Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 06:04 PM EDT

PDB ID	:	4R1Q
Title	:	Crystal Structure of Thermophilic Geobacillus kaustophilus L-Arabinose isomerase in complex with L-arabitol
Authors	:	Choi, J.M.; Lee, Y.J.; Lee, D.W.; Lee, S.H.
Deposited on	:	2014-08-07
Resolution	:	2.25 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 (i) 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 (i)) were used in the production of this report:

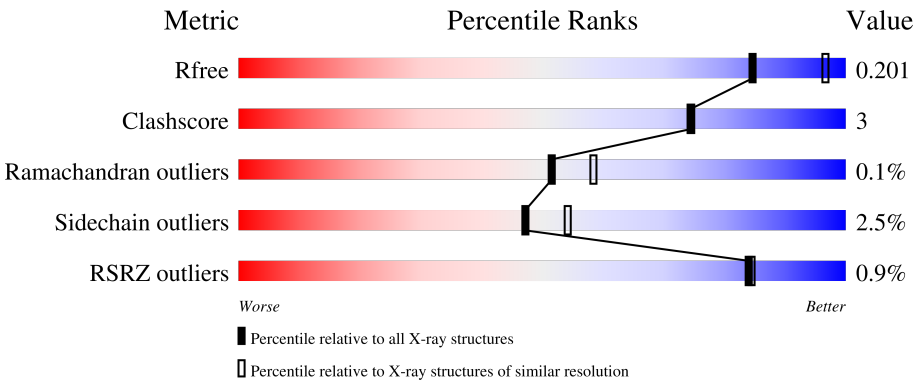
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.25 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	497	92% 8%
1	B	497	89% 10%
1	C	497	93% 5% •
1	D	497	.% 91% 8% •
1	E	497	2% 92% 8% •

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Mol	Chain	Length	Quality of chain
1	F	497	3% 88% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SST	A	502	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25396 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.

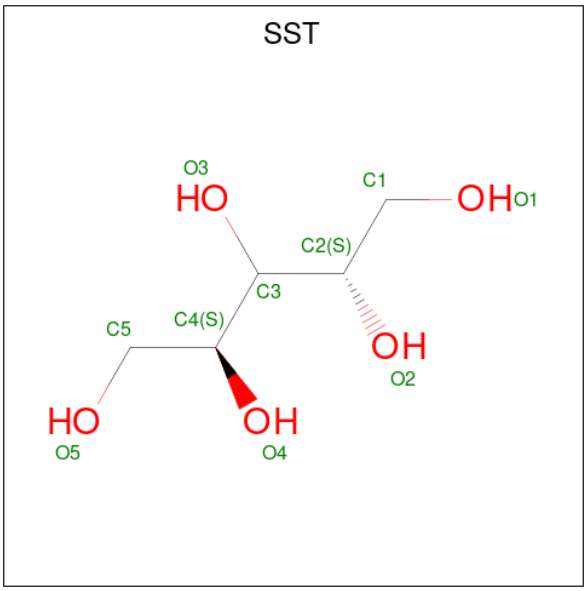
- Molecule 1 is a protein called L-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	495	3942	2508	689	723	22	0	0	0
1	B	495	3945	2509	692	723	21	0	0	0
1	C	495	3953	2514	695	723	21	0	1	0
1	D	496	3950	2513	690	724	23	0	0	0
1	E	496	3953	2514	693	724	22	0	0	0
1	F	495	3942	2508	689	723	22	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	SEE REMARK 999	UNP Q5KYP7
B	1	MET	-	SEE REMARK 999	UNP Q5KYP7
C	1	MET	-	SEE REMARK 999	UNP Q5KYP7
D	1	MET	-	SEE REMARK 999	UNP Q5KYP7
E	1	MET	-	SEE REMARK 999	UNP Q5KYP7
F	1	MET	-	SEE REMARK 999	UNP Q5KYP7

- Molecule 2 is L-arabinitol (three-letter code: SST) (formula: $C_5H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 5 5	0	0
2	A	1	Total C O 10 5 5	0	0
2	B	1	Total C O 10 5 5	0	0
2	C	1	Total C O 10 5 5	0	0
2	C	1	Total C O 10 5 5	0	0
2	E	1	Total C O 10 5 5	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is water.

