Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 11:19 pm BST

PDB ID	:	3HVZ
Title	:	Crystal Structure of the TGS domain of the CLOLEP_03100 protein from Clostridium leptum, Northeast Structural Genomics Consortium Target QlR13A
Authors	:	Forouhar, F.; Lew, S.; Seetharaman, J.; Sahdev, S.; Xiao, R.; Ciccosanti, C.; Lee, D.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2009-06-16
Resolution	:	2.20 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 following versions of software and data (see references (1)) were used in the production of this report:

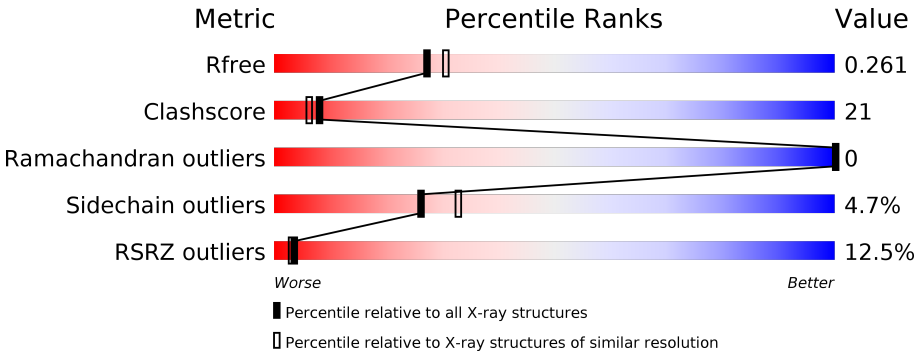
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	78	4% 59% 18% 5% 18%
1	B	78	4% 53% 27% • 18%
1	C	78	4% 53% 27% • 18%
1	D	78	4% 60% 19% • 18%
1	E	78	41% 47% 32% 21%
1	F	78	4% 53% 27% • 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3029 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	64	Total	C	N	O	Se	0	0	0
			486	316	78	91	1			
1	B	64	Total	C	N	O	Se	0	0	0
			486	316	78	91	1			
1	C	64	Total	C	N	O	Se	0	0	0
			486	316	78	91	1			
1	D	64	Total	C	N	O	Se	0	0	0
			486	316	78	91	1			
1	E	62	Total	C	N	O	Se	0	0	0
			468	305	75	87	1			
1	F	64	Total	C	N	O	Se	0	0	0
			486	316	78	91	1			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	MSE	-	INITIATING METHIONINE	UNP A7VWX7
A	461	LEU	-	EXPRESSION TAG	UNP A7VWX7
A	462	GLU	-	EXPRESSION TAG	UNP A7VWX7
A	463	HIS	-	EXPRESSION TAG	UNP A7VWX7
A	464	HIS	-	EXPRESSION TAG	UNP A7VWX7
A	465	HIS	-	EXPRESSION TAG	UNP A7VWX7
A	466	HIS	-	EXPRESSION TAG	UNP A7VWX7
A	467	HIS	-	EXPRESSION TAG	UNP A7VWX7
A	468	HIS	-	EXPRESSION TAG	UNP A7VWX7
B	391	MSE	-	INITIATING METHIONINE	UNP A7VWX7
B	461	LEU	-	EXPRESSION TAG	UNP A7VWX7
B	462	GLU	-	EXPRESSION TAG	UNP A7VWX7
