WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2022 – 03:40 pm GMT

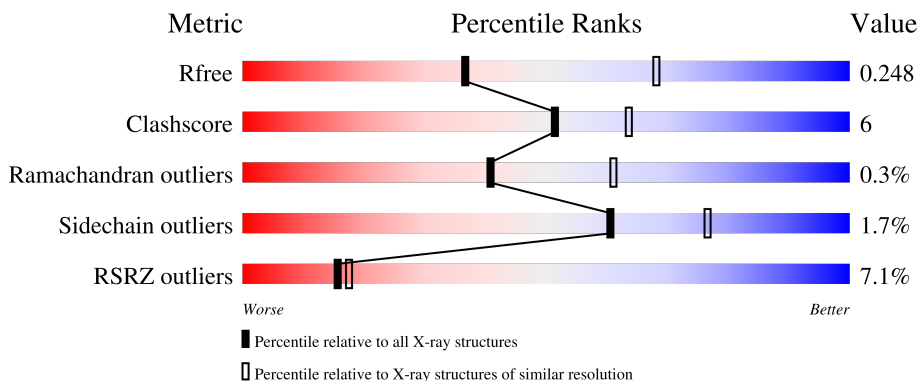|		
PDB ID	:	7QNM
Title	:	Crystallization and structural analyses of ZgHAD, a L-2-haloacid dehalogenase from the marine Flavobacterium Zobellia galactanivorans
Authors	:	Grigorian, E.; Roret, T.; Leblanc, C.; Delage, L.; Czjzek, M.
Deposited on	:	2021-12-21
Resolution	:	2.73 Å(reported)

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 2.73 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	Percentile Ranks	Value
Rfree		0.248
Clashscore		6
Ramachandran outliers		0.3%
Sidechain outliers		1.7%
RSRZ outliers		7.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (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 <=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	5% 87% 10% ••
1	B	227	3% 88% 8% •••
1	C	227	6% 81% 16% ••
1	D	227	17% 81% 14% •••
1	E	227	19% 83% 13% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	227	13% 79% 17%
1	G	227	2% 78% 19%
1	H	227	4% 86% 11%
1	I	227	3% 87% 10%
1	J	227	% 83% 13%
1	K	227	% 86% 11%
1	L	227	2% 86% 10%
1	M	227	6% 81% 14%
1	N	227	3% 87% 9%
1	O	227	% 85% 11%
1	P	227	3% 84% 12%
1	Q	227	5% 79% 17%
1	R	227	7% 82% 13%
1	S	227	11% 82% 14%
1	T	227	7% 87% 9%
1	U	227	7% 83% 12%
1	V	227	9% 83% 13%
1	W	227	12% 78% 17%
1	X	227	6% 84% 13%
1	Y	227	11% 82% 15%
1	Z	227	16% 83% 13%

2 Entry composition (i)

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 1720	C 1102	N 290	O 321	S 7	0	0	0
1	B	221	Total 1720	C 1102	N 290	O 321	S 7	0	0	0
1	C	222	Total 1729	C 1108	N 292	O 322	S 7	0	0	0
1	D	221	Total 1720	C 1102	N 290	O 321	S 7	0	0	0
1	E	221	Total 1720	C 1102	N 290	O 321	S 7	0	0	0
1	F	221	Total 1720	C 1102	N 290	O 321	S 7	0	0	0
1	G	222	Total 1729	C 1108	N 292	O 322	S 7	0	0	0
1	H	222	Total 1729	C 1108	N 292	O 322	S 7	0	0	0
1	I	222	Total 1729	C 1108	N 292	O 322	S 7	0	0	0
1	J	222	Total 1729	C 1108	N 292	O 322	S 7	0	0	0
1	K	222	Total 1729	C 1108	N 292	O 322	S 7	0	0	0
1	L	221	Total 1720	C 1102	N 290	O 321	S 7	0	0	0
1	M	221	Total 1720	C 1102	N 290	O 321	S 7	0	0	0
1	N	222	Total 1729	C 1108	N 292	O 322	S 7	0	0	0
1	O	221	Total 1720	C 1102	N 290	O 321	S 7	0	0	0
1	P	222	Total 1729	C 1108	N 292	O 322	S 7	0	0	0

Continued on next page...

Continued from previous page...

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

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 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 (three-letter code: PO4) (formula: O_4P).
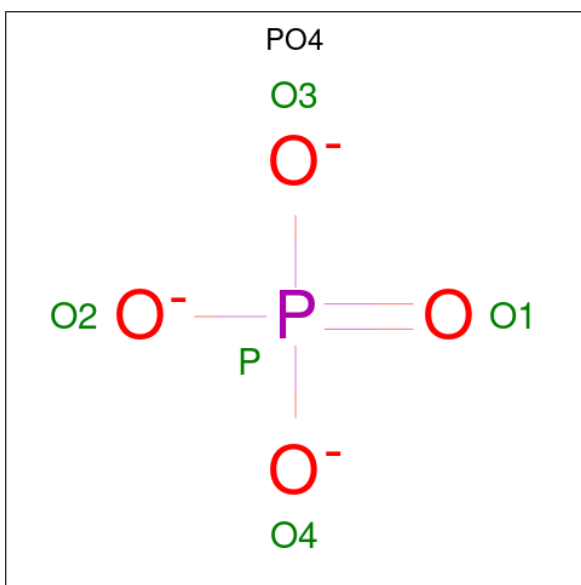
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0
2	E	1	Total 5	O 4	P 1	0	0
2	F	1	Total 5	O 4	P 1	0	0
2	G	1	Total 5	O 4	P 1	0	0
2	H	1	Total 5	O 4	P 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is water.

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

Continued on next page...

Continued from previous page...

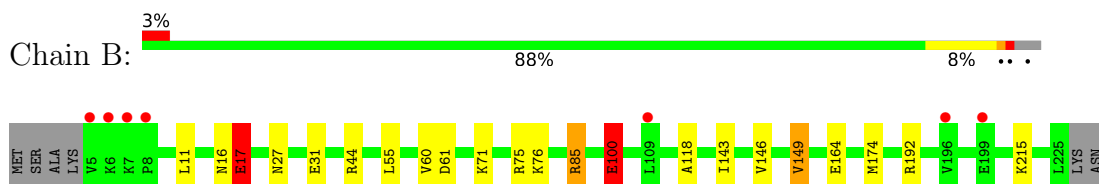| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	O 1	0	0
3	D	2	Total 2	O 2	0	0
3	F	1	Total 1	O 1	0	0
3	G	3	Total 3	O 3	0	0
3	H	4	Total 4	O 4	0	0
3	I	3	Total 3	O 3	0	0
3	J	2	Total 2	O 2	0	0
3	K	6	Total 6	O 6	0	0
3	L	1	Total 1	O 1	0	0
3	M	1	Total 1	O 1	0	0
3	N	2	Total 2	O 2	0	0
3	O	4	Total 4	O 4	0	0
3	P	7	Total 7	O 7	0	0
3	Q	2	Total 2	O 2	0	0
3	R	2	Total 2	O 2	0	0
3	T	2	Total 2	O 2	0	0
3	U	2	Total 2	O 2	0	0
3	W	1	Total 1	O 1	0	0
3	X	2	Total 2	O 2	0	0
3	Y	1	Total 1	O 1	0	0
3	Z	1	Total 1	O 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.
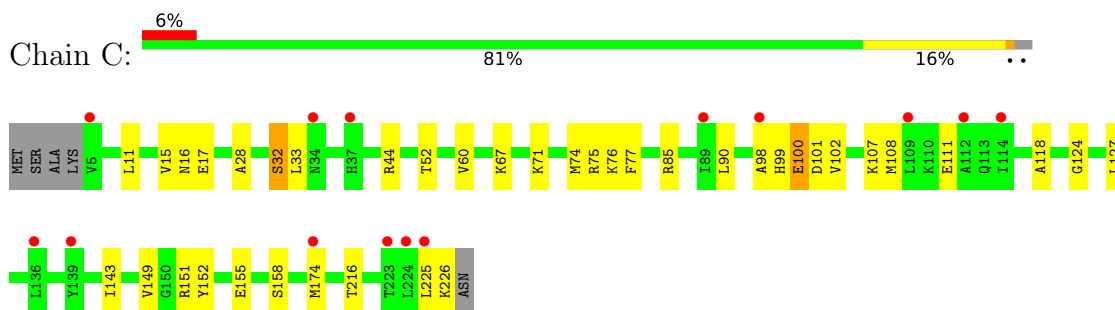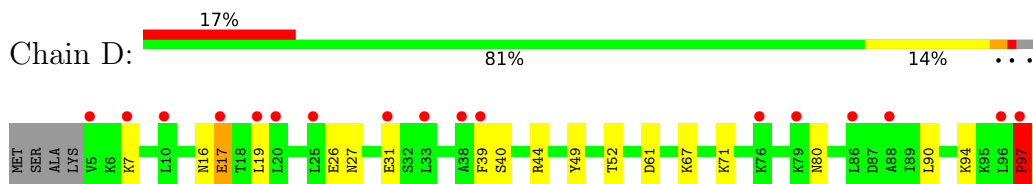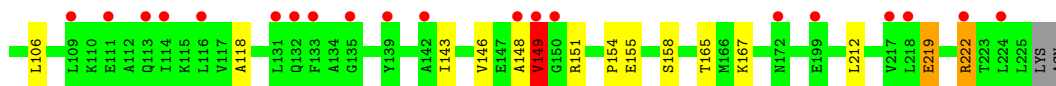
- Molecule 1: (S)-2-haloacid dehalogenase