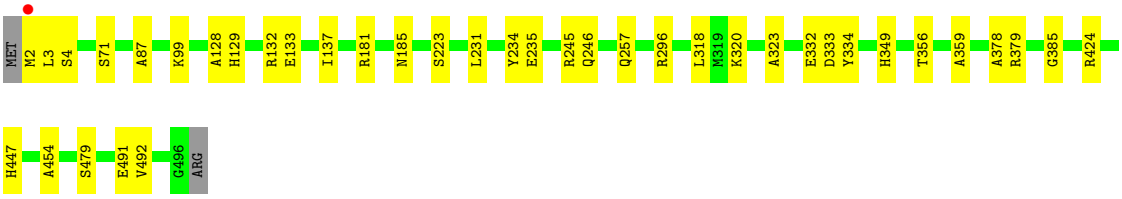
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	321	Total O 321 321	0	0
4	B	324	Total O 324 324	0	0
4	C	288	Total O 288 288	0	0
4	D	281	Total O 281 281	0	0
4	E	224	Total O 224 224	0	0
4	F	207	Total O 207 207	0	0

3 Residue-property plots (i)

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

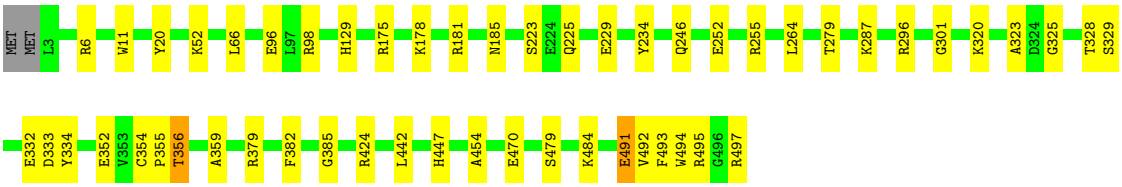
• Molecule 1: L-arabinose isomerase

Chain A:



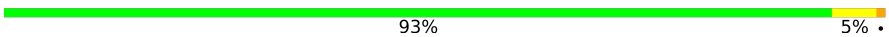
• Molecule 1: L-arabinose isomerase

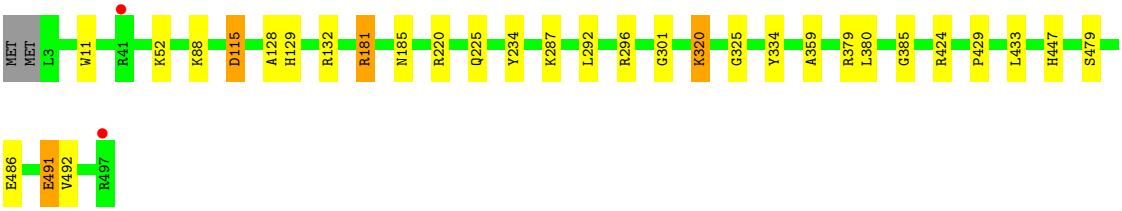
Chain B:



• Molecule 1: L-arabinose isomerase

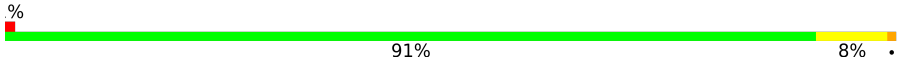
Chain C:





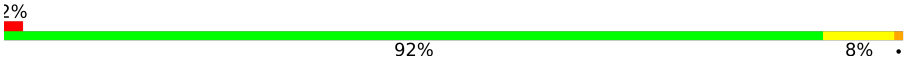
• Molecule 1: L-arabinose isomerase

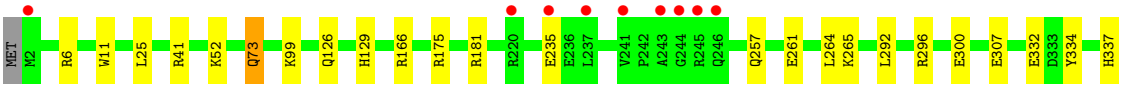
Chain D:



• Molecule 1: L-arabinose isomerase

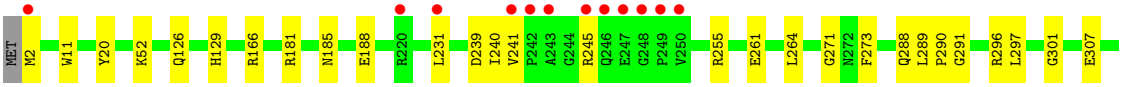
Chain E:





• Molecule 1: L-arabinose isomerase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.51Å 146.26Å 215.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 2.25 49.08 – 2.25	Depositor EDS
% Data completeness (in resolution range)	90.3 (49.08-2.25) 90.3 (49.08-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	7.59 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.154 , 0.201 0.154 , 0.201	Depositor DCC
R_{free} test set	8051 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25396	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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

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	0.43	0/4041	0.57	2/5472 (0.0%)
1	B	0.43	0/4044	0.56	0/5476
1	C	0.40	0/4055	0.54	1/5490 (0.0%)
1	D	0.40	0/4049	0.54	1/5482 (0.0%)
1	E	0.38	0/4052	0.52	0/5486
1	F	0.36	0/4041	0.52	1/5472 (0.0%)
All	All	0.40	0/24282	0.54	5/32878 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	318	LEU	CA-CB-CG	8.90	135.78	115.30
1	A	318	LEU	CB-CG-CD1	-5.78	101.17	111.00
1	C	181	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	F	318	LEU	CA-CB-CG	5.27	127.42	115.30
1	D	264	LEU	CA-CB-CG	5.09	127.01	115.30

