	0.47
1:V:60:VAL:O	1:V:152:TYR:OH	2.26	0.47
1:Y:206:LEU:HD13	1:Z:60:VAL:HG11	1.96	0.47
1:L:16:ASN:O	1:L:22:MET:SD	2.72	0.47
1:Y:68:ALA:HB1	1:Z:205:PRO:HG2	1.97	0.47
1:A:101:ASP:CG	1:A:216:THR:HB	2.40	0.47
1:P:165:THR:HA	1:Q:143:ILE:O	2.14	0.47
1:E:71:LYS:O	1:E:75:ARG:HG2	2.15	0.47
1:G:224:LEU:C	1:G:226:LYS:H	2.23	0.46
1:J:127:LEU:CD2	1:J:143:ILE:HG22	2.44	0.46
1:M:67:LYS:HA	1:M:90:LEU:HD11	1.98	0.46
1:R:16:ASN:O	1:R:17:GLU:HB2	2.16	0.46
1:H:214:ALA:HB1	1:H:219:GLU:HB3	1.97	0.46
1:Q:17:GLU:CD	1:Q:201:HIS:NE2	2.72	0.46
1:R:11:LEU:HD23	1:R:174:MET:HB3	1.97	0.46
1:S:119:LEU:HG	1:S:153:LYS:HD3	1.97	0.46
1:U:44:ARG:HG3	1:V:44:ARG:HG3	1.97	0.46
1:X:165:THR:HA	1:Y:143:ILE:O	2.15	0.46
1:H:118:ALA:HB3	1:H:143:ILE:HG22	1.95	0.46
1:D:146:VAL:HA	1:D:149:VAL:HG12	1.98	0.46
1:F:60:VAL:O	1:F:152:TYR:OH	2.32	0.46
1:M:16:ASN:O	1:M:17:GLU:CB	2.63	0.46
1:O:206:LEU:HD13	1:P:60:VAL:HG11	1.97	0.46
1:G:90:LEU:O	1:G:93:ILE:HG22	2.14	0.46
1:H:71:LYS:O	1:H:75:ARG:HG2	2.15	0.46
1:R:17:GLU:OE2	1:R:22:MET:CG	2.61	0.46
1:S:127:LEU:HD23	1:S:143:ILE:HG22	1.98	0.46
1:T:127:LEU:CD2	1:T:143:ILE:HG22	2.45	0.46
1:F:11:LEU:HD23	1:F:174:MET:HB3	1.97	0.46
1:C:33:LEU:HD12	1:C:77:PHE:HB2	1.98	0.46
1:D:71:LYS:NZ	1:G:83:GLU:OE1	2.39	0.46
1:P:83:GLU:HG2	1:S:83:GLU:CD	2.41	0.46
1:S:131:LEU:HD12	1:S:143:ILE:HD13	1.98	0.46
1:E:131:LEU:HD12	1:E:143:ILE:HD13	1.98	0.46
1:P:101:ASP:OD2	1:P:216:THR:HB	2.16	0.46
1:W:5:VAL:O	1:W:6:LYS:C	2.49	0.46
1:G:221:ALA:O	1:G:225:LEU:HG	2.17	0.45
1:M:151:ARG:HD3	1:M:155:GLU:OE1	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:71:LYS:O	1:T:75:ARG:HG3	2.16	0.45
1:V:61:ASP:OD1	1:V:123:ASN:ND2	2.49	0.45
1:A:206:LEU:HD13	1:B:60:VAL:HG11	1.98	0.45
1:C:44:ARG:HG3	1:D:44:ARG:HG3	1.97	0.45
1:C:60:VAL:O	1:C:152:TYR:OH	2.29	0.45
1:J:80:ASN:HD21	1:M:82:SER:CB	2.29	0.45
1:O:33:LEU:HD12	1:O:38:ALA:HB1	1.98	0.45
1:Q:146:VAL:HA	1:Q:149:VAL:CG2	2.46	0.45
1:D:67:LYS:HA	1:D:90:LEU:HD11	1.99	0.45
1:M:154:PRO:HG3	1:N:52:THR:HG23	1.97	0.45
1:Y:40:SER:CB	1:Z:76:LYS:HZ1	2.27	0.45
1:Y:151:ARG:HD3	1:Y:155:GLU:OE1	2.16	0.45
1:G:120:SER:HB3	1:G:127:LEU:HD22	1.99	0.45
1:N:167:LYS:CG	1:O:143:ILE:HD12	2.47	0.45
1:O:127:LEU:CD2	1:O:143:ILE:HG22	2.46	0.45
1:P:61:ASP:OD1	1:P:64:THR:OG1	2.28	0.45
1:S:101:ASP:CG	1:S:216:THR:HB	2.42	0.45
1:Y:61:ASP:OD1	1:Y:123:ASN:ND2	2.49	0.45
1:D:27:ASN:O	1:D:31:GLU:HG3	2.17	0.45
1:N:33:LEU:HD12	1:N:38:ALA:HB1	1.98	0.45
1:U:101:ASP:CG	1:U:216:THR:HB	2.41	0.45
1:V:90:LEU:O	1:V:93:ILE:HG22	2.17	0.45
1:B:16:ASN:O	1:B:17:GLU:CB	2.58	0.45
1:D:98:ALA:HB1	1:D:102:VAL:CG2	2.47	0.45
1:D:151:ARG:HE	1:D:155:GLU:CD	2.23	0.45
1:U:163:LEU:HD11	1:U:191:LEU:HD11	1.99	0.45
1:Y:98:ALA:HB1	1:Y:102:VAL:CG2	2.46	0.45
1:J:42:TRP:HB2	1:J:73:THR:HG21	1.98	0.45
