Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 11:12 PM EST

PDB ID	:	8GQG
Title	:	Crystal structure of Thioloase from Pseudomonas aeruginosa PAO1
Authors	:	Hong, J.; Son, H.F.; Kim, K.J.
Deposited on	:	2022-08-30
Resolution	:	1.80 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:

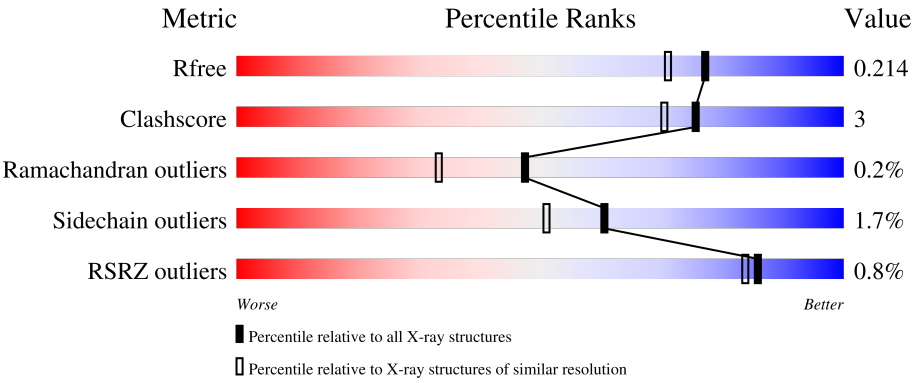
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.80 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.



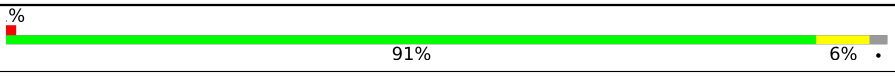
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	402	89% 6%
1	B	402	90% 7%
1	C	402	90% 5%
1	D	402	90% 8%
1	E	402	88% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	402	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19363 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 Thiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	1	0
			2903	1808	519	556	20			
1	B	394	Total	C	N	O	S	0	1	0
			2953	1836	527	570	20			
1	C	388	Total	C	N	O	S	0	1	0
			2912	1813	520	559	20			
1	D	394	Total	C	N	O	S	0	1	0
			2953	1836	527	570	20			
1	E	388	Total	C	N	O	S	0	1	0
			2912	1813	520	559	20			
1	F	394	Total	C	N	O	S	0	1	0
			2953	1836	527	570	20			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	395	LEU	-	expression tag	UNP Q9HYF2
A	396	GLU	-	expression tag	UNP Q9HYF2
A	397	HIS	-	expression tag	UNP Q9HYF2
A	398	HIS	-	expression tag	UNP Q9HYF2
A	399	HIS	-	expression tag	UNP Q9HYF2
A	400	HIS	-	expression tag	UNP Q9HYF2
A	401	HIS	-	expression tag	UNP Q9HYF2
A	402	HIS	-	expression tag	UNP Q9HYF2
B	395	LEU	-	expression tag	UNP Q9HYF2
B	396	GLU	-	expression tag	UNP Q9HYF2
B	397	HIS	-	expression tag	UNP Q9HYF2
B	398	HIS	-	expression tag	UNP Q9HYF2
B	399	HIS	-	expression tag	UNP Q9HYF2
B	400	HIS	-	expression tag	UNP Q9HYF2
B	401	HIS	-	expression tag	UNP Q9HYF2
B	402	HIS	-	expression tag	UNP Q9HYF2
C	395	LEU	-	expression tag	UNP Q9HYF2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	396	GLU	-	expression tag	UNP Q9HYF2
C	397	HIS	-	expression tag	UNP Q9HYF2
C	398	HIS	-	expression tag	UNP Q9HYF2
C	399	HIS	-	expression tag	UNP Q9HYF2
C	400	HIS	-	expression tag	UNP Q9HYF2
C	401	HIS	-	expression tag	UNP Q9HYF2
C	402	HIS	-	expression tag	UNP Q9HYF2
D	395	LEU	-	expression tag	UNP Q9HYF2
D	396	GLU	-	expression tag	UNP Q9HYF2
D	397	HIS	-	expression tag	UNP Q9HYF2
D	398	HIS	-	expression tag	UNP Q9HYF2
D	399	HIS	-	expression tag	UNP Q9HYF2
D	400	HIS	-	expression tag	UNP Q9HYF2
D	401	HIS	-	expression tag	UNP Q9HYF2
D	402	HIS	-	expression tag	UNP Q9HYF2
E	395	LEU	-	expression tag	UNP Q9HYF2
E	396	GLU	-	expression tag	UNP Q9HYF2
E	397	HIS	-	expression tag	UNP Q9HYF2
E	398	HIS	-	expression tag	UNP Q9HYF2
E	399	HIS	-	expression tag	UNP Q9HYF2
E	400	HIS	-	expression tag	UNP Q9HYF2
E	401	HIS	-	expression tag	UNP Q9HYF2
E	402	HIS	-	expression tag	UNP Q9HYF2
F	395	LEU	-	expression tag	UNP Q9HYF2
F	396	GLU	-	expression tag	UNP Q9HYF2
F	397	HIS	-	expression tag	UNP Q9HYF2
F	398	HIS	-	expression tag	UNP Q9HYF2
F	399	HIS	-	expression tag	UNP Q9HYF2
F	400	HIS	-	expression tag	UNP Q9HYF2
F	401	HIS	-	expression tag	UNP Q9HYF2
F	402	HIS	-	expression tag	UNP Q9HYF2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	317	Total O 317 317	0	0
2	B	284	Total O 284 284	0	0
2	C	321	Total O 321 321	0	0
2	D	270	Total O 270 270	0	0