B	463	HIS	-	EXPRESSION TAG	UNP A7VWX7
B	464	HIS	-	EXPRESSION TAG	UNP A7VWX7
B	465	HIS	-	EXPRESSION TAG	UNP A7VWX7
B	466	HIS	-	EXPRESSION TAG	UNP A7VWX7
B	467	HIS	-	EXPRESSION TAG	UNP A7VWX7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	468	HIS	-	EXPRESSION TAG	UNP A7VWX7
C	391	MSE	-	INITIATING METHIONINE	UNP A7VWX7
C	461	LEU	-	EXPRESSION TAG	UNP A7VWX7
C	462	GLU	-	EXPRESSION TAG	UNP A7VWX7
C	463	HIS	-	EXPRESSION TAG	UNP A7VWX7
C	464	HIS	-	EXPRESSION TAG	UNP A7VWX7
C	465	HIS	-	EXPRESSION TAG	UNP A7VWX7
C	466	HIS	-	EXPRESSION TAG	UNP A7VWX7
C	467	HIS	-	EXPRESSION TAG	UNP A7VWX7
C	468	HIS	-	EXPRESSION TAG	UNP A7VWX7
D	391	MSE	-	INITIATING METHIONINE	UNP A7VWX7
D	461	LEU	-	EXPRESSION TAG	UNP A7VWX7
D	462	GLU	-	EXPRESSION TAG	UNP A7VWX7
D	463	HIS	-	EXPRESSION TAG	UNP A7VWX7
D	464	HIS	-	EXPRESSION TAG	UNP A7VWX7
D	465	HIS	-	EXPRESSION TAG	UNP A7VWX7
D	466	HIS	-	EXPRESSION TAG	UNP A7VWX7
D	467	HIS	-	EXPRESSION TAG	UNP A7VWX7
D	468	HIS	-	EXPRESSION TAG	UNP A7VWX7
E	391	MSE	-	INITIATING METHIONINE	UNP A7VWX7
E	461	LEU	-	EXPRESSION TAG	UNP A7VWX7
E	462	GLU	-	EXPRESSION TAG	UNP A7VWX7
E	463	HIS	-	EXPRESSION TAG	UNP A7VWX7
E	464	HIS	-	EXPRESSION TAG	UNP A7VWX7
E	465	HIS	-	EXPRESSION TAG	UNP A7VWX7
E	466	HIS	-	EXPRESSION TAG	UNP A7VWX7
E	467	HIS	-	EXPRESSION TAG	UNP A7VWX7
E	468	HIS	-	EXPRESSION TAG	UNP A7VWX7
F	391	MSE	-	INITIATING METHIONINE	UNP A7VWX7
F	461	LEU	-	EXPRESSION TAG	UNP A7VWX7
F	462	GLU	-	EXPRESSION TAG	UNP A7VWX7
F	463	HIS	-	EXPRESSION TAG	UNP A7VWX7
F	464	HIS	-	EXPRESSION TAG	UNP A7VWX7
F	465	HIS	-	EXPRESSION TAG	UNP A7VWX7
F	466	HIS	-	EXPRESSION TAG	UNP A7VWX7
F	467	HIS	-	EXPRESSION TAG	UNP A7VWX7
F	468	HIS	-	EXPRESSION TAG	UNP A7VWX7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	19	Total O 19 19	0	0