1:N:167:LYS:HG2	1:O:143:ILE:HD12	1.98	0.45
1:O:71:LYS:O	1:O:75:ARG:HG2	2.16	0.45
1:V:98:ALA:HB1	1:V:102:VAL:HG21	1.99	0.45
1:V:143:ILE:O	1:W:165:THR:HA	2.17	0.45
1:Y:98:ALA:HB1	1:Y:102:VAL:HG21	1.98	0.45
1:D:101:ASP:CG	1:D:216:THR:HB	2.42	0.45
1:G:206:LEU:HD13	1:H:60:VAL:HG11	1.99	0.45
1:I:11:LEU:HD23	1:I:174:MET:HB3	1.99	0.45
1:R:225:LEU:O	1:R:226:LYS:CG	2.65	0.45
1:I:101:ASP:CG	1:I:216:THR:HB	2.42	0.45
1:V:27:ASN:O	1:V:31:GLU:HG2	2.17	0.45
1:Z:29:ILE:HD13	1:Z:42:TRP:CE3	2.52	0.45
1:F:144:PHE:CE2	1:F:162:VAL:HG13	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:121:ASN:HA	1:Q:146:VAL:HG13	1.99	0.44
1:R:167:LYS:NZ	1:S:140:PHE:O	2.31	0.44
1:Y:101:ASP:CG	1:Y:216:THR:HB	2.42	0.44
1:Z:149:VAL:HG12	1:Z:161:ALA:CB	2.47	0.44
1:J:151:ARG:HD3	1:J:155:GLU:CD	2.43	0.44
1:P:167:LYS:HG2	1:Q:143:ILE:HD11	1.99	0.44
1:Q:76:LYS:HZ1	1:R:40:SER:CB	2.26	0.44
1:B:11:LEU:HD23	1:B:174:MET:HB3	1.99	0.44
1:C:108:MET:HG2	1:C:225:LEU:HD12	1.98	0.44
1:W:214:ALA:HB1	1:W:219:GLU:HB3	1.99	0.44
1:G:33:LEU:HD12	1:G:38:ALA:HB1	1.99	0.44
1:R:71:LYS:O	1:R:75:ARG:HG2	2.18	0.44
1:V:146:VAL:HA	1:V:149:VAL:HG12	2.00	0.44
1:W:5:VAL:CG1	1:W:6:LYS:HG2	2.36	0.44
1:D:49:TYR:HA	1:D:52:THR:HB	1.98	0.44
1:O:131:LEU:HD12	1:O:143:ILE:HD13	2.00	0.44
1:V:33:LEU:HD12	1:V:38:ALA:HB1	1.99	0.44
1:K:71:LYS:O	1:K:75:ARG:HG2	2.17	0.44
1:N:151:ARG:HE	1:N:155:GLU:CD	2.26	0.44
1:Z:16:ASN:O	1:Z:17:GLU:HB2	2.18	0.44
1:B:174:MET:HA	1:B:192:ARG:O	2.18	0.44
1:H:174:MET:HA	1:H:192:ARG:O	2.18	0.44
1:X:101:ASP:CG	1:X:216:THR:HB	2.43	0.44
1:Y:17:GLU:CD	1:Y:201:HIS:NE2	2.76	0.44
1:J:80:ASN:ND2	1:M:82:SER:CB	2.81	0.44
1:N:165:THR:HA	1:O:143:ILE:O	2.17	0.44
1:W:98:ALA:HB1	1:W:102:VAL:CG2	2.47	0.44
1:X:195:PHE:HB2	1:X:210:PRO:HG3	2.00	0.44
1:F:143:ILE:CD1	1:G:167:LYS:HG2	2.48	0.43
1:Q:67:LYS:HA	1:Q:90:LEU:HD11	1.98	0.43
1:Q:195:PHE:CD2	1:Q:203:ILE:HD11	2.53	0.43
1:Q:60:VAL:O	1:Q:152:TYR:OH	2.34	0.43
1:D:148:ALA:O	1:E:148:ALA:O	2.36	0.43
1:F:143:ILE:O	1:G:165:THR:HA	2.18	0.43
1:J:101:ASP:CG	1:J:216:THR:HB	2.43	0.43
1:X:109:LEU:HD21	1:X:221:ALA:HA	1.99	0.43
1:E:76:LYS:NZ	1:F:40:SER:OG	2.39	0.43
1:J:226:LYS:HA	1:J:226:LYS:HD3	1.80	0.43
1:Q:101:ASP:OD1	1:Q:198:ARG:NH1	2.47	0.43
1:B:146:VAL:HA	1:B:149:VAL:HG12	2.00	0.43
1:K:33:LEU:HD12	1:K:38:ALA:HB1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:17:GLU:OE1	1:Q:22:MET:HG3	2.18	0.43
1:V:151:ARG:HE	1:V:155:GLU:CD	2.27	0.43
1:W:44:ARG:HH12	2:W:301:PO4:P	2.42	0.43
1:G:109:LEU:HD21	1:G:221:ALA:HA	2.01	0.43
1:J:27:ASN:O	1:J:31:GLU:HG2	2.19	0.43
1:K:67:LYS:HA	1:K:90:LEU:HD11	2.00	0.43
1:O:40:SER:CB	1:P:76:LYS:NZ	2.78	0.43
1:O:174:MET:HA	1:O:192:ARG:O	2.18	0.43
1:J:67:LYS:HA	1:J:90:LEU:HD11	2.00	0.43
1:V:101:ASP:CG	1:V:216:THR:HB	2.43	0.43