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	3942	0	3833	20	0
1	B	3945	0	3837	32	0
1	C	3953	0	3850	20	0
1	D	3950	0	3845	30	0
1	E	3953	0	3846	29	0
1	F	3942	0	3833	33	0
2	A	20	0	22	1	0
2	B	10	0	11	1	0
2	C	20	0	23	2	0
2	E	10	0	11	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	321	0	0	2	0
4	B	324	0	0	7	0
4	C	288	0	0	2	0
4	D	281	0	0	4	0
4	E	224	0	0	3	0
4	F	207	0	0	2	0
All	All	25396	0	23111	149	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (149) 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:E:400:ARG:HH21	1:E:491:GLU:HG2	1.25	0.98
1:B:320:LYS:HE3	1:B:325:GLY:HA2	1.57	0.84
1:E:400:ARG:NH2	1:E:491:GLU:HG2	1.98	0.78
1:A:447:HIS:HB2	1:E:129:HIS:HB2	1.71	0.73
1:D:129:HIS:HB2	1:E:447:HIS:HB2	1.71	0.73
1:A:492:VAL:HG11	1:E:492:VAL:HG12	1.71	0.73
1:C:129:HIS:HB2	1:F:447:HIS:HB2	1.75	0.69
1:E:400:ARG:HH21	1:E:491:GLU:CG	2.05	0.67
1:D:278:THR:HG21	4:D:605:HOH:O	1.94	0.67
1:B:225:GLN:NE2	1:B:229:GLU:OE2	2.28	0.66
1:B:356:THR:HG21	4:B:885:HOH:O	1.96	0.64
1:A:129:HIS:HB2	1:D:447:HIS:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:HIS:HB2	1:C:447:HIS:HB2	1.80	0.64
1:D:128:ALA:O	1:D:132:ARG:HD2	1.97	0.64
1:E:491:GLU:HB3	4:E:823:HOH:O	1.96	0.64
1:B:246:GLN:OE1	4:B:884:HOH:O	2.15	0.64
1:D:430:ARG:HD3	1:D:476:GLU:HG3	1.79	0.63
1:C:492:VAL:HG12	1:F:492:VAL:HG11	1.82	0.62
1:B:252:GLU:OE1	1:B:255:ARG:NH1	2.27	0.61
1:F:420:LEU:HD12	1:F:421:PRO:HD2	1.83	0.60
1:E:11:TRP:CD2	1:E:52:LYS:HE3	2.35	0.60
1:B:359:ALA:HB2	1:B:385:GLY:HA2	1.83	0.60
1:F:239:ASP:HB2	1:F:363:ARG:HG3	1.83	0.59
1:B:181:ARG:NH2	1:B:185:ASN:OD1	2.36	0.59
2:E:501:SST:H9	2:E:501:SST:H11	1.84	0.59
1:F:289:LEU:HD12	1:F:290:PRO:HD2	1.84	0.59
1:B:98:ARG:NH2	4:B:822:HOH:O	2.32	0.58
1:A:359:ALA:HB2	1:A:385:GLY:HA2	1.85	0.57
1:D:234:TYR:CE2	1:D:296:ARG:HD2	2.40	0.56
1:F:359:ALA:HB2	1:F:385:GLY:HA2	1.86	0.56
1:B:447:HIS:HB2	1:F:129:HIS:HB2	1.86	0.56
1:A:492:VAL:HG12	1:D:492:VAL:HG11	1.87	0.56
1:C:359:ALA:HB2	1:C:385:GLY:HA2	1.88	0.55
1:A:4:SER:HA	4:A:895:HOH:O	2.06	0.55
1:D:234:TYR:HE2	1:D:296:ARG:HD2	1.70	0.55
1:A:332:GLU:OE1	1:A:447:HIS:HD2	1.88	0.55
1:D:434:ARG:NH1	1:D:435:ASP:OD1	2.39	0.54
1:B:492:VAL:HG12	1:C:492:VAL:HG11	1.88	0.54
1:D:359:ALA:HB2	1:D:385:GLY:HA2	1.91	0.53
1:C:128:ALA:O	1:C:132:ARG:HD2	2.09	0.53
4:A:889:HOH:O	1:C:181:ARG:HD3	2.08	0.53
2:A:501:SST:H9	2:A:501:SST:H11	1.91	0.52
1:E:332:GLU:OE2	1:E:447:HIS:HD2	1.91	0.52
1:C:115:ASP:OD1	1:C:115:ASP:N	2.36	0.52
1:D:482:SER:O	1:D:486:GLU:HG3	2.10	0.52
1:B:301:GLY:HA2	1:B:320:LYS:HE2	1.93	0.51
1:D:332:GLU:OE2	1:D:447:HIS:HD2	1.94	0.51
1:C:11:TRP:CD2	1:C:52:LYS:HE3	2.46	0.51
1:E:307:GLU:OE2	2:E:501:SST:O2	2.24	0.51
1:F:231:LEU:HD11	1:F:255:ARG:HA	1.92	0.51
1:E:181:ARG:HD3	4:F:636:HOH:O	2.11	0.50
1:E:359:ALA:HB2	1:E:385:GLY:HA2	1.92	0.50
1:A:320:LYS:NZ	1:A:356:THR:HG21	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:TRP:CE3	1:D:52:LYS:HD2	2.47	0.50
4:B:801:HOH:O	1:D:181:ARG:HD3	2.11	0.50
1:F:126:GLN:HB2	1:F:129:HIS:CE1	2.46	0.50
1:B:332:GLU:OE1	1:B:447:HIS:HD2	1.94	0.50
1:A:128:ALA:O	1:A:132:ARG:HD2	2.11	0.49
1:D:264:LEU:HB3	1:D:297:LEU:HD11	1.93	0.49
1:A:257:GLN:HG3	1:A:378:ALA:HB3	1.94	0.49
1:E:166:ARG:NE	4:E:631:HOH:O	2.34	0.49
1:B:66:LEU:HD13	1:B:96:GLU:HG2	1.94	0.48
1:D:492:VAL:HG12	1:E:492:VAL:HG11	1.94	0.48
1:E:126:GLN:HB2	1:E:129:HIS:CE1	2.48	0.48
1:F:447:HIS:H	1:F:447:HIS:CD2	2.31	0.48
1:B:492:VAL:HG11	1:F:492:VAL:HG12	1.95	0.48
1:F:393:SER:HB2	4:F:780:HOH:O	2.13	0.48
1:B:11:TRP:CE3	1:B:52:LYS:HD2	2.49	0.47
2:B:501:SST:H7	1:F:20:TYR:OH	2.14	0.47
1:C:287:LYS:NZ	4:C:871:HOH:O	2.47	0.47
1:C:234:TYR:CE2	1:C:296:ARG:HD2	2.50	0.47
1:D:315:LEU:HD12	1:D:318:LEU:HD11	1.97	0.47
1:A:320:LYS:HZ3	1:A:356:THR:HG21	1.80	0.47
1:C:491:GLU:HB2	4:C:853:HOH:O	2.14	0.47
1:D:491:GLU:HB2	4:D:763:HOH:O	2.14	0.47
1:F:241:VAL:HG23	1:F:364:VAL:O	2.14	0.47
1:D:216:VAL:O	1:D:220:ARG:HG3	2.16	0.46
