Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 01:33 AM JST

PDB ID	:	6INT
Title	:	xylose isomerase from Paenibacillus sp. R4
Authors	:	Lee, J.H.; Lee, C.W.; Park, S.
Deposited on	:	2018-10-26
Resolution	:	1.94 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:

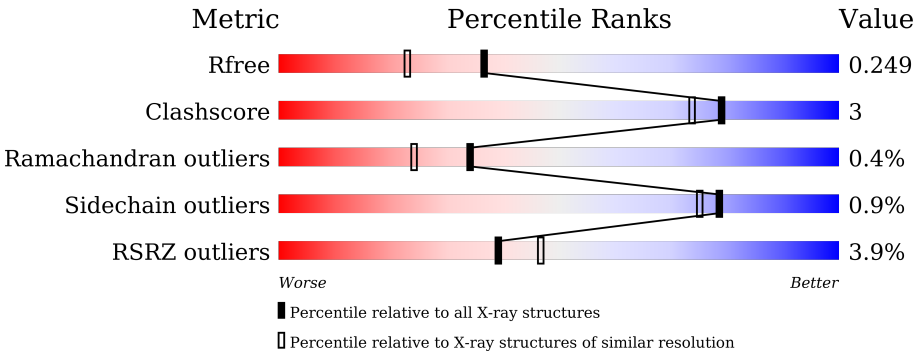
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	438	5% 89% 5% 6%
1	B	438	4% 86% 8% 6%
1	C	438	4% 89% 5% 6%
1	D	438	3% 89% 5% 6%
1	E	438	2% 88% 6% 6%
1	F	438	3% 87% 7% 6%

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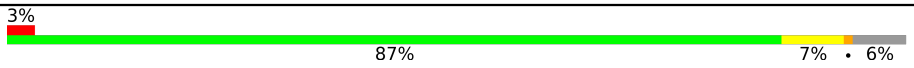
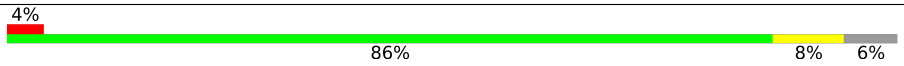
Mol	Chain	Length	Quality of chain
1	G	438	
1	H	438	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 28563 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 Xylose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3269	2083	560	618	8			
1	B	412	Total	C	N	O	S	0	0	0
			3257	2074	559	616	8			
1	C	413	Total	C	N	O	S	0	0	0
			3269	2083	560	618	8			
1	D	413	Total	C	N	O	S	0	0	0
			3269	2083	560	618	8			
1	E	412	Total	C	N	O	S	0	0	0
			3257	2074	559	616	8			
1	F	413	Total	C	N	O	S	0	0	0
			3269	2083	560	618	8			
1	G	413	Total	C	N	O	S	0	0	0
			3269	2083	560	618	8			
1	H	413	Total	C	N	O	S	0	0	0
			3269	2083	560	618	8			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		
2	B	3	Total	Ca	0	0
			3	3		
2	C	3	Total	Ca	0	0
			3	3		
2	D	3	Total	Ca	0	0
			3	3		
2	E	3	Total	Ca	0	0
			3	3		
2	F	3	Total	Ca	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	3	Total Ca 3 3	0	0
2	H	3	Total Ca 3 3	0	0

- Molecule 3 is water.

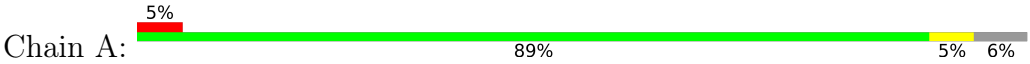
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	275	Total O 275 275	0	0
3	B	249	Total O 249 249	0	0
3	C	289	Total O 289 289	0	0
3	D	309	Total O 309 309	0	0
3	E	358	Total O 358 358	0	0
3	F	341	Total O 341 341	0	0
3	G	279	Total O 279 279	0	0
3	H	311	Total O 311 311	0	0

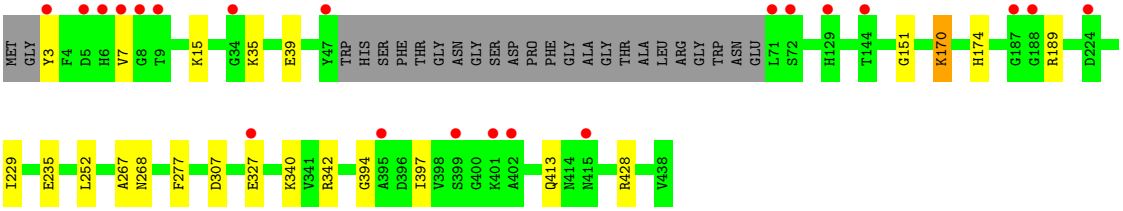
3 Residue-property plots (i)