1:Z:174:MET:HA	1:Z:192:ARG:O	2.19	0.43
1:C:52:THR:HG23	1:D:154:PRO:HG3	2.01	0.43
1:C:98:ALA:HB1	1:C:102:VAL:HG21	2.01	0.43
1:D:26:GLU:HA	1:D:39:PHE:CD1	2.54	0.43
1:F:101:ASP:CG	1:F:216:THR:HB	2.44	0.43
1:H:82:SER:HA	1:K:80:ASN:ND2	2.34	0.43
1:N:67:LYS:HA	1:N:90:LEU:HD11	2.01	0.43
1:P:127:LEU:CD2	1:P:143:ILE:HG22	2.49	0.43
1:U:200:GLY:O	1:V:76:LYS:HE2	2.17	0.43
1:D:165:THR:HA	1:E:143:ILE:O	2.19	0.43
1:R:119:LEU:HG	1:R:153:LYS:HD3	2.01	0.43
1:X:67:LYS:HA	1:X:90:LEU:HD11	2.00	0.43
1:R:225:LEU:C	1:R:226:LYS:HG3	2.44	0.42
1:D:7:LYS:HE3	1:D:7:LYS:HB3	1.74	0.42
1:E:119:LEU:HG	1:E:153:LYS:HD3	2.01	0.42
1:F:118:ALA:HB3	1:F:143:ILE:HG22	2.01	0.42
1:Q:29:ILE:HG13	1:Q:89:ILE:CG2	2.50	0.42
1:A:11:LEU:HD23	1:A:174:MET:HB3	2.02	0.42
1:Q:146:VAL:O	1:Q:150:GLY:N	2.51	0.42
1:R:80:ASN:HD21	1:U:82:SER:CB	2.31	0.42
1:S:101:ASP:OD1	1:S:198:ARG:NH2	2.53	0.42
1:F:163:LEU:HD11	1:F:191:LEU:HD11	2.01	0.42
1:I:26:GLU:HA	1:I:39:PHE:CD1	2.55	0.42
1:M:18:THR:OG1	1:M:178:ALA:N	2.47	0.42
1:P:120:SER:HB3	1:P:127:LEU:HD22	2.01	0.42
1:T:214:ALA:HB1	1:T:219:GLU:HB3	2.02	0.42
1:T:167:LYS:HD3	1:U:143:ILE:HG13	2.01	0.42
1:Y:11:LEU:HD23	1:Y:174:MET:HB3	2.01	0.42
1:W:5:VAL:CG1	1:W:6:LYS:HG3	2.33	0.42
1:C:16:ASN:O	1:C:17:GLU:HB2	2.19	0.42
1:X:14:ASP:O	1:X:18:THR:HB	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:163:LEU:HD11	1:X:191:LEU:HD11	2.02	0.42
1:Z:121:ASN:HA	1:Z:146:VAL:HG13	2.02	0.42
1:A:44:ARG:HG3	1:B:44:ARG:HG3	2.01	0.42
1:F:148:ALA:O	1:G:148:ALA:O	2.38	0.42
1:K:108:MET:HE2	1:K:225:LEU:HD12	2.01	0.42
1:L:121:ASN:HA	1:L:146:VAL:HG13	2.02	0.42
1:Q:15:VAL:HG21	1:Q:127:LEU:HD11	2.02	0.42
1:Q:174:MET:HA	1:Q:192:ARG:O	2.20	0.42
1:Z:101:ASP:CG	1:Z:216:THR:HB	2.44	0.42
1:G:150:GLY:O	3:G:401:HOH:O	2.21	0.42
1:J:143:ILE:HG13	1:K:167:LYS:HD3	2.01	0.42
1:K:144:PHE:CE2	1:K:162:VAL:HG13	2.55	0.42
1:N:101:ASP:OD2	1:N:216:THR:HB	2.20	0.42
1:Q:33:LEU:HD12	1:Q:38:ALA:HB1	2.02	0.42
1:D:102:VAL:O	1:D:106:LEU:HD23	2.20	0.41
1:H:101:ASP:CG	1:H:216:THR:HB	2.44	0.41
1:N:202:ALA:O	2:N:301:PO4:O4	2.38	0.41
1:W:19:LEU:HA	1:W:102:VAL:HG11	2.02	0.41
1:C:11:LEU:HD23	1:C:174:MET:HB3	2.02	0.41
1:M:155:GLU:HG3	1:N:55:LEU:HD22	2.02	0.41
1:Q:184:LEU:HD22	1:Q:204:TYR:CD2	2.55	0.41
1:W:15:VAL:HG21	1:W:127:LEU:HD11	2.02	0.41
1:A:61:ASP:OD1	1:A:61:ASP:C	2.63	0.41
1:G:16:ASN:O	1:G:17:GLU:HB2	2.20	0.41
1:B:61:ASP:OD1	1:B:61:ASP:C	2.63	0.41
1:J:99:HIS:CE1	1:J:198:ARG:HD2	2.55	0.41
1:P:29:ILE:HD13	1:P:42:TRP:CE3	2.55	0.41
1:T:7:LYS:HA	1:T:8:PRO:HD3	1.87	0.41
1:W:101:ASP:OD2	1:W:216:THR:HB	2.21	0.41
1:Y:14:ASP:O	1:Y:18:THR:HB	2.21	0.41
1:D:19:LEU:HA	1:D:102:VAL:HG11	2.02	0.41
1:D:60:VAL:O	1:D:152:TYR:OH	2.37	0.41
1:G:11:LEU:HD23	1:G:174:MET:HB3	2.02	0.41
1:G:55:LEU:HD22	1:H:155:GLU:HG3	2.03	0.41