Continued on next page...

Continued from previous page...

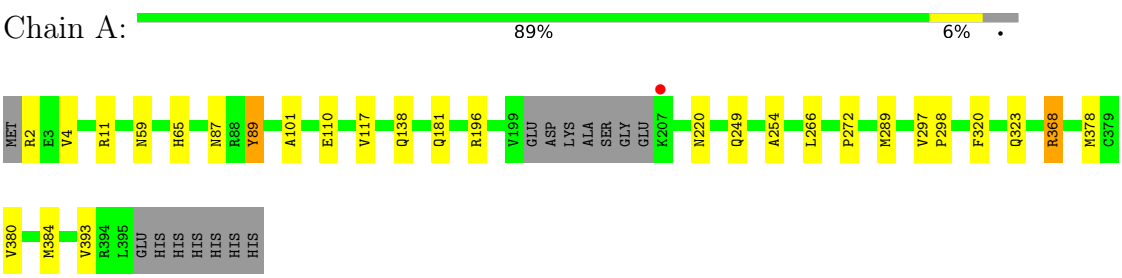
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	312	Total O 312 312	0	0
2	F	273	Total O 273 273	0	0

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.

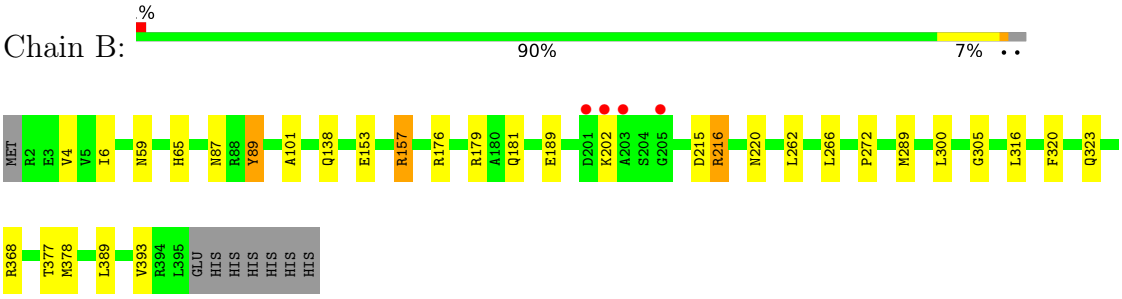
- Molecule 1: Thiolase

Chain A:



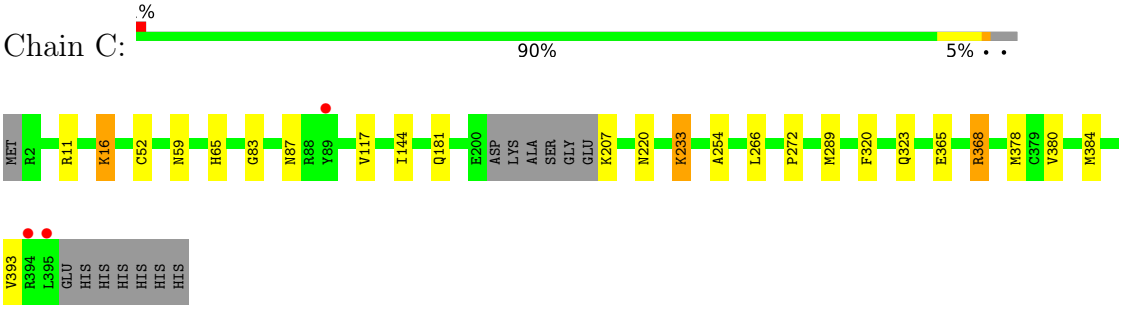
- Molecule 1: Thiolase

Chain B:



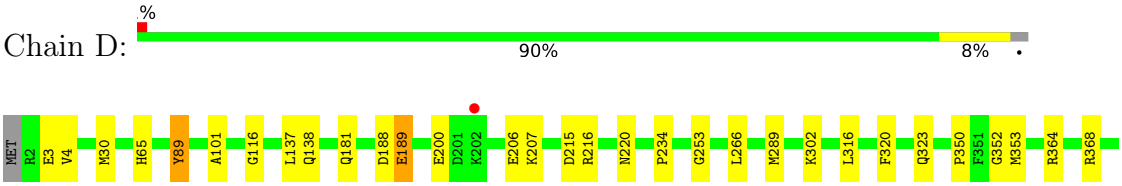
- Molecule 1: Thiolase

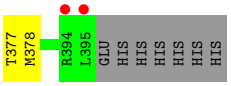
Chain C:



- Molecule 1: Thiolase

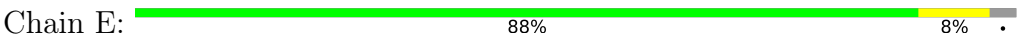
Chain D:

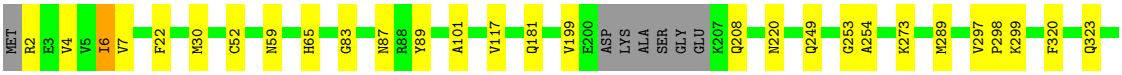


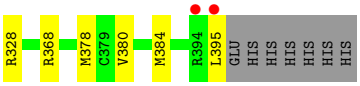


• Molecule 1: Thiolase

Chain E:

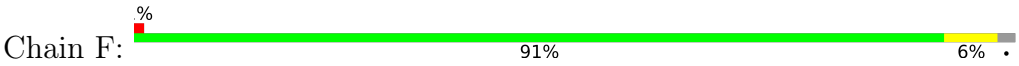


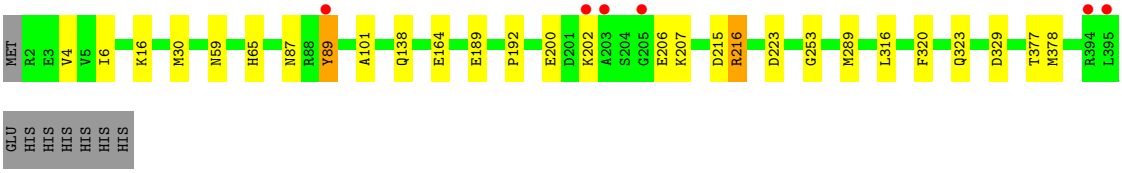




• Molecule 1: Thiolase

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.22Å 204.78Å 262.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.65 – 1.80 31.63 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.2 (31.65-1.80) 95.1 (31.63-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.172 , 0.207 0.182 , 0.214	Depositor DCC
R_{free} test set	13813 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.487 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.487 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19363	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 2.82% 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