Continued on next page...

Continued from previous page...

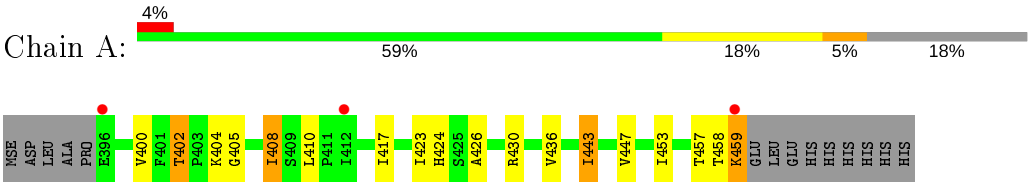
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	25	Total O 25 25	0	0
2	C	24	Total O 24 24	0	0
2	D	37	Total O 37 37	0	0
2	E	4	Total O 4 4	0	0
2	F	22	Total O 22 22	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

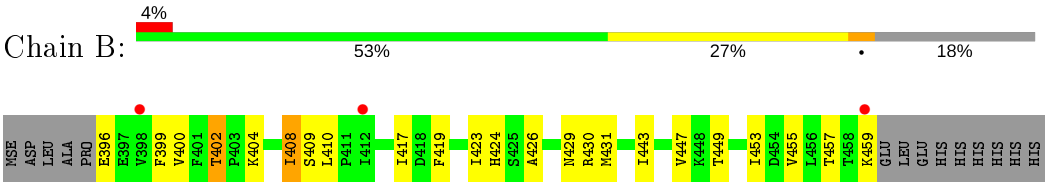
- Molecule 1: Uncharacterized protein

Chain A:



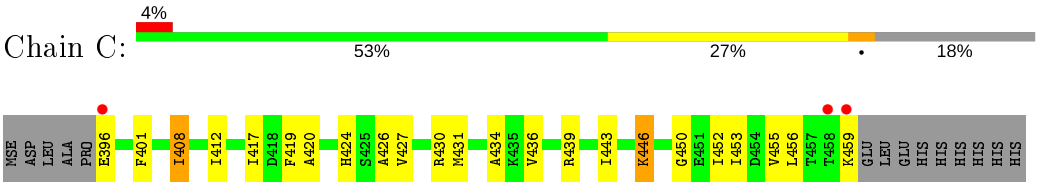
- Molecule 1: Uncharacterized protein

Chain B:



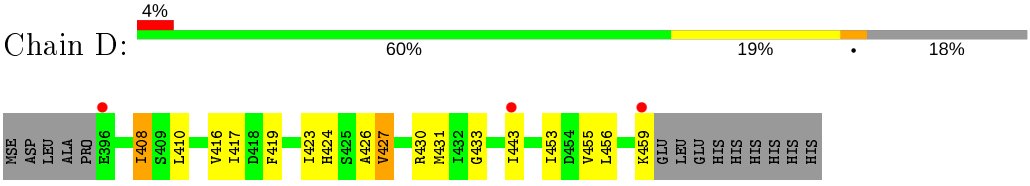
- Molecule 1: Uncharacterized protein

Chain C:



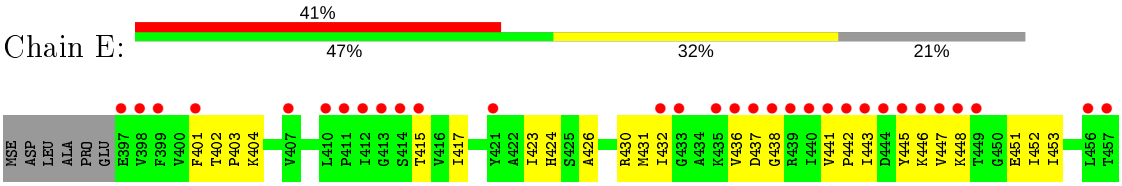
- Molecule 1: Uncharacterized protein

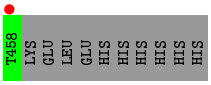
Chain D:



- Molecule 1: Uncharacterized protein

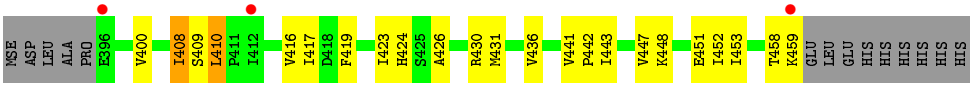
Chain E:





- Molecule 1: Uncharacterized protein

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	107.77Å 110.40Å 107.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.70 – 2.20 29.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	85.7 (19.70-2.20) 98.3 (29.93-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.20Å)	Xtriage
Refinement program	CNS 1.2 & XtalView, REFMAC	Depositor
R, R_{free}	0.224 , 0.254 0.234 , 0.261	Depositor DCC
R_{free} test set	3131 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3029	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.01% 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	0.40	0/493	0.61	0/667
1	B	0.39	0/493	0.60	0/667
1	C	0.36	0/493	0.58	0/667
1	D	0.40	0/493	0.65	0/667
1	E	0.31	0/475	0.50	0/644
1	F	0.35	0/493	0.58	0/667
All	All	0.37	0/2940	0.59	0/3979