1:E:379:ARG:NH1	1:E:421:PRO:O	2.46	0.46
1:B:20:TYR:OH	2:C:501:SST:H7	2.16	0.46
1:F:181:ARG:NH2	1:F:185:ASN:OD1	2.49	0.46
1:D:475:ASN:HB2	1:D:476:GLU:OE1	2.16	0.46
1:D:59:GLU:H	1:D:59:GLU:CD	2.18	0.46
1:B:329:SER:HB2	1:B:354:CYS:HB3	1.97	0.45
1:E:344:LEU:HD13	1:E:426:LEU:HG	1.98	0.45
1:A:181:ARG:NH2	1:A:185:ASN:OD1	2.49	0.45
1:A:231:LEU:O	1:A:235:GLU:HG3	2.16	0.45
1:F:11:TRP:CD2	1:F:52:LYS:HE3	2.50	0.45
1:F:301:GLY:HA2	1:F:320:LYS:HD3	1.99	0.45
1:A:447:HIS:CB	1:E:129:HIS:HB2	2.45	0.45
1:B:491:GLU:HB2	4:B:693:HOH:O	2.17	0.45
1:B:442:LEU:HD13	1:B:484:LYS:HG2	1.99	0.45
1:D:1:MET:CE	1:D:320:LYS:HB3	2.47	0.45
1:B:6:ARG:NH1	4:B:891:HOH:O	2.50	0.44
1:B:320:LYS:HD2	1:B:328:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:318:LEU:HD11	1:F:463:PHE:CZ	2.52	0.44
1:F:337:HIS:O	1:F:343:GLU:HA	2.17	0.44
1:F:354:CYS:O	1:F:357:ILE:HG12	2.17	0.44
1:B:234:TYR:CE2	1:B:296:ARG:HD2	2.53	0.44
1:B:323:ALA:HB1	1:B:454:ALA:HB3	1.98	0.44
1:B:355:PRO:HA	1:B:382:PHE:CZ	2.52	0.44
1:D:288:GLN:OE1	1:D:377:PRO:HA	2.17	0.44
1:C:429:PRO:HG2	1:C:433:LEU:HA	2.00	0.43
2:C:502:SST:O2	1:F:307:GLU:OE2	2.35	0.43
1:F:271:GLY:HA3	1:F:273:PHE:CE2	2.53	0.43
1:C:129:HIS:HB2	1:F:447:HIS:CB	2.47	0.43
1:D:181:ARG:NH2	1:D:185:ASN:OD1	2.50	0.43
1:C:181:ARG:NH2	1:C:185:ASN:OD1	2.52	0.43
1:D:66:LEU:HD12	1:D:66:LEU:HA	1.88	0.43
1:D:367:HIS:O	1:D:377:PRO:HD2	2.18	0.43
1:F:261:GLU:OE1	1:F:296:ARG:HD3	2.18	0.43
1:B:352:GLU:OE1	1:B:352:GLU:N	2.50	0.43
1:B:470:GLU:HB2	1:B:494:TRP:CD1	2.54	0.43
1:C:292:LEU:HD13	1:C:380:LEU:HG	2.00	0.43
1:B:495:ARG:HG3	4:B:707:HOH:O	2.19	0.43
1:E:337:HIS:HB3	1:E:344:LEU:HG	2.02	0.42
1:A:234:TYR:CE2	1:A:296:ARG:HD2	2.55	0.42
1:B:493:PHE:O	1:B:497:ARG:NH1	2.51	0.42
1:F:352:GLU:OE1	1:F:352:GLU:N	2.44	0.42
1:B:181:ARG:HD3	4:D:602:HOH:O	2.18	0.42
1:E:261:GLU:OE2	1:E:296:ARG:NH1	2.50	0.42
1:D:19:LEU:N	4:D:749:HOH:O	2.53	0.42
1:D:134:TYR:O	1:D:137:ILE:HG22	2.20	0.42
1:E:482:SER:O	1:E:486:GLU:HG3	2.20	0.42
1:F:314:ALA:O	1:F:318:LEU:HB2	2.19	0.42
1:C:88:LYS:HE3	1:F:188:GLU:HA	2.02	0.41
1:C:301:GLY:HA2	1:C:320:LYS:HD3	2.01	0.41
1:E:257:GLN:HG3	1:E:378:ALA:HB3	2.02	0.41
1:E:265:LYS:NZ	1:E:300:GLU:OE1	2.36	0.41
1:E:99:LYS:HA	1:E:99:LYS:HD3	1.92	0.41
1:E:292:LEU:HD13	1:E:380:LEU:HG	2.02	0.41
1:F:288:GLN:OE1	1:F:377:PRO:HA	2.19	0.41
1:A:137:ILE:HD12	1:A:137:ILE:HA	1.93	0.41
1:B:178:LYS:HB3	1:B:178:LYS:HE2	1.80	0.41
1:E:6:ARG:HH21	1:E:73:GLN:HB3	1.85	0.41
1:F:52:LYS:HA	1:F:52:LYS:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:470:GLU:HB2	1:F:494:TRP:CD1	2.56	0.41
1:A:323:ALA:HB1	1:A:454:ALA:HB3	2.03	0.41
1:B:234:TYR:HE2	1:B:296:ARG:HD2	1.85	0.41
1:C:486:GLU:HG2	1:F:489:TRP:CH2	2.55	0.41
1:D:126:GLN:HB2	1:D:129:HIS:CE1	2.55	0.41
1:F:240:ILE:HB	1:F:245:ARG:HG2	2.03	0.41
1:C:320:LYS:NZ	1:C:325:GLY:HA2	2.36	0.41
1:E:41:ARG:NE	4:E:737:HOH:O	2.28	0.41
1:A:71:SER:O	1:A:99:LYS:NZ	2.54	0.40
1:E:25:LEU:HD23	1:E:25:LEU:HA	1.95	0.40
1:A:332:GLU:OE2	1:A:349:HIS:CD2	2.74	0.40
1:F:332:GLU:OE1	1:F:447:HIS:ND1	2.47	0.40
1:A:87:ALA:HB2	1:A:133:GLU:HG3	2.03	0.40
1:D:112:ILE:HG13	1:E:337:HIS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	493/497 (99%)	479 (97%)	13 (3%)	1 (0%)	47	53
1	B	493/497 (99%)	482 (98%)	11 (2%)	0	100	100
1	C	494/497 (99%)	482 (98%)	12 (2%)	0	100	100
1	D	494/497 (99%)	481 (97%)	13 (3%)	0	100	100
1	E	494/497 (99%)	482 (98%)	12 (2%)	0	100	100
1	F	493/497 (99%)	477 (97%)	15 (3%)	1 (0%)	47	53
All	All	2961/2982 (99%)	2883 (97%)	76 (3%)	2 (0%)	51	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	F	291	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/415 (100%)	403 (98%)	10 (2%)	49	55
1	B	413/415 (100%)	401 (97%)	12 (3%)	42	48
1	C	414/415 (100%)	405 (98%)	9 (2%)	52	59
1	D	414/415 (100%)	405 (98%)	9 (2%)	52	59
1	E	414/415 (100%)	404 (98%)	10 (2%)	49	55
1	F	413/415 (100%)	402 (97%)	11 (3%)	44	51
All	All	2481/2490 (100%)	2420 (98%)	61 (2%)	47	54