5.1 Standard geometry

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	0.75	0/2944	0.90	1/3982 (0.0%)
1	B	0.77	0/2995	0.90	2/4051 (0.0%)
1	C	0.75	0/2953	0.88	2/3994 (0.1%)
1	D	0.78	0/2995	0.89	0/4051
1	E	0.75	0/2953	0.90	2/3994 (0.1%)
1	F	0.79	0/2995	0.90	0/4051
All	All	0.77	0/17835	0.89	7/24123 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	11	ARG	CG-CD-NE	5.70	123.76	111.80
1	E	368	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	11	ARG	CG-CD-NE	5.43	123.21	111.80
1	B	157	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	368	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	E	328	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	368	ARG	NE-CZ-NH1	5.12	122.86	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	2903	0	2905	20	0
1	B	2953	0	2948	20	0
1	C	2912	0	2911	17	0
1	D	2953	0	2948	22	0
1	E	2912	0	2911	20	0
1	F	2953	0	2948	19	0
2	A	317	0	0	6	0
2	B	284	0	0	2	0
2	C	321	0	0	5	0
2	D	270	0	0	3	0
2	E	312	0	0	4	0
2	F	273	0	0	5	0
All	All	19363	0	17571	108	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 (108) 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:F:30:MET:HE1	1:F:253:GLY:HA2	1.54	0.88
1:D:30:MET:HE1	1:D:253:GLY:HA2	1.55	0.88
1:B:305:GLY:HA2	2:D:631:HOH:O	1.76	0.85
1:D:189:GLU:HB3	2:D:610:HOH:O	1.83	0.76
1:F:164:GLU:HG2	2:F:756:HOH:O	1.84	0.76
1:A:368:ARG:HD2	2:A:720:HOH:O	1.87	0.74
1:F:30:MET:CE	1:F:253:GLY:HA2	2.18	0.72
1:D:138:GLN:NE2	2:D:501:HOH:O	2.22	0.71
1:B:215:ASP:OD1	1:B:216:ARG:NH2	2.23	0.70
1:E:181:GLN:HE22	1:E:220:ASN:HD21	1.40	0.69
1:D:30:MET:CE	1:D:253:GLY:HA2	2.23	0.68
1:A:138:GLN:CG	2:A:703:HOH:O	2.42	0.67
1:F:138:GLN:NE2	2:F:502:HOH:O	2.28	0.67
1:B:59:ASN:HD21	1:B:87:ASN:HB2	1.61	0.66
1:C:181:GLN:HE22	1:C:220:ASN:HD21	1.41	0.66
1:F:320:PHE:H	1:F:323:GLN:HE21	1.45	0.65
1:A:138:GLN:HG2	2:A:703:HOH:O	1.96	0.65
1:D:181:GLN:HE22	1:D:220:ASN:HD21	1.45	0.64
1:A:266:LEU:HD11	1:D:266:LEU:HD11	1.80	0.64
1:B:320:PHE:H	1:B:323:GLN:HE21	1.46	0.63
1:F:215:ASP:OD1	1:F:216:ARG:NH2	2.31	0.63
1:D:320:PHE:H	1:D:323:GLN:HE21	1.46	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:MET:HE1	1:D:253:GLY:CA	2.29	0.61
