



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 01:58 PM EDT

PDB ID : 6QZ2
Title : Structure of MHETase from Ideonella sakaiensis
Authors : Allen, M.D.; Johnson, C.W.; Knott, B.C.; Beckham, G.T.; McGeehan, J.E.
Deposited on : 2019-03-10
Resolution : 1.90 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:

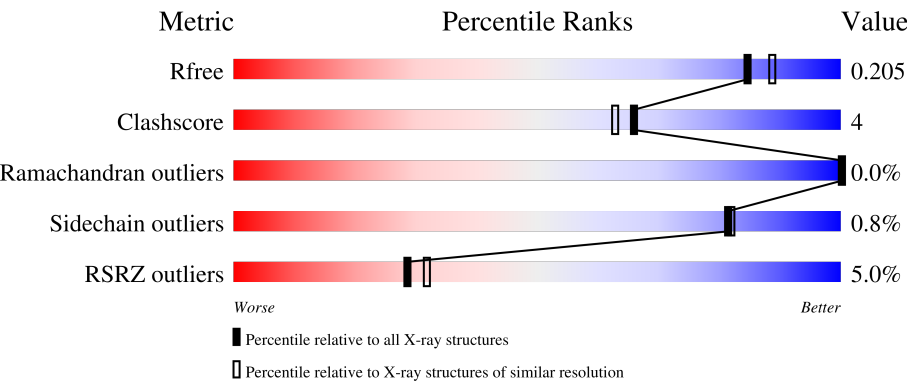
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	611	<div><div>%</div><div>87%5%8%</div></div>
1	B	611	<div><div>%</div><div>88%.8%</div></div>
1	C	611	<div><div>%</div><div>86%5%8%</div></div>
1	D	611	<div><div>%</div><div>88%.8%</div></div>
1	E	611	<div><div></div><div>85%7%8%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	611	<div><div>%</div><div><div></div><div>87%</div><div>5%</div><div>8%</div></div></div>
1	G	611	<div><div>%</div><div><div></div><div>85%</div><div>7%</div><div>8%</div></div></div>
1	H	611	<div><div>4%</div><div><div></div><div>84%</div><div>8%</div><div>8%</div></div></div>
1	I	611	<div><div>16%</div><div><div></div><div>82%</div><div>9%</div><div>8%</div></div></div>
1	J	611	<div><div>22%</div><div><div></div><div>73%</div><div>18%</div><div>8%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47549 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 Mono(2-hydroxyethyl) terephthalate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4147	2597	729	793	28			
1	B	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	C	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	D	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	E	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	F	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	G	562	Total	C	N	O	S	0	0	0
			4147	2597	729	793	28			
1	H	562	Total	C	N	O	S	0	0	0
			4147	2597	729	793	28			
1	I	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	J	560	Total	C	N	O	S	0	0	0
			4133	2587	727	791	28			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	604	LEU	-	expression tag	UNP A0A0K8P8E7
A	605	GLU	-	expression tag	UNP A0A0K8P8E7
A	606	HIS	-	expression tag	UNP A0A0K8P8E7
A	607	HIS	-	expression tag	UNP A0A0K8P8E7
A	608	HIS	-	expression tag	UNP A0A0K8P8E7
A	609	HIS	-	expression tag	UNP A0A0K8P8E7
A	610	HIS	-	expression tag	UNP A0A0K8P8E7
A	611	HIS	-	expression tag	UNP A0A0K8P8E7
B	604	LEU	-	expression tag	UNP A0A0K8P8E7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	GLU	-	expression tag	UNP A0A0K8P8E7
B	606	HIS	-	expression tag	UNP A0A0K8P8E7
B	607	HIS	-	expression tag	UNP A0A0K8P8E7
B	608	HIS	-	expression tag	UNP A0A0K8P8E7
B	609	HIS	-	expression tag	UNP A0A0K8P8E7
B	610	HIS	-	expression tag	UNP A0A0K8P8E7
B	611	HIS	-	expression tag	UNP A0A0K8P8E7
C	604	LEU	-	expression tag	UNP A0A0K8P8E7
C	605	GLU	-	expression tag	UNP A0A0K8P8E7
C	606	HIS	-	expression tag	UNP A0A0K8P8E7
C	607	HIS	-	expression tag	UNP A0A0K8P8E7
C	608	HIS	-	expression tag	UNP A0A0K8P8E7
C	609	HIS	-	expression tag	UNP A0A0K8P8E7
C	610	HIS	-	expression tag	UNP A0A0K8P8E7
C	611	HIS	-	expression tag	UNP A0A0K8P8E7
D	604	LEU	-	expression tag	UNP A0A0K8P8E7
D	605	GLU	-	expression tag	UNP A0A0K8P8E7
D	606	HIS	-	expression tag	UNP A0A0K8P8E7
D	607	HIS	-	expression tag	UNP A0A0K8P8E7
D	608	HIS	-	expression tag	UNP A0A0K8P8E7
D	609	HIS	-	expression tag	UNP A0A0K8P8E7
D	610	HIS	-	expression tag	UNP A0A0K8P8E7
D	611	HIS	-	expression tag	UNP A0A0K8P8E7
E	604	LEU	-	expression tag	UNP A0A0K8P8E7
E	605	GLU	-	expression tag	UNP A0A0K8P8E7
E	606	HIS	-	expression tag	UNP A0A0K8P8E7
E	607	HIS	-	expression tag	UNP A0A0K8P8E7
E	608	HIS	-	expression tag	UNP A0A0K8P8E7
E	609	HIS	-	expression tag	UNP A0A0K8P8E7
E	610	HIS	-	expression tag	UNP A0A0K8P8E7
E	611	HIS	-	expression tag	UNP A0A0K8P8E7
F	604	LEU	-	expression tag	UNP A0A0K8P8E7
F	605	GLU	-	expression tag	UNP A0A0K8P8E7
F	606	HIS	-	expression tag	UNP A0A0K8P8E7
F	607	HIS	-	expression tag	UNP A0A0K8P8E7
F	608	HIS	-	expression tag	UNP A0A0K8P8E7
F	609	HIS	-	expression tag	UNP A0A0K8P8E7
F	610	HIS	-	expression tag	UNP A0A0K8P8E7
F	611	HIS	-	expression tag	UNP A0A0K8P8E7
G	604	LEU	-	expression tag	UNP A0A0K8P8E7
G	605	GLU	-	expression tag	UNP A0A0K8P8E7
G	606	HIS	-	expression tag	UNP A0A0K8P8E7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	607	HIS	-	expression tag	UNP A0A0K8P8E7
G	608	HIS	-	expression tag	UNP A0A0K8P8E7
G	609	HIS	-	expression tag	UNP A0A0K8P8E7
G	610	HIS	-	expression tag	UNP A0A0K8P8E7
G	611	HIS	-	expression tag	UNP A0A0K8P8E7
H	604	LEU	-	expression tag	UNP A0A0K8P8E7
H	605	GLU	-	expression tag	UNP A0A0K8P8E7
H	606	HIS	-	expression tag	UNP A0A0K8P8E7
H	607	HIS	-	expression tag	UNP A0A0K8P8E7
H	608	HIS	-	expression tag	UNP A0A0K8P8E7
H	609	HIS	-	expression tag	UNP A0A0K8P8E7
H	610	HIS	-	expression tag	UNP A0A0K8P8E7
H	611	HIS	-	expression tag	UNP A0A0K8P8E7
I	604	LEU	-	expression tag	UNP A0A0K8P8E7
I	605	GLU	-	expression tag	UNP A0A0K8P8E7
I	606	HIS	-	expression tag	UNP A0A0K8P8E7
I	607	HIS	-	expression tag	UNP A0A0K8P8E7
I	608	HIS	-	expression tag	UNP A0A0K8P8E7
I	609	HIS	-	expression tag	UNP A0A0K8P8E7
I	610	HIS	-	expression tag	UNP A0A0K8P8E7
I	611	HIS	-	expression tag	UNP A0A0K8P8E7
J	604	LEU	-	expression tag	UNP A0A0K8P8E7
J	605	GLU	-	expression tag	UNP A0A0K8P8E7
J	606	HIS	-	expression tag	UNP A0A0K8P8E7
J	607	HIS	-	expression tag	UNP A0A0K8P8E7
J	608	HIS	-	expression tag	UNP A0A0K8P8E7
J	609	HIS	-	expression tag	UNP A0A0K8P8E7
J	610	HIS	-	expression tag	UNP A0A0K8P8E7
J	611	HIS	-	expression tag	UNP A0A0K8P8E7