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	223	SER
1	A	245	ARG
1	A	246	GLN
1	A	333	ASP
1	A	334	TYR
1	A	379	ARG
1	A	424	ARG
1	A	479	SER
1	A	491	GLU
1	B	175	ARG
1	B	223	SER
1	B	264	LEU
1	B	279	THR
1	B	287	LYS
1	B	333	ASP
1	B	334	TYR

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Mol	Chain	Res	Type
1	B	356	THR
1	B	379	ARG
1	B	424	ARG
1	B	479	SER
1	B	491	GLU
1	C	115	ASP
1	C	220	ARG
1	C	225	GLN
1	C	320	LYS
1	C	334	TYR
1	C	379	ARG
1	C	424	ARG
1	C	479	SER
1	C	491	GLU
1	D	30	GLU
1	D	66	LEU
1	D	241	VAL
1	D	264	LEU
1	D	278	THR
1	D	334	TYR
1	D	379	ARG
1	D	424	ARG
1	D	491	GLU
1	E	73	GLN
1	E	175	ARG
1	E	235	GLU
1	E	264	LEU
1	E	334	TYR
1	E	379	ARG
1	E	405	VAL
1	E	424	ARG
1	E	479	SER
1	E	491	GLU
1	F	2	MET
1	F	166	ARG
1	F	264	LEU
1	F	297	LEU
1	F	326	LYS
1	F	333	ASP
1	F	334	TYR
1	F	363	ARG
1	F	379	ARG

