Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:50 AM GMT

PDB ID	:	3G7S
Title	:	Crystal structure of a long-chain-fatty-acid-CoA ligase (FadD1) from Archaeoglobus fulgidus
Authors	:	Palani, K.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-02-10
Resolution	:	2.15 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
http://wwpdb.org/validation/2016/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:

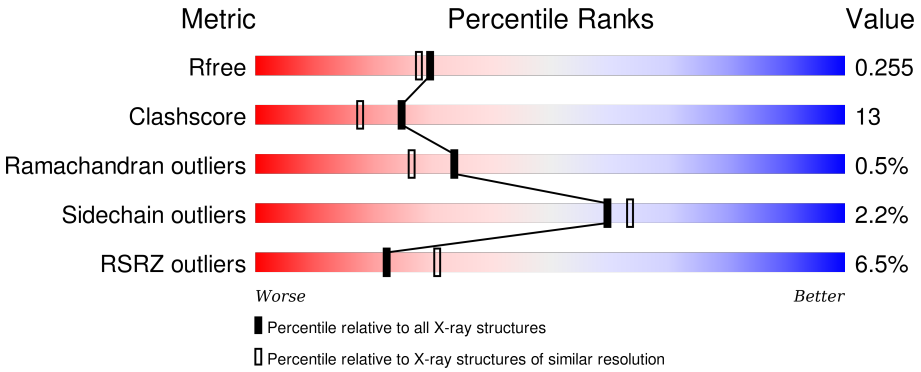
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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. 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	549	8% 67% 22% • 9%
1	B	549	4% 66% 22% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8080 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 Long-chain-fatty-acid--CoA ligase (FadD-1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	Se	0	0	0
			3926	2524	641	737	6	18			
1	B	496	Total	C	N	O	S	Se	0	0	0
			3924	2526	641	732	6	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	EXPRESSION TAG	UNP O30147
A	0	SER	-	EXPRESSION TAG	UNP O30147
A	1	LEU	-	EXPRESSION TAG	UNP O30147
A	541	GLY	-	EXPRESSION TAG	UNP O30147
A	542	HIS	-	EXPRESSION TAG	UNP O30147
A	543	HIS	-	EXPRESSION TAG	UNP O30147
A	544	HIS	-	EXPRESSION TAG	UNP O30147
A	545	HIS	-	EXPRESSION TAG	UNP O30147
A	546	HIS	-	EXPRESSION TAG	UNP O30147
A	547	HIS	-	EXPRESSION TAG	UNP O30147
B	-1	MSE	-	EXPRESSION TAG	UNP O30147
B	0	SER	-	EXPRESSION TAG	UNP O30147
B	1	LEU	-	EXPRESSION TAG	UNP O30147
B	541	GLY	-	EXPRESSION TAG	UNP O30147
B	542	HIS	-	EXPRESSION TAG	UNP O30147
B	543	HIS	-	EXPRESSION TAG	UNP O30147
B	544	HIS	-	EXPRESSION TAG	UNP O30147
B	545	HIS	-	EXPRESSION TAG	UNP O30147
B	546	HIS	-	EXPRESSION TAG	UNP O30147
B	547	HIS	-	EXPRESSION TAG	UNP O30147

- Molecule 2 is water.