1:N:203:ILE:CD1	1:N:213:GLU:OE2	2.68	0.41
1:R:195:PHE:HB2	1:R:210:PRO:HG3	2.03	0.41
1:Y:17:GLU:HG2	1:Y:201:HIS:NE2	2.36	0.41
1:Q:149:VAL:HG12	1:Q:161:ALA:HB3	2.03	0.41
1:S:60:VAL:O	1:S:152:TYR:OH	2.37	0.41
1:F:183:ILE:HD12	1:F:193:THR:HB	2.02	0.41
1:R:5:VAL:HG11	1:R:192:ARG:NH2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:19:LEU:HA	1:Y:102:VAL:HG11	2.03	0.41
1:D:98:ALA:HB1	1:D:102:VAL:HG21	2.01	0.41
1:G:27:ASN:O	1:G:31:GLU:HG2	2.21	0.41
1:J:101:ASP:OD2	1:J:216:THR:HB	2.21	0.41
1:K:17:GLU:HG2	1:K:201:HIS:CE1	2.56	0.41
1:L:32:SER:OG	1:L:89:ILE:HD11	2.21	0.41
1:N:137:ALA:O	1:O:167:LYS:NZ	2.52	0.41
1:P:151:ARG:HE	1:P:155:GLU:CD	2.28	0.41
1:P:167:LYS:HE3	1:P:167:LYS:HB2	1.95	0.41
1:P:202:ALA:O	2:P:301:PO4:O4	2.38	0.41
1:Q:101:ASP:CG	1:Q:216:THR:HB	2.46	0.41
1:S:49:TYR:HA	1:S:52:THR:HB	2.03	0.41
1:T:226:LYS:HA	1:T:226:LYS:HD2	1.86	0.41
1:U:16:ASN:O	1:U:17:GLU:CB	2.62	0.41
1:U:17:GLU:HG2	1:U:201:HIS:NE2	2.35	0.41
1:W:33:LEU:HD12	1:W:38:ALA:HB1	2.02	0.41
1:W:61:ASP:OD1	1:W:123:ASN:ND2	2.45	0.41
1:S:61:ASP:OD1	1:S:61:ASP:C	2.63	0.41
1:T:151:ARG:HE	1:T:155:GLU:CD	2.28	0.41
1:U:60:VAL:HG11	1:V:206:LEU:HD13	2.02	0.41
1:H:33:LEU:HD12	1:H:38:ALA:HB1	2.03	0.40
1:J:196:VAL:HG12	1:J:198:ARG:HG2	2.03	0.40
1:M:17:GLU:CG	1:M:201:HIS:NE2	2.84	0.40
1:Y:121:ASN:HA	1:Y:146:VAL:HG13	2.02	0.40
1:C:107:LYS:O	1:C:111:GLU:HG2	2.20	0.40
1:F:33:LEU:HD12	1:F:38:ALA:HB1	2.02	0.40
1:M:44:ARG:HG3	1:N:44:ARG:HG3	2.03	0.40
1:N:226:LYS:HB2	1:N:226:LYS:HE2	1.74	0.40
1:O:143:ILE:HD13	1:O:143:ILE:HG21	1.82	0.40
1:L:101:ASP:CG	1:L:216:THR:HB	2.46	0.40
1:M:11:LEU:HD23	1:M:174:MET:HB3	2.01	0.40
1:U:33:LEU:HD12	1:U:77:PHE:HB2	2.03	0.40
1:Z:42:TRP:HB2	1:Z:73:THR:HG21	2.02	0.40
1:Z:98:ALA:HB1	1:Z:102:VAL:HG21	2.04	0.40
1:E:127:LEU:CD2	1:E:143:ILE:HG22	2.50	0.40
1:F:195:PHE:CD2	1:F:203:ILE:HD11	2.57	0.40
1:K:60:VAL:O	1:K:152:TYR:OH	2.31	0.40
1:K:151:ARG:HD3	1:K:155:GLU:CD	2.47	0.40
1:Q:16:ASN:O	1:Q:17:GLU:HB2	2.22	0.40
1:C:15:VAL:HG21	1:C:127:LEU:HD11	2.04	0.40
1:E:123:ASN:OD1	1:E:123:ASN:N	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:163:LEU:HD11	1:S:191:LEU:HD11	2.02	0.40
1:Y:17:GLU:CG	1:Y:201:HIS:NE2	2.85	0.40

All (21) 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)
1:C:111:GLU:OE1	1:S:7:LYS:NZ[2_646]	1.24	0.96
1:A:83:GLU:OE2	1:X:83:GLU:OE2[1_556]	1.47	0.73
1:G:219:GLU:OE1	1:N:103:LYS:NZ[2_646]	1.79	0.41
1:D:97:PRO:CG	1:F:222:ARG:NE[1_455]	1.81	0.39
1:K:111:GLU:OE1	1:L:7:LYS:NZ[1_655]	1.87	0.33
1:C:85:ARG:NH1	1:V:222:ARG:NH2[2_546]	1.94	0.26
1:D:97:PRO:CB	1:F:222:ARG:NH2[1_455]	1.97	0.23
1:A:103:LYS:NZ	1:X:219:GLU:OE2[2_656]	1.98	0.22
1:I:7:LYS:NZ	1:J:111:GLU:OE1[1_455]	1.99	0.21
1:G:31:GLU:O	1:Q:79:LYS:NZ[2_546]	2.01	0.19
1:A:83:GLU:CD	1:X:83:GLU:OE2[1_556]	2.02	0.18