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total 1	Ca 1	0	0
2	G	1	Total 1	Ca 1	0	0
2	H	1	Total 1	Ca 1	0	0
2	I	1	Total 1	Ca 1	0	0
2	J	1	Total 1	Ca 1	0	0

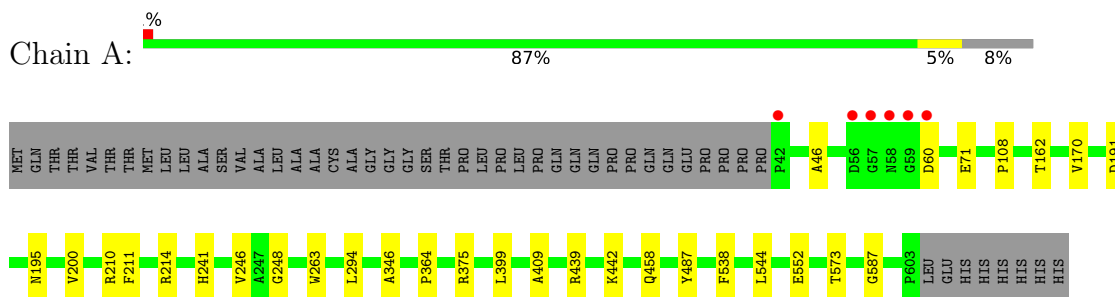
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	777	Total 777	O 777	0	0
3	B	759	Total 759	O 759	0	0
3	C	785	Total 785	O 785	0	0
3	D	706	Total 706	O 706	0	0
3	E	724	Total 724	O 724	0	0
3	F	773	Total 773	O 773	0	0
3	G	567	Total 567	O 567	0	0
3	H	461	Total 461	O 461	0	0
3	I	341	Total 341	O 341	0	0
3	J	232	Total 232	O 232	0	0

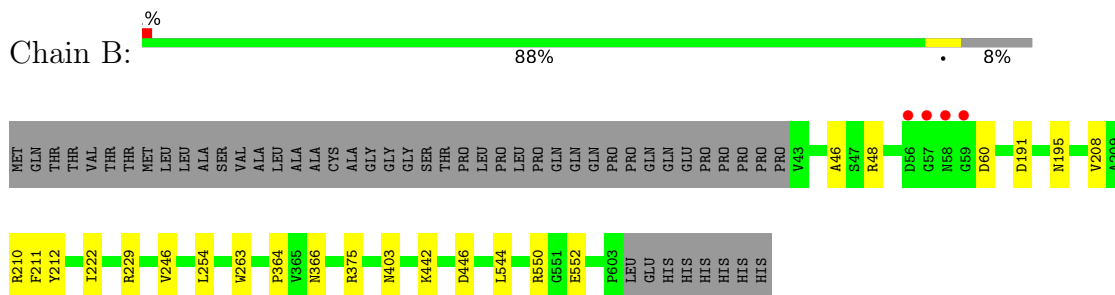
3 Residue-property plots

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.

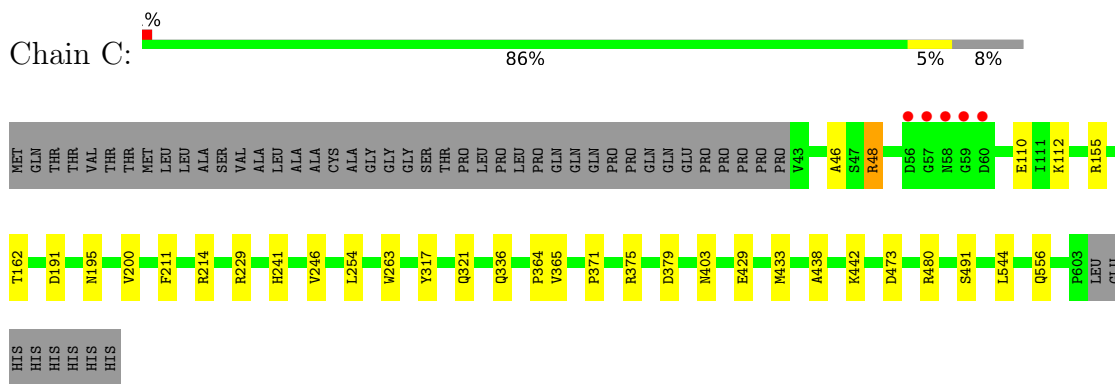
- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase



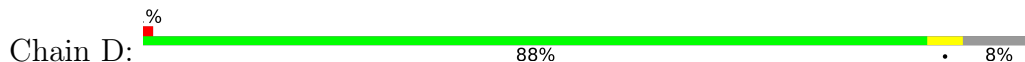
- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

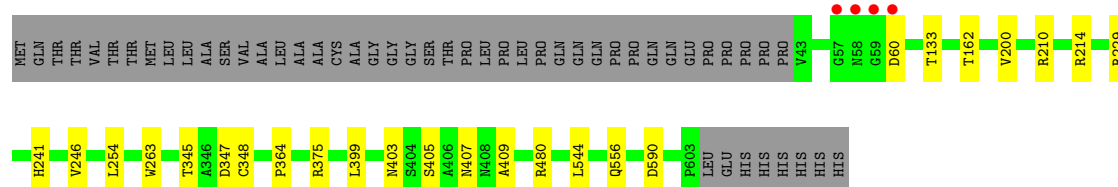


- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase



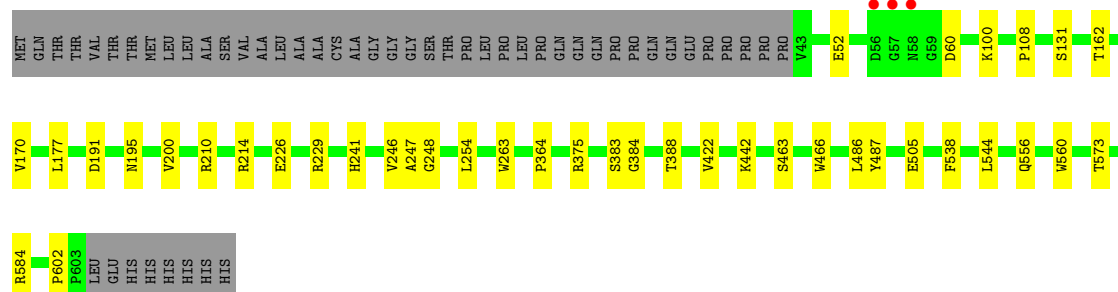
- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase





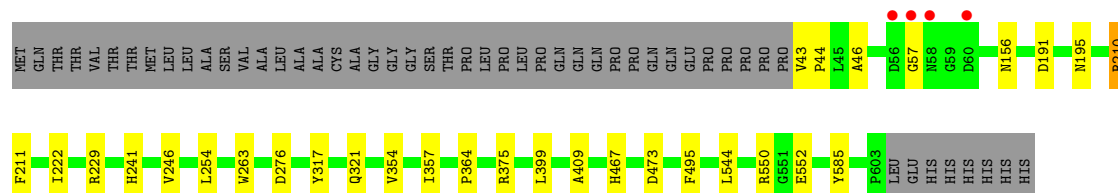
- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain E: 85% 7% 8%



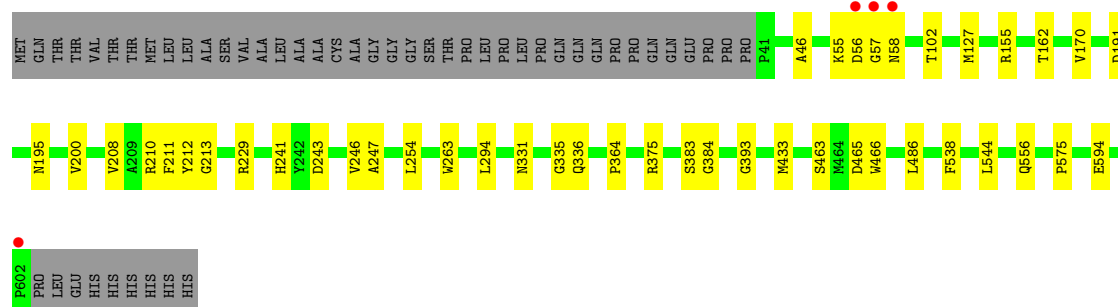
- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain F: 87% 5% 8%