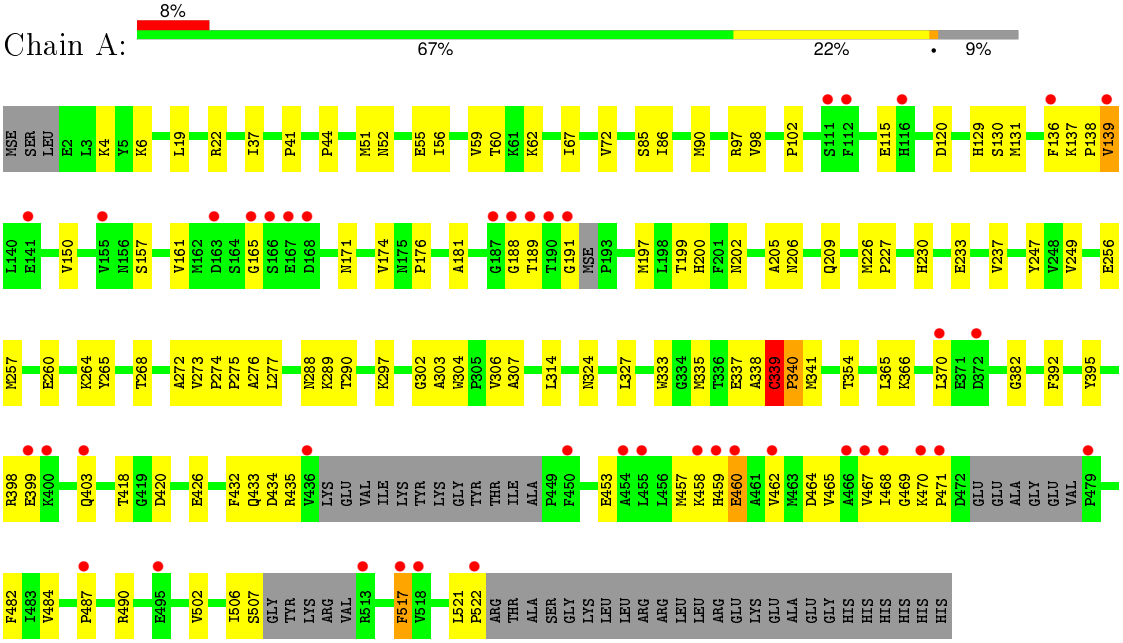
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	92	Total O 92 92	0	0
2	B	138	Total O 138 138	0	0

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 errors 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.

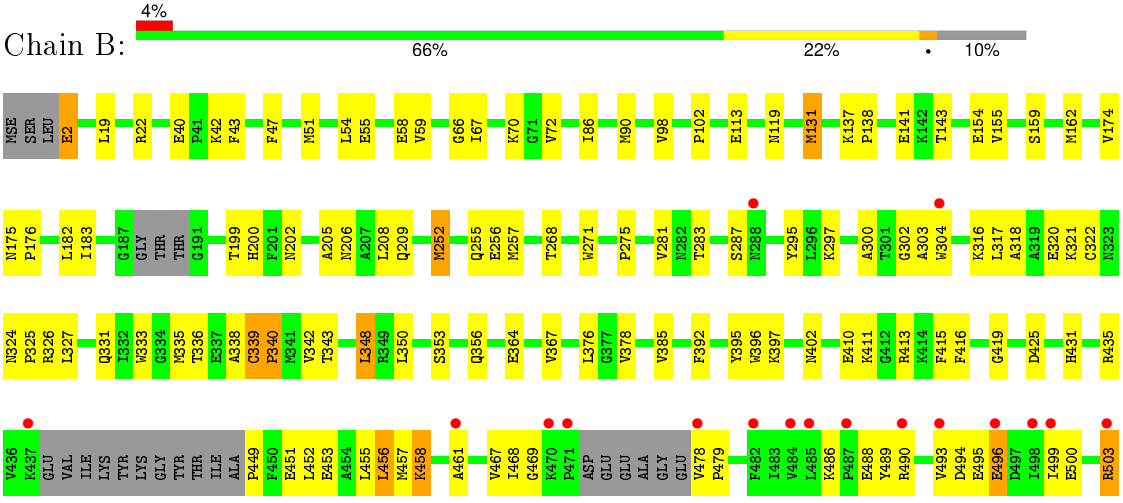
- Molecule 1: Long-chain-fatty-acid--CoA ligase (FadD-1)

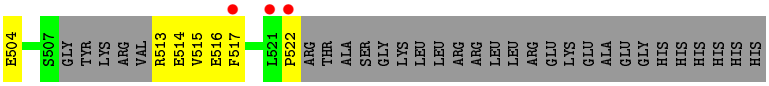
Chain A:



- Molecule 1: Long-chain-fatty-acid--CoA ligase (FadD-1)

Chain B:




E504
S507
GLY
TYR
LYS
ARG
VAL
R513
E514
V515
E516
F517
L521
P522
ARG
THR
ALA
SER
GLY
LYS
LEU
LEU
ARG
ARG
LEU
LEU
ARG
GLU
LYS
GLU
ALA
GLU
GLY
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.04Å 105.07Å 182.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.57 – 2.15 48.96 – 2.15	Depositor EDS
% Data completeness (in resolution range)	85.8 (45.57-2.15) 85.9 (48.96-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.256 0.222 , 0.255	Depositor DCC
R_{free} test set	2667 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.846	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 55377 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8080	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.39	0/3998	0.63	1/5382 (0.0%)
1	B	0.42	0/3995	0.65	1/5376 (0.0%)
All	All	0.40	0/7993	0.64	2/10758 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	175	ASN	N-CA-C	-5.18	97.01	111.00
1	A	339	CYS	N-CA-C	5.09	124.75	111.00

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	3926	0	3900	101	0
1	B	3924	0	3908	100	0
2	A	92	0	0	3	0
2	B	138	0	0	6	0
All	All	8080	0	7808	200	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 13.

All (200) 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:A:457:MSE:HE2	1:A:465:VAL:HG12	1.32	1.07
1:A:457:MSE:HE1	1:A:464:ASP:HA	1.31	1.07
1:A:457:MSE:HE1	1:A:464:ASP:CA	1.95	0.96
1:A:137:LYS:HB3	1:A:138:PRO:HD3	1.48	0.95
1:B:395:TYR:N	1:B:402:ASN:HD21	1.71	0.89
1:B:395:TYR:H	1:B:402:ASN:ND2	1.71	0.88
1:A:51:MSE:HE1	1:A:59:VAL:HG21	1.56	0.88
1:B:338:ALA:C	1:B:340:PRO:HA	1.94	0.88
1:B:19:LEU:H	1:B:200:HIS:HD2	1.22	0.87
1:B:40:GLU:HB2	1:B:257:MSE:HE2	1.58	0.85
1:B:395:TYR:H	1:B:402:ASN:HD21	0.88	0.85
1:A:457:MSE:CE	1:A:465:VAL:HG12	2.06	0.84
1:A:129:HIS:CD2	1:A:131:MSE:HG2	2.12	0.83
1:A:19:LEU:H	1:A:200:HIS:HD2	1.29	0.77
1:B:339:CYS:N	1:B:340:PRO:HA	1.99	0.77
1:B:335:MSE:O	1:B:340:PRO:HB2	1.88	0.74
1:A:56:ILE:HG23	1:A:90:MSE:HE1	1.70	0.73
1:A:199:THR:H	1:A:202:ASN:HD22	1.37	0.71
1:B:40:GLU:HB2	1:B:257:MSE:CE	2.19	0.71
1:A:174:VAL:O	1:A:176:PRO:HD3	1.90	0.70
1:A:457:MSE:HE2	1:A:465:VAL:CG1	2.19	0.69
1:B:452:LEU:HD22	1:B:515:VAL:HG23	1.74	0.69
1:B:324:ASN:ND2	1:B:327:LEU:HB2	2.07	0.69
1:B:503:ARG:HD2	1:B:514:GLU:OE1	1.94	0.67
1:A:129:HIS:HD2	1:A:131:MSE:HG2	1.60	0.66
1:A:457:MSE:CE	1:A:465:VAL:N	2.59	0.65
1:B:479:PRO:HG2	1:B:515:VAL:HA	1.79	0.65
1:A:19:LEU:H	1:A:200:HIS:CD2	2.14	0.65
1:B:19:LEU:H	1:B:200:HIS:CD2	2.10	0.65
1:A:470:LYS:HG2	1:A:471:PRO:HD2	1.80	0.65