1:B:85:ARG:CZ	1:D:222:ARG:NH1[1_655]	2.02	0.18
1:A:219:GLU:OE2	1:T:31:GLU:OE1[2_656]	2.03	0.17
1:B:85:ARG:NH1	1:D:222:ARG:NH1[1_655]	2.03	0.17
1:B:215:LYS:NZ	1:Z:31:GLU:O[1_656]	2.06	0.14
1:F:77:PHE:O	1:P:85:ARG:NH2[2_656]	2.06	0.14
1:C:85:ARG:NH2	1:V:222:ARG:NH1[2_546]	2.07	0.13
1:B:85:ARG:NH1	1:D:222:ARG:CZ[1_655]	2.13	0.07
1:C:85:ARG:CZ	1:V:222:ARG:CZ[2_546]	2.17	0.03
1:F:77:PHE:O	1:P:85:ARG:CZ[2_656]	2.17	0.03
1:I:112:ALA:O	1:J:111:GLU:OE1[1_455]	2.17	0.03

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	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	B	219/227 (96%)	209 (95%)	8 (4%)	2 (1%)	14	26
1	C	220/227 (97%)	212 (96%)	8 (4%)	0	100	100
1	D	219/227 (96%)	212 (97%)	5 (2%)	2 (1%)	14	26
1	E	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	F	219/227 (96%)	212 (97%)	6 (3%)	1 (0%)	24	40
1	G	220/227 (97%)	210 (96%)	9 (4%)	1 (0%)	24	40
1	H	220/227 (97%)	215 (98%)	5 (2%)	0	100	100
1	I	220/227 (97%)	214 (97%)	4 (2%)	2 (1%)	14	26
1	J	220/227 (97%)	212 (96%)	6 (3%)	2 (1%)	14	26
1	K	220/227 (97%)	216 (98%)	4 (2%)	0	100	100
1	L	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	M	219/227 (96%)	211 (96%)	7 (3%)	1 (0%)	24	40
1	N	220/227 (97%)	216 (98%)	4 (2%)	0	100	100
1	O	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	P	220/227 (97%)	216 (98%)	4 (2%)	0	100	100
1	Q	220/227 (97%)	213 (97%)	6 (3%)	1 (0%)	24	40
1	R	220/227 (97%)	212 (96%)	7 (3%)	1 (0%)	24	40
1	S	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	T	220/227 (97%)	212 (96%)	8 (4%)	0	100	100
1	U	219/227 (96%)	209 (95%)	8 (4%)	2 (1%)	14	26
1	V	219/227 (96%)	210 (96%)	7 (3%)	2 (1%)	14	26
1	W	219/227 (96%)	212 (97%)	6 (3%)	1 (0%)	24	40
1	X	219/227 (96%)	217 (99%)	2 (1%)	0	100	100
1	Y	219/227 (96%)	212 (97%)	6 (3%)	1 (0%)	24	40
1	Z	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
All	All	5705/5902 (97%)	5535 (97%)	151 (3%)	19 (0%)	36	54

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	17	GLU
1	U	17	GLU
1	W	6	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	17	GLU
1	D	17	GLU
1	F	17	GLU
1	J	17	GLU
1	R	17	GLU
1	V	149	VAL
1	Y	17	GLU
1	M	17	GLU
1	G	17	GLU
1	J	16	ASN
1	U	149	VAL
1	I	17	GLU
1	I	23	GLY
1	V	17	GLU
1	B	149	VAL
1	D	149	VAL

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	182/187 (97%)	178 (98%)	4 (2%)	45	65
1	B	182/187 (97%)	179 (98%)	3 (2%)	55	72
1	C	183/187 (98%)	181 (99%)	2 (1%)	65	79
1	D	182/187 (97%)	174 (96%)	8 (4%)	25	45
1	E	182/187 (97%)	177 (97%)	5 (3%)	39	61
1	F	182/187 (97%)	177 (97%)	5 (3%)	39	61
1	G	183/187 (98%)	179 (98%)	4 (2%)	45	65
1	H	183/187 (98%)	181 (99%)	2 (1%)	65	79
1	I	183/187 (98%)	179 (98%)	4 (2%)	45	65
1	J	183/187 (98%)	179 (98%)	4 (2%)	45	65