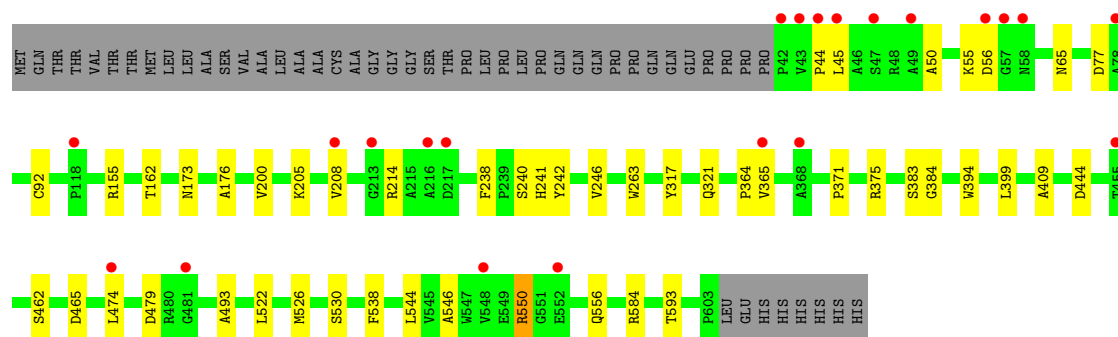
- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain G: 85% 7% 8%

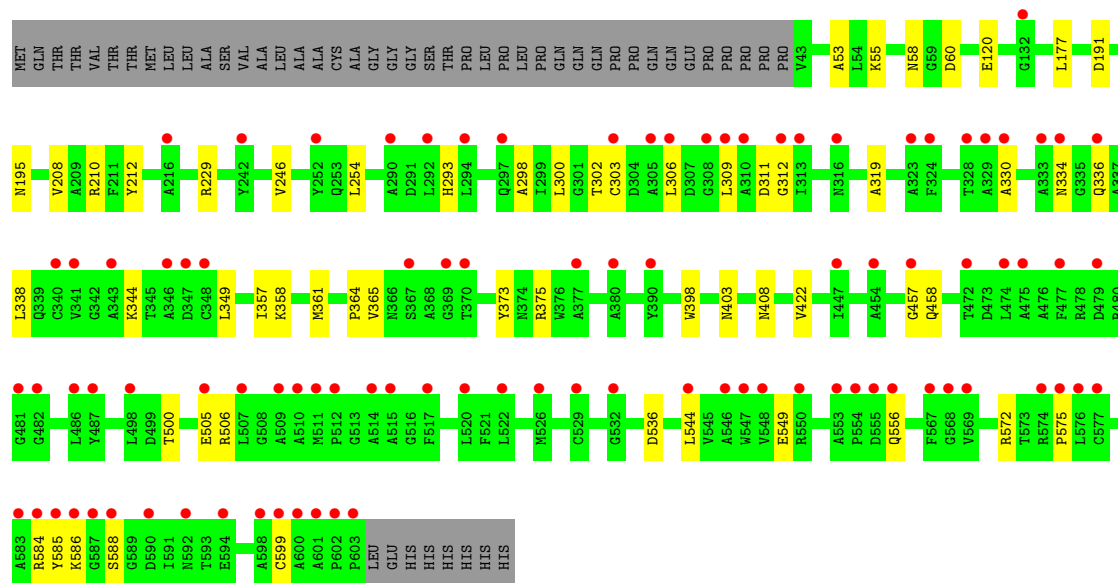
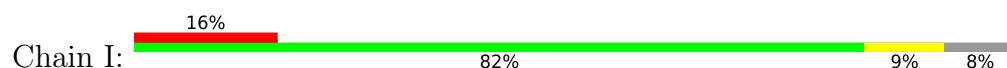


- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

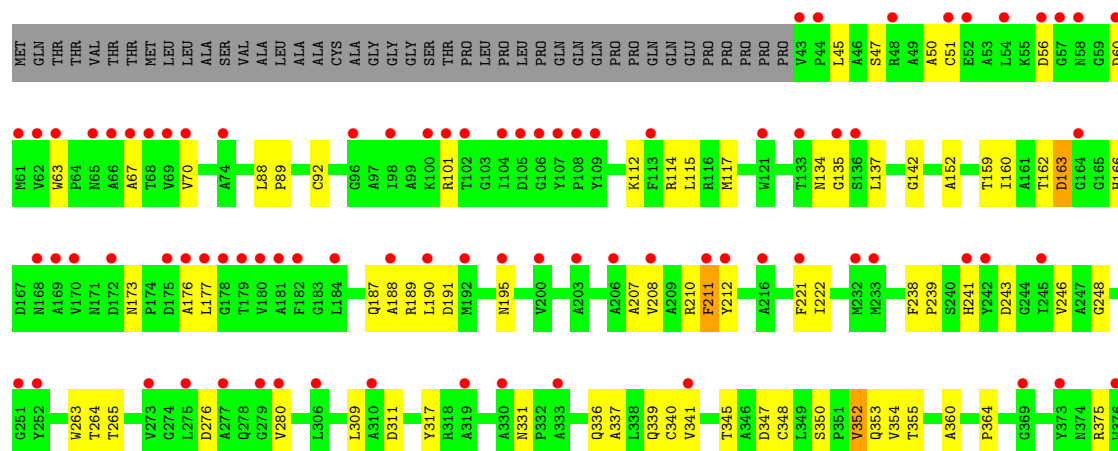
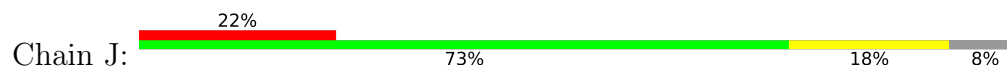
Chain H: 84% 8% 8%

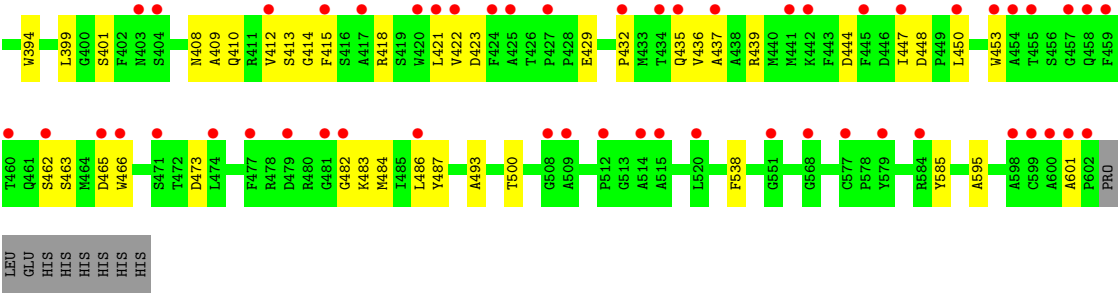


• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase



• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	110.49Å 135.63Å 138.15Å 83.09° 67.91° 67.57°	Depositor
Resolution (Å)	57.62 – 1.90 88.35 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (57.62-1.90) 93.7 (88.35-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.185 , 0.205 0.185 , 0.205	Depositor DCC
R_{free} test set	24892 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for h,l,h-k 0.016 for h,h-l,k 0.023 for h,h-k,h-l 0.017 for -h,-h+k,-l 0.017 for -h,-k,-h+l 0.023 for -h,-l,-k 0.055 for -h,-h+l,-h+k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	47549	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.26	0/4256	0.46	0/5796
1	B	0.27	0/4248	0.47	0/5785
1	C	0.27	0/4248	0.47	0/5785
1	D	0.26	0/4248	0.47	0/5785
1	E	0.26	0/4248	0.46	0/5785
1	F	0.26	0/4248	0.47	0/5785
1	G	0.26	0/4256	0.45	0/5796
1	H	0.26	0/4256	0.46	0/5796
1	I	0.28	0/4248	0.47	0/5785
1	J	0.28	0/4240	0.49	0/5773
All	All	0.27	0/42496	0.47	0/57871

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4147	0	3937	19	0
1	B	4140	0	3929	16	0
1	C	4140	0	3929	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4140	0	3929	24	0
1	E	4140	0	3929	27	0
1	F	4140	0	3929	22	0
1	G	4147	0	3937	31	0
1	H	4147	0	3937	32	0
1	I	4140	0	3929	50	0
1	J	4133	0	3922	85	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	777	0	0	7	4
3	B	759	0	0	7	1
3	C	785	0	0	11	3
3	D	706	0	0	14	3
3	E	724	0	0	14	8
3	F	773	0	0	8	1
3	G	567	0	0	16	4
3	H	461	0	0	14	3
3	I	341	0	0	25	0
3	J	232	0	0	29	1
All	All	47549	0	39307	326	14

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 4.

