wwPDB X-ray Structure Validation Summary Report (i)

Feb 8, 2024 – 09:18 AM EST

PDB ID	:	2HQT
Title	:	Crystal structures of the interacting domains from yeast glutamyl-tRNA synthetase and tRNA aminoacylation and nuclear export cofactor Arc1p reveal a novel function for an old fold
Authors	:	Simader, H.; Hothorn, M.; Suck, D.
Deposited on	:	2006-07-19
Resolution	:	1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

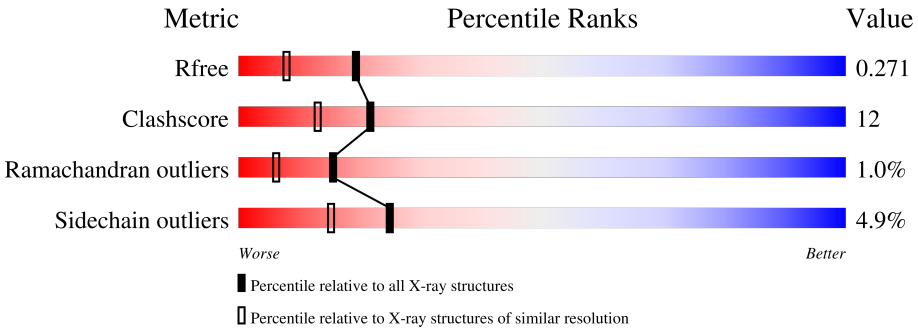
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.90 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)

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%

Mol	Chain	Length	Quality of chain
1	A	124	65% 22% 5% • 7%
1	B	124	79% 16% • •
1	C	124	67% 21% • 8%
1	D	124	81% 15% • •
1	E	124	73% 18% • 6%
1	F	124	70% 22% 5% •
1	G	124	83% 11% • • •

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Mol	Chain	Length	Quality of chain
1	H	124	
1	I	124	
1	J	124	
1	K	124	
1	L	124	
1	M	124	
1	N	124	
1	O	124	
1	P	124	
1	Q	124	
1	R	124	
1	S	124	
1	T	124	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19976 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 GU4 nucleic-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	0	0
			911	584	148	178	1			
1	B	120	Total	C	N	O	S	0	0	0
			954	614	154	185	1			
1	C	114	Total	C	N	O	S	0	0	0
			887	570	145	171	1			
1	D	120	Total	C	N	O	S	0	0	0
			957	615	155	186	1			
1	E	116	Total	C	N	O	S	0	0	0
			902	579	148	174	1			
1	F	120	Total	C	N	O	S	0	0	0
			953	613	153	185	2			
1	G	120	Total	C	N	O	S	0	0	0
			940	604	153	182	1			
1	H	111	Total	C	N	O	S	0	0	0
			864	560	141	162	1			
1	I	116	Total	C	N	O	S	0	0	0
			902	578	148	175	1			
1	J	121	Total	C	N	O	S	0	0	0
			955	615	154	185	1			
1	K	117	Total	C	N	O	S	0	0	0
			919	591	151	176	1			
1	L	119	Total	C	N	O	S	0	0	0
			950	611	154	184	1			
1	M	117	Total	C	N	O	S	0	0	0
			938	604	151	181	2			
1	N	119	Total	C	N	O	S	0	0	0
			921	593	151	176	1			
1	O	119	Total	C	N	O	S	0	0	0
			936	601	154	180	1			
1	P	119	Total	C	N	O	S	0	0	0
			944	608	153	181	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	117	Total	C	N	O	S	0	0	0
			927	596	151	178	2			
1	R	119	Total	C	N	O	S	0	0	0
			941	606	153	181	1			
1	S	116	Total	C	N	O	S	0	0	0
			895	577	147	170	1			
1	T	121	Total	C	N	O	S	0	0	0
			965	621	156	186	2			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P46672
A	2	HIS	-	cloning artifact	UNP P46672
B	1	GLY	-	cloning artifact	UNP P46672
B	2	HIS	-	cloning artifact	UNP P46672
C	1	GLY	-	cloning artifact	UNP P46672
C	2	HIS	-	cloning artifact	UNP P46672
D	1	GLY	-	cloning artifact	UNP P46672
D	2	HIS	-	cloning artifact	UNP P46672
E	1	GLY	-	cloning artifact	UNP P46672
E	2	HIS	-	cloning artifact	UNP P46672
F	1	GLY	-	cloning artifact	UNP P46672
F	2	HIS	-	cloning artifact	UNP P46672
G	1	GLY	-	cloning artifact	UNP P46672
G	2	HIS	-	cloning artifact	UNP P46672
H	1	GLY	-	cloning artifact	UNP P46672
H	2	HIS	-	cloning artifact	UNP P46672
I	1	GLY	-	cloning artifact	UNP P46672
I	2	HIS	-	cloning artifact	UNP P46672
J	1	GLY	-	cloning artifact	UNP P46672
J	2	HIS	-	cloning artifact	UNP P46672
K	1	GLY	-	cloning artifact	UNP P46672
K	2	HIS	-	cloning artifact	UNP P46672
L	1	GLY	-	cloning artifact	UNP P46672
L	2	HIS	-	cloning artifact	UNP P46672
M	1	GLY	-	cloning artifact	UNP P46672
M	2	HIS	-	cloning artifact	UNP P46672
N	1	GLY	-	cloning artifact	UNP P46672
N	2	HIS	-	cloning artifact	UNP P46672
O	1	GLY	-	cloning artifact	UNP P46672
O	2	HIS	-	cloning artifact	UNP P46672
P	1	GLY	-	cloning artifact	UNP P46672