1	K	183/187 (98%)	181 (99%)	2 (1%)	65	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	182/187 (97%)	180 (99%)	2 (1%)	65	79
1	M	182/187 (97%)	181 (100%)	1 (0%)	81	88
1	N	183/187 (98%)	179 (98%)	4 (2%)	45	65
1	O	182/187 (97%)	181 (100%)	1 (0%)	81	88
1	P	183/187 (98%)	181 (99%)	2 (1%)	65	79
1	Q	183/187 (98%)	181 (99%)	2 (1%)	65	79
1	R	183/187 (98%)	178 (97%)	5 (3%)	39	61
1	S	182/187 (97%)	179 (98%)	3 (2%)	55	72
1	T	183/187 (98%)	176 (96%)	7 (4%)	29	51
1	U	182/187 (97%)	177 (97%)	5 (3%)	39	61
1	V	182/187 (97%)	182 (100%)	0	100	100
1	W	182/187 (97%)	178 (98%)	4 (2%)	45	65
1	X	182/187 (97%)	179 (98%)	3 (2%)	55	72
1	Y	182/187 (97%)	178 (98%)	4 (2%)	45	65
1	Z	182/187 (97%)	179 (98%)	3 (2%)	55	72
All	All	4743/4862 (98%)	4654 (98%)	89 (2%)	50	68

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	155	GLU
1	A	192	ARG
1	A	209	THR
1	B	17	GLU
1	B	61	ASP
1	B	100	GLU
1	C	29	ILE
1	C	32	SER
1	D	34	ASN
1	D	61	ASP
1	D	94	LYS
1	D	97	PRO
1	D	102	VAL
1	D	149	VAL
1	D	212	LEU
1	D	219	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	5	VAL
1	E	17	GLU
1	E	33	LEU
1	E	50	SER
1	E	123	ASN
1	F	32	SER
1	F	85	ARG
1	F	179	ASN
1	F	209	THR
1	F	222	ARG
1	G	34	ASN
1	G	83	GLU
1	G	199	GLU
1	G	209	THR
1	H	155	GLU
1	H	219	GLU
1	I	17	GLU
1	I	61	ASP
1	I	209	THR
1	I	219	GLU
1	J	17	GLU
1	J	32	SER
1	J	50	SER
1	J	61	ASP
1	K	17	GLU
1	K	61	ASP
1	L	17	GLU
1	L	209	THR
1	M	17	GLU
1	N	5	VAL
1	N	17	GLU
1	N	61	ASP
1	N	149	VAL
1	O	151	ARG
1	P	85	ARG
1	P	155	GLU
1	Q	34	ASN
1	Q	212	LEU
1	R	17	GLU
1	R	34	ASN
1	R	179	ASN
1	R	199	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	212	LEU
1	S	17	GLU
1	S	61	ASP
1	S	198	ARG
1	T	5	VAL
1	T	17	GLU
1	T	32	SER
1	T	61	ASP
1	T	132	GLN
1	T	212	LEU
1	T	219	GLU
1	U	17	GLU
1	U	29	ILE
1	U	32	SER
1	U	61	ASP
1	U	222	ARG
1	W	7	LYS
1	W	17	GLU
1	W	32	SER
1	W	219	GLU
1	X	17	GLU
1	X	209	THR
1	X	212	LEU
1	Y	17	GLU
1	Y	100	GLU
1	Y	179	ASN
1	Y	209	THR
1	Z	31	GLU
1	Z	116	LEU
1	Z	219	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	130	GLN
1	D	80	ASN
1	E	34	ASN
1	E	130	GLN
1	E	201	HIS
1	F	16	ASN
1	F	123	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	130	GLN
1	G	92	ASN
1	G	130	GLN
1	H	179	ASN
1	K	80	ASN
1	K	123	ASN
1	L	37	HIS
1	L	113	GLN
1	L	172	ASN
1	L	179	ASN
1	M	16	ASN
1	M	130	GLN
1	P	172	ASN
1	Q	130	GLN
1	R	80	ASN
1	R	130	GLN
1	R	172	ASN
1	S	130	GLN
1	T	179	ASN
1	U	80	ASN
1	W	37	HIS
1	Z	16	ASN
1	Z	130	GLN

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](#)

26 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	S	301	-	4,4,4	0.76	0	6,6,6	0.53	0
2	PO4	Q	301	-	4,4,4	0.82	0	6,6,6	0.45	0
2	PO4	T	301	-	4,4,4	0.87	0	6,6,6	0.41	0
2	PO4	X	301	-	4,4,4	0.96	0	6,6,6	0.43	0
2	PO4	A	301	-	4,4,4	0.63	0	6,6,6	0.55	0
2	PO4	E	301	-	4,4,4	0.65	0	6,6,6	0.48	0