All (326) 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:H:92:CYS:SG	3:H:1295:HOH:O	2.21	0.98
1:J:345:THR:HG23	1:J:347:ASP:H	1.26	0.98
1:E:602:PRO:O	3:E:901:HOH:O	1.87	0.91
1:G:58:ASN:N	3:G:901:HOH:O	2.02	0.90
1:F:57:GLY:N	3:F:902:HOH:O	2.05	0.89
1:D:345:THR:HG23	1:D:347:ASP:H	1.37	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:549:GLU:OE2	3:I:901:HOH:O	1.93	0.86
1:J:117:MET:SD	3:J:1108:HOH:O	2.33	0.86
1:I:336:GLN:NE2	3:I:902:HOH:O	1.94	0.85
1:F:354:VAL:O	3:F:901:HOH:O	1.96	0.84
1:B:442:LYS:CE	3:B:924:HOH:O	2.26	0.83
1:J:317:TYR:OH	3:J:901:HOH:O	1.96	0.82
1:D:405:SER:OG	3:D:901:HOH:O	1.86	0.82
1:J:422:VAL:O	3:J:902:HOH:O	1.97	0.81
1:I:588:SER:O	3:I:904:HOH:O	1.98	0.81
1:E:131:SER:HA	3:E:907:HOH:O	1.83	0.79
1:I:536:ASP:OD2	3:I:903:HOH:O	1.97	0.79
1:C:473:ASP:OD2	3:C:902:HOH:O	1.99	0.79
1:D:60:ASP:O	1:D:210:ARG:NH2	2.16	0.79
1:J:473:ASP:OD1	3:J:903:HOH:O	2.01	0.79
1:J:101:ARG:NE	3:J:912:HOH:O	2.17	0.77
1:J:190:LEU:N	3:J:910:HOH:O	2.16	0.76
1:J:177:LEU:HD12	1:J:422:VAL:HG23	1.66	0.76
1:J:221:PHE:O	3:J:904:HOH:O	2.04	0.75
1:C:48:ARG:NH1	3:C:901:HOH:O	1.90	0.75
1:H:526:MET:HE2	1:H:530:SER:HA	1.69	0.74
1:J:337:ALA:O	3:J:905:HOH:O	2.06	0.73
1:I:506:ARG:NH1	3:I:915:HOH:O	2.22	0.73
1:G:55:LYS:O	3:G:901:HOH:O	2.05	0.73
1:H:77:ASP:O	3:H:901:HOH:O	2.06	0.73
1:H:45:LEU:O	3:H:902:HOH:O	2.06	0.73
1:G:56:ASP:OD2	3:G:903:HOH:O	2.06	0.73
1:G:393:GLY:HA3	3:G:1138:HOH:O	1.88	0.72
1:G:335:GLY:O	3:G:902:HOH:O	2.06	0.72
1:H:546:ALA:HA	1:H:550:ARG:HH21	1.56	0.71
1:J:246:VAL:N	3:J:904:HOH:O	2.18	0.71
1:I:120:GLU:OE2	3:I:905:HOH:O	2.08	0.70
1:J:191:ASP:HA	1:J:195:ASN:HB3	1.74	0.70
1:I:556:GLN:HG2	1:I:599:CYS:SG	2.31	0.70
1:J:340:CYS:O	3:J:907:HOH:O	2.09	0.69
1:I:229:ARG:HD3	1:I:254:LEU:HD12	1.72	0.69
1:C:429:GLU:OE2	3:C:903:HOH:O	2.10	0.69
1:G:213:GLY:N	3:G:905:HOH:O	2.19	0.69
1:F:585:TYR:OH	3:F:903:HOH:O	2.10	0.69
1:E:226:GLU:N	3:E:907:HOH:O	2.26	0.67
1:I:303:CYS:HA	1:I:306:LEU:HD13	1.75	0.67
1:F:473:ASP:OD1	3:F:904:HOH:O	2.13	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:345:THR:HG23	1:J:347:ASP:N	2.04	0.67
1:B:403:ASN:OD1	3:B:901:HOH:O	2.10	0.67
1:J:429:GLU:OE1	3:J:908:HOH:O	2.13	0.67
1:I:330:ALA:O	3:I:906:HOH:O	2.12	0.67
1:A:71:GLU:OE2	3:A:903:HOH:O	2.11	0.67
1:H:479:ASP:OD2	3:H:904:HOH:O	2.13	0.66
1:D:407:ASN:ND2	3:D:905:HOH:O	2.28	0.66
1:G:556:GLN:OE1	3:G:904:HOH:O	2.13	0.66
1:I:408:ASN:O	3:I:907:HOH:O	2.13	0.66
1:I:457:GLY:HA3	3:I:931:HOH:O	1.95	0.66
1:B:550:ARG:HB2	1:B:552:GLU:HG3	1.78	0.66
1:J:500:THR:OG1	3:J:906:HOH:O	2.09	0.66
1:C:403:ASN:ND2	3:C:909:HOH:O	2.24	0.66
1:J:115:LEU:HB2	1:J:160:ILE:HD13	1.78	0.66
1:I:549:GLU:O	3:I:908:HOH:O	2.14	0.66
1:C:556:GLN:NE2	3:C:914:HOH:O	2.29	0.66
1:E:388:THR:N	3:E:902:HOH:O	1.92	0.66
1:B:442:LYS:HE3	3:B:924:HOH:O	1.89	0.65
1:E:214:ARG:NH1	3:E:903:HOH:O	2.00	0.65
1:J:56:ASP:OD1	3:J:909:HOH:O	2.15	0.65
1:G:246:VAL:HG23	1:G:544:LEU:HD22	1.77	0.65
1:J:409:ALA:HB3	1:J:412:VAL:HG22	1.79	0.64
1:B:210:ARG:NH1	3:B:903:HOH:O	2.28	0.64
1:D:246:VAL:HG23	1:D:544:LEU:HD22	1.79	0.64
1:B:60:ASP:O	3:B:903:HOH:O	2.16	0.64
1:F:357:ILE:N	3:F:901:HOH:O	2.30	0.64
1:J:345:THR:HG22	1:J:348:CYS:SG	2.38	0.64
1:B:229:ARG:HD3	1:B:254:LEU:HD12	1.80	0.63
1:C:336:GLN:OE1	3:C:906:HOH:O	2.16	0.63
1:D:214:ARG:NE	3:D:903:HOH:O	2.23	0.63
1:E:229:ARG:HD3	1:E:254:LEU:HD12	1.81	0.63
1:C:473:ASP:OD1	3:C:905:HOH:O	2.15	0.63
1:I:584:ARG:HH22	1:I:586:LYS:HA	1.64	0.63
1:J:188:ALA:C	3:J:910:HOH:O	2.36	0.63
1:J:309:LEU:HD12	1:J:585:TYR:HB2	1.81	0.63
1:I:309:LEU:HD12	1:I:585:TYR:HB2	1.81	0.62
1:G:229:ARG:HD3	1:G:254:LEU:HD12	1.82	0.62
1:E:505:GLU:OE1	3:E:904:HOH:O	2.16	0.62
1:I:246:VAL:HG23	1:I:544:LEU:HD22	1.81	0.62
1:J:191:ASP:N	3:J:910:HOH:O	2.33	0.62
1:A:458:GLN:NE2	3:A:912:HOH:O	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:VAL:HG23	1:E:544:LEU:HD22	1.82	0.62
1:J:309:LEU:HD22	1:J:311:ASP:HB3	1.82	0.61
1:I:458:GLN:NE2	3:I:924:HOH:O	2.33	0.61
1:D:214:ARG:NH2	3:D:903:HOH:O	2.17	0.61
1:B:48:ARG:NH2	3:B:902:HOH:O	2.11	0.60
1:F:246:VAL:HG23	1:F:544:LEU:HD22	1.83	0.60
1:H:546:ALA:HA	1:H:550:ARG:NH2	2.15	0.60
1:I:364:PRO:O	3:I:909:HOH:O	2.17	0.59
1:C:155:ARG:NH1	3:C:918:HOH:O	2.34	0.59
1:G:336:GLN:NE2	3:G:914:HOH:O	2.35	0.59
1:F:550:ARG:NH1	3:F:911:HOH:O	2.34	0.59
1:A:214:ARG:NH2	3:A:907:HOH:O	2.26	0.59
1:E:210:ARG:NH1	3:E:911:HOH:O	2.36	0.59
1:J:453:TRP:O	3:J:911:HOH:O	2.17	0.59
1:J:47:SER:H	1:J:211:PHE:HE1	1.49	0.59
1:D:590:ASP:OD2	3:D:902:HOH:O	2.16	0.58
1:A:294:LEU:HD11	1:A:346:ALA:O	2.03	0.58
1:B:246:VAL:HG23	1:B:544:LEU:HD22	1.86	0.58
1:A:60:ASP:O	1:A:210:ARG:NH2	2.35	0.58
1:E:247:ALA:HB3	1:E:486:LEU:HD23	1.84	0.58
1:J:462:SER:HB3	1:J:465:ASP:HB2	1.85	0.58
1:D:556:GLN:NE2	3:D:909:HOH:O	2.37	0.58
1:A:246:VAL:HG23	1:A:544:LEU:HD22	1.87	0.57
1:C:214:ARG:NH1	3:C:920:HOH:O	2.37	0.57
1:A:573:THR:HB	3:A:1168:HOH:O	2.04	0.57
1:F:222:ILE:HG12	1:F:246:VAL:HB	1.86	0.56
1:I:584:ARG:HG2	1:I:584:ARG:HH21	1.70	0.56
1:H:321:GLN:O	3:H:905:HOH:O	2.18	0.56
1:D:214:ARG:NH1	3:D:910:HOH:O	2.37	0.56
1:F:229:ARG:NE	1:F:467:HIS:CE1	2.74	0.56
1:J:173:ASN:HB3	1:J:176:ALA:HB3	1.87	0.56
1:D:345:THR:HG22	1:D:348:CYS:SG	2.45	0.55
1:D:214:ARG:NH2	3:D:910:HOH:O	2.39	0.55
1:I:60:ASP:OD1	1:I:210:ARG:NH2	2.38	0.55
1:J:189:ARG:NE	3:J:902:HOH:O	2.27	0.55
1:H:205:LYS:HA	1:H:208:VAL:HG22	1.87	0.55
1:H:214:ARG:HD2	3:H:916:HOH:O	2.07	0.55
1:E:226:GLU:HB3	3:E:907:HOH:O	2.07	0.55
1:J:412:VAL:HG23	1:J:413:SER:H	1.72	0.55
1:C:246:VAL:HG23	1:C:544:LEU:HD22	1.89	0.54
1:H:556:GLN:O	3:H:906:HOH:O	2.19	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:306:LEU:HD23	1:I:319:ALA:HB1	1.89	0.53
1:J:177:LEU:HD22	1:J:418:ARG:HG2	1.90	0.53
1:D:403:ASN:ND2	3:D:914:HOH:O	2.40	0.53
1:E:556:GLN:NE2	3:E:905:HOH:O	2.21	0.53
1:J:177:LEU:HD12	1:J:422:VAL:CG2	2.37	0.53
1:I:338:LEU:O	1:I:349:LEU:N	2.42	0.53
1:E:442:LYS:HE2	3:E:1188:HOH:O	2.09	0.53
1:I:584:ARG:NH2	1:I:585:TYR:O	2.42	0.53
1:F:276:ASP:HB2	3:F:1330:HOH:O	2.08	0.52
1:I:311:ASP:HB2	1:I:572:ARG:HH12	1.75	0.52
1:C:229:ARG:HD3	1:C:254:LEU:HD12	1.91	0.52
1:E:100:LYS:HG3	3:E:1284:HOH:O	2.10	0.52
1:C:438:ALA:O	1:C:442:LYS:HG3	2.09	0.52
1:G:247:ALA:HB3	1:G:486:LEU:HD23	1.92	0.52
1:A:552:GLU:OE2	3:A:905:HOH:O	2.19	0.52
1:H:246:VAL:HG23	1:H:544:LEU:HD22	1.92	0.52
1:F:254:LEU:HD21	1:F:495:PHE:CZ	2.45	0.52
1:J:67:ALA:O	3:J:914:HOH:O	2.19	0.52
1:A:214:ARG:NH1	3:A:902:HOH:O	2.10	0.51
1:J:187:GLN:O	3:J:910:HOH:O	2.19	0.51
1:D:133:THR:HG23	3:D:923:HOH:O	2.10	0.51
1:J:601:ALA:HB1	3:J:933:HOH:O	2.11	0.51
1:G:465:ASP:O	3:G:906:HOH:O	2.19	0.51
1:H:162:THR:HB	1:H:200:VAL:HG21	1.93	0.50
1:I:344:LYS:HZ1	1:I:349:LEU:HA	1.75	0.50
1:J:421:LEU:HD21	1:J:439:ARG:HG2	1.92	0.50
1:G:393:GLY:CA	3:G:1138:HOH:O	2.51	0.50
1:H:242:TYR:N	3:H:903:HOH:O	2.12	0.50
1:J:92:CYS:CB	1:J:211:PHE:HE2	2.24	0.50
1:C:403:ASN:ND2	3:C:924:HOH:O	2.44	0.50
1:I:55:LYS:HE3	3:I:1108:HOH:O	2.12	0.50
1:D:556:GLN:NE2	3:D:912:HOH:O	2.39	0.50
1:I:365:VAL:O	3:I:911:HOH:O	2.19	0.50
1:J:447:ILE:HA	1:J:450:LEU:HD12	1.93	0.50