1:E:320:PHE:H	1:E:323:GLN:HE21	1.49	0.61
1:C:320:PHE:H	1:C:323:GLN:HE21	1.50	0.60
1:D:215:ASP:OD1	1:D:216:ARG:NH2	2.35	0.58
1:A:320:PHE:H	1:A:323:GLN:HE21	1.49	0.57
1:B:181:GLN:HE22	1:B:220:ASN:HD21	1.51	0.57
1:A:196:ARG:HD3	2:A:686:HOH:O	2.05	0.57
1:B:138:GLN:NE2	2:B:501:HOH:O	2.22	0.57
1:E:7:VAL:O	1:E:273:LYS:HD2	2.05	0.56
1:E:30:MET:CE	1:E:253:GLY:HA2	2.35	0.56
1:C:117:VAL:HG23	1:C:254:ALA:HB2	1.87	0.55
1:B:266:LEU:HD13	1:C:266:LEU:HD11	1.88	0.55
1:A:59:ASN:HD21	1:A:87:ASN:HB2	1.72	0.54
1:D:188:ASP:OD2	1:D:364:ARG:NH2	2.35	0.54
1:C:272:PRO:HB2	1:C:393:VAL:HG21	1.89	0.54
1:A:272:PRO:HB2	1:A:393:VAL:HG21	1.89	0.54
1:A:181:GLN:HE22	1:A:220:ASN:HD21	1.56	0.54
1:E:117:VAL:HG23	1:E:254:ALA:HB2	1.91	0.53
1:A:266:LEU:CD1	1:D:266:LEU:HD11	2.38	0.53
1:F:59:ASN:HD21	1:F:87:ASN:HB2	1.73	0.53
1:A:2:ARG:NH2	1:A:110:GLU:OE1	2.41	0.53
1:E:299:LYS:NZ	2:E:505:HOH:O	2.43	0.52
1:B:65:HIS:HD2	2:B:743:HOH:O	1.93	0.51
1:F:192:PRO:HG3	2:F:750:HOH:O	2.09	0.51
2:E:768:HOH:O	1:F:65:HIS:HD2	1.94	0.51
1:B:6:ILE:HD12	1:B:6:ILE:N	2.25	0.50
1:A:138:GLN:HG3	2:A:703:HOH:O	2.09	0.50
1:B:262:LEU:HD11	1:C:266:LEU:HD12	1.94	0.50
1:C:365:GLU:OE2	1:C:368:ARG:NH1	2.43	0.50
1:C:16:LYS:NZ	2:C:505:HOH:O	2.45	0.49
1:F:189:GLU:HB3	2:F:572:HOH:O	2.12	0.49
1:E:249:GLN:NE2	2:E:509:HOH:O	2.46	0.49
1:A:117:VAL:HG23	1:A:254:ALA:HB2	1.95	0.48
1:F:200:GLU:HA	1:F:206:GLU:O	2.13	0.48
1:A:297:VAL:HB	1:A:298:PRO:HD3	1.95	0.47
1:B:153:GLU:HG3	1:B:157:ARG:HD2	1.95	0.47
1:B:272:PRO:HB2	1:B:393:VAL:HG21	1.97	0.47
1:D:181:GLN:NE2	1:D:220:ASN:HD21	2.11	0.47
2:C:777:HOH:O	1:D:65:HIS:HD2	1.98	0.47
1:C:233:LYS:HA	1:C:233:LYS:HD3	1.69	0.46
1:E:181:GLN:NE2	1:E:220:ASN:HD21	2.11	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:ILE:HD13	1:E:6:ILE:N	2.31	0.46
1:E:59:ASN:HD21	1:E:87:ASN:HB2	1.81	0.46
1:C:59:ASN:HD21	1:C:87:ASN:HB2	1.81	0.46
1:F:4:VAL:HG11	1:F:101:ALA:HA	1.97	0.46
1:F:30:MET:HE1	1:F:253:GLY:CA	2.35	0.45
1:F:329:ASP:OD2	2:F:501:HOH:O	2.21	0.45
1:A:380:VAL:HB	1:A:384:MET:HB2	1.98	0.45
1:B:181:GLN:NE2	1:B:220:ASN:HD21	2.12	0.45
1:B:316:LEU:HG	1:B:377:THR:HG23	1.97	0.45
1:C:16:LYS:HE2	2:C:519:HOH:O	2.16	0.45