2	PO4	Z	301	-	4,4,4	0.76	0	6,6,6	0.47	0
2	PO4	O	301	-	4,4,4	0.75	0	6,6,6	0.56	0
2	PO4	L	301	-	4,4,4	0.77	0	6,6,6	0.49	0
2	PO4	C	301	-	4,4,4	0.66	0	6,6,6	0.48	0
2	PO4	N	301	-	4,4,4	1.02	0	6,6,6	0.40	0
2	PO4	V	301	-	4,4,4	0.62	0	6,6,6	0.54	0
2	PO4	B	301	-	4,4,4	0.75	0	6,6,6	0.51	0
2	PO4	D	301	-	4,4,4	0.58	0	6,6,6	0.58	0
2	PO4	M	301	-	4,4,4	0.83	0	6,6,6	0.44	0
2	PO4	U	301	-	4,4,4	0.72	0	6,6,6	0.45	0
2	PO4	K	301	-	4,4,4	0.74	0	6,6,6	0.51	0
2	PO4	G	301	-	4,4,4	1.03	0	6,6,6	0.37	0
2	PO4	R	301	-	4,4,4	0.69	0	6,6,6	0.53	0
2	PO4	F	301	-	4,4,4	0.68	0	6,6,6	0.49	0
2	PO4	P	301	-	4,4,4	0.74	0	6,6,6	0.58	0
2	PO4	Y	301	-	4,4,4	0.62	0	6,6,6	0.52	0
2	PO4	J	301	-	4,4,4	0.98	0	6,6,6	0.42	0
2	PO4	W	301	-	4,4,4	1.05	0	6,6,6	0.48	0
2	PO4	H	301	-	4,4,4	0.73	0	6,6,6	0.54	0
2	PO4	I	301	-	4,4,4	0.55	0	6,6,6	0.53	0

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	301	PO4	1	0
2	P	301	PO4	1	0
2	W	301	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	221/227 (97%)	0.09	3 (1%) 73 72	61, 84, 123, 138	0
1	B	221/227 (97%)	0.06	4 (1%) 67 64	64, 85, 116, 135	0
1	C	222/227 (97%)	0.09	2 (0%) 81 81	67, 92, 120, 139	0
1	D	221/227 (97%)	0.53	10 (4%) 38 37	72, 108, 144, 190	0
1	E	221/227 (97%)	0.51	5 (2%) 61 58	72, 100, 136, 168	0
1	F	221/227 (97%)	0.38	4 (1%) 67 64	72, 89, 121, 172	0
1	G	222/227 (97%)	-0.04	4 (1%) 67 64	59, 78, 110, 147	0
1	H	222/227 (97%)	-0.06	3 (1%) 73 72	58, 76, 106, 157	0
1	I	222/227 (97%)	0.00	4 (1%) 67 64	56, 72, 99, 123	0
1	J	222/227 (97%)	-0.06	2 (0%) 81 81	59, 76, 112, 139	0
1	K	222/227 (97%)	-0.12	4 (1%) 67 64	54, 72, 102, 121	0
1	L	221/227 (97%)	-0.06	1 (0%) 87 87	54, 73, 98, 117	0
1	M	221/227 (97%)	0.09	5 (2%) 61 58	61, 83, 118, 164	0
1	N	222/227 (97%)	0.01	4 (1%) 67 64	60, 75, 108, 132	0
1	O	221/227 (97%)	-0.21	1 (0%) 87 87	52, 66, 99, 134	0
1	P	222/227 (97%)	-0.16	2 (0%) 81 81	52, 68, 98, 117	0
1	Q	222/227 (97%)	0.08	1 (0%) 87 87	56, 83, 115, 139	0
1	R	222/227 (97%)	0.08	2 (0%) 81 81	63, 90, 121, 147	0
1	S	221/227 (97%)	0.56	8 (3%) 46 44	66, 97, 126, 153	0
1	T	222/227 (97%)	0.17	3 (1%) 73 72	69, 93, 125, 144	0
1	U	221/227 (97%)	0.20	4 (1%) 67 64	65, 90, 118, 145	0
1	V	221/227 (97%)	0.23	3 (1%) 73 72	65, 96, 129, 140	0
1	W	221/227 (97%)	0.34	5 (2%) 61 58	68, 97, 131, 161	0
1	X	221/227 (97%)	0.24	7 (3%) 50 48	68, 92, 124, 154	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	221/227 (97%)	0.26	2 (0%) 81 81	73, 100, 131, 142	0
1	Z	221/227 (97%)	0.24	2 (0%) 81 81	67, 98, 135, 157	0
All	All	5757/5902 (97%)	0.13	95 (1%) 69 66	52, 85, 124, 190	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	ALA	4.9
1	P	148	ALA	4.4
1	X	148	ALA	4.2
1	B	148	ALA	4.0
1	V	148	ALA	3.9
1	H	148	ALA	3.9
1	D	148	ALA	3.8
1	M	225	LEU	3.7
1	W	225	LEU	3.7
1	X	149	VAL	3.5