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

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

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

L106 L109 K110 E111 A112 Q113 I114 K115 L116 V117 A118 L131 Q132 F133 A134 G135 Y139 A142 I143 V146 E147 A148 V149 G150 R151 P154 E155 S158 T165 M166 K167 N172 E199 L212 V217 L218 E219 R222 T223 L224 L225 LYS ASN

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

Chain E:

19%

83%   13%

MET SER ALA LYS V5 K6 K7 P8 L11 I12 F13 D14 V15 N16 E17 T18 L19 L20 N27 E31 S32 L33 H37 S50 L51 T52 V60 K67 K71 M74 R75 K76 D84 L90 K95 L96 P97 A98 H99 E100 D101 V102 L106 K107 M108 E111

A112 Q113 I114 K115 L116 L119 N123 L127 N128 A129 Q130 L131 Q132 F133 L136 Y139 F140 D141 A142 I143 A148 V149 Y152 K153 S158 M174 M175 V176 A177 T193 E199 G200 H201 L206 P210 T216 V217 L218 E219 V220 A221 R222 T223 L224 L225 LYS

ASN

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

Chain F:

13%

79%   17%

MET SER ALA LYS V5 P8 E9 L10 L11 N16 E17 T18 L19 L20 P24 S32 L33 A38 F39 S40 V60 T73 M74 R75 K76 F77 D84 R85 A88 I93 A98 M108 L109 K110 E111 A112 Q113 I114 A118 S122 K125 A129 Q132

A142 I143 F144 A148 V149 G150 R151 Y152 K153 P154 S158 Y159 R160 A161 V162 L163 E164 T165 M166 K167 M174 N179 I183 L191 R192 T193 A194 F195 E199 I203 L206 T209 P210 V217 L218 A221 R222 L225 LYS ASN
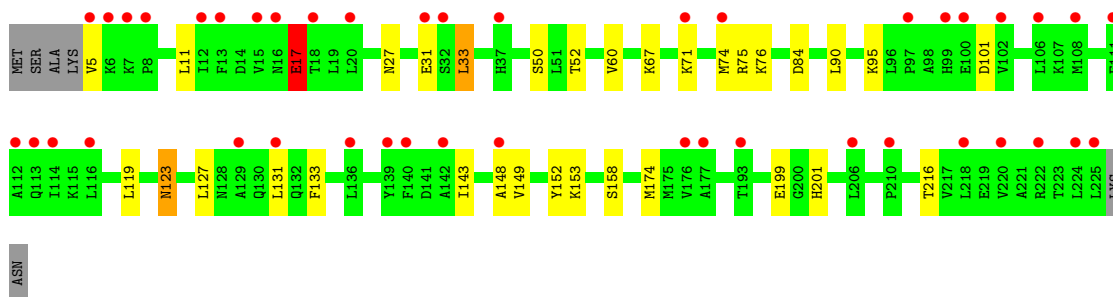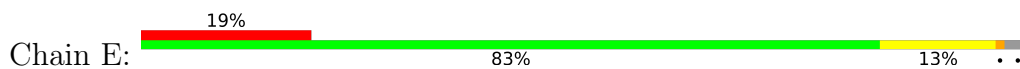
• Molecule 1: (S)-2-haloacid dehalogenase

Chain G:

2%

78%   19%

MET SER ALA LYS V5 L11 N16 E17 N27 E31 S32 L33 N34 A38 R44 L55 V60 K71 R75 S82 E83 D84 R85 L90 I93 D101 L109 I114 L119 S120 L127 L131 A137 I143 A148 V149 G150 R151
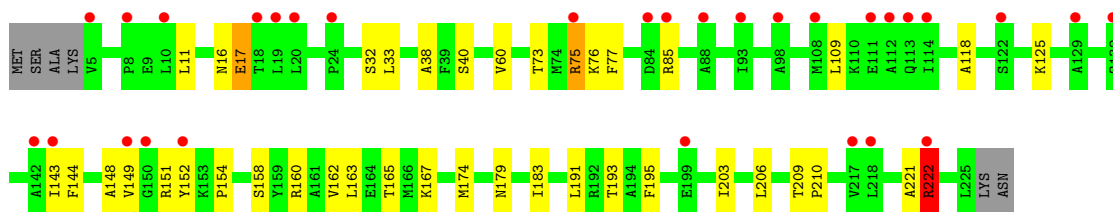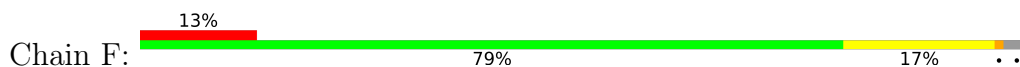
Y152 K153 S158 E164 T165 M166 K167 M174 E199 L206 T209 T216 E219 V220 A221 L224 L225 K226 ASN

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

Chain H:

4%

86%   11%

MET SER ALA LYS V5 K6 L11 D14 L33 E36 H37 A38 R44 V60 K71 R75 S82 E83 D84 M108 I114 A118 L119 F140 I143 V149 G150 R151 Y152 K153 P154 E155 S158 L163 V168 M174 N179 R192

A214 E219 K226 ASN

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

Chain I:

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

Chain J:

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

Chain K:

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

Chain L:
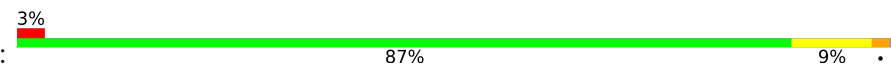
• Molecule 1: (S)-2-haloacid dehalogenase

Chain M:
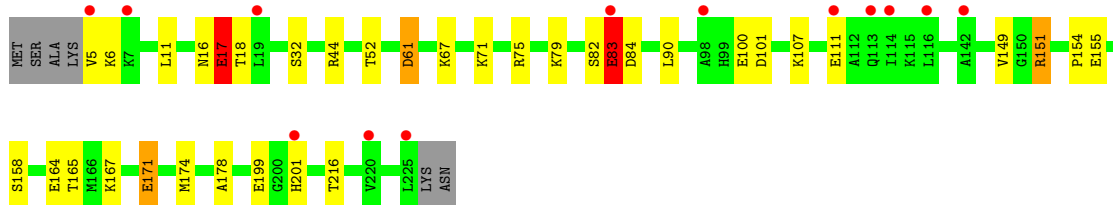
• Molecule 1: (S)-2-haloacid dehalogenase

Chain N:

• Molecule 1: (S)-2-haloacid dehalogenase
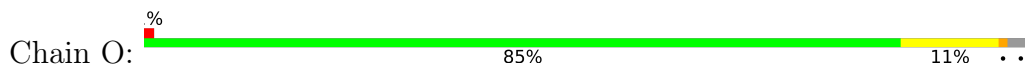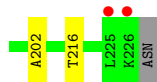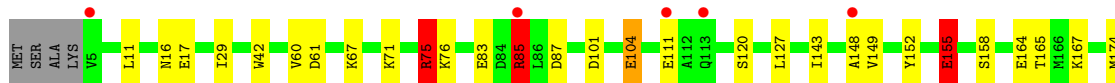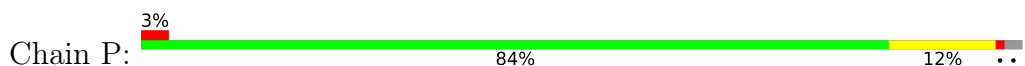
Chain O:

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

Chain P:

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

Chain Q:

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

Chain R:

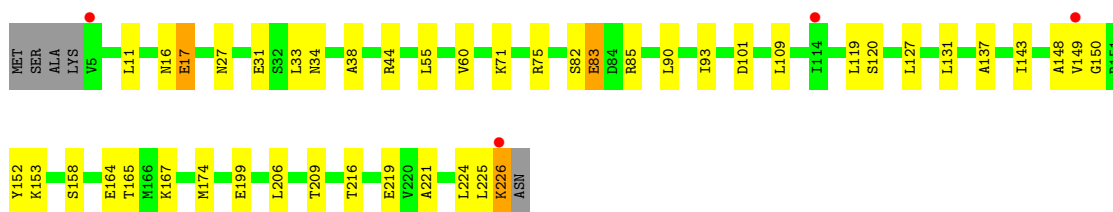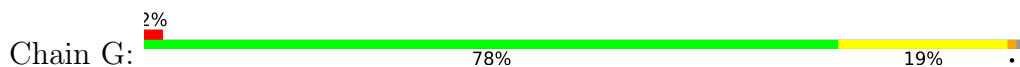• Molecule 1: (S)-2-haloacid dehalogenase
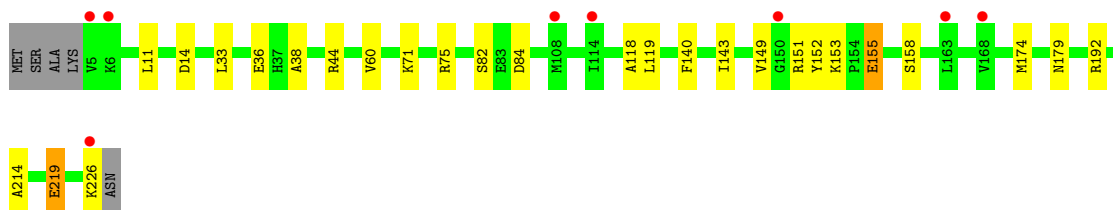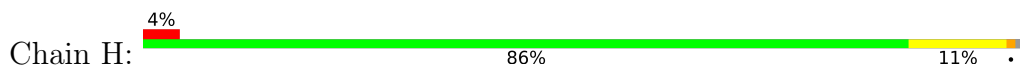
Chain S:

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

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

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

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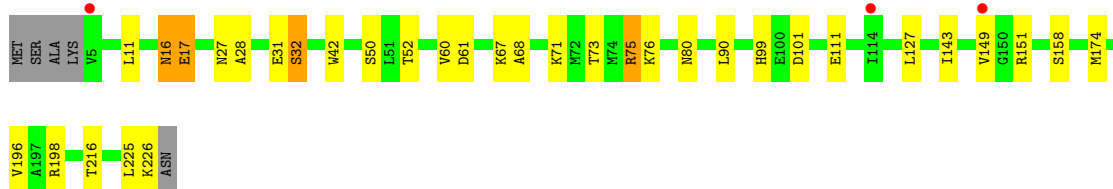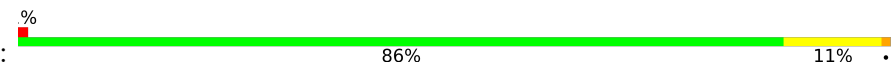
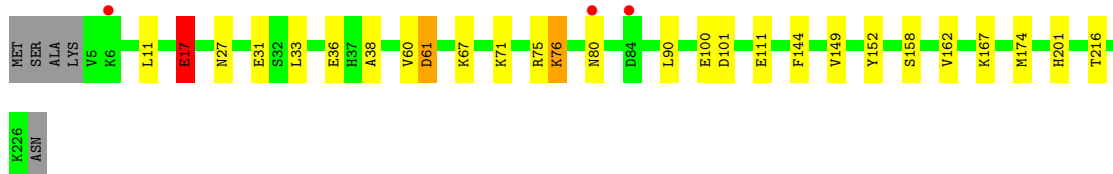• Molecule 1: (S)-2-haloacid dehalogenase

Chain X:

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

Chain Y:

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

Chain Z:
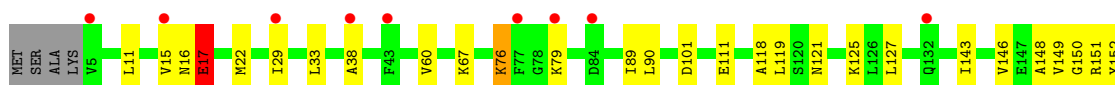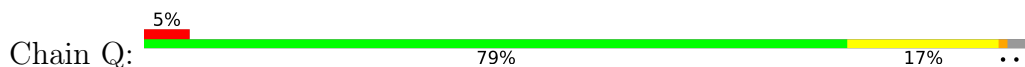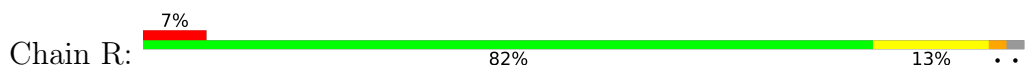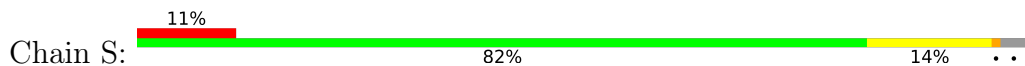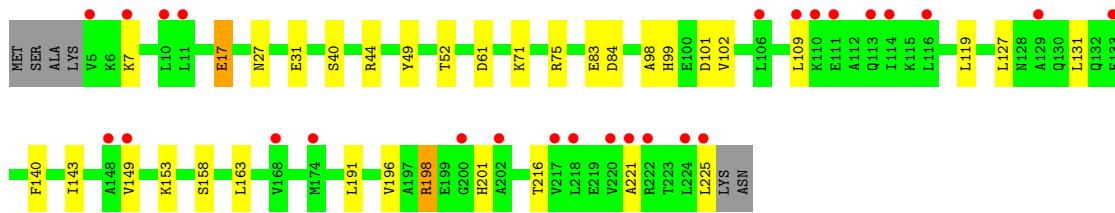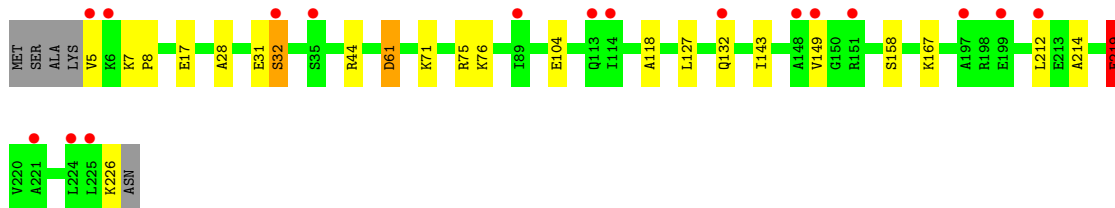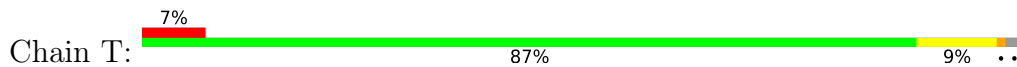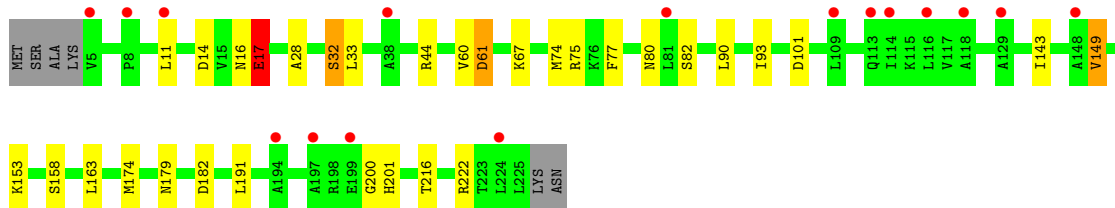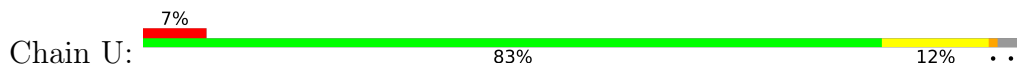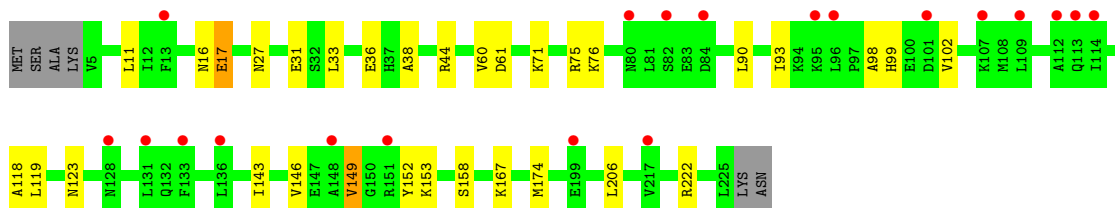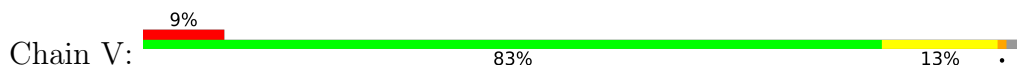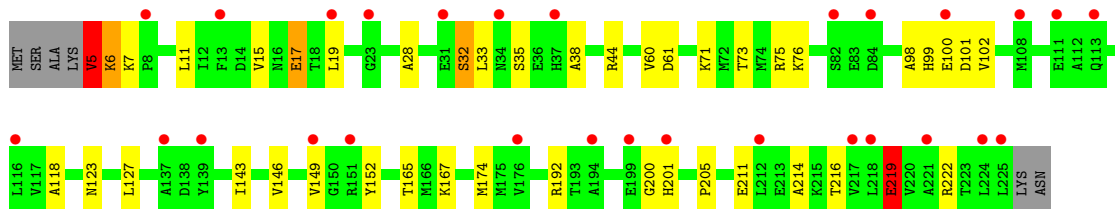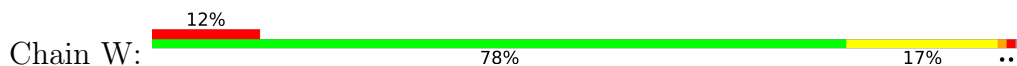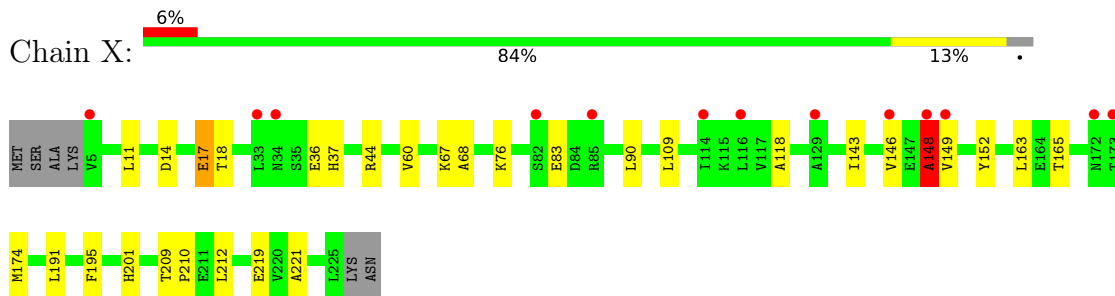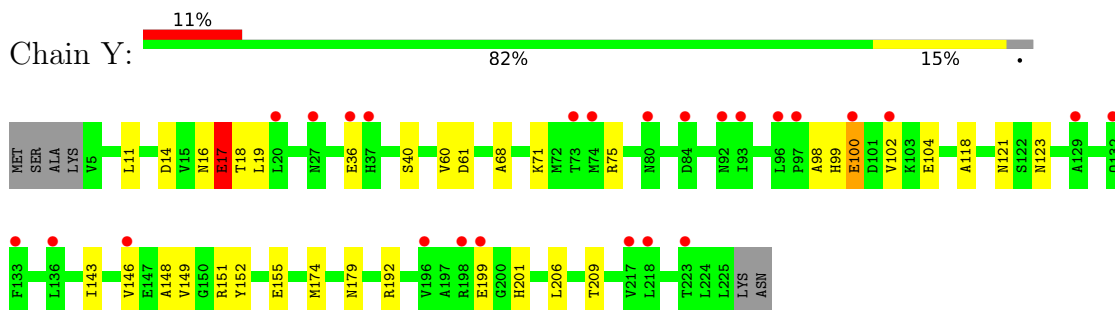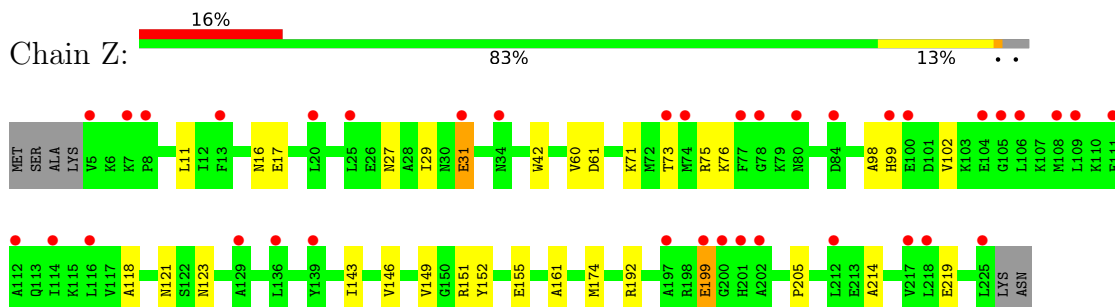
4 Data and refinement statistics ⓘ