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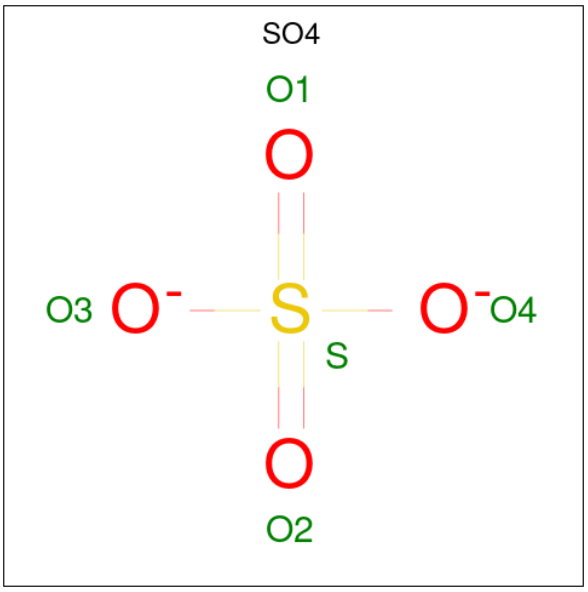
Chain	Residue	Modelled	Actual	Comment	Reference
P	2	HIS	-	cloning artifact	UNP P46672
Q	1	GLY	-	cloning artifact	UNP P46672
Q	2	HIS	-	cloning artifact	UNP P46672
R	1	GLY	-	cloning artifact	UNP P46672
R	2	HIS	-	cloning artifact	UNP P46672
S	1	GLY	-	cloning artifact	UNP P46672
S	2	HIS	-	cloning artifact	UNP P46672
T	1	GLY	-	cloning artifact	UNP P46672
T	2	HIS	-	cloning artifact	UNP P46672

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	N	1	Total O S 5 4 1	0	0
2	Q	1	Total O S 5 4 1	0	0
2	S	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	75	Total O 75 75	0	0
3	B	97	Total O 97 97	0	0
3	C	40	Total O 40 40	0	0
3	D	82	Total O 82 82	0	0
3	E	61	Total O 61 61	0	0
3	F	55	Total O 55 55	0	0
3	G	86	Total O 86 86	0	0
3	H	44	Total O 44 44	0	0
3	I	57	Total O 57 57	0	0
3	J	77	Total O 77 77	0	0
3	K	49	Total O 49 49	0	0
3	L	56	Total O 56 56	0	0
3	M	64	Total O 64 64	0	0
3	N	52	Total O 52 52	0	0
3	O	80	Total O 80 80	0	0
3	P	77	Total O 77 77	0	0