1:F:30:MET:CE	1:F:253:GLY:CA	2.94	0.45
1:A:249:GLN:NE2	2:A:510:HOH:O	2.51	0.44
1:A:4:VAL:HG11	1:A:101:ALA:HA	1.98	0.44
1:A:266:LEU:HD11	1:D:266:LEU:CD1	2.45	0.44
1:C:52:CYS:O	1:C:83:GLY:HA2	2.18	0.44
1:C:368:ARG:CD	2:C:643:HOH:O	2.65	0.44
1:E:22:PHE:CE2	1:E:30:MET:HE3	2.53	0.44
1:B:4:VAL:HG11	1:B:101:ALA:HA	2.00	0.43
1:E:4:VAL:HG11	1:E:101:ALA:HA	2.00	0.43
1:E:30:MET:HE2	1:E:253:GLY:HA2	2.00	0.43
1:E:199:VAL:HG23	1:E:208:GLN:HG2	1.99	0.43
1:B:316:LEU:HA	1:B:377:THR:O	2.19	0.43
1:B:300:LEU:HD21	1:B:389:LEU:HB2	2.00	0.43
1:D:137:LEU:HD23	1:D:137:LEU:HA	1.88	0.43
1:B:176:ARG:HG2	1:B:179:ARG:HH22	1.84	0.43
1:C:368:ARG:HD2	2:C:643:HOH:O	2.19	0.43
1:D:316:LEU:HA	1:D:377:THR:O	2.19	0.43
1:F:316:LEU:HA	1:F:377:THR:O	2.19	0.43
1:C:65:HIS:HA	1:D:89[A]:TYR:OH	2.19	0.42
1:C:144:ILE:O	1:D:65:HIS:HE1	2.03	0.42
1:D:4:VAL:HG11	1:D:101:ALA:HA	2.01	0.42
1:E:395:LEU:O	2:E:501:HOH:O	2.22	0.42
1:E:52:CYS:O	1:E:83:GLY:HA2	2.19	0.42
1:A:65:HIS:HA	1:B:89[A]:TYR:OH	2.20	0.42
1:D:116:GLY:HA3	1:D:352:GLY:O	2.19	0.42
1:D:200:GLU:HA	1:D:206:GLU:O	2.19	0.42
1:E:65:HIS:HA	1:F:89[A]:TYR:OH	2.20	0.42
1:A:89[B]:TYR:OH	1:B:65:HIS:HA	2.19	0.42
1:E:380:VAL:HB	1:E:384:MET:HB2	2.01	0.42
1:F:316:LEU:HG	1:F:377:THR:HG23	2.02	0.41
1:D:350:PRO:O	1:D:353:MET:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:MET:HE1	1:E:253:GLY:HA2	2.03	0.40
1:F:223:ASP:OD1	1:F:223:ASP:N	2.52	0.40
1:C:380:VAL:HB	1:C:384:MET:HB2	2.02	0.40
1:E:297:VAL:HB	1:E:298:PRO:HD3	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	384/402 (96%)	370 (96%)	12 (3%)	2 (0%)	29	15
1	B	393/402 (98%)	380 (97%)	11 (3%)	2 (0%)	29	15
1	C	385/402 (96%)	374 (97%)	11 (3%)	0	100	100
1	D	393/402 (98%)	379 (96%)	12 (3%)	2 (0%)	29	15
1	E	385/402 (96%)	373 (97%)	10 (3%)	2 (0%)	29	15
1	F	393/402 (98%)	381 (97%)	10 (2%)	2 (0%)	29	15
All	All	2333/2412 (97%)	2257 (97%)	66 (3%)	10 (0%)	47	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	89[A]	TYR
1	B	89[B]	TYR
1	D	89[A]	TYR
1	D	89[B]	TYR
1	F	89[A]	TYR
1	F	89[B]	TYR
1	E	89[A]	TYR
1	E	89[B]	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	89[A]	TYR
1	A	89[B]	TYR