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 49.46 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.51-2.73) 98.9 (49.46-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 0.206 , 0.248	Depositor DCC
R_{free} test set	7202 reflections (5.00%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	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.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.71	1/1749 (0.1%)	0.81	1/2363 (0.0%)
1	B	0.91	2/1749 (0.1%)	0.86	2/2363 (0.1%)
1	C	0.94	1/1758 (0.1%)	0.81	2/2374 (0.1%)
1	D	0.69	1/1749 (0.1%)	0.82	2/2363 (0.1%)
1	E	0.76	1/1749 (0.1%)	0.81	1/2363 (0.0%)
1	F	0.82	2/1749 (0.1%)	0.91	6/2363 (0.3%)
1	G	0.69	1/1758 (0.1%)	0.84	3/2374 (0.1%)
1	H	0.74	1/1758 (0.1%)	0.80	0/2374
1	I	0.68	0/1758	0.78	1/2374 (0.0%)
1	J	0.68	0/1758	0.82	2/2374 (0.1%)
1	K	0.70	0/1758	0.82	4/2374 (0.2%)
1	L	0.74	1/1749 (0.1%)	0.86	4/2363 (0.2%)
1	M	1.12	6/1749 (0.3%)	1.00	5/2363 (0.2%)
1	N	0.80	1/1758 (0.1%)	1.13	3/2374 (0.1%)
1	O	0.91	1/1749 (0.1%)	0.81	3/2363 (0.1%)
1	P	0.78	3/1758 (0.2%)	0.85	3/2374 (0.1%)
1	Q	0.79	2/1758 (0.1%)	1.12	6/2374 (0.3%)
1	R	0.82	3/1758 (0.2%)	0.87	4/2374 (0.2%)
1	S	0.69	0/1749	0.79	0/2363
1	T	0.71	2/1758 (0.1%)	0.78	0/2374
1	U	0.69	0/1749	0.77	0/2363
1	V	0.70	1/1749 (0.1%)	0.82	0/2363
1	W	0.88	4/1749 (0.2%)	0.87	4/2363 (0.2%)
1	X	0.92	2/1749 (0.1%)	0.83	3/2363 (0.1%)
1	Y	1.32	5/1749 (0.3%)	0.90	7/2363 (0.3%)
1	Z	1.02	1/1749 (0.1%)	0.81	1/2363 (0.0%)
All	All	0.83	42/45573 (0.1%)	0.86	67/61559 (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 (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	17	GLU	CD-OE2	35.74	1.65	1.25
1	Z	199	GLU	CD-OE2	31.51	1.60	1.25
1	C	100	GLU	CD-OE2	28.11	1.56	1.25
1	O	100	GLU	CD-OE2	25.29	1.53	1.25
1	X	17	GLU	CD-OE2	23.42	1.51	1.25
1	B	100	GLU	CD-OE1	22.97	1.50	1.25
1	M	17	GLU	CD-OE2	22.55	1.50	1.25
1	W	5	VAL	C-O	-18.41	0.88	1.23
1	Y	17	GLU	CD-OE1	-18.11	1.05	1.25
1	M	83	GLU	CD-OE2	17.57	1.45	1.25
1	Y	100	GLU	CD-OE2	16.59	1.44	1.25
1	N	85	ARG	CZ-NH2	16.23	1.54	1.33
1	Q	17	GLU	CD-OE1	-15.48	1.08	1.25
1	F	75	ARG	CZ-NH2	14.55	1.51	1.33
1	Y	36	GLU	CD-OE2	14.44	1.41	1.25
1	M	199	GLU	CD-OE2	14.43	1.41	1.25
1	M	17	GLU	CD-OE1	-12.94	1.11	1.25
1	P	104	GLU	CD-OE2	12.67	1.39	1.25
1	E	199	GLU	CD-OE1	12.50	1.39	1.25
1	R	31	GLU	CD-OE2	12.15	1.39	1.25
1	R	17	GLU	CD-OE1	11.75	1.38	1.25
1	L	17	GLU	CD-OE2	11.12	1.37	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	199	GLU	CD-OE2	11.04	1.37	1.25
1	F	160	ARG	CZ-NH1	10.33	1.46	1.33
1	M	171	GLU	CD-OE2	10.17	1.36	1.25
1	B	100	GLU	CD-OE2	-9.10	1.15	1.25
1	W	100	GLU	CD-OE2	8.90	1.35	1.25
1	V	36	GLU	CD-OE2	7.64	1.34	1.25
1	R	100	GLU	CD-OE1	7.22	1.33	1.25
1	X	36	GLU	CD-OE1	7.15	1.33	1.25
1	T	104	GLU	CD-OE2	6.91	1.33	1.25
1	H	36	GLU	CD-OE1	-6.83	1.18	1.25
1	M	100	GLU	CD-OE2	6.66	1.32	1.25
1	G	85	ARG	CZ-NH2	6.48	1.41	1.33
1	D	219	GLU	CD-OE2	6.30	1.32	1.25
1	P	155	GLU	CD-OE1	-6.29	1.18	1.25
1	W	5	VAL	CA-CB	5.98	1.67	1.54
1	W	5	VAL	N-CA	-5.90	1.34	1.46
1	T	219	GLU	CD-OE1	-5.43	1.19	1.25
1	P	104	GLU	CD-OE1	-5.35	1.19	1.25
1	Q	17	GLU	CD-OE2	5.19	1.31	1.25
1	A	100	GLU	CD-OE2	5.01	1.31	1.25