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Mol	Chain	Res	Type
1	F	424	ARG
1	F	491	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	SST	A	502	3	9,9,9	1.49	2 (22%)	11,11,11	1.72	3 (27%)
2	SST	E	501	3	9,9,9	1.32	2 (22%)	11,11,11	0.83	0
2	SST	C	501	3	9,9,9	1.38	2 (22%)	11,11,11	2.16	3 (27%)
2	SST	A	501	3	9,9,9	1.34	2 (22%)	11,11,11	0.78	0
2	SST	B	501	3	9,9,9	1.26	1 (11%)	11,11,11	2.00	4 (36%)
2	SST	C	502	3	9,9,9	1.35	2 (22%)	11,11,11	0.81	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SST	A	502	3	-	8/12/12/12	-
2	SST	E	501	3	-	8/12/12/12	-
2	SST	C	501	3	-	5/12/12/12	-
2	SST	A	501	3	-	3/12/12/12	-
2	SST	B	501	3	-	0/12/12/12	-
2	SST	C	502	3	-	8/12/12/12	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	SST	O4-C4	-2.45	1.38	1.43
2	C	501	SST	O4-C4	-2.29	1.38	1.43
2	C	501	SST	O3-C3	-2.28	1.37	1.43
2	C	502	SST	O2-C2	-2.26	1.38	1.43
2	A	501	SST	O2-C2	-2.22	1.38	1.43
2	A	502	SST	O4-C4	-2.22	1.38	1.43
2	E	501	SST	O4-C4	-2.22	1.38	1.43
2	A	502	SST	O2-C2	-2.17	1.38	1.43
2	E	501	SST	O2-C2	-2.14	1.38	1.43
2	A	501	SST	O4-C4	-2.14	1.38	1.43
2	B	501	SST	O2-C2	-2.06	1.39	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	SST	C2-C3-C4	4.30	122.30	113.36
2	B	501	SST	C2-C3-C4	3.87	121.42	113.36
2	B	501	SST	O4-C4-C3	3.71	118.12	109.10
2	C	501	SST	O2-C2-C3	3.64	117.96	109.10
2	A	502	SST	C5-C4-C3	-3.11	105.66	112.41
2	C	501	SST	O4-C4-C3	2.95	116.26	109.10
2	B	501	SST	O2-C2-C3	2.85	116.03	109.10
2	A	502	SST	C1-C2-C3	-2.60	106.78	112.41
2	B	501	SST	O5-C5-C4	-2.22	106.24	111.07
2	A	502	SST	O3-C3-C4	2.09	113.85	108.81