1:H:444:ASP:OD2	3:H:908:HOH:O	2.20	0.50
1:J:135:GLY:HA2	1:J:166:HIS:O	2.12	0.49
1:J:264:THR:HG22	1:J:360:ALA:HB1	1.95	0.49
1:E:60:ASP:CB	1:E:210:ARG:HH12	2.26	0.49
1:E:162:THR:HB	1:E:200:VAL:HG21	1.94	0.48
1:I:309:LEU:HD22	1:I:311:ASP:HB3	1.93	0.48
1:A:108:PRO:HG2	1:A:170:VAL:HG11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ARG:HA	1:A:442:LYS:HE3	1.96	0.48
1:A:263:TRP:CD2	1:A:364:PRO:HA	2.49	0.48
1:J:222:ILE:HG12	1:J:246:VAL:HB	1.95	0.48
1:J:399:LEU:C	1:J:409:ALA:HB2	2.33	0.48
1:G:383:SER:OG	1:G:384:GLY:N	2.47	0.48
1:J:208:VAL:HA	3:J:1108:HOH:O	2.14	0.48
1:J:63:TRP:CH2	1:J:207:ALA:HB2	2.49	0.48
1:I:373:TYR:OH	3:I:912:HOH:O	2.20	0.48
1:F:263:TRP:CD2	1:F:364:PRO:HA	2.49	0.47
1:E:442:LYS:HG2	3:E:1188:HOH:O	2.13	0.47
1:C:480:ARG:NH2	3:C:904:HOH:O	2.14	0.47
1:E:52:GLU:HG3	3:E:1023:HOH:O	2.14	0.47
1:F:156:ASN:ND2	3:F:925:HOH:O	2.47	0.47
1:G:208:VAL:HG13	1:G:212:TYR:HD2	1.78	0.47
1:I:575:PRO:O	3:I:913:HOH:O	2.20	0.47
1:G:210:ARG:C	3:G:905:HOH:O	2.52	0.47
1:J:263:TRP:CD2	1:J:364:PRO:HA	2.50	0.47
1:H:263:TRP:HB2	1:H:364:PRO:HB3	1.95	0.47
1:H:263:TRP:CD2	1:H:364:PRO:HA	2.50	0.47
1:J:45:LEU:HD23	1:J:212:TYR:O	2.15	0.47
1:D:263:TRP:CD2	1:D:364:PRO:HA	2.50	0.47
1:H:474:LEU:HA	3:H:1141:HOH:O	2.13	0.47
1:H:55:LYS:HE3	1:H:56:ASP:HB2	1.97	0.47
1:E:383:SER:OG	1:E:384:GLY:N	2.46	0.46
1:I:293:HIS:CE1	3:I:935:HOH:O	2.68	0.46
1:I:506:ARG:CZ	3:I:915:HOH:O	2.62	0.46
1:D:162:THR:HB	1:D:200:VAL:HG21	1.96	0.46
1:A:162:THR:HB	1:A:200:VAL:HG21	1.97	0.46
1:D:480:ARG:NH2	3:D:904:HOH:O	2.19	0.46
1:J:88:LEU:HA	1:J:89:PRO:HD3	1.80	0.46
1:J:595:ALA:HB2	3:J:987:HOH:O	2.15	0.46
1:H:44:PRO:O	1:H:50:ALA:HB2	2.16	0.46
1:C:110:GLU:OE2	1:C:112:LYS:NZ	2.45	0.46
1:C:162:THR:HB	1:C:200:VAL:HG21	1.97	0.46
1:D:210:ARG:HH21	1:F:210:ARG:HH12	1.63	0.46
1:I:300:LEU:HD22	1:I:312:GLY:HA2	1.96	0.46
1:I:344:LYS:NZ	1:I:349:LEU:HA	2.32	0.45
1:J:401:SER:N	1:J:408:ASN:OD1	2.46	0.45
1:B:46:ALA:HA	1:B:211:PHE:CZ	2.51	0.45
1:C:46:ALA:HA	1:C:211:PHE:CZ	2.52	0.45
1:J:114:ARG:O	1:J:160:ILE:HD12	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:560:TRP:HB3	1:E:573:THR:HG22	1.99	0.45
1:H:462:SER:O	1:H:465:ASP:HB2	2.16	0.45
1:J:56:ASP:OD2	1:J:70:VAL:N	2.48	0.45
1:J:248:GLY:HA3	1:J:487:TYR:CZ	2.51	0.45
1:D:229:ARG:HD3	1:D:254:LEU:HD12	1.98	0.45
1:H:593:THR:HG21	3:H:1283:HOH:O	2.17	0.45
1:I:53:ALA:HB3	3:I:971:HOH:O	2.16	0.45
1:J:412:VAL:HG23	1:J:413:SER:N	2.30	0.45
1:F:550:ARG:HB2	1:F:552:GLU:HG3	1.99	0.45
1:G:433:MET:HG3	3:G:1098:HOH:O	2.16	0.45
1:H:65:ASN:HB2	3:H:1139:HOH:O	2.16	0.44
1:I:298:ALA:O	1:I:302:THR:HG23	2.17	0.44
1:I:500:THR:HG22	3:I:996:HOH:O	2.16	0.44
1:J:162:THR:OG1	1:J:163:ASP:N	2.50	0.44
1:J:238:PHE:HB3	1:J:241:HIS:CD2	2.52	0.44
1:I:505:GLU:OE2	3:I:914:HOH:O	2.21	0.44
1:C:317:TYR:O	1:C:321:GLN:HG2	2.18	0.44
1:D:210:ARG:NH1	3:D:938:HOH:O	2.51	0.44
1:G:57:GLY:N	3:G:901:HOH:O	2.49	0.44
1:I:357:ILE:O	1:I:361:MET:HG2	2.18	0.44
1:J:423:ASP:HA	3:J:902:HOH:O	2.17	0.44
1:G:243:ASP:HA	3:G:938:HOH:O	2.17	0.44
1:H:394:TRP:CD1	1:H:493:ALA:HB2	2.53	0.44
1:J:341:VAL:C	3:J:907:HOH:O	2.55	0.44
1:G:191:ASP:HA	1:G:195:ASN:HB3	2.00	0.44
1:G:46:ALA:HA	1:G:211:PHE:CZ	2.52	0.44
1:A:587:GLY:O	1:G:170:VAL:HG22	2.18	0.43
1:G:162:THR:HB	1:G:200:VAL:HG21	2.00	0.43
1:D:214:ARG:CZ	3:D:910:HOH:O	2.66	0.43
1:F:263:TRP:HB2	1:F:364:PRO:HB3	2.00	0.43
1:J:331:ASN:N	1:J:336:GLN:O	2.47	0.43
1:J:410:GLN:OE1	1:J:415:PHE:HB2	2.18	0.43
1:J:410:GLN:HA	1:J:414:GLY:HA3	2.00	0.43
1:J:483:LYS:NZ	3:J:919:HOH:O	2.27	0.43
1:B:222:ILE:HG12	1:B:246:VAL:HB	1.98	0.43
1:I:398:TRP:CD1	1:I:398:TRP:N	2.85	0.43
1:I:506:ARG:NH2	3:I:940:HOH:O	2.43	0.43
1:J:142:GLY:HA3	1:J:152:ALA:HB3	1.99	0.43
3:A:1460:HOH:O	1:G:102:THR:HG21	2.18	0.43
1:H:155:ARG:NH1	3:H:915:HOH:O	2.38	0.43
1:I:334:ASN:HA	3:I:1003:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:383:SER:OG	1:H:384:GLY:N	2.49	0.43
1:E:108:PRO:HG2	1:E:170:VAL:HG11	2.00	0.43
1:J:463:SER:HA	1:J:466:TRP:CE2	2.54	0.43
1:C:263:TRP:HB2	1:C:364:PRO:HB3	2.01	0.42
1:C:365:VAL:HG12	1:C:371:PRO:HA	2.01	0.42
1:E:177:LEU:HD12	1:E:422:VAL:HG23	2.01	0.42
1:H:584:ARG:NE	3:H:920:HOH:O	2.42	0.42
1:J:115:LEU:HD12	1:J:159:THR:O	2.18	0.42
1:E:463:SER:HA	1:E:466:TRP:CE2	2.54	0.42
1:G:127:MET:HE2	3:G:1021:HOH:O	2.17	0.42
1:J:394:TRP:CD1	1:J:493:ALA:HB2	2.53	0.42
1:A:46:ALA:HA	1:A:211:PHE:CZ	2.54	0.42
1:F:399:LEU:C	1:F:409:ALA:HB2	2.40	0.42
1:G:263:TRP:CD2	1:G:364:PRO:HA	2.54	0.42
1:J:339:GLN:HG3	1:J:354:VAL:HG21	2.01	0.42
1:J:432:PRO:HD2	1:J:435:GLN:OE1	2.19	0.42
1:A:191:ASP:HA	1:A:195:ASN:HB3	2.00	0.42
1:G:575:PRO:HD3	1:G:594:GLU:HG3	2.01	0.42
1:I:208:VAL:HG13	1:I:212:TYR:HD2	1.85	0.42
1:I:53:ALA:HA	1:I:58:ASN:HB3	2.02	0.42
1:J:166:HIS:HE1	3:J:972:HOH:O	2.03	0.42
1:J:444:ASP:O	1:J:448:ASP:HB2	2.19	0.42
1:H:238:PHE:HB3	1:H:241:HIS:CD2	2.55	0.42
1:J:177:LEU:HD13	1:J:418:ARG:HA	2.00	0.42
1:A:399:LEU:C	1:A:409:ALA:HB2	2.40	0.42
1:I:191:ASP:HA	1:I:195:ASN:HB3	2.01	0.42
1:I:403:ASN:HB3	3:I:925:HOH:O	2.20	0.42
1:J:134:ASN:HB3	1:J:163:ASP:O	2.20	0.42
1:J:189:ARG:NH2	3:J:902:HOH:O	2.49	0.42
1:J:265:THR:HG23	1:J:412:VAL:HG12	2.01	0.42
1:E:191:ASP:HA	1:E:195:ASN:HB3	2.01	0.41
1:E:248:GLY:HA3	1:E:487:TYR:CZ	2.56	0.41
1:I:336:GLN:NE2	3:I:921:HOH:O	2.25	0.41
1:J:51:CYS:HB2	1:J:211:PHE:CE2	2.55	0.41
1:J:421:LEU:HD23	1:J:421:LEU:HA	1.95	0.41
1:F:46:ALA:HA	1:F:211:PHE:CZ	2.56	0.41
1:F:191:ASP:HA	1:F:195:ASN:HB3	2.01	0.41
1:I:311:ASP:OD1	1:I:311:ASP:N	2.54	0.41
1:J:276:ASP:CG	1:J:280:VAL:HG22	2.41	0.41
1:B:442:LYS:NZ	3:B:924:HOH:O	2.49	0.41
1:G:294:LEU:HD11	1:G:331:ASN:ND2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:177:LEU:HD12	1:I:422:VAL:HG23	2.02	0.41
1:J:421:LEU:HD12	1:J:436:VAL:HG13	2.02	0.41
1:D:263:TRP:HB2	1:D:364:PRO:HB3	2.03	0.41
1:G:463:SER:HA	1:G:466:TRP:CE2	2.56	0.41
1:E:263:TRP:CD2	1:E:364:PRO:HA	2.55	0.41
1:H:173:ASN:HB3	1:H:176:ALA:HB3	2.02	0.41
1:J:239:PRO:HB3	3:J:977:HOH:O	2.20	0.41
1:J:352:VAL:HA	1:J:355:THR:HG22	2.02	0.41
1:B:366:ASN:HB2	1:B:446:ASP:OD1	2.21	0.41
1:C:191:ASP:HA	1:C:195:ASN:HB3	2.02	0.41
1:E:584:ARG:HD3	3:E:1427:HOH:O	2.21	0.41
1:G:155:ARG:NH1	3:G:939:HOH:O	2.53	0.41
1:G:263:TRP:HB2	1:G:364:PRO:HB3	2.03	0.41
1:I:208:VAL:HG13	1:I:212:TYR:CD2	2.56	0.41
1:J:114:ARG:HB2	1:J:137:LEU:HD21	2.02	0.41
1:B:208:VAL:HG13	1:B:212:TYR:HD2	1.85	0.41
1:B:263:TRP:CD2	1:B:364:PRO:HA	2.56	0.41
1:J:280:VAL:HG21	1:J:437:ALA:HB1	2.03	0.41
1:A:248:GLY:HA3	1:A:487:TYR:CZ	2.56	0.40
1:F:43:VAL:HA	1:F:44:PRO:HD3	1.94	0.40
1:F:254:LEU:CD2	1:F:495:PHE:CE1	3.04	0.40
1:H:399:LEU:C	1:H:409:ALA:HB2	2.41	0.40
1:A:263:TRP:HB2	1:A:364:PRO:HB3	2.03	0.40
1:B:191:ASP:HA	1:B:195:ASN:HB3	2.02	0.40
1:C:379:ASP:OD2	1:C:491:SER:OG	2.34	0.40
1:H:317:TYR:CZ	1:H:522:LEU:HD12	2.56	0.40
1:F:317:TYR:O	1:F:321:GLN:HG2	2.22	0.40
1:H:365:VAL:HG12	1:H:371:PRO:HA	2.04	0.40
1:J:350:SER:HB2	1:J:353:GLN:H	1.87	0.40
1:J:208:VAL:HG22	3:J:1108:HOH:O	2.21	0.40
1:J:243:ASP:O	1:J:482:GLY:HA2	2.21	0.40
1:J:484:MET:SD	1:J:486:LEU:HD21	2.62	0.40
1:D:399:LEU:C	1:D:409:ALA:HB2	2.41	0.40