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	17	GLU	OE1-CD-OE2	-34.49	81.91	123.30
1	N	85	ARG	NE-CZ-NH2	34.39	137.50	120.30
1	M	83	GLU	OE1-CD-OE2	-24.27	94.17	123.30
1	N	85	ARG	NH1-CZ-NH2	-14.36	103.61	119.40
1	F	222	ARG	NE-CZ-NH2	13.44	127.02	120.30
1	R	17	GLU	OE1-CD-OE2	-12.88	107.84	123.30
1	X	17	GLU	OE1-CD-OE2	11.73	137.38	123.30
1	G	85	ARG	NE-CZ-NH2	11.32	125.96	120.30
1	Q	17	GLU	CG-CD-OE1	11.26	140.83	118.30
1	M	171	GLU	OE1-CD-OE2	-11.23	109.82	123.30
1	Y	17	GLU	OE1-CD-OE2	11.09	136.61	123.30
1	B	100	GLU	OE1-CD-OE2	-11.08	110.00	123.30
1	Y	100	GLU	OE1-CD-OE2	-11.07	110.02	123.30
1	F	75	ARG	NE-CZ-NH2	-10.31	115.15	120.30
1	A	75	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	L	17	GLU	OE1-CD-OE2	9.08	134.20	123.30
1	M	83	GLU	CG-CD-OE2	8.68	135.65	118.30
1	W	5	VAL	O-C-N	-8.63	108.90	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	100	GLU	OE1-CD-OE2	-8.32	113.31	123.30
1	Y	36	GLU	OE1-CD-OE2	8.24	133.19	123.30
1	P	85	ARG	CG-CD-NE	-7.82	95.37	111.80
1	X	17	GLU	CG-CD-OE2	-7.79	102.73	118.30
1	Y	17	GLU	CG-CD-OE2	-7.62	103.06	118.30
1	Y	100	GLU	CG-CD-OE2	7.40	133.10	118.30
1	Q	198	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	D	97	PRO	N-CA-CB	-6.97	94.93	102.60
1	W	5	VAL	CA-CB-CG1	6.82	121.13	110.90
1	W	5	VAL	CA-C-O	6.58	133.92	120.10
1	F	222	ARG	NH1-CZ-NH2	-6.53	112.22	119.40
1	C	100	GLU	OE1-CD-OE2	-6.48	115.52	123.30
1	Q	226	LYS	CA-C-O	-6.38	106.70	120.10
1	R	75	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	P	104	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	O	100	GLU	N-CA-CB	-6.23	99.39	110.60
1	G	226	LYS	CA-C-O	-6.22	107.03	120.10
1	N	85	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	E	17	GLU	OE1-CD-OE2	-6.10	115.98	123.30
1	R	226	LYS	CB-CA-C	-6.08	98.24	110.40
1	K	17	GLU	CG-CD-OE1	-5.90	106.50	118.30
1	L	17	GLU	CG-CD-OE2	-5.87	106.57	118.30
1	O	100	GLU	CG-CD-OE2	-5.79	106.73	118.30
1	C	100	GLU	N-CA-CB	-5.76	100.22	110.60
1	J	151	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	J	75	ARG	CB-CG-CD	-5.74	96.67	111.60
1	Y	104	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	G	85	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
1	Y	36	GLU	CG-CD-OE2	-5.58	107.13	118.30
1	O	75	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	Q	76	LYS	N-CA-CB	-5.53	100.64	110.60
1	D	222	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	M	151	ARG	CG-CD-NE	-5.46	100.34	111.80
1	Z	199	GLU	CG-CD-OE2	-5.45	107.39	118.30
1	R	6	LYS	CB-CA-C	-5.44	99.52	110.40
1	W	219	GLU	OE1-CD-OE2	-5.38	116.85	123.30
1	B	85	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	K	36	GLU	N-CA-CB	-5.31	101.04	110.60
1	F	151	ARG	CG-CD-NE	-5.31	100.66	111.80
1	M	100	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	Q	198	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	X	148	ALA	O-C-N	-5.21	114.37	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	75	ARG	CG-CD-NE	-5.16	100.97	111.80
1	F	75	ARG	CB-CG-CD	-5.14	98.23	111.60
1	L	100	GLU	N-CA-CB	-5.14	101.34	110.60
1	P	75	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	K	76	LYS	N-CA-CB	-5.10	101.42	110.60
1	F	160	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	K	100	GLU	N-CA-CB	-5.04	101.53	110.60

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1720	0	1763	17	4
1	B	1720	0	1763	16	4

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1729	0	1776	25	4
1	D	1720	0	1763	23	5
1	E	1720	0	1763	22	0
1	F	1720	0	1763	24	4
1	G	1729	0	1776	29	2
1	H	1729	0	1776	20	0
1	I	1729	0	1776	15	2
1	J	1729	0	1775	30	2
1	K	1729	0	1776	18	1
1	L	1720	0	1763	19	1
1	M	1720	0	1763	30	0
1	N	1729	0	1776	19	1
1	O	1720	0	1763	25	0
1	P	1729	0	1776	33	2
1	Q	1729	0	1776	36	1
1	R	1729	0	1776	32	0
1	S	1720	0	1763	33	1
1	T	1729	0	1776	13	1
1	U	1720	0	1763	26	0
1	V	1720	0	1763	21	3
1	W	1720	0	1763	39	0
1	X	1720	0	1763	18	3
1	Y	1720	0	1763	28	0
1	Z	1720	0	1763	24	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
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

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	509	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 (509) 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:J:75:ARG:NH2	1:M:84:ASP:OD1	1.57	1.34
1:Y:17:GLU:CD	1:Y:17:GLU:OE2	1.65	1.32
1:H:84:ASP:OD2	1:K:75:ARG:NH2	1.68	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:71:LYS:NZ	1:M:83:GLU:OE2	1.85	1.07
1:P:83:GLU:OE2	1:S:83:GLU:OE2	1.74	1.04
1:J:75:ARG:NH2	1:M:84:ASP:CG	2.12	1.03
1:P:83:GLU:CD	1:S:83:GLU:OE2	1.97	1.02
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: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
1:J:71:LYS:CE	1:M:83:GLU:OE2	2.33	0.77
1:H:84:ASP:CG	1:K:75:ARG:NH2	2.38	0.76
1:P:75:ARG:HH21	1:S:84:ASP:CG	1.87	0.76
1:K:149:VAL:HG11	1:K:158:SER:HA	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:75:ARG:HH22	1:O:84:ASP:CG	1.93	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:W:35:SER:HG	1:X:37:HIS:CD2	2.17	0.62
1:Q:151:ARG:HD3	1:Q:155:GLU:CD	2.19	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:Y:17:GLU:OE2	1:Y:17:GLU:CG	2.49	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: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:I:61:ASP:OD1	1:I:61:ASP:C	2.40	0.59
1:U:14:ASP:OD2	1:U:179:ASN:ND2	2.36	0.59
1:L:80:ASN:HD21	1:O:82:SER:HA	1.67	0.59
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:P:148:ALA:O	1:Q:148:ALA:C	2.41	0.57
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:X:60:VAL:O	1:X:152:TYR:OH	2.19	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: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:C:151:ARG:HD3	1:C:155:GLU:CD	2.28	0.54
1:P:149:VAL:HG11	1:P:158:SER:HA	1.90	0.54
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