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: Xylose isomerase

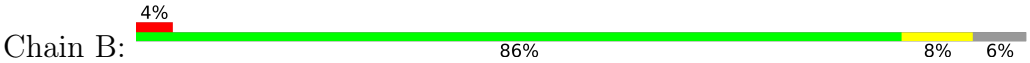
Chain A:

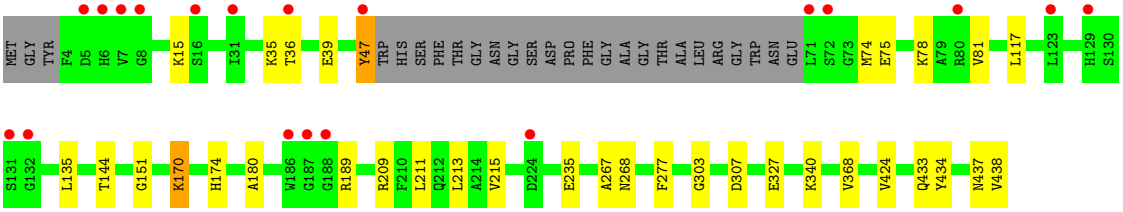




- Molecule 1: Xylose isomerase

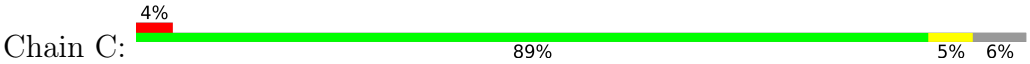
Chain B:

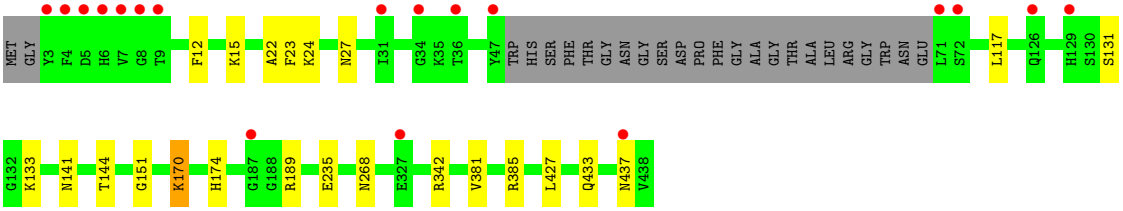




- Molecule 1: Xylose isomerase

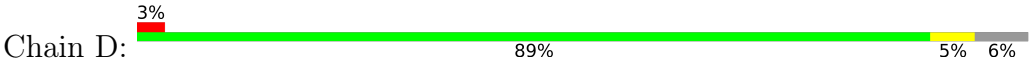
Chain C:

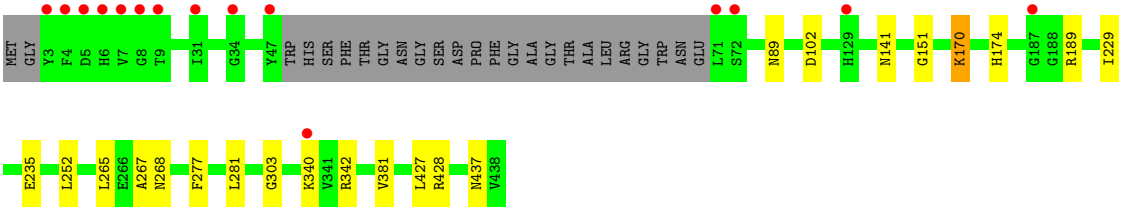




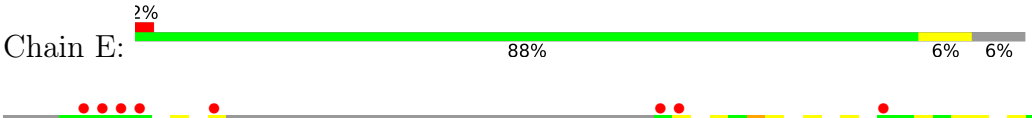
- Molecule 1: Xylose isomerase

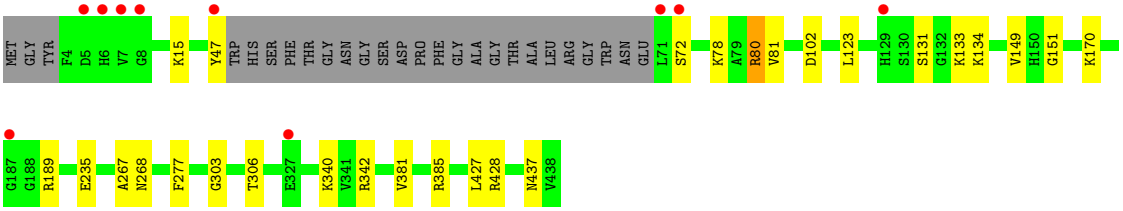
Chain D:



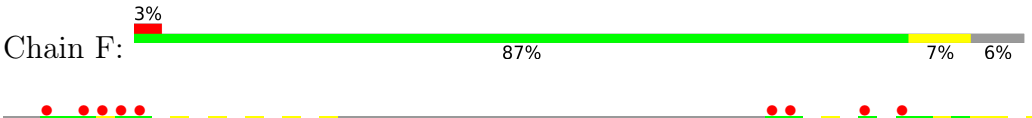


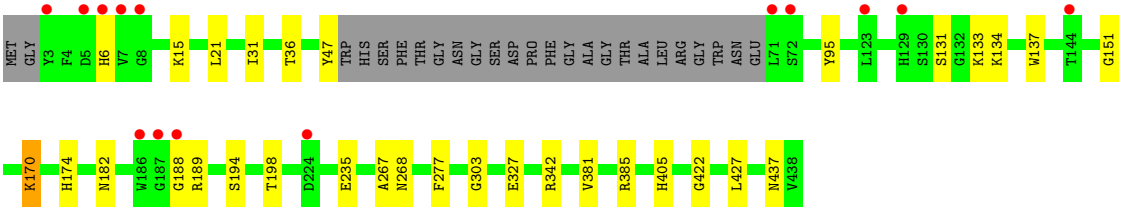
• Molecule 1: Xylose isomerase



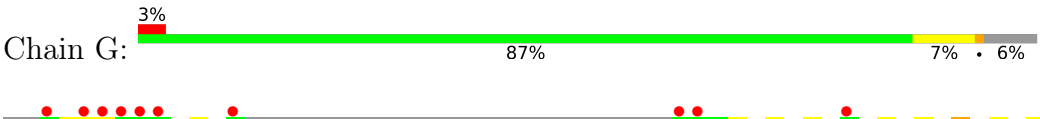


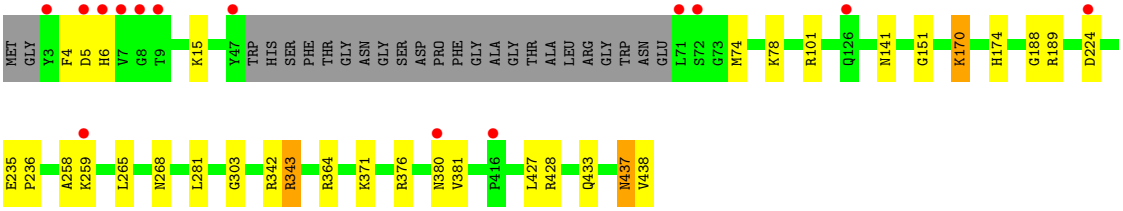
• Molecule 1: Xylose isomerase



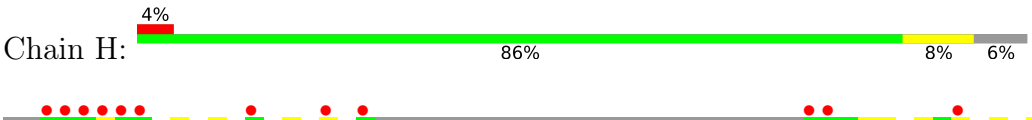


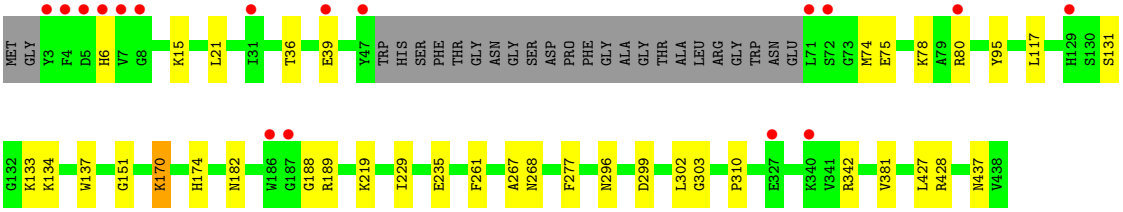
• Molecule 1: Xylose isomerase





• Molecule 1: Xylose isomerase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.28Å 124.04Å 315.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.83 – 1.94 23.83 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.9 (23.83-1.94) 98.9 (23.83-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.23 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???), REFMAC	Depositor
R, R_{free}	0.204 , 0.249 0.204 , 0.249	Depositor DCC
R_{free} test set	12775 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	16.6	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 53.8	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	0.95	EDS
Total number of atoms	28563	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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 54.09 % 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 3.8405e-05. 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: 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	0.38	0/3339	0.53	0/4516
1	B	0.38	0/3326	0.53	0/4498
1	C	0.37	0/3339	0.53	0/4516
1	D	0.39	0/3339	0.53	0/4516
1	E	0.40	0/3326	0.58	1/4498 (0.0%)
1	F	0.39	0/3339	0.55	0/4516
1	G	0.38	0/3339	0.53	0/4516
1	H	0.37	0/3339	0.53	0/4516
All	All	0.38	0/26686	0.54	1/36092 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	80	ARG	NE-CZ-NH2	-7.46	116.57	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3269	0	3178	16	0
1	B	3257	0	3169	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3269	0	3178	14	0
1	D	3269	0	3178	17	0
1	E	3257	0	3169	19	0
1	F	3269	0	3178	23	0
1	G	3269	0	3178	24	0
1	H	3269	0	3178	26	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
3	A	275	0	0	4	1
3	B	249	0	0	1	0
3	C	289	0	0	0	0
3	D	309	0	0	3	0
3	E	358	0	0	4	0
3	F	341	0	0	1	0
3	G	279	0	0	4	0
3	H	311	0	0	3	0
All	All	28563	0	25406	143	1