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	486	0	506	25	0
1	B	486	0	506	26	0
1	C	486	0	506	21	0
1	D	486	0	506	18	0
1	E	468	0	487	23	0
1	F	486	0	506	23	0
2	A	19	0	0	1	0
2	B	25	0	0	2	0
2	C	24	0	0	0	0
2	D	37	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	4	0	0	0	0
2	F	22	0	0	0	0
All	All	3029	0	3017	126	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 21.

All (126) 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:431:MSE:HE2	1:F:443:ILE:HD11	1.50	0.93
1:A:424:HIS:HD2	1:A:426:ALA:H	1.12	0.90
1:B:402:THR:HG21	2:B:565:HOH:O	1.71	0.89
1:B:417:ILE:HD11	1:B:443:ILE:HG23	1.53	0.88
1:C:424:HIS:HD2	1:C:426:ALA:H	1.18	0.88
1:B:424:HIS:HD2	1:B:426:ALA:H	1.22	0.85
1:A:402:THR:HG21	2:A:563:HOH:O	1.77	0.84
1:E:423:ILE:HG23	1:F:423:ILE:HG22	1.60	0.83
1:F:417:ILE:HD11	1:F:443:ILE:HG23	1.62	0.81
1:F:447:VAL:HG21	1:F:453:ILE:HD11	1.63	0.80
1:E:402:THR:HG22	1:E:404:LYS:H	1.48	0.79
1:B:408:ILE:HG21	1:B:423:ILE:HD11	1.66	0.76
1:B:402:THR:HG22	1:B:404:LYS:H	1.49	0.75
1:A:402:THR:HG23	1:A:404:LYS:H	1.54	0.73
1:E:442:PRO:HG2	1:E:445:TYR:HB2	1.70	0.73
1:D:416:VAL:HG22	1:D:443:ILE:O	1.90	0.72
1:B:400:VAL:HG11	1:B:447:VAL:HG21	1.72	0.72
1:B:429:ASN:HB3	2:B:549:HOH:O	1.91	0.70
1:A:457:THR:HG22	1:A:459:LYS:H	1.57	0.70
1:F:416:VAL:HG22	1:F:443:ILE:O	1.93	0.69
1:C:424:HIS:CD2	1:C:426:ALA:H	2.07	0.68
1:E:417:ILE:HG23	1:E:431:MSE:HE1	1.76	0.68
1:D:424:HIS:HD2	1:D:426:ALA:H	1.40	0.67
1:C:417:ILE:HD11	1:C:443:ILE:HB	1.75	0.67
1:D:408:ILE:HD11	1:D:410:LEU:HD21	1.75	0.67
1:A:459:LYS:HB2	1:B:430:ARG:HH12	1.59	0.66
1:C:431:MSE:HE3	1:C:455:VAL:HG13	1.76	0.66
1:B:400:VAL:HG11	1:B:447:VAL:CG2	2.24	0.66
1:E:430:ARG:NH1	1:F:430:ARG:HG2	2.11	0.65
1:E:447:VAL:HG21	1:E:453:ILE:HD11	1.79	0.64
1:D:417:ILE:HD11	1:D:443:ILE:HG22	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:THR:CG2	1:B:404:LYS:H	2.11	0.63
1:A:423:ILE:CG2	1:B:423:ILE:HG23	2.29	0.63
1:A:424:HIS:CD2	1:A:426:ALA:H	2.04	0.62
1:E:423:ILE:HG23	1:F:423:ILE:CG2	2.29	0.61
1:F:419:PHE:O	1:F:423:ILE:HG12	2.00	0.61
1:B:424:HIS:CD2	1:B:426:ALA:H	2.12	0.60
1:F:431:MSE:HE2	1:F:443:ILE:CD1	2.28	0.60
1:C:396:GLU:OE2	1:C:396:GLU:HA	2.00	0.60
1:C:446:LYS:HB2	1:C:446:LYS:HZ2	1.67	0.60