1	D	149	VAL	3.5
1	I	149	VAL	3.4
1	S	148	ALA	3.4
1	S	149	VAL	3.3
1	X	33	LEU	3.1
1	F	149	VAL	3.1
1	G	148	ALA	3.1
1	X	150	GLY	3.1
1	W	149	VAL	3.0
1	Z	78	GLY	3.0
1	U	148	ALA	2.9
1	S	109	LEU	2.9
1	M	148	ALA	2.9
1	J	149	VAL	2.9
1	S	224	LEU	2.9
1	N	148	ALA	2.9
1	U	5	VAL	2.9
1	S	225	LEU	2.8
1	S	114	ILE	2.8
1	D	196	VAL	2.8
1	N	150	GLY	2.8
1	N	149	VAL	2.8
1	D	102	VAL	2.7
1	I	148	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	V	150	GLY	2.7
1	F	150	GLY	2.7
1	M	5	VAL	2.6
1	B	149	VAL	2.6
1	Q	5	VAL	2.6
1	N	222	ARG	2.6
1	O	150	GLY	2.6
1	M	149	VAL	2.6
1	A	149	VAL	2.5
1	D	109	LEU	2.5
1	B	150	GLY	2.5
1	R	148	ALA	2.5
1	D	150	GLY	2.4
1	H	5	VAL	2.4
1	W	148	ALA	2.4
1	V	149	VAL	2.4
1	B	5	VAL	2.4
1	E	149	VAL	2.4
1	T	148	ALA	2.4
1	D	10	LEU	2.4
1	M	150	GLY	2.4
1	W	217	VAL	2.4
1	U	224	LEU	2.3
1	I	5	VAL	2.3
1	A	78	GLY	2.3
1	H	150	GLY	2.3
1	G	149	VAL	2.3
1	D	224	LEU	2.3
1	F	148	ALA	2.3
1	E	224	LEU	2.2
1	P	81	LEU	2.2
1	K	149	VAL	2.2
1	L	149	VAL	2.2
1	Y	80	ASN	2.2
1	X	76	LYS	2.2
1	C	5	VAL	2.2
1	D	97	PRO	2.2
1	T	150	GLY	2.2
1	K	148	ALA	2.1
1	U	38	ALA	2.1
1	G	5	VAL	2.1
1	R	5	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	225	LEU	2.1
1	S	106	LEU	2.1
1	Y	33	LEU	2.1
1	W	150	GLY	2.1
1	T	149	VAL	2.1
1	F	62	PHE	2.1
1	C	148	ALA	2.1
1	D	220	VAL	2.1
1	E	98	ALA	2.1
1	E	5	VAL	2.1
1	X	5	VAL	2.1
1	K	17	GLU	2.0
1	G	226	LYS	2.0
1	S	11	LEU	2.0
1	I	150	GLY	2.0
1	J	5	VAL	2.0
1	Z	148	ALA	2.0
1	K	150	GLY	2.0
1	X	34	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	PO4	F	301	5/5	0.44	0.15	126,153,162,167	0
2	PO4	E	301	5/5	0.76	0.12	130,143,144,153	0
2	PO4	W	301	5/5	0.79	0.14	91,97,109,119	0
2	PO4	Q	301	5/5	0.81	0.11	101,139,142,144	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	D	301	5/5	0.83	0.10	92,104,111,127	0
2	PO4	Z	301	5/5	0.84	0.10	110,126,133,139	0
2	PO4	Y	301	5/5	0.85	0.11	126,137,146,154	0
2	PO4	I	301	5/5	0.86	0.14	73,98,118,124	0
2	PO4	M	301	5/5	0.87	0.10	97,123,130,140	0
2	PO4	B	301	5/5	0.89	0.10	94,99,103,107	0
2	PO4	N	301	5/5	0.89	0.09	98,105,112,122	0
2	PO4	C	301	5/5	0.90	0.10	101,120,122,128	0
2	PO4	J	301	5/5	0.90	0.11	107,114,117,123	0
2	PO4	X	301	5/5	0.91	0.13	90,99,107,108	0
2	PO4	K	301	5/5	0.91	0.14	77,106,113,119	0
2	PO4	P	301	5/5	0.91	0.14	76,77,92,97	0
2	PO4	L	301	5/5	0.92	0.14	93,103,111,112	0
2	PO4	T	301	5/5	0.92	0.10	101,103,106,108	0
2	PO4	G	301	5/5	0.93	0.15	77,82,88,102	0
2	PO4	V	301	5/5	0.93	0.09	82,82,92,98	0
2	PO4	O	301	5/5	0.94	0.12	76,82,94,96	0
2	PO4	R	301	5/5	0.94	0.09	99,100,109,114	0
2	PO4	S	301	5/5	0.94	0.08	96,99,105,109	0
2	PO4	A	301	5/5	0.94	0.09	76,89,92,99	0
2	PO4	U	301	5/5	0.94	0.12	88,94,102,103	0
2	PO4	H	301	5/5	0.96	0.07	74,86,86,89	0

6.5 Other polymers ⓘ

There are no such residues in this entry.