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 (143) 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:170:LYS:HE2	1:H:174:HIS:CE1	1.88	1.09
1:G:259:LYS:NZ	3:G:601:HOH:O	1.93	1.02
1:D:170:LYS:HE2	1:D:174:HIS:CE1	2.05	0.91
1:G:364:ARG:HH12	1:G:438:VAL:HG22	1.34	0.89
1:B:170:LYS:HE2	1:B:174:HIS:CE1	2.09	0.88
1:A:327:GLU:OE2	3:A:601:HOH:O	1.89	0.87
1:B:303:GLY:HA3	1:D:303:GLY:HA3	1.58	0.82
1:F:303:GLY:HA3	1:H:303:GLY:HA3	1.64	0.80
1:E:437:ASN:ND2	1:H:15:LYS:O	2.16	0.78
1:A:170:LYS:HE2	1:A:174:HIS:CE1	2.20	0.77
1:A:15:LYS:O	1:D:437:ASN:ND2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:342:ARG:NH1	3:G:602:HOH:O	2.19	0.76
1:B:35:LYS:HG3	1:B:39:GLU:HG3	1.68	0.74
1:D:265:LEU:HD12	1:D:281:LEU:HD23	1.70	0.73
1:H:170:LYS:HE2	1:H:174:HIS:NE2	2.05	0.72
1:E:385:ARG:NH2	3:E:602:HOH:O	2.21	0.72
1:F:170:LYS:HE2	1:F:174:HIS:CE1	2.25	0.71
1:E:151:GLY:HA2	1:E:189:ARG:HB2	1.72	0.70
1:B:151:GLY:HA2	1:B:189:ARG:HB2	1.75	0.69
1:G:170:LYS:HE2	1:G:174:HIS:CE1	2.28	0.69
1:F:381:VAL:HG21	1:F:427:LEU:HD21	1.76	0.68
1:C:170:LYS:HE2	1:C:174:HIS:CE1	2.28	0.68
1:H:151:GLY:HA2	1:H:189:ARG:HB2	1.75	0.67
1:A:39:GLU:OE1	3:A:602:HOH:O	2.12	0.66
1:D:141:ASN:ND2	3:D:601:HOH:O	2.28	0.65
1:D:428:ARG:NH1	3:D:602:HOH:O	2.29	0.65
1:G:437:ASN:O	1:G:438:VAL:HB	1.98	0.63
1:H:6:HIS:HD2	1:H:21:LEU:HD13	1.64	0.63
1:E:428:ARG:NH2	1:H:342:ARG:HH12	1.96	0.62
1:G:265:LEU:HD12	1:G:281:LEU:HD23	1.81	0.62
1:A:413:GLN:NE2	3:A:607:HOH:O	2.32	0.62
1:E:15:LYS:O	1:H:437:ASN:ND2	2.33	0.62
1:F:198:THR:HG22	3:F:838:HOH:O	1.98	0.62
1:B:437:ASN:ND2	1:C:15:LYS:O	2.31	0.62
1:C:151:GLY:HA2	1:C:189:ARG:HB2	1.82	0.61
1:F:194:SER:O	1:F:198:THR:HG23	2.01	0.60
1:G:151:GLY:HA2	1:G:189:ARG:HB2	1.83	0.60
1:D:170:LYS:HE2	1:D:174:HIS:NE2	2.17	0.60
1:E:428:ARG:HH22	1:H:342:ARG:HH12	1.50	0.59
1:F:15:LYS:HD2	1:G:437:ASN:HD21	1.67	0.58
1:B:170:LYS:HE2	1:B:174:HIS:NE2	2.18	0.58
1:E:131:SER:OG	1:E:133:LYS:HG2	2.03	0.58
1:E:80:ARG:NH2	3:E:601:HOH:O	2.17	0.58
1:D:151:GLY:HA2	1:D:189:ARG:HB2	1.86	0.56
1:F:151:GLY:HA2	1:F:189:ARG:HB2	1.87	0.55
1:B:36:THR:OG1	1:B:39:GLU:HG2	2.08	0.54