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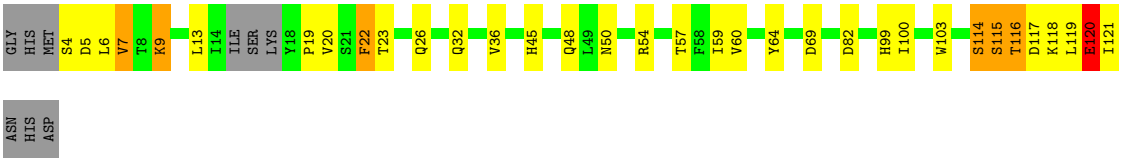
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Q	84	Total O 84 84	0	0
3	R	93	Total O 93 93	0	0
3	S	62	Total O 62 62	0	0
3	T	74	Total O 74 74	0	0

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. 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. 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.

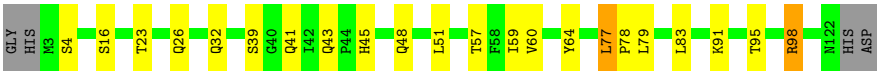
• Molecule 1: GU4 nucleic-binding protein 1

Chain A:



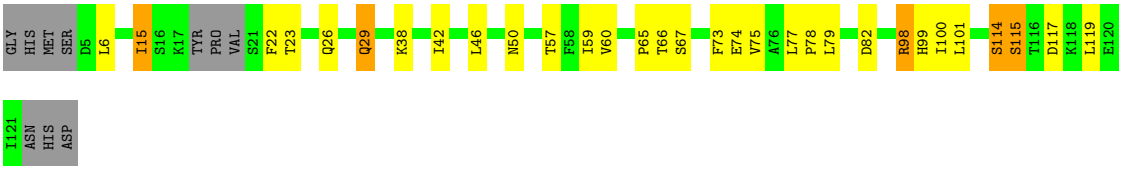
• Molecule 1: GU4 nucleic-binding protein 1

Chain B:



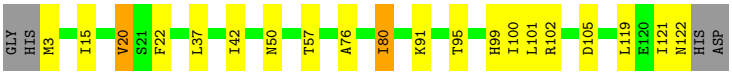
• Molecule 1: GU4 nucleic-binding protein 1

Chain C:



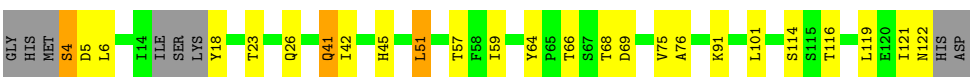
• Molecule 1: GU4 nucleic-binding protein 1

Chain D:



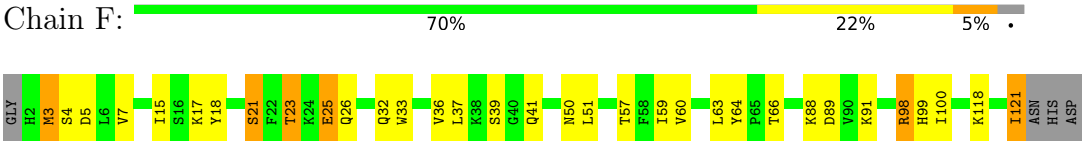
• Molecule 1: GU4 nucleic-binding protein 1

Chain E:



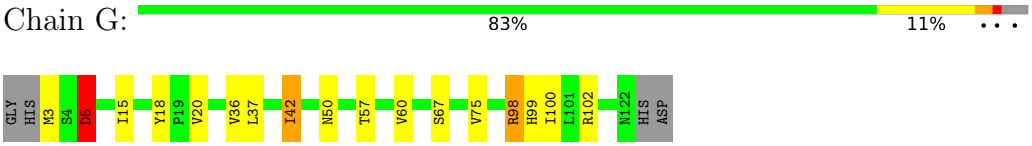
• Molecule 1: GU4 nucleic-binding protein 1