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	306/318 (96%)	303 (99%)	3 (1%)	76	71
1	B	311/318 (98%)	306 (98%)	5 (2%)	62	54
1	C	307/318 (96%)	302 (98%)	5 (2%)	62	54
1	D	311/318 (98%)	303 (97%)	8 (3%)	46	32
1	E	307/318 (96%)	303 (99%)	4 (1%)	69	62
1	F	311/318 (98%)	304 (98%)	7 (2%)	50	37
All	All	1853/1908 (97%)	1821 (98%)	32 (2%)	60	51

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	289	MET
1	A	368	ARG
1	A	378	MET
1	B	189	GLU
1	B	202	LYS
1	B	216	ARG
1	B	289	MET
1	B	378	MET
1	C	16	LYS
1	C	207	LYS
1	C	233	LYS
1	C	289	MET
1	C	378	MET
1	D	3	GLU
1	D	189	GLU
1	D	207	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	234	PRO
1	D	289	MET
1	D	302	LYS
1	D	368	ARG
1	D	378	MET
1	E	2	ARG
1	E	6	ILE
1	E	289	MET
1	E	378	MET
1	F	6	ILE
1	F	16	LYS
1	F	202	LYS
1	F	207	LYS
1	F	216	ARG
1	F	289	MET
1	F	378	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	59	ASN
1	A	65	HIS
1	A	131	HIS
1	A	181	GLN
1	A	208	GLN
1	A	249	GLN
1	A	323	GLN
1	A	370	ASN
1	B	59	ASN
1	B	65	HIS
1	B	131	HIS
1	B	181	GLN
1	B	323	GLN
1	B	341	ASN
1	C	42	ASN
1	C	59	ASN
1	C	65	HIS
1	C	131	HIS
1	C	166	GLN
1	C	181	GLN
1	C	323	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	370	ASN
1	D	42	ASN
1	D	65	HIS
1	D	131	HIS
1	D	166	GLN
1	D	181	GLN
1	D	323	GLN
1	D	341	ASN
1	E	42	ASN
1	E	59	ASN
1	E	65	HIS
1	E	131	HIS
1	E	166	GLN
1	E	181	GLN
1	E	323	GLN
1	E	370	ASN
1	F	42	ASN
1	F	59	ASN
1	F	65	HIS
1	F	66	ASN
1	F	323	GLN
1	F	341	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

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	387/402 (96%)	-0.40	1 (0%)	94	92	15, 24, 42, 75	0
1	B	394/402 (98%)	-0.26	4 (1%)	82	80	17, 25, 47, 80	0
1	C	388/402 (96%)	-0.40	3 (0%)	86	84	15, 24, 41, 81	0
1	D	394/402 (98%)	-0.30	3 (0%)	86	84	16, 25, 48, 84	0
1	E	388/402 (96%)	-0.39	2 (0%)	91	89	15, 24, 41, 79	0
1	F	394/402 (98%)	-0.22	6 (1%)	73	70	16, 25, 47, 83	0
All	All	2345/2412 (97%)	-0.33	19 (0%)	86	84	15, 25, 46, 84	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	395	LEU	4.7
1	F	202	LYS	4.1
1	D	395	LEU	4.0
1	B	205	GLY	3.5
1	C	395	LEU	3.3
1	D	394	ARG	3.0
1	F	394	ARG	2.7
1	D	202	LYS	2.7
1	F	205	GLY	2.7
1	E	395	LEU	2.7
1	F	89[A]	TYR	2.6
1	E	394	ARG	2.6
1	A	207	LYS	2.6
1	B	202	LYS	2.5
1	C	394	ARG	2.3
1	B	203	ALA	2.2
1	F	203	ALA	2.1
1	B	201	ASP	2.1
1	C	89[A]	TYR	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.