1:A:307:ASP:HB2	1:A:340:LYS:HD2	1.90	0.54
1:F:137:TRP:HB3	1:F:182:ASN:HB2	1.91	0.53
1:E:303:GLY:HA3	1:G:303:GLY:HA3	1.90	0.52
1:H:36:THR:OG1	1:H:39:GLU:HG2	2.09	0.52
1:B:15:LYS:HD3	1:C:437:ASN:ND2	2.25	0.52
1:G:381:VAL:HG21	1:G:427:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:VAL:HG23	1:G:343:ARG:HD3	1.92	0.51
1:H:219:LYS:NZ	3:H:611:HOH:O	2.44	0.51
1:G:74:MET:O	1:G:78:LYS:HG3	2.11	0.51
1:A:428:ARG:NH1	3:A:613:HOH:O	2.44	0.50
1:A:428:ARG:NH2	1:D:342:ARG:HH12	2.10	0.50
1:C:131:SER:OG	1:C:133:LYS:HG2	2.10	0.50
1:H:381:VAL:HG21	1:H:427:LEU:HD21	1.94	0.50
1:H:6:HIS:CD2	1:H:21:LEU:HD13	2.46	0.50
1:C:381:VAL:HG21	1:C:427:LEU:HD21	1.93	0.50
1:A:170:LYS:HE2	1:A:174:HIS:NE2	2.26	0.49
1:C:22:ALA:O	1:C:24:LYS:NZ	2.43	0.49
1:G:376:ARG:NE	1:G:380:ASN:OD1	2.43	0.49
1:D:381:VAL:HG21	1:D:427:LEU:HD21	1.96	0.48
1:E:381:VAL:HG21	1:E:427:LEU:HD21	1.97	0.47
1:F:6:HIS:CD2	1:F:21:LEU:HD22	2.49	0.47
1:C:151:GLY:HA2	1:C:189:ARG:CB	2.44	0.47
1:E:342:ARG:HH22	1:H:428:ARG:NH2	2.13	0.47
1:F:6:HIS:CD2	1:F:21:LEU:HD13	2.49	0.47
1:F:170:LYS:HE2	1:F:174:HIS:NE2	2.30	0.47
1:E:267:ALA:HA	1:E:277:PHE:CD1	2.50	0.47
1:E:47:TYR:OH	1:E:81:VAL:HG22	2.15	0.47
1:H:117:LEU:HG	1:H:174:HIS:CE1	2.50	0.47
1:B:368:VAL:HG13	1:B:434:TYR:HB3	1.97	0.46
1:F:327:GLU:O	1:F:327:GLU:HG3	2.15	0.46
1:H:75:GLU:OE2	3:H:601:HOH:O	2.21	0.46
1:E:306:THR:O	1:E:340:LYS:HE2	2.15	0.46
1:A:267:ALA:HA	1:A:277:PHE:CD1	2.51	0.45
1:B:209:ARG:O	1:B:213:LEU:HG	2.16	0.45
1:B:75:GLU:H	1:B:75:GLU:CD	2.20	0.45
1:C:433:GLN:HG2	1:C:437:ASN:OD1	2.16	0.45
1:B:117:LEU:HG	1:B:174:HIS:CE1	2.52	0.45
1:B:267:ALA:HA	1:B:277:PHE:CD1	2.52	0.45
1:F:385:ARG:HD2	1:F:422:GLY:HA2	1.99	0.45
1:G:4:PHE:C	1:G:6:HIS:H	2.20	0.45
1:B:327:GLU:O	1:B:327:GLU:HG3	2.17	0.45
1:B:433:GLN:O	1:B:437:ASN:HB2	2.17	0.44
1:B:434:TYR:O	1:B:438:VAL:HG13	2.17	0.44
1:A:394:GLY:HA2	1:A:397:ILE:HD12	2.00	0.44
1:F:131:SER:OG	1:F:133:LYS:HG2	2.17	0.44
1:G:224:ASP:HB3	3:G:822:HOH:O	2.16	0.44
1:B:135:LEU:HD23	1:B:180:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:MET:O	1:H:78:LYS:HG3	2.17	0.44