Chain F:



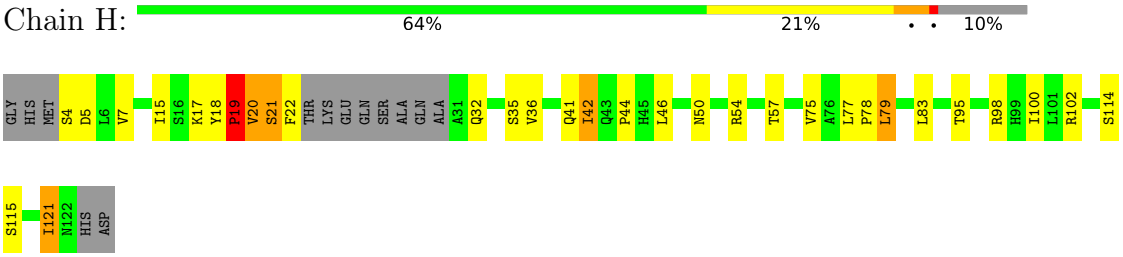
• Molecule 1: GU4 nucleic-binding protein 1

Chain G:



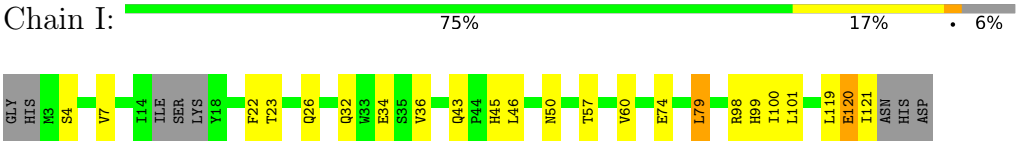
• Molecule 1: GU4 nucleic-binding protein 1

Chain H:



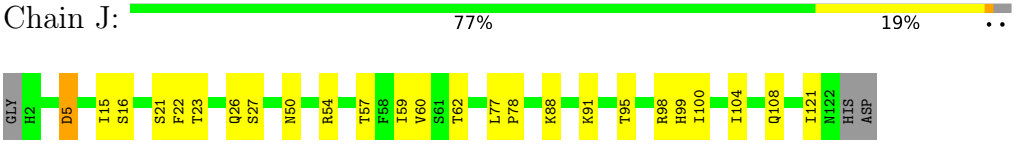
• Molecule 1: GU4 nucleic-binding protein 1

Chain I:



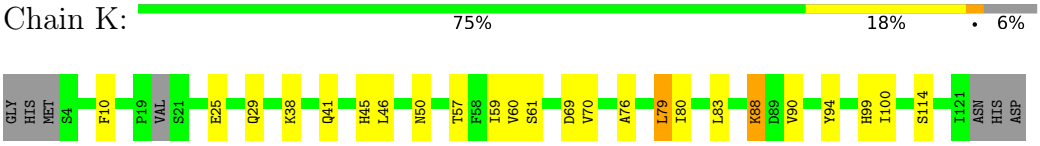
• Molecule 1: GU4 nucleic-binding protein 1

Chain J:



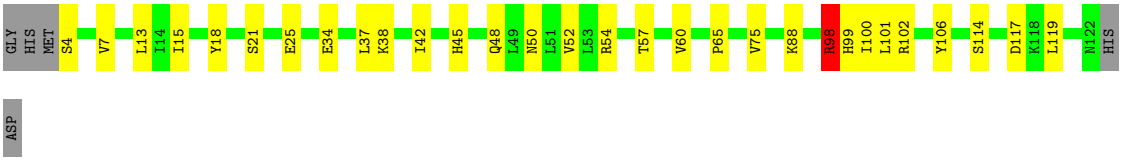
• Molecule 1: GU4 nucleic-binding protein 1

Chain K:



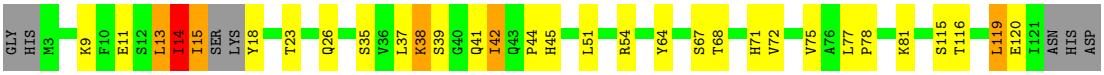
• Molecule 1: GU4 nucleic-binding protein 1

Chain L:



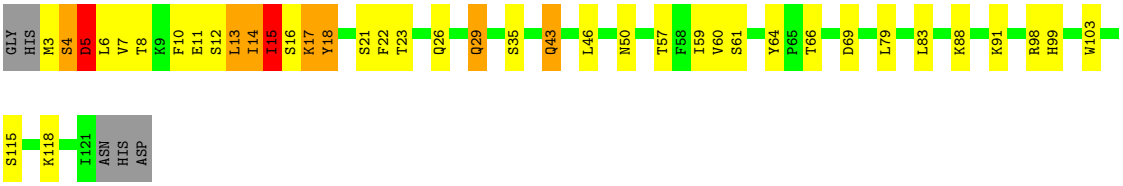
• Molecule 1: GU4 nucleic-binding protein 1

Chain M:



• Molecule 1: GU4 nucleic-binding protein 1

Chain N:

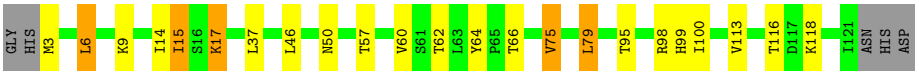


• Molecule 1: GU4 nucleic-binding protein 1

Chain O:

• Molecule 1: GU4 nucleic-binding protein 1

Chain P:



• Molecule 1: GU4 nucleic-binding protein 1

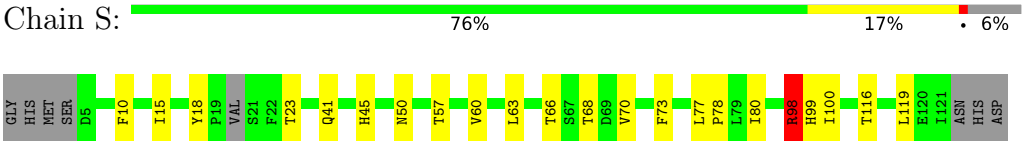
Chain Q:

• Molecule 1: GU4 nucleic-binding protein 1

Chain R:

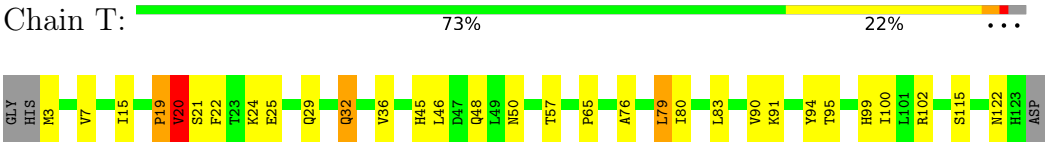
• Molecule 1: GU4 nucleic-binding protein 1

Chain S:



• Molecule 1: GU4 nucleic-binding protein 1

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	222.32Å 89.46Å 126.79Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 45.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-1.90) 97.0 (45.04-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.262 0.221 , 0.271	Depositor DCC
R_{free} test set	9383 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 59.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19976	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 52.55 % 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 4.7859e-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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.70	0/928	0.74	1/1265 (0.1%)
1	B	0.77	0/973	0.81	1/1327 (0.1%)
1	C	0.63	0/903	0.74	1/1233 (0.1%)
1	D	0.70	0/976	0.74	1/1331 (0.1%)
1	E	0.69	1/919 (0.1%)	0.66	0/1255
1	F	0.70	0/972	0.75	1/1326 (0.1%)
1	G	0.73	0/958	0.80	2/1307 (0.2%)
1	H	0.64	0/881	0.73	1/1204 (0.1%)
1	I	0.60	0/918	0.68	0/1252
1	J	0.75	0/974	0.77	0/1329
1	K	0.59	0/936	0.65	0/1275
1	L	0.68	1/969 (0.1%)	0.72	2/1320 (0.2%)
1	M	0.62	0/956	0.71	0/1301
1	N	0.61	0/940	0.72	1/1285 (0.1%)
1	O	0.70	0/953	0.90	4/1298 (0.3%)
1	P	0.60	0/963	0.63	0/1313
1	Q	0.75	0/944	0.78	2/1285 (0.2%)
1	R	0.77	0/960	0.75	0/1310
1	S	0.67	0/912	0.75	1/1246 (0.1%)
1	T	0.71	0/984	0.75	1/1340 (0.1%)
All	All	0.68	2/18919 (0.0%)	0.74	19/25802 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	1
1	E	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	2
1	H	0	1
1	M	0	2
1	N	0	2
1	O	0	1
1	S	0	1
1	T	0	3
All	All	0	17