All (14) 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)
3:E:1449:HOH:O	3:H:1218:HOH:O[1_655]	1.83	0.37
3:D:1450:HOH:O	3:E:1566:HOH:O[1_455]	1.92	0.28

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1307:HOH:O	3:G:1262:HOH:O[1_655]	1.93	0.27
3:A:1530:HOH:O	3:G:1310:HOH:O[1_655]	2.01	0.19
3:D:1176:HOH:O	3:E:1039:HOH:O[1_455]	2.02	0.18
3:E:1548:HOH:O	3:H:1292:HOH:O[1_655]	2.02	0.18
3:C:1669:HOH:O	3:D:1586:HOH:O[1_645]	2.05	0.15
3:C:1188:HOH:O	3:E:1226:HOH:O[1_545]	2.06	0.14
3:B:1369:HOH:O	3:F:1518:HOH:O[1_556]	2.08	0.12
3:E:1591:HOH:O	3:H:1342:HOH:O[1_655]	2.09	0.11
3:E:904:HOH:O	3:J:1039:HOH:O[1_655]	2.13	0.07
3:C:1261:HOH:O	3:E:1262:HOH:O[1_545]	2.18	0.02
3:A:1307:HOH:O	3:G:1372:HOH:O[1_655]	2.19	0.01
3:A:1480:HOH:O	3:G:1347:HOH:O[1_655]	2.19	0.01