1:E:424:HIS:HD2	1:E:426:ALA:H	1.49	0.59
1:E:402:THR:HG23	1:E:403:PRO:HD2	1.85	0.59
1:B:417:ILE:HD11	1:B:443:ILE:CG2	2.31	0.58
1:F:459:LYS:H	1:F:459:LYS:HD2	1.69	0.57
1:E:441:VAL:HB	1:E:442:PRO:HD2	1.85	0.57
1:B:447:VAL:HG23	1:B:453:ILE:HD11	1.87	0.57
1:D:443:ILE:HG12	2:D:570:HOH:O	2.03	0.57
1:C:446:LYS:H	1:C:446:LYS:HZ1	1.53	0.56
1:D:424:HIS:CD2	1:D:426:ALA:H	2.22	0.56
1:B:402:THR:HG22	1:B:404:LYS:N	2.19	0.56
1:F:409:SER:O	1:F:410:LEU:HD13	2.05	0.56
1:B:457:THR:O	1:B:459:LYS:HG3	2.05	0.56
1:C:431:MSE:HE2	1:C:434:ALA:HB2	1.88	0.56
1:A:423:ILE:HG23	1:B:423:ILE:HG23	1.86	0.56
1:C:446:LYS:NZ	1:C:446:LYS:H	2.04	0.56
1:A:402:THR:HG22	1:A:405:GLY:H	1.71	0.55
1:D:459:LYS:HD2	1:D:459:LYS:N	2.22	0.54
1:D:408:ILE:HD11	1:D:410:LEU:CD2	2.37	0.53
1:F:441:VAL:HB	1:F:442:PRO:HD2	1.90	0.53
1:A:459:LYS:HB2	1:B:430:ARG:NH1	2.23	0.53
1:D:423:ILE:HG13	1:D:427:VAL:HG11	1.90	0.53
1:A:400:VAL:HG11	1:A:447:VAL:CG2	2.39	0.53
1:D:431:MSE:HE2	1:D:443:ILE:HD12	1.90	0.53
1:C:401:PHE:HE1	1:C:450:GLY:HA2	1.75	0.52
1:D:433:GLY:HA2	1:D:443:ILE:HD11	1.92	0.52
1:E:415:THR:HA	1:E:446:LYS:HA	1.92	0.52
1:F:459:LYS:N	1:F:459:LYS:HD2	2.24	0.52
1:E:424:HIS:CD2	1:E:426:ALA:H	2.28	0.51
1:B:447:VAL:CG2	1:B:453:ILE:HD11	2.41	0.51
1:C:417:ILE:HD13	1:C:431:MSE:SE	2.61	0.50
1:F:400:VAL:HG11	1:F:447:VAL:HG21	1.93	0.50
1:D:424:HIS:O	1:D:427:VAL:HG13	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:VAL:HG11	1:A:447:VAL:HG21	1.93	0.49
1:F:448:LYS:HG2	1:F:451:GLU:CD	2.32	0.49
1:A:430:ARG:HB3	1:A:457:THR:HG23	1.94	0.49
1:A:436:VAL:HG22	1:A:453:ILE:HD12	1.94	0.49
1:C:419:PHE:CZ	1:C:453:ILE:HB	2.48	0.49
1:A:447:VAL:HG23	1:A:453:ILE:HD11	1.94	0.49
1:A:459:LYS:HA	1:A:459:LYS:HE3	1.94	0.48
1:B:408:ILE:HD11	1:B:410:LEU:HG	1.95	0.48
1:B:417:ILE:HG13	1:B:443:ILE:O	2.13	0.48
1:D:456:LEU:N	1:D:456:LEU:HD12	2.28	0.48
1:C:456:LEU:HD12	1:C:456:LEU:N	2.29	0.47
1:E:402:THR:C	1:E:404:LYS:H	2.17	0.47
1:C:401:PHE:HB2	1:C:452:ILE:HD13	1.96	0.47
1:F:436:VAL:HA	1:F:452:ILE:O	2.15	0.47
1:C:408:ILE:O	1:C:408:ILE:HG13	2.15	0.46
1:C:424:HIS:HE1	1:D:455:VAL:O	1.99	0.46
1:F:419:PHE:CD2	1:F:453:ILE:HD12	2.51	0.46
1:D:424:HIS:HB3	1:D:427:VAL:HG12	1.97	0.45
1:A:402:THR:CG2	1:A:404:LYS:H	2.24	0.45