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:40:SER:CB	1:Z:76:LYS:NZ	2.71	0.54
1:Z:151:ARG:HD3	1:Z:155:GLU:CD	2.27	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: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: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: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:B:75:ARG:HH12	1:E:84:ASP:CG	2.11	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:Q:151:ARG:HD3	1:Q:155:GLU:OE1	2.11	0.51
1:W:11:LEU:HD23	1:W:174:MET:HB3	1.92	0.51
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:V:98:ALA:HB1	1:V:102:VAL:CG2	2.40	0.51
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:Z:98:ALA:HB1	1:Z:102:VAL:CG2	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:LEU:HG	1:H:153:LYS:HD3	1.93	0.50
1:K:61:ASP:OD1	1:K:61:ASP:C	2.49	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: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: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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:119:LEU:HG	1:V:153:LYS:HD3	1.95	0.48
1:R:17:GLU:CD	1:R:201:HIS:HE2	2.14	0.48
1:P:75:ARG:NH2	1:S:84:ASP:CG	2.63	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: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:N:101:ASP:CG	1:N:216:THR:HB	2.34	0.48
1:P:83:GLU:OE2	1:S:83:GLU:CD	2.49	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: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:P:71:LYS:HD3	1:S:83:GLU:OE1	2.15	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
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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:VAL:HA	1:D:149:VAL:HG12	1.98	0.46
1:G:101:ASP:CG	1:G:216:THR:HB	2.35	0.46
1:X:148:ALA:O	1:Y:148:ALA:C	2.53	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:N:61:ASP:OD1	1:N:61:ASP:C	2.54	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:E:60:VAL:O	1:E:152:TYR:OH	2.27	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:M:61:ASP:OD1	1:M:61:ASP:C	2.54	0.46
1:D:71:LYS:NZ	1:G:83:GLU:OE1	2.39	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: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
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:R:101:ASP:CG	1:R:216:THR:HB	2.37	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: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:V:90:LEU:O	1:V:93:ILE:HG22	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:T:61:ASP:C	1:T:61:ASP:OD1	2.55	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: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: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
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:Z:149:VAL:HG12	1:Z:161:ALA:CB	2.47	0.44
1:K:101:ASP:CG	1:K:216:THR:HB	2.38	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:P:101:ASP:CG	1:P:216:THR:HB	2.37	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:O:101:ASP:CG	1:O:216:THR:HB	2.38	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:U:61:ASP:OD1	1:U:61:ASP:C	2.56	0.43
1:X:109:LEU:HD21	1:X:221:ALA:HA	1.99	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:U:153:LYS:NZ	1:U:182:ASP:OD2	2.42	0.43
1:B:146:VAL:HA	1:B:149:VAL:HG12	2.00	0.43
1:C:101:ASP:CG	1:C:216:THR:HB	2.39	0.43
1:K:33:LEU:HD12	1:K:38:ALA:HB1	2.00	0.43
1:Q:17:GLU:OE1	1:Q:22:MET:HG3	2.18	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: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: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:E:101:ASP:CG	1:E:216:THR:HB	2.39	0.42
1:D:7:LYS:HE3	1:D:7:LYS:HB3	1.74	0.42
1:M:101:ASP:CG	1:M:216:THR:HB	2.40	0.42
1:W:101:ASP:CG	1:W:216:THR:HB	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:60:VAL:O	1:F:152:TYR:OH	2.32	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:A:101:ASP:CG	1:A:216:THR:HB	2.40	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
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: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: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:17:GLU:CD	1:Q:201:HIS:NE2	2.72	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: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:G:16:ASN:O	1:G:17:GLU:HB2	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:224:LEU:C	1:G:226:LYS:H	2.23	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:E:76:LYS:NZ	1:F:40:SER:OG	2.39	0.41
1:P:83:GLU:HG2	1:S:83:GLU:CD	2.41	0.41
1:Q:149:VAL:HG12	1:Q:161:ALA:HB3	2.03	0.41
1:W:5:VAL:O	1:W:6:LYS:C	2.49	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
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: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: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: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:S:101:ASP:CG	1:S:216:THR:HB	2.42	0.40
1:U:101:ASP:CG	1:U:216:THR:HB	2.41	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ARG:HE	1:D:155:GLU:CD	2.23	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: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
1:L:140:PHE:O	1:M:167:LYS:NZ	2.33	0.40
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%)	17	32
1	C	220/227 (97%)	212 (96%)	8 (4%)	0	100	100
1	D	219/227 (96%)	212 (97%)	5 (2%)	2 (1%)	17	32
1	E	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	F	219/227 (96%)	212 (97%)	6 (3%)	1 (0%)	29	48
1	G	220/227 (97%)	210 (96%)	9 (4%)	1 (0%)	29	48
1	H	220/227 (97%)	215 (98%)	5 (2%)	0	100	100
1	I	220/227 (97%)	214 (97%)	4 (2%)	2 (1%)	17	32
1	J	220/227 (97%)	212 (96%)	6 (3%)	2 (1%)	17	32
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%)	29	48
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%)	29	48
1	R	220/227 (97%)	212 (96%)	7 (3%)	1 (0%)	29	48
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%)	17	32
1	V	219/227 (96%)	210 (96%)	7 (3%)	2 (1%)	17	32
1	W	219/227 (96%)	212 (97%)	6 (3%)	1 (0%)	29	48
1	X	219/227 (96%)	217 (99%)	2 (1%)	0	100	100
1	Y	219/227 (96%)	212 (97%)	6 (3%)	1 (0%)	29	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
All	All	5705/5902 (97%)	5535 (97%)	151 (3%)	19 (0%)	41	61

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	17	GLU
1	U	17	GLU
1	W	6	LYS
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%)	52	71
1	B	182/187 (97%)	179 (98%)	3 (2%)	62	78
1	C	183/187 (98%)	182 (100%)	1 (0%)	88	92
1	D	182/187 (97%)	175 (96%)	7 (4%)	33	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	182/187 (97%)	177 (97%)	5 (3%)	44	65
1	F	182/187 (97%)	177 (97%)	5 (3%)	44	65
1	G	183/187 (98%)	179 (98%)	4 (2%)	52	71
1	H	183/187 (98%)	181 (99%)	2 (1%)	73	84
1	I	183/187 (98%)	181 (99%)	2 (1%)	73	84
1	J	183/187 (98%)	180 (98%)	3 (2%)	62	78
1	K	183/187 (98%)	181 (99%)	2 (1%)	73	84
1	L	182/187 (97%)	180 (99%)	2 (1%)	73	84
1	M	182/187 (97%)	180 (99%)	2 (1%)	73	84
1	N	183/187 (98%)	179 (98%)	4 (2%)	52	71
1	O	182/187 (97%)	181 (100%)	1 (0%)	88	92
1	P	183/187 (98%)	180 (98%)	3 (2%)	62	78
1	Q	183/187 (98%)	181 (99%)	2 (1%)	73	84
1	R	183/187 (98%)	179 (98%)	4 (2%)	52	71
1	S	182/187 (97%)	179 (98%)	3 (2%)	62	78
1	T	183/187 (98%)	176 (96%)	7 (4%)	33	54
1	U	182/187 (97%)	178 (98%)	4 (2%)	52	71
1	V	182/187 (97%)	182 (100%)	0	100	100
1	W	182/187 (97%)	177 (97%)	5 (3%)	44	65
1	X	182/187 (97%)	180 (99%)	2 (1%)	73	84
1	Y	182/187 (97%)	178 (98%)	4 (2%)	52	71
1	Z	182/187 (97%)	181 (100%)	1 (0%)	88	92
All	All	4743/4862 (98%)	4661 (98%)	82 (2%)	60	76

All (82) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	32	SER
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
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	61	ASP
1	I	209	THR
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	M	61	ASP
1	N	5	VAL
1	N	17	GLU
1	N	61	ASP
1	N	149	VAL
1	O	151	ARG
1	P	61	ASP
1	P	85	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	155	GLU
1	Q	111	GLU
1	Q	212	LEU
1	R	17	GLU
1	R	34	ASN
1	R	179	ASN
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	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	W	222	ARG
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

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

Mol	Chain	Res	Type
1	D	80	ASN
1	F	130	GLN
1	H	179	ASN
1	K	80	ASN
1	L	34	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	80	ASN
1	R	80	ASN
1	T	179	ASN
1	U	80	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	Q	301	-	4,4,4	0.76	0	6,6,6	0.42	0
2	PO4	K	301	-	4,4,4	0.69	0	6,6,6	0.48	0
2	PO4	G	301	-	4,4,4	0.97	0	6,6,6	0.34	0
2	PO4	B	301	-	4,4,4	0.71	0	6,6,6	0.47	0
2	PO4	C	301	-	4,4,4	0.61	0	6,6,6	0.45	0
2	PO4	V	301	-	4,4,4	0.57	0	6,6,6	0.50	0
2	PO4	F	301	-	4,4,4	0.64	0	6,6,6	0.46	0
2	PO4	Z	301	-	4,4,4	0.71	0	6,6,6	0.44	0
2	PO4	U	301	-	4,4,4	0.67	0	6,6,6	0.42	0
2	PO4	P	301	-	4,4,4	0.69	0	6,6,6	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PO4	E	301	-	4,4,4	0.61	0	6,6,6	0.44	0
2	PO4	T	301	-	4,4,4	0.81	0	6,6,6	0.38	0
2	PO4	D	301	-	4,4,4	0.53	0	6,6,6	0.55	0
2	PO4	J	301	-	4,4,4	0.92	0	6,6,6	0.39	0
2	PO4	Y	301	-	4,4,4	0.57	0	6,6,6	0.49	0
2	PO4	H	301	-	4,4,4	0.68	0	6,6,6	0.51	0
2	PO4	W	301	-	4,4,4	0.99	0	6,6,6	0.45	0
2	PO4	S	301	-	4,4,4	0.71	0	6,6,6	0.50	0
2	PO4	N	301	-	4,4,4	0.96	0	6,6,6	0.37	0
2	PO4	O	301	-	4,4,4	0.70	0	6,6,6	0.52	0
2	PO4	A	301	-	4,4,4	0.58	0	6,6,6	0.52	0
2	PO4	L	301	-	4,4,4	0.72	0	6,6,6	0.45	0
2	PO4	R	301	-	4,4,4	0.65	0	6,6,6	0.50	0
2	PO4	I	301	-	4,4,4	0.51	0	6,6,6	0.50	0
2	PO4	M	301	-	4,4,4	0.77	0	6,6,6	0.41	0
2	PO4	X	301	-	4,4,4	0.90	0	6,6,6	0.40	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	P	301	PO4	1	0
2	W	301	PO4	1	0
2	N	301	PO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.59	12 (5%)	25	29	61, 84, 123, 138	0
1	B	221/227 (97%)	0.48	7 (3%)	47	54	64, 85, 116, 135	0
1	C	222/227 (97%)	0.66	14 (6%)	20	22	67, 92, 120, 139	0
1	D	221/227 (97%)	1.01	38 (17%)	1	1	72, 108, 144, 190	0
1	E	221/227 (97%)	1.12	43 (19%)	1	1	72, 100, 136, 168	0
1	F	221/227 (97%)	0.88	30 (13%)	3	3	72, 89, 121, 172	0
1	G	222/227 (97%)	0.47	4 (1%)	68	74	59, 78, 110, 147	0
1	H	222/227 (97%)	0.52	8 (3%)	42	47	58, 76, 106, 157	0
1	I	222/227 (97%)	0.50	6 (2%)	54	61	56, 72, 99, 123	0
1	J	222/227 (97%)	0.42	3 (1%)	75	80	59, 76, 112, 139	0
1	K	222/227 (97%)	0.37	3 (1%)	75	80	54, 72, 102, 121	0
1	L	221/227 (97%)	0.38	4 (1%)	68	74	54, 73, 98, 117	0
1	M	221/227 (97%)	0.59	13 (5%)	22	25	61, 83, 118, 164	0
1	N	222/227 (97%)	0.47	7 (3%)	47	54	60, 75, 108, 132	0
1	O	221/227 (97%)	0.38	2 (0%)	84	88	52, 66, 99, 134	0
1	P	222/227 (97%)	0.48	7 (3%)	47	54	52, 68, 98, 117	0
1	Q	222/227 (97%)	0.56	11 (4%)	28	32	56, 83, 115, 139	0
1	R	222/227 (97%)	0.73	16 (7%)	15	17	63, 90, 121, 147	0
1	S	221/227 (97%)	0.82	26 (11%)	4	4	66, 97, 126, 153	0
1	T	222/227 (97%)	0.67	17 (7%)	13	15	69, 93, 125, 144	0
1	U	221/227 (97%)	0.62	16 (7%)	15	17	65, 90, 118, 145	0
1	V	221/227 (97%)	0.72	20 (9%)	9	10	65, 96, 129, 140	0
1	W	221/227 (97%)	0.89	28 (12%)	3	3	68, 97, 131, 161	0
1	X	221/227 (97%)	0.73	13 (5%)	22	25	68, 92, 124, 154	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	Y	221/227 (97%)	0.88	25 (11%)	5	5	73, 100, 131, 142	0
1	Z	221/227 (97%)	1.00	37 (16%)	1	1	67, 98, 135, 157	0
All	All	5757/5902 (97%)	0.65	410 (7%)	16	17	52, 85, 124, 190	0