1:A:342:ARG:HH12	1:D:428:ARG:NH2	2.15	0.44
1:C:141:ASN:OD1	1:C:144:THR:HG23	2.18	0.44
1:D:229:ILE:HD12	1:D:252:LEU:HD21	1.99	0.43
1:B:307:ASP:HB2	1:B:340:LYS:HD2	2.00	0.43
1:E:78:LYS:HG2	1:E:123:LEU:HD11	1.99	0.43
3:E:748:HOH:O	1:F:405:HIS:HD2	2.01	0.43
1:A:15:LYS:C	1:D:437:ASN:HD21	2.18	0.43
1:F:6:HIS:HD2	1:F:21:LEU:HD22	1.83	0.43
1:G:170:LYS:HE2	1:G:174:HIS:NE2	2.32	0.43
1:B:47:TYR:OH	1:B:81:VAL:HG22	2.17	0.43
1:F:342:ARG:HH12	1:G:428:ARG:NH2	2.16	0.43
1:G:433:GLN:O	1:G:437:ASN:HB2	2.18	0.43
1:C:117:LEU:HG	1:C:174:HIS:CE1	2.54	0.43
1:D:102:ASP:HB2	3:D:625:HOH:O	2.18	0.43
1:F:267:ALA:HA	1:F:277:PHE:CD1	2.54	0.43
1:G:258:ALA:N	3:G:601:HOH:O	2.35	0.42
1:H:131:SER:HB3	1:H:133:LYS:HG2	2.01	0.42
1:F:437:ASN:HD21	1:G:15:LYS:HB2	1.84	0.42
1:H:151:GLY:HA2	1:H:189:ARG:CB	2.45	0.42
1:H:267:ALA:HA	1:H:277:PHE:CD1	2.55	0.42
1:C:12:PHE:HA	1:C:23:PHE:HB2	2.01	0.42
1:F:342:ARG:HA	1:F:342:ARG:HD2	1.91	0.42
1:D:340:LYS:HB3	1:D:340:LYS:HE2	1.85	0.42
1:E:170:LYS:HD3	1:E:170:LYS:HA	1.84	0.42
1:F:95:TYR:OH	1:F:134:LYS:HE2	2.20	0.42
1:A:229:ILE:HD12	1:A:252:LEU:HD21	2.02	0.42
1:C:170:LYS:HE2	1:C:174:HIS:NE2	2.35	0.42
1:E:80:ARG:NH2	1:E:102:ASP:O	2.53	0.42
1:H:229:ILE:HG13	1:H:261:PHE:CD2	2.54	0.42
1:H:137:TRP:HB3	1:H:182:ASN:HB2	2.02	0.41
1:H:428:ARG:NH1	3:H:622:HOH:O	2.52	0.41
1:H:95:TYR:CZ	1:H:134:LYS:HE3	2.55	0.41
1:H:296:ASN:HA	1:H:310:PRO:HD3	2.02	0.41
1:B:144:THR:HG22	3:B:847:HOH:O	2.19	0.41
1:F:31:ILE:HD13	1:F:36:THR:HG22	2.03	0.41
1:B:424:VAL:HG11	1:C:342:ARG:HD2	2.01	0.41
1:A:151:GLY:HA2	1:A:189:ARG:HB2	2.04	0.40
1:D:89:ASN:HD22	1:D:89:ASN:HA	1.75	0.40
1:D:267:ALA:HA	1:D:277:PHE:CD1	2.56	0.40
1:G:189:ARG:NH1	1:G:236:PRO:HG3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:371:LYS:HD2	1:G:371:LYS:HA	1.91	0.40
1:H:299:ASP:HB3	1:H:302:LEU:HD12	2.03	0.40
1:F:95:TYR:CZ	1:F:134:LYS:HE2	2.56	0.40
1:G:101:ARG:HB2	1:G:141:ASN:HB3	2.03	0.40
1:A:35:LYS:HG3	1:A:39:GLU:HB3	2.02	0.40
1:B:211:LEU:O	1:B:215:VAL:HG23	2.20	0.40
1:E:134:LYS:HG3	3:E:873:HOH:O	2.20	0.40
1:B:74:MET:O	1:B:78:LYS:HG3	2.21	0.40
1:G:364:ARG:NH1	1:G:438:VAL:HG22	2.18	0.40