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	560/611 (92%)	544 (97%)	16 (3%)	0	100	100
1	B	559/611 (92%)	543 (97%)	16 (3%)	0	100	100
1	C	559/611 (92%)	544 (97%)	15 (3%)	0	100	100
1	D	559/611 (92%)	541 (97%)	18 (3%)	0	100	100
1	E	559/611 (92%)	545 (98%)	14 (2%)	0	100	100
1	F	559/611 (92%)	544 (97%)	15 (3%)	0	100	100
1	G	560/611 (92%)	547 (98%)	13 (2%)	0	100	100
1	H	560/611 (92%)	544 (97%)	16 (3%)	0	100	100
1	I	559/611 (92%)	540 (97%)	19 (3%)	0	100	100
1	J	558/611 (91%)	536 (96%)	21 (4%)	1 (0%)	47	38
All	All	5592/6110 (92%)	5428 (97%)	163 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	50	ALA

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	408/449 (91%)	405 (99%)	3 (1%)	84	84
1	B	407/449 (91%)	406 (100%)	1 (0%)	93	94
1	C	407/449 (91%)	403 (99%)	4 (1%)	76	76
1	D	407/449 (91%)	405 (100%)	2 (0%)	88	89
1	E	407/449 (91%)	404 (99%)	3 (1%)	84	84
1	F	407/449 (91%)	404 (99%)	3 (1%)	84	84
1	G	408/449 (91%)	405 (99%)	3 (1%)	84	84
1	H	408/449 (91%)	404 (99%)	4 (1%)	76	76
1	I	407/449 (91%)	405 (100%)	2 (0%)	88	89
1	J	406/449 (90%)	398 (98%)	8 (2%)	55	51
All	All	4072/4490 (91%)	4039 (99%)	33 (1%)	81	82

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	HIS
1	A	375	ARG
1	A	538	PHE
1	B	375	ARG
1	C	48	ARG
1	C	241	HIS
1	C	375	ARG
1	C	433	MET
1	D	241	HIS
1	D	375	ARG
1	E	241	HIS
1	E	375	ARG
1	E	538	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	210	ARG
1	F	241	HIS
1	F	375	ARG
1	G	241	HIS
1	G	375	ARG
1	G	538	PHE
1	H	240	SER
1	H	375	ARG
1	H	538	PHE
1	H	550	ARG
1	I	358	LYS
1	I	375	ARG
1	J	60	ASP
1	J	112	LYS
1	J	163	ASP
1	J	210	ARG
1	J	211	PHE
1	J	352	VAL
1	J	375	ARG
1	J	538	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	403	ASN
1	J	241	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	562/611 (91%)	-0.09	6 (1%) 80 82	13, 20, 33, 63	0
1	B	561/611 (91%)	0.00	4 (0%) 87 88	12, 19, 31, 57	0
1	C	561/611 (91%)	-0.11	5 (0%) 84 85	11, 19, 31, 53	0
1	D	561/611 (91%)	-0.03	4 (0%) 87 88	14, 21, 33, 61	0
1	E	561/611 (91%)	0.04	3 (0%) 91 92	14, 21, 33, 59	0
1	F	561/611 (91%)	-0.16	4 (0%) 87 88	11, 20, 33, 57	0
1	G	562/611 (91%)	-0.11	4 (0%) 87 88	18, 27, 38, 66	0
1	H	562/611 (91%)	0.35	22 (3%) 39 42	21, 31, 50, 70	0
1	I	561/611 (91%)	0.98	95 (16%) 1 1	26, 41, 59, 72	0
1	J	560/611 (91%)	1.25	136 (24%) 0 0	28, 49, 64, 80	0
All	All	5612/6110 (91%)	0.21	283 (5%) 28 32	11, 24, 54, 80	0