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	SST	O3-C3-C4-O4
2	A	502	SST	C2-C3-C4-O4
2	A	502	SST	O2-C2-C3-O3
2	A	502	SST	C1-C2-C3-O3
2	A	502	SST	C1-C2-C3-C4
2	C	501	SST	O4-C4-C5-O5
2	C	501	SST	C3-C4-C5-O5
2	C	502	SST	O1-C1-C2-O2
2	C	502	SST	O1-C1-C2-C3
2	E	501	SST	O1-C1-C2-O2
2	A	502	SST	O2-C2-C3-C4
2	A	502	SST	O3-C3-C4-C5
2	A	502	SST	C2-C3-C4-C5
2	C	502	SST	C1-C2-C3-C4
2	E	501	SST	O1-C1-C2-C3
2	C	502	SST	O2-C2-C3-C4
2	C	501	SST	C1-C2-C3-O3
2	E	501	SST	C2-C3-C4-O4
2	C	502	SST	C2-C3-C4-O4
2	E	501	SST	C1-C2-C3-C4
2	C	501	SST	O2-C2-C3-O3
2	A	501	SST	C1-C2-C3-C4
2	C	501	SST	C1-C2-C3-C4
2	E	501	SST	C2-C3-C4-C5
2	E	501	SST	O2-C2-C3-C4
2	C	502	SST	C1-C2-C3-O3
2	C	502	SST	C2-C3-C4-C5
2	E	501	SST	O4-C4-C5-O5
2	E	501	SST	C3-C4-C5-O5
2	A	501	SST	C2-C3-C4-O4
2	C	502	SST	O2-C2-C3-O3
2	A	501	SST	C2-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	SST	2	0
2	C	501	SST	1	0
2	A	501	SST	1	0
2	B	501	SST	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	SST	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	495/497 (99%)	-0.66	1 (0%)	95	96	12, 20, 36, 52	0
1	B	495/497 (99%)	-0.72	0	100	100	11, 18, 32, 51	0
1	C	495/497 (99%)	-0.66	2 (0%)	92	93	12, 22, 38, 52	0
1	D	496/497 (99%)	-0.60	3 (0%)	89	89	12, 22, 37, 54	0
1	E	496/497 (99%)	-0.39	9 (1%)	68	69	14, 25, 48, 67	0
1	F	495/497 (99%)	-0.23	13 (2%)	56	57	15, 28, 52, 71	0
All	All	2972/2982 (99%)	-0.55	28 (0%)	84	84	11, 22, 42, 71	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	246	GLN	4.2
1	F	249	PRO	4.2
1	E	237	LEU	3.8
1	F	220	ARG	3.6
1	C	497	ARG	3.5
1	E	241	VAL	3.4
1	F	250	VAL	3.2
1	F	243	ALA	3.2
1	E	244	GLY	3.2
1	A	2	MET	3.2
1	D	26	LYS	3.0
1	E	245	ARG	2.8
1	E	246	GLN	2.7
1	F	241	VAL	2.6
1	F	248	GLY	2.5
1	F	247	GLU	2.4
1	E	243	ALA	2.4
1	E	2	MET	2.4
1	D	246	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	30	GLU	2.3
1	F	245	ARG	2.2
1	E	235	GLU	2.2
1	F	231	LEU	2.2
1	F	242	PRO	2.2
1	C	41	ARG	2.0
1	F	412	LYS	2.0
1	E	220	ARG	2.0
1	F	2	MET	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	SST	C	501	10/10	0.92	0.14	25,29,33,35	0
2	SST	B	501	10/10	0.93	0.16	25,30,35,42	0
2	SST	C	502	10/10	0.94	0.17	36,41,43,47	0
2	SST	A	502	10/10	0.95	0.11	23,29,33,36	0
2	SST	A	501	10/10	0.96	0.12	27,28,33,34	0
2	SST	E	501	10/10	0.96	0.12	34,36,43,49	0
3	MN	E	502	1/1	0.98	0.07	36,36,36,36	0
3	MN	D	501	1/1	0.99	0.07	28,28,28,28	0
3	MN	F	501	1/1	0.99	0.07	39,39,39,39	0
3	MN	A	503	1/1	1.00	0.06	27,27,27,27	0
3	MN	B	502	1/1	1.00	0.06	26,26,26,26	0
3	MN	C	503	1/1	1.00	0.10	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.