All (1) 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:A:615:HOH:O	3:A:703:HOH:O[4_597]	2.17	0.03

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	409/438 (93%)	399 (98%)	8 (2%)	2 (0%)	29	17
1	B	408/438 (93%)	400 (98%)	7 (2%)	1 (0%)	47	39
1	C	409/438 (93%)	398 (97%)	10 (2%)	1 (0%)	47	39
1	D	409/438 (93%)	401 (98%)	7 (2%)	1 (0%)	47	39
1	E	408/438 (93%)	398 (98%)	9 (2%)	1 (0%)	47	39
1	F	409/438 (93%)	399 (98%)	8 (2%)	2 (0%)	29	17
1	G	409/438 (93%)	397 (97%)	9 (2%)	3 (1%)	22	11
1	H	409/438 (93%)	399 (98%)	8 (2%)	2 (0%)	29	17
All	All	3270/3504 (93%)	3191 (98%)	66 (2%)	13 (0%)	34	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	H	188	GLY
1	F	188	GLY
1	A	235	GLU
1	B	235	GLU
1	C	235	GLU
1	D	235	GLU
1	E	235	GLU
1	F	235	GLU
1	G	5	ASP
1	G	235	GLU
1	H	235	GLU
1	G	188	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	338/355 (95%)	335 (99%)	3 (1%)	78	75
1	B	337/355 (95%)	334 (99%)	3 (1%)	78	75
1	C	338/355 (95%)	334 (99%)	4 (1%)	71	64
1	D	338/355 (95%)	336 (99%)	2 (1%)	86	85
1	E	337/355 (95%)	335 (99%)	2 (1%)	86	85
1	F	338/355 (95%)	335 (99%)	3 (1%)	78	75
1	G	338/355 (95%)	334 (99%)	4 (1%)	71	64
1	H	338/355 (95%)	335 (99%)	3 (1%)	78	75
All	All	2702/2840 (95%)	2678 (99%)	24 (1%)	78	75

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	TYR

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Mol	Chain	Res	Type
1	A	170	LYS
1	A	268	ASN
1	B	47	TYR
1	B	170	LYS
1	B	268	ASN
1	C	27	ASN
1	C	170	LYS
1	C	268	ASN
1	C	385	ARG
1	D	170	LYS
1	D	268	ASN
1	E	72	SER
1	E	268	ASN
1	F	47	TYR
1	F	170	LYS
1	F	268	ASN
1	G	170	LYS
1	G	268	ASN
1	G	343	ARG
1	G	437	ASN
1	H	80	ARG
1	H	170	LYS
1	H	268	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	437	ASN
1	C	27	ASN
1	D	89	ASN
1	E	89	ASN
1	E	240	GLN
1	F	6	HIS
1	F	240	GLN
1	G	89	ASN
1	G	126	GLN
1	G	437	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