All (283) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	43	VAL	7.3
1	E	57	GLY	6.9
1	I	603	PRO	6.8
1	J	63	TRP	6.3
1	I	602	PRO	6.2
1	J	177	LEU	5.9
1	I	585	TYR	5.6
1	I	584	ARG	5.3
1	F	57	GLY	5.2
1	J	184	LEU	5.2
1	H	57	GLY	5.1
1	J	514	ALA	5.0
1	I	341	VAL	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	308	GLY	5.0
1	A	42	PRO	4.8
1	J	164	GLY	4.8
1	C	57	GLY	4.7
1	B	57	GLY	4.7
1	C	58	ASN	4.6
1	H	45	LEU	4.6
1	I	600	ALA	4.5
1	J	43	VAL	4.4
1	F	58	ASN	4.4
1	J	57	GLY	4.3
1	I	598	ALA	4.3
1	J	169	ALA	4.3
1	H	44	PRO	4.2
1	I	305	ALA	4.2
1	I	512	PRO	4.2
1	J	188	ALA	4.1
1	J	600	ALA	4.1
1	H	368	ALA	4.1
1	J	369	GLY	4.1
1	J	51	CYS	4.0
1	I	309	LEU	4.0
1	J	102	THR	4.0
1	J	69	VAL	4.0
1	I	380	ALA	4.0
1	I	457	GLY	3.9
1	I	514	ALA	3.9
1	D	57	GLY	3.9
1	J	447	ILE	3.8
1	J	211	PHE	3.8
1	J	457	GLY	3.8
1	J	412	VAL	3.8
1	F	56	ASP	3.8
1	J	56	ASP	3.7
1	J	459	PHE	3.6
1	J	109	TYR	3.6
1	I	583	ALA	3.6
1	J	62	VAL	3.6
1	I	377	ALA	3.5
1	G	58	ASN	3.5
1	J	584	ARG	3.5
1	I	529	CYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	42	PRO	3.5
1	J	279	GLY	3.5
1	I	588	SER	3.5
1	J	422	VAL	3.4
1	J	403	ASN	3.4
1	I	313	ILE	3.4
1	I	340	CYS	3.4
1	J	341	VAL	3.4
1	H	208	VAL	3.3
1	I	312	GLY	3.3
1	I	550	ARG	3.3
1	J	417	ALA	3.3
1	J	482	GLY	3.3
1	J	598	ALA	3.3
1	I	336	GLN	3.3
1	J	241	HIS	3.3
1	J	458	GLN	3.3
1	J	104	ILE	3.3
1	I	454	ALA	3.3
1	J	415	PHE	3.2
1	J	106	GLY	3.2
1	J	180	VAL	3.2
1	J	481	GLY	3.2
1	J	176	ALA	3.2
1	I	294	LEU	3.1
1	A	57	GLY	3.1
1	C	59	GLY	3.1
1	I	548	VAL	3.1
1	I	515	ALA	3.1
1	J	551	GLY	3.1
1	I	510	ALA	3.0
1	I	553	ALA	3.0
1	I	369	GLY	3.0
1	I	310	ALA	3.0
1	I	329	ALA	3.0
1	I	306	LEU	3.0
1	J	58	ASN	3.0
1	J	107	TYR	3.0
1	I	567	PHE	2.9
1	C	60	ASP	2.9
1	J	44	PRO	2.9
1	I	599	CYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	474	LEU	2.9
1	J	474	LEU	2.9
1	J	477	PHE	2.9
1	J	466	TRP	2.9
1	J	200	VAL	2.9
1	J	61	MET	2.9
1	J	437	ALA	2.9
1	I	556	GLN	2.9
1	I	587	GLY	2.9
1	I	522	LEU	2.9
1	A	60	ASP	2.9
1	J	105	ASP	2.9
1	J	203	ALA	2.9
1	J	450	LEU	2.8
1	J	66	ALA	2.8
1	J	101	ARG	2.8
1	I	486	LEU	2.8
1	J	121	TRP	2.8
1	J	190	LEU	2.8
1	I	601	ALA	2.8
1	B	59	GLY	2.8
1	H	56	ASP	2.8
1	I	568	GLY	2.8
1	D	59	GLY	2.8
1	G	57	GLY	2.8
1	I	482	GLY	2.8
1	I	348	CYS	2.8
1	H	49	ALA	2.7
1	C	56	ASP	2.7
1	I	367	SER	2.7
1	J	181	ALA	2.7
1	I	333	ALA	2.7
1	J	65	ASN	2.7
1	J	275	LEU	2.7
1	I	509	ALA	2.7
1	J	70	VAL	2.7
1	J	54	LEU	2.7
1	I	594	GLU	2.7
1	H	481	GLY	2.7
1	J	454	ALA	2.6
1	I	575	PRO	2.6
1	H	58	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	442	LYS	2.6
1	J	175	ASP	2.6
1	J	108	PRO	2.6
1	J	602	PRO	2.6
1	J	170	VAL	2.6
1	J	206	ALA	2.6
1	E	56	ASP	2.6
1	J	427	PRO	2.6
1	J	179	THR	2.6
1	E	58	ASN	2.6
1	J	195	ASN	2.6
1	J	421	LEU	2.6
1	J	515	ALA	2.6
1	I	547	TRP	2.6
1	J	462	SER	2.6
1	J	98	ILE	2.6
1	H	47	SER	2.5
1	A	56	ASP	2.5
1	J	208	VAL	2.5
1	I	517	PHE	2.5
1	J	216	ALA	2.5
1	J	242	TYR	2.5
1	J	330	ALA	2.5
1	J	373	TYR	2.5
1	H	552	GLU	2.5
1	I	347	ASP	2.5
1	I	303	CYS	2.5
1	I	555	ASP	2.5
1	I	592	ASN	2.5
1	J	465	ASP	2.5
1	I	576	LEU	2.5
1	J	306	LEU	2.5
1	J	136	SER	2.5
1	J	376	TRP	2.5
1	I	323	ALA	2.5
1	J	96	GLY	2.5
1	J	434	THR	2.5
1	B	56	ASP	2.5
1	J	319	ALA	2.5
1	J	273	VAL	2.5
1	I	324	PHE	2.5
1	J	455	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	435	GLN	2.4
1	J	277	ALA	2.4
1	I	574	ARG	2.4
1	J	599	CYS	2.4
1	H	216	ALA	2.4
1	J	310	ALA	2.4
1	A	58	ASN	2.4
1	J	48	ARG	2.4
1	I	586	LYS	2.4
1	I	334	ASN	2.4
1	I	511	MET	2.4
1	I	292	LEU	2.4
1	I	346	ALA	2.4
1	J	333	ALA	2.4
1	J	60	ASP	2.4
1	I	569	VAL	2.4
1	F	60	ASP	2.4
1	J	67	ALA	2.4
1	H	455	THR	2.4
1	J	178	GLY	2.4
1	J	512	PRO	2.4
1	I	290	ALA	2.3
1	J	252	TYR	2.3
1	J	509	ALA	2.3
1	B	58	ASN	2.3
1	I	297	GLN	2.3
1	D	58	ASN	2.3
1	I	242	TYR	2.3
1	J	479	ASP	2.3
1	J	420	TRP	2.3
1	J	135	GLY	2.3
1	J	432	PRO	2.3
1	I	507	LEU	2.3
1	J	280	VAL	2.3
1	G	602	PRO	2.3
1	I	447	ILE	2.3
1	J	601	ALA	2.3
1	I	477	PHE	2.2
1	J	113	PHE	2.2
1	J	192	MET	2.2
1	I	316	ASN	2.2
1	J	74	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	100	LYS	2.2
1	J	486	LEU	2.2
1	I	481	GLY	2.2
1	I	505	GLU	2.2
1	H	217	ASP	2.2
1	I	330	ALA	2.2
1	I	520	LEU	2.2
1	I	370	THR	2.2
1	I	475	ALA	2.2
1	J	182	PHE	2.2
1	J	577	CYS	2.2
1	J	232	MET	2.2
1	J	68	THR	2.2
1	I	487	TYR	2.2
1	J	508	GLY	2.2
1	J	221	PHE	2.2
1	H	474	LEU	2.1
1	J	133	THR	2.1
1	J	460	THR	2.1
1	I	343	ALA	2.1
1	J	453	TRP	2.1
1	I	390	TYR	2.1
1	J	212	TYR	2.1
1	H	548	VAL	2.1
1	J	52	GLU	2.1
1	I	132	GLY	2.1
1	I	532	GLY	2.1
1	H	365	VAL	2.1
1	J	441	MET	2.1
1	I	577	CYS	2.1
1	H	78	ALA	2.1
1	I	216	ALA	2.1
1	I	544	LEU	2.1
1	J	425	ALA	2.1
1	J	579	TYR	2.1
1	J	251	GLY	2.1
1	J	233	MET	2.1
1	J	445	PHE	2.1
1	J	245	ILE	2.1
1	J	404	SER	2.1
1	J	172	ASP	2.1
1	A	59	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	546	ALA	2.1
1	J	168	ASN	2.1
1	I	554	PRO	2.1
1	I	252	TYR	2.0
1	J	424	PHE	2.0
1	H	118	PRO	2.0
1	H	213	GLY	2.0
1	J	568	GLY	2.0
1	J	520	LEU	2.0
1	D	60	ASP	2.0
1	I	479	ASP	2.0
1	I	472	THR	2.0
1	I	526	MET	2.0
1	G	56	ASP	2.0
1	I	590	ASP	2.0
1	I	498	LEU	2.0
1	I	328	THR	2.0
1	J	471	SER	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	CA	I	801	1/1	0.91	0.07	47,47,47,47	0
2	CA	B	801	1/1	0.97	0.37	51,51,51,51	0
2	CA	J	801	1/1	0.98	0.05	44,44,44,44	0
2	CA	F	801	1/1	0.99	0.11	23,23,23,23	0
2	CA	G	801	1/1	0.99	0.08	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	H	801	1/1	0.99	0.09	26,26,26,26	0
2	CA	A	801	1/1	0.99	0.12	21,21,21,21	0
2	CA	C	801	1/1	0.99	0.08	19,19,19,19	0
2	CA	E	801	1/1	1.00	0.10	21,21,21,21	0
2	CA	D	801	1/1	1.00	0.15	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.