1:E:447:VAL:HG11	1:E:453:ILE:HD11	1.97	0.45
1:A:417:ILE:HD11	1:A:443:ILE:HG23	1.99	0.44
1:A:408:ILE:HD12	1:A:408:ILE:C	2.38	0.44
1:F:408:ILE:HD11	1:F:410:LEU:HD21	1.99	0.44
1:C:417:ILE:HG12	1:C:443:ILE:O	2.17	0.44
1:E:437:ASP:OD2	1:E:451:GLU:HG2	2.17	0.44
1:C:436:VAL:O	1:C:436:VAL:HG23	2.18	0.44
1:A:408:ILE:HD11	1:A:410:LEU:HG	1.99	0.43
1:F:400:VAL:HG11	1:F:447:VAL:CG2	2.47	0.43
1:A:408:ILE:O	1:A:408:ILE:HG13	2.17	0.43
1:E:436:VAL:HG22	1:E:441:VAL:HG11	1.99	0.43
1:A:457:THR:CG2	1:A:458:THR:N	2.81	0.43
1:B:408:ILE:HD12	1:B:419:PHE:CD2	2.53	0.43
1:E:436:VAL:C	1:E:438:GLY:H	2.22	0.43
1:A:408:ILE:HD11	1:A:410:LEU:CD2	2.49	0.43
1:D:426:ALA:O	1:D:430:ARG:HD3	2.19	0.43
1:F:430:ARG:HB3	1:F:458:THR:HG22	2.01	0.43
1:F:417:ILE:HG13	1:F:443:ILE:O	2.20	0.42
1:E:417:ILE:HG13	1:E:443:ILE:O	2.19	0.42
1:E:447:VAL:HG22	1:E:448:LYS:N	2.35	0.42
1:B:431:MSE:HE3	1:B:455:VAL:HG13	2.02	0.41
1:E:432:ILE:C	1:E:432:ILE:HD12	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:PHE:CE1	1:B:409:SER:HB3	2.56	0.41
1:F:424:HIS:CD2	1:F:426:ALA:HB3	2.55	0.41
1:A:408:ILE:HD11	1:A:410:LEU:HD21	2.01	0.41
1:C:420:ALA:O	1:C:427:VAL:HG13	2.20	0.41
1:E:401:PHE:HB2	1:E:452:ILE:CD1	2.51	0.41
1:F:424:HIS:HD2	1:F:426:ALA:HB3	1.86	0.41
1:D:419:PHE:CE1	1:D:453:ILE:HB	2.55	0.41
1:A:424:HIS:HE1	1:B:455:VAL:O	2.04	0.41
1:E:402:THR:C	1:E:404:LYS:N	2.74	0.41
1:C:430:ARG:NH1	1:D:430:ARG:HG2	2.36	0.40
1:E:436:VAL:HG23	1:E:436:VAL:O	2.21	0.40
1:C:436:VAL:HG23	1:C:439:ARG:NH1	2.36	0.40
1:B:399:PHE:O	1:B:449:THR:HA	2.21	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	62/78 (80%)	61 (98%)	1 (2%)	0	100	100
1	B	62/78 (80%)	59 (95%)	3 (5%)	0	100	100
1	C	62/78 (80%)	60 (97%)	2 (3%)	0	100	100
1	D	62/78 (80%)	61 (98%)	1 (2%)	0	100	100
1	E	60/78 (77%)	54 (90%)	6 (10%)	0	100	100
1	F	62/78 (80%)	61 (98%)	1 (2%)	0	100	100
All	All	370/468 (79%)	356 (96%)	14 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	54/65 (83%)	50 (93%)	4 (7%)	13	14
1	B	54/65 (83%)	51 (94%)	3 (6%)	21	25
1	C	54/65 (83%)	50 (93%)	4 (7%)	13	14
1	D	54/65 (83%)	52 (96%)	2 (4%)	34	43
1	E	52/65 (80%)	52 (100%)	0	100	100
1	F	54/65 (83%)	52 (96%)	2 (4%)	34	43
All	All	322/390 (83%)	307 (95%)	15 (5%)	26	33