Of 24 ligands modelled in this entry, 24 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, 95^{th} 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	413/438 (94%)	0.33	21 (5%)	28	35	12, 19, 32, 79	0
1	B	412/438 (94%)	0.44	19 (4%)	32	39	13, 21, 33, 68	0
1	C	413/438 (94%)	0.29	18 (4%)	34	41	9, 18, 34, 77	0
1	D	413/438 (94%)	0.13	15 (3%)	42	50	9, 15, 28, 59	0
1	E	412/438 (94%)	0.11	10 (2%)	59	66	10, 16, 28, 62	0
1	F	413/438 (94%)	0.13	14 (3%)	45	53	11, 17, 28, 54	0
1	G	413/438 (94%)	0.23	14 (3%)	45	53	11, 19, 34, 62	0
1	H	413/438 (94%)	0.15	17 (4%)	37	44	10, 18, 31, 55	0
All	All	3302/3504 (94%)	0.23	128 (3%)	39	47	9, 18, 32, 79	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	TYR	9.9
1	C	7	VAL	9.1
1	G	71	LEU	8.8
1	C	3	TYR	8.5
1	B	7	VAL	8.5
1	B	71	LEU	8.0
1	G	7	VAL	7.8
1	E	7	VAL	7.4
1	F	71	LEU	6.9
1	C	71	LEU	6.8
1	D	71	LEU	6.8
1	H	7	VAL	6.6
1	A	7	VAL	6.4
1	G	3	TYR	6.3
1	D	7	VAL	6.3
1	A	71	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
1	H	71	LEU	6.1
1	F	3	TYR	5.8
1	E	71	LEU	5.8
1	H	3	TYR	5.6
1	F	7	VAL	5.4
1	D	3	TYR	5.1
1	G	47	TYR	5.1
1	B	8	GLY	5.1
1	E	5	ASP	4.8
1	A	8	GLY	4.4
1	C	187	GLY	4.4
1	G	5	ASP	4.4
1	H	187	GLY	4.3
1	C	47	TYR	4.2
1	D	8	GLY	4.1
1	B	129	HIS	4.1
1	B	47	TYR	4.1
1	C	6	HIS	4.0
1	E	72	SER	4.0
1	C	8	GLY	3.9
1	C	5	ASP	3.9
1	D	72	SER	3.9
1	F	188	GLY	3.8
1	H	5	ASP	3.7
1	H	6	HIS	3.6
1	A	327	GLU	3.6
1	B	187	GLY	3.6
1	A	6	HIS	3.5
1	A	5	ASP	3.5
1	B	5	ASP	3.5
1	H	129	HIS	3.5
1	H	72	SER	3.4
1	B	6	HIS	3.4
1	C	129	HIS	3.3
1	F	129	HIS	3.3
1	E	6	HIS	3.3
1	C	31	ILE	3.3
1	F	187	GLY	3.3
1	D	5	ASP	3.2
1	C	4	PHE	3.2
1	F	72	SER	3.2
1	B	186	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	9	THR	3.1
1	F	6	HIS	3.1
1	H	8	GLY	3.1
1	E	8	GLY	3.0
1	H	327	GLU	3.0
1	A	34	GLY	2.9
1	F	8	GLY	2.9
1	C	72	SER	2.9
1	A	129	HIS	2.9
1	E	187	GLY	2.8
1	G	259	LYS	2.8
1	G	6	HIS	2.8
1	F	5	ASP	2.8
1	H	4	PHE	2.7
1	B	72	SER	2.7
1	G	72	SER	2.7
1	B	224	ASP	2.7
1	G	9	THR	2.7
1	B	31	ILE	2.6
1	F	144	THR	2.6
1	A	72	SER	2.5
1	F	186	TRP	2.5
1	A	144	THR	2.5
1	D	9	THR	2.5
1	A	395	ALA	2.5
1	D	6	HIS	2.5
1	H	340	LYS	2.5
1	E	327	GLU	2.5
1	G	380	ASN	2.4
1	A	47	TYR	2.4
1	D	47	TYR	2.4
1	D	129	HIS	2.4
1	A	9	THR	2.4
1	A	399	SER	2.4
1	H	47	TYR	2.4
1	G	8	GLY	2.4
1	A	402	ALA	2.3
1	A	187	GLY	2.3
1	D	34	GLY	2.3
1	G	126	GLN	2.3
1	D	187	GLY	2.3
1	B	123	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	4	PHE	2.3
1	A	224	ASP	2.3
1	D	31	ILE	2.3
1	F	224	ASP	2.3
1	G	416	PRO	2.3
1	F	123	LEU	2.2
1	H	80	ARG	2.2
1	A	188	GLY	2.2
1	C	327	GLU	2.2
1	B	36	THR	2.1
1	B	132	GLY	2.1
1	D	340	LYS	2.1
1	H	31	ILE	2.1
1	E	129	HIS	2.1
1	A	415	ASN	2.1
1	C	437	ASN	2.1
1	C	126	GLN	2.1
1	B	131	SER	2.1
1	B	188	GLY	2.1
1	C	34	GLY	2.1
1	E	47	TYR	2.1
1	B	80	ARG	2.1
1	C	36	THR	2.1
1	H	39	GLU	2.0
1	H	186	TRP	2.0
1	A	401	LYS	2.0
1	G	224	ASP	2.0
1	B	16	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, 95^{th} 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	A	503	1/1	0.95	0.06	17,17,17,17	0
2	CA	B	501	1/1	0.97	0.05	19,19,19,19	0
2	CA	A	501	1/1	0.98	0.06	16,16,16,16	0
2	CA	A	502	1/1	0.98	0.04	17,17,17,17	0
2	CA	B	502	1/1	0.98	0.05	20,20,20,20	0
2	CA	B	503	1/1	0.98	0.05	16,16,16,16	0
2	CA	C	501	1/1	0.98	0.05	17,17,17,17	0
2	CA	C	502	1/1	0.98	0.04	15,15,15,15	0
2	CA	C	503	1/1	0.98	0.06	11,11,11,11	0
2	CA	D	502	1/1	0.98	0.05	13,13,13,13	0
2	CA	E	502	1/1	0.98	0.05	15,15,15,15	0
2	CA	F	503	1/1	0.98	0.07	13,13,13,13	0
2	CA	E	501	1/1	0.99	0.05	16,16,16,16	0
2	CA	D	501	1/1	0.99	0.03	15,15,15,15	0
2	CA	E	503	1/1	0.99	0.07	13,13,13,13	0
2	CA	F	501	1/1	0.99	0.04	18,18,18,18	0
2	CA	F	502	1/1	0.99	0.03	19,19,19,19	0
2	CA	D	503	1/1	0.99	0.08	14,14,14,14	0
2	CA	G	501	1/1	0.99	0.06	18,18,18,18	0
2	CA	G	502	1/1	0.99	0.05	16,16,16,16	0
2	CA	G	503	1/1	0.99	0.06	14,14,14,14	0
2	CA	H	501	1/1	0.99	0.07	16,16,16,16	0
2	CA	H	502	1/1	0.99	0.03	17,17,17,17	0
2	CA	H	503	1/1	1.00	0.07	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.