All (410) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	5	VAL	16.3
1	R	5	VAL	12.7
1	Z	5	VAL	10.2
1	D	114	ILE	8.9
1	M	5	VAL	8.6
1	G	5	VAL	7.7
1	E	5	VAL	6.9
1	X	33	LEU	6.6
1	W	224	LEU	6.6
1	A	78	GLY	5.2
1	D	131	LEU	5.1
1	Y	84	ASP	5.1
1	Z	78	GLY	5.0
1	Z	199	GLU	4.8
1	L	5	VAL	4.8
1	Z	31	GLU	4.7
1	S	168	VAL	4.7
1	E	114	ILE	4.7
1	R	31	GLU	4.6
1	S	5	VAL	4.5
1	I	150	GLY	4.5
1	S	129	ALA	4.4
1	Z	112	ALA	4.4
1	X	114	ILE	4.4
1	E	218	LEU	4.3
1	E	112	ALA	4.3
1	N	149	VAL	4.3
1	Y	100	GLU	4.3
1	A	113	GLN	4.3
1	E	225	LEU	4.2
1	W	149	VAL	4.2
1	M	220	VAL	4.2
1	W	225	LEU	4.2
1	Z	20	LEU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	109	LEU	4.1
1	E	222	ARG	4.1
1	D	96	LEU	4.1
1	E	97	PRO	4.1
1	F	18	THR	4.0
1	X	5	VAL	4.0
1	U	114	ILE	4.0
1	Z	139	TYR	4.0
1	R	136	LEU	4.0
1	E	111	GLU	4.0
1	I	149	VAL	4.0
1	P	148	ALA	4.0
1	X	173	THR	4.0
1	S	114	ILE	3.9
1	A	148	ALA	3.9
1	Q	5	VAL	3.9
1	E	16	ASN	3.9
1	C	37	HIS	3.9
1	Z	201	HIS	3.8
1	U	5	VAL	3.8
1	S	110	LYS	3.8
1	M	114	ILE	3.8
1	Z	108	MET	3.8
1	D	5	VAL	3.7
1	D	97	PRO	3.7
1	Z	77	PHE	3.7
1	V	109	LEU	3.7
1	E	31	GLU	3.7
1	S	225	LEU	3.7
1	X	172	ASN	3.6
1	E	139	TYR	3.6
1	Q	84	ASP	3.6
1	V	113	GLN	3.6
1	X	85	ARG	3.6
1	U	129	ALA	3.6
1	E	71	LYS	3.6
1	V	133	PHE	3.6
1	E	7	LYS	3.6
1	V	128	ASN	3.5
1	C	109	LEU	3.5
1	T	6	LYS	3.5
1	W	23	GLY	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	100	GLU	3.5
1	N	199	GLU	3.5
1	E	8	PRO	3.5
1	J	5	VAL	3.5
1	D	111	GLU	3.4
1	X	148	ALA	3.4
1	P	226	LYS	3.4
1	T	114	ILE	3.4
1	W	137	ALA	3.4
1	V	114	ILE	3.4
1	Y	73	THR	3.4
1	F	85	ARG	3.4
1	E	224	LEU	3.4
1	C	139	TYR	3.4
1	Y	97	PRO	3.4
1	M	83	GLU	3.4
1	T	199	GLU	3.4
1	Z	114	ILE	3.3
1	D	218	LEU	3.3
1	R	131	LEU	3.3
1	S	106	LEU	3.3
1	T	224	LEU	3.3
1	Z	109	LEU	3.3
1	Y	129	ALA	3.2
1	W	212	LEU	3.2
1	D	113	GLN	3.2
1	M	113	GLN	3.2
1	X	149	VAL	3.2
1	D	7	LYS	3.2
1	S	111	GLU	3.2
1	S	217	VAL	3.2
1	W	113	GLN	3.2
1	X	34	ASN	3.2
1	E	116	LEU	3.2
1	Y	198	ARG	3.2
1	Q	77	PHE	3.2
1	Z	217	VAL	3.2
1	T	113	GLN	3.2
1	F	84	ASP	3.1
1	Z	218	LEU	3.1
1	F	93	ILE	3.1
1	D	139	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	148	ALA	3.1
1	M	142	ALA	3.1
1	K	84	ASP	3.1
1	S	224	LEU	3.1
1	F	129	ALA	3.1
1	W	221	ALA	3.1
1	S	116	LEU	3.1
1	E	108	MET	3.0
1	Y	20	LEU	3.0
1	A	132	GLN	3.0
1	Z	74	MET	3.0
1	N	5	VAL	3.0
1	D	10	LEU	3.0
1	X	129	ALA	3.0
1	W	82	SER	3.0
1	O	5	VAL	3.0
1	W	218	LEU	3.0
1	D	133	PHE	3.0
1	N	150	GLY	3.0
1	W	100	GLU	3.0
1	W	151	ARG	3.0
1	S	174	MET	3.0
1	C	34	ASN	3.0
1	I	80	ASN	3.0
1	P	111	GLU	3.0
1	E	177	ALA	3.0
1	D	79	LYS	2.9
1	Z	105	GLY	2.9
1	Q	29	ILE	2.9
1	R	109	LEU	2.9
1	S	221	ALA	2.9
1	L	199	GLU	2.9
1	F	8	PRO	2.9
1	Y	80	ASN	2.9
1	F	217	VAL	2.9
1	E	6	LYS	2.9
1	Z	34	ASN	2.9
1	D	135	GLY	2.9
1	E	15	VAL	2.9
1	C	224	LEU	2.9
1	D	217	VAL	2.9
1	X	146	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Z	212	LEU	2.8
1	V	84	ASP	2.8
1	E	74	MET	2.8
1	Z	111	GLU	2.8
1	W	217	VAL	2.8
1	P	113	GLN	2.8
1	Q	43	PHE	2.8
1	B	109	LEU	2.8
1	U	197	ALA	2.8
1	W	201	HIS	2.8
1	Y	27	ASN	2.8
1	U	8	PRO	2.8
1	Z	84	ASP	2.8
1	S	11	LEU	2.8
1	E	176	VAL	2.7
1	Z	100	GLU	2.7
1	U	109	LEU	2.7
1	X	116	LEU	2.7
1	Q	132	GLN	2.7
1	Z	129	ALA	2.7
1	F	218	LEU	2.7
1	E	193	THR	2.7
1	A	5	VAL	2.7
1	U	81	LEU	2.7
1	U	199	GLU	2.7
1	Z	8	PRO	2.7
1	T	5	VAL	2.7
1	S	218	LEU	2.7
1	F	111	GLU	2.7
1	R	17	GLU	2.7
1	D	149	VAL	2.7
1	E	113	GLN	2.7
1	V	96	LEU	2.7
1	Z	104	GLU	2.7
1	M	7	LYS	2.7
1	D	224	LEU	2.7
1	R	104	GLU	2.7
1	F	75	ARG	2.7
1	J	114	ILE	2.7
1	Y	223	THR	2.7
1	Y	132	GLN	2.6
1	P	5	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	19	LEU	2.6
1	E	142	ALA	2.6
1	V	112	ALA	2.6
1	Y	36	GLU	2.6
1	F	114	ILE	2.6
1	D	33	LEU	2.6
1	I	151	ARG	2.6
1	F	113	GLN	2.6
1	W	108	MET	2.6
1	E	99	HIS	2.6
1	T	221	ALA	2.6
1	V	136	LEU	2.6
1	E	140	PHE	2.6
1	Z	73	THR	2.6
1	Y	102	VAL	2.6
1	W	111	GLU	2.6
1	C	114	ILE	2.5
1	D	132	GLN	2.5
1	S	7	LYS	2.5
1	A	225	LEU	2.5
1	D	19	LEU	2.5
1	D	150	GLY	2.5
1	E	102	VAL	2.5
1	S	200	GLY	2.5
1	T	225	LEU	2.5
1	F	122	SER	2.5
1	W	31	GLU	2.5
1	P	85	ARG	2.5
1	C	136	LEU	2.5
1	M	225	LEU	2.5
1	Z	116	LEU	2.5
1	T	35	SER	2.5
1	V	107	LYS	2.5
1	R	86	LEU	2.5
1	A	107	LYS	2.5
1	W	194	ALA	2.5
1	W	84	ASP	2.5
1	E	129	ALA	2.5
1	F	199	GLU	2.5