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	114	SER	CB-OG	5.47	1.49	1.42
1	L	106	TYR	CE2-CZ	-5.19	1.31	1.38

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	98	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	T	102	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	O	102	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	S	98	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	O	102	ARG	NE-CZ-NH1	6.88	123.74	120.30

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	SER	Peptide
1	A	120	GLU	Peptide
1	D	3	MET	Peptide
1	E	18	TYR	Peptide
1	E	4	SER	Peptide

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	911	0	902	27	0
1	B	954	0	952	13	0
1	C	887	0	861	23	0
1	D	957	0	956	13	0
1	E	902	0	877	24	0
1	F	953	0	948	37	0
1	G	940	0	929	13	0
1	H	864	0	846	27	0
1	I	902	0	876	15	0
1	J	955	0	948	19	0
1	K	919	0	913	16	0
1	L	950	0	952	25	0
1	M	938	0	940	34	0
1	N	921	0	898	49	0
1	O	936	0	932	31	0
1	P	944	0	941	19	0
1	Q	927	0	929	26	0
1	R	941	0	934	17	0
1	S	895	0	868	17	0
1	T	965	0	970	35	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	E	10	0	0	1	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	Q	5	0	0	0	0
2	S	5	0	0	0	0
3	A	75	0	0	0	0
3	B	97	0	0	1	0
3	C	40	0	0	0	0
3	D	82	0	0	0	0
3	E	61	0	0	0	0
3	F	55	0	0	3	0
3	G	86	0	0	0	0
3	H	44	0	0	0	0
3	I	57	0	0	0	0
3	J	77	0	0	1	0
3	K	49	0	0	1	0
3	L	56	0	0	0	0
3	M	64	0	0	1	0
3	N	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	80	0	0	4	0
3	P	77	0	0	1	0
3	Q	84	0	0	2	0
3	R	93	0	0	2	0
3	S	62	0	0	1	0
3	T	74	0	0	0	0
All	All	19976	0	18372	439	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 12.

The worst 5 of 439 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:T:20:VAL:HG12	1:T:21:SER:CA	1.37	1.54
1:H:20:VAL:HA	1:H:21:SER:CB	1.46	1.38
1:T:19:PRO:O	1:T:20:VAL:HG23	1.23	1.27
1:N:10:PHE:O	1:N:13:LEU:HD23	1.39	1.19
1:N:15:ILE:N	1:N:15:ILE:HD12	1.60	1.15