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	THR
1	A	408	ILE
1	A	443	ILE
1	A	459	LYS
1	B	396	GLU
1	B	402	THR
1	B	408	ILE
1	C	408	ILE
1	C	412	ILE
1	C	446	LYS
1	C	459	LYS
1	D	408	ILE
1	D	427	VAL
1	F	408	ILE
1	F	410	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	HIS
1	B	424	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	429	ASN
1	C	424	HIS
1	D	424	HIS
1	D	429	ASN
1	E	424	HIS
1	E	429	ASN
1	F	429	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	63/78 (80%)	0.27	3 (4%) 30 29	15, 29, 46, 75	0
1	B	63/78 (80%)	0.30	3 (4%) 30 29	18, 29, 48, 76	0
1	C	63/78 (80%)	0.21	3 (4%) 30 29	21, 33, 56, 74	0
1	D	63/78 (80%)	0.19	3 (4%) 30 29	15, 24, 38, 71	0
1	E	61/78 (78%)	2.14	32 (52%) 0 0	49, 76, 88, 94	0
1	F	63/78 (80%)	0.30	3 (4%) 30 29	24, 37, 56, 74	0
All	All	376/468 (80%)	0.56	47 (12%) 3 3	15, 33, 82, 94	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	459	LYS	6.8
1	E	412	ILE	6.8
1	E	443	ILE	6.3
1	E	440	ILE	5.8
1	E	432	ILE	5.1
1	E	399	PHE	4.4
1	E	458	THR	4.3
1	E	445	TYR	4.1
1	B	412	ILE	4.0
1	E	413	GLY	3.9
1	E	414	SER	3.7
1	E	444	ASP	3.6
1	A	412	ILE	3.5
1	D	459	LYS	3.4
1	E	436	VAL	3.3
1	E	456	LEU	3.3
1	F	396	GLU	3.3
1	C	396	GLU	3.3
1	E	449	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	459	LYS	3.1
1	E	447	VAL	3.1
1	E	397	GLU	3.1
1	B	398	VAL	3.0
1	E	411	PRO	2.9
1	E	437	ASP	2.9
1	E	398	VAL	2.9
1	F	412	ILE	2.9
1	E	448	LYS	2.8
1	E	435	LYS	2.7
1	E	410	LEU	2.6
1	E	439	ARG	2.5
1	E	457	THR	2.5
1	E	442	PRO	2.4
1	E	415	THR	2.4
1	C	458	THR	2.4
1	E	401	PHE	2.4
1	E	441	VAL	2.4
1	C	459	LYS	2.3
1	E	421	TYR	2.3
1	A	459	LYS	2.3
1	E	446	LYS	2.2
1	D	396	GLU	2.2
1	D	443	ILE	2.2
1	A	396	GLU	2.1
1	E	438	GLY	2.1
1	E	407	VAL	2.0
1	E	433	GLY	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 carbohydrates 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.