1	T	132	GLN	2.5
1	C	225	LEU	2.5
1	D	116	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	U	11	LEU	2.5
1	W	13	PHE	2.5
1	Z	13	PHE	2.5
1	V	151	ARG	2.5
1	D	25	LEU	2.4
1	W	139	TYR	2.4
1	H	6	LYS	2.4
1	T	197	ALA	2.4
1	U	38	ALA	2.4
1	R	6	LYS	2.4
1	D	20	LEU	2.4
1	F	143	ILE	2.4
1	Z	80	ASN	2.4
1	V	148	ALA	2.4
1	Y	199	GLU	2.4
1	Z	200	GLY	2.4
1	F	24	PRO	2.4
1	Z	99	HIS	2.4
1	U	224	LEU	2.4
1	F	132	GLN	2.4
1	T	32	SER	2.4
1	X	82	SER	2.4
1	S	149	VAL	2.4
1	Q	226	LYS	2.4
1	S	113	GLN	2.4
1	Z	106	LEU	2.4
1	C	89	ILE	2.4
1	V	101	ASP	2.4
1	I	128	ASN	2.4
1	L	17	GLU	2.4
1	W	19	LEU	2.4
1	T	89	ILE	2.4
1	F	5	VAL	2.4
1	W	8	PRO	2.3
1	D	88	ALA	2.3
1	E	148	ALA	2.3
1	I	148	ALA	2.3
1	S	222	ARG	2.3
1	B	5	VAL	2.3
1	B	196	VAL	2.3
1	Z	225	LEU	2.3
1	Y	93	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	31	GLU	2.3
1	E	100	GLU	2.3
1	Y	218	LEU	2.3
1	W	199	GLU	2.3
1	H	163	LEU	2.3
1	S	109	LEU	2.3
1	U	118	ALA	2.3
1	Y	92	ASN	2.3
1	V	95	LYS	2.3
1	R	217	VAL	2.3
1	C	174	MET	2.3
1	E	210	PRO	2.3
1	R	225	LEU	2.3
1	F	98	ALA	2.3
1	Q	79	LYS	2.3
1	Y	217	VAL	2.3
1	M	98	ALA	2.3
1	D	199	GLU	2.3
1	V	199	GLU	2.3
1	V	13	PHE	2.3
1	Y	133	PHE	2.3
1	D	172	ASN	2.3
1	Y	74	MET	2.3
1	F	142	ALA	2.3
1	U	148	ALA	2.3
1	S	133	PHE	2.3
1	E	106	LEU	2.2
1	K	80	ASN	2.2
1	H	108	MET	2.2
1	M	19	LEU	2.2
1	R	34	ASN	2.2
1	W	116	LEU	2.2
1	C	98	ALA	2.2
1	S	202	ALA	2.2
1	B	6	LYS	2.2
1	D	76	LYS	2.2
1	E	131	LEU	2.2
1	U	116	LEU	2.2
1	W	37	HIS	2.2
1	Y	96	LEU	2.2
1	A	62	PHE	2.2
1	N	84	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	217	VAL	2.2
1	L	100	GLU	2.2
1	A	116	LEU	2.2
1	T	212	LEU	2.2
1	T	148	ALA	2.2
1	H	114	ILE	2.2
1	Q	199	GLU	2.2
1	H	168	VAL	2.2
1	W	176	VAL	2.2
1	B	8	PRO	2.2
1	D	142	ALA	2.2
1	F	112	ALA	2.2
1	C	5	VAL	2.2
1	Q	15	VAL	2.2
1	T	151	ARG	2.2
1	Y	37	HIS	2.2
1	B	7	LYS	2.2
1	D	17	GLU	2.2
1	M	111	GLU	2.2
1	R	223	THR	2.2
1	A	128	ASN	2.2
1	V	82	SER	2.2
1	W	34	ASN	2.2
1	F	20	LEU	2.2
1	H	226	LYS	2.2
1	H	150	GLY	2.2
1	C	112	ALA	2.2
1	Z	197	ALA	2.2
1	D	39	PHE	2.2
1	K	6	LYS	2.1
1	F	149	VAL	2.1
1	G	149	VAL	2.1
1	R	113	GLN	2.1
1	F	88	ALA	2.1
1	E	12	ILE	2.1
1	T	149	VAL	2.1
1	D	86	LEU	2.1
1	C	223	THR	2.1
1	E	18	THR	2.1
1	B	199	GLU	2.1
1	E	13	PHE	2.1
1	E	220	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	V	217	VAL	2.1
1	Y	146	VAL	2.1
1	Y	196	VAL	2.1
1	E	136	LEU	2.1
1	O	150	GLY	2.1
1	R	105	GLY	2.1
1	Z	136	LEU	2.1
1	G	226	LYS	2.1
1	U	113	GLN	2.1
1	E	20	LEU	2.1
1	G	114	ILE	2.1
1	S	10	LEU	2.1
1	Q	38	ALA	2.1
1	S	148	ALA	2.1
1	V	80	ASN	2.1
1	D	222	ARG	2.1
1	A	212	LEU	2.1
1	E	206	LEU	2.1
1	M	201	HIS	2.1
1	R	149	VAL	2.1
1	Z	202	ALA	2.1
1	F	108	MET	2.1
1	F	222	ARG	2.1
1	F	10	LEU	2.1
1	M	116	LEU	2.1
1	Z	7	LYS	2.1
1	D	38	ALA	2.1
1	V	131	LEU	2.0
1	E	37	HIS	2.0
1	P	225	LEU	2.0
1	Y	136	LEU	2.0
1	Z	25	LEU	2.0
1	F	152	TYR	2.0
1	N	111	GLU	2.0
1	U	194	ALA	2.0
1	J	149	VAL	2.0
1	E	32	SER	2.0
1	F	150	GLY	2.0
1	N	75	ARG	2.0
1	S	220	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	F	301	5/5	0.69	0.34	126,153,162,167	0
2	PO4	D	301	5/5	0.83	0.24	92,104,111,127	0
2	PO4	Y	301	5/5	0.83	0.38	126,137,146,154	0
2	PO4	J	301	5/5	0.86	0.40	107,114,117,123	0
2	PO4	L	301	5/5	0.86	0.35	93,103,111,112	0
2	PO4	E	301	5/5	0.86	0.34	130,143,144,153	0
2	PO4	Z	301	5/5	0.86	0.54	110,126,133,139	0
2	PO4	Q	301	5/5	0.87	0.28	101,139,142,144	0
2	PO4	X	301	5/5	0.87	0.23	90,99,107,108	0
2	PO4	I	301	5/5	0.88	0.21	73,98,118,124	0
2	PO4	W	301	5/5	0.90	0.15	91,97,109,119	0
2	PO4	C	301	5/5	0.90	0.20	101,120,122,128	0
2	PO4	M	301	5/5	0.90	0.25	97,123,130,140	0
2	PO4	K	301	5/5	0.90	0.32	77,106,113,119	0
2	PO4	V	301	5/5	0.92	0.15	82,82,92,98	0
2	PO4	T	301	5/5	0.93	0.16	101,103,106,108	0
2	PO4	B	301	5/5	0.93	0.21	94,99,103,107	0
2	PO4	R	301	5/5	0.93	0.22	99,100,109,114	0
2	PO4	U	301	5/5	0.94	0.28	88,94,102,103	0
2	PO4	N	301	5/5	0.94	0.23	98,105,112,122	0
2	PO4	A	301	5/5	0.94	0.15	76,89,92,99	0
2	PO4	P	301	5/5	0.95	0.20	76,77,92,97	0
2	PO4	S	301	5/5	0.95	0.20	96,99,105,109	0
2	PO4	G	301	5/5	0.95	0.20	77,82,88,102	0
2	PO4	O	301	5/5	0.96	0.23	76,82,94,96	0
2	PO4	H	301	5/5	0.96	0.17	74,86,86,89	0

6.5 Other polymers (i)

There are no such residues in this entry.