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	111/124 (90%)	106 (96%)	2 (2%)	3 (3%)	5 1
1	B	118/124 (95%)	116 (98%)	2 (2%)	0	100 100
1	C	110/124 (89%)	103 (94%)	6 (6%)	1 (1%)	17 7
1	D	118/124 (95%)	114 (97%)	4 (3%)	0	100 100
1	E	112/124 (90%)	107 (96%)	4 (4%)	1 (1%)	17 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	118/124 (95%)	116 (98%)	1 (1%)	1 (1%)	19 9
1	G	118/124 (95%)	114 (97%)	3 (2%)	1 (1%)	19 9
1	H	107/124 (86%)	102 (95%)	2 (2%)	3 (3%)	5 1
1	I	112/124 (90%)	109 (97%)	3 (3%)	0	100 100
1	J	119/124 (96%)	115 (97%)	4 (3%)	0	100 100
1	K	113/124 (91%)	110 (97%)	3 (3%)	0	100 100
1	L	117/124 (94%)	114 (97%)	3 (3%)	0	100 100
1	M	113/124 (91%)	106 (94%)	4 (4%)	3 (3%)	5 1
1	N	117/124 (94%)	109 (93%)	4 (3%)	4 (3%)	3 0
1	O	117/124 (94%)	112 (96%)	2 (2%)	3 (3%)	5 1
1	P	117/124 (94%)	113 (97%)	4 (3%)	0	100 100
1	Q	113/124 (91%)	110 (97%)	1 (1%)	2 (2%)	8 2
1	R	117/124 (94%)	115 (98%)	2 (2%)	0	100 100
1	S	112/124 (90%)	107 (96%)	4 (4%)	1 (1%)	17 7
1	T	119/124 (96%)	114 (96%)	4 (3%)	1 (1%)	19 9
All	All	2298/2480 (93%)	2212 (96%)	62 (3%)	24 (1%)	15 6

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	120	GLU
1	C	22	PHE
1	E	5	ASP
1	F	3	MET

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	105/117 (90%)	98 (93%)	7 (7%)	16 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	110/117 (94%)	105 (96%)	5 (4%)	27 18
1	C	98/117 (84%)	89 (91%)	9 (9%)	9 3
1	D	111/117 (95%)	108 (97%)	3 (3%)	44 38
1	E	100/117 (86%)	97 (97%)	3 (3%)	41 33
1	F	110/117 (94%)	103 (94%)	7 (6%)	17 8
1	G	106/117 (91%)	102 (96%)	4 (4%)	33 24
1	H	95/117 (81%)	88 (93%)	7 (7%)	13 6
1	I	100/117 (86%)	96 (96%)	4 (4%)	31 22
1	J	109/117 (93%)	103 (94%)	6 (6%)	21 12
1	K	104/117 (89%)	100 (96%)	4 (4%)	33 24
1	L	110/117 (94%)	106 (96%)	4 (4%)	35 26
1	M	109/117 (93%)	103 (94%)	6 (6%)	21 12
1	N	102/117 (87%)	91 (89%)	11 (11%)	6 2
1	O	106/117 (91%)	103 (97%)	3 (3%)	43 36
1	P	108/117 (92%)	100 (93%)	8 (7%)	13 6
1	Q	107/117 (92%)	103 (96%)	4 (4%)	34 25
1	R	107/117 (92%)	103 (96%)	4 (4%)	34 25
1	S	97/117 (83%)	96 (99%)	1 (1%)	76 76
1	T	112/117 (96%)	108 (96%)	4 (4%)	35 26
All	All	2106/2340 (90%)	2002 (95%)	104 (5%)	25 15

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	88	LYS
1	N	13	LEU
1	S	98	ARG
1	L	21	SER
1	M	15	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	26	GLN

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Mol	Chain	Res	Type
1	S	50	ASN
1	L	29	GLN
1	R	50	ASN
1	T	48	GLN

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)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	E	2004	-	4,4,4	0.30	0	6,6,6	0.47	0
2	SO4	Q	2009	-	4,4,4	0.13	0	6,6,6	0.38	0
2	SO4	B	2001	-	4,4,4	0.16	0	6,6,6	0.41	0
2	SO4	N	2007	-	4,4,4	0.10	0	6,6,6	0.67	0
2	SO4	J	2006	-	4,4,4	0.17	0	6,6,6	0.47	0
2	SO4	M	2008	-	4,4,4	0.18	0	6,6,6	0.31	0
2	SO4	I	2005	-	4,4,4	0.18	0	6,6,6	0.41	0
2	SO4	A	2002	-	4,4,4	0.18	0	6,6,6	0.55	0
2	SO4	E	2003	-	4,4,4	0.21	0	6,6,6	0.51	0
2	SO4	S	2010	-	4,4,4	0.15	0	6,6,6	0.71	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2004	SO4	1	0
2	B	2001	SO4	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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.