1:A:470:LYS:HZ1	1:A:517:PHE:HD1	1.45	0.64
1:A:370:LEU:CD2	1:A:382:GLY:HA2	2.27	0.64
1:A:256:GLU:O	1:A:260:GLU:HG3	1.98	0.63
1:B:159:SER:HA	1:B:162:MSE:HE3	1.80	0.63
1:A:67:ILE:HD12	1:A:72:VAL:HB	1.81	0.62
1:A:468:ILE:HD12	1:A:482:PHE:CE1	2.35	0.62
1:A:502:VAL:O	1:A:506:ILE:HG22	1.99	0.62
1:A:324:ASN:ND2	1:A:327:LEU:HB2	2.15	0.62
1:B:411:LYS:HD2	1:B:413:ARG:NH2	2.15	0.61
1:B:2:GLU:HG3	1:B:378:VAL:HB	1.82	0.61
1:B:43:PHE:CD1	1:B:131:MSE:HE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:MSE:C	1:B:340:PRO:HB2	2.22	0.59
1:B:86:ILE:O	1:B:90:MSE:HG2	2.02	0.59
1:B:396:TRP:CE2	1:B:397:LYS:HG2	2.38	0.59
1:B:40:GLU:CB	1:B:257:MSE:HE2	2.29	0.59
1:A:129:HIS:HD2	1:A:131:MSE:H	1.51	0.59
1:B:154:GLU:HG2	1:B:155:VAL:HG23	1.85	0.59
1:B:119:ASN:HD21	1:B:143:THR:HA	1.68	0.59
1:B:335:MSE:O	1:B:340:PRO:CB	2.52	0.58
1:A:457:MSE:CE	1:A:464:ASP:HA	2.21	0.56
1:B:453:GLU:HG2	1:B:467:VAL:HG23	1.88	0.56
1:A:335:MSE:HE2	1:A:418:THR:HB	1.88	0.56
1:B:419:GLY:HA3	1:B:435:ARG:HH21	1.71	0.56
1:B:287:SER:O	1:B:321:LYS:NZ	2.39	0.56
1:A:399:GLU:O	1:A:403:GLN:HG3	2.06	0.56
1:B:490:ARG:NH2	1:B:522:PRO:HG3	2.21	0.55
1:A:289:LYS:HE2	1:A:290:THR:O	2.06	0.55
1:B:449:PRO:HG2	2:B:549:HOH:O	2.06	0.55
1:A:136:PHE:O	1:A:139:VAL:HG12	2.06	0.55
1:B:478:VAL:HG13	1:B:516:GLU:HG3	1.89	0.55
1:A:457:MSE:CE	1:A:465:VAL:H	2.20	0.54
1:A:51:MSE:HE1	1:A:59:VAL:CG2	2.35	0.54
1:B:98:VAL:O	1:B:98:VAL:HG12	2.07	0.54
1:A:420:ASP:OD1	1:A:435:ARG:HG2	2.07	0.54
1:B:47:PHE:HE1	1:B:59:VAL:HG11	1.72	0.54
1:B:268:THR:HB	1:B:297:LYS:HE2	1.89	0.54
1:B:331:GLN:NE2	1:B:356:GLN:HE21	2.06	0.54
1:A:86:ILE:O	1:A:90:MSE:HG2	2.07	0.54
1:A:189:THR:HG22	1:A:191:GLY:H	1.74	0.53
1:B:495:GLU:O	1:B:499:ILE:HG12	2.09	0.52
1:B:455:LEU:HA	1:B:458:LYS:HD2	1.90	0.52
1:A:482:PHE:HD2	1:A:521:LEU:HD12	1.74	0.52
1:B:205:ALA:O	1:B:209:GLN:HG3	2.10	0.52
1:A:67:ILE:HG22	1:A:161:VAL:HG11	1.92	0.52
1:B:202:ASN:HB3	1:B:339:CYS:SG	2.50	0.51
1:A:226:MSE:HE1	1:A:276:ALA:HB2	1.93	0.51
1:B:367:VAL:HG12	1:B:376:LEU:HD12	1.92	0.51
1:B:411:LYS:HD2	1:B:413:ARG:HH21	1.76	0.51
1:A:470:LYS:HG2	1:A:471:PRO:CD	2.41	0.51
1:A:19:LEU:N	1:A:200:HIS:HD2	2.06	0.50
1:A:370:LEU:HD21	1:A:382:GLY:HA2	1.92	0.50
1:A:115:GLU:HB2	1:A:139:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:THR:HB	1:A:297:LYS:HE2	1.92	0.50
1:B:425:ASP:OD2	1:B:431:HIS:HE1	1.95	0.50
1:A:339:CYS:N	1:A:340:PRO:HA	2.27	0.50
1:B:51:MSE:HE2	1:B:55:GLU:HB3	1.94	0.50
1:B:453:GLU:O	1:B:457:MSE:HB2	2.11	0.50
1:B:51:MSE:CE	1:B:55:GLU:HB3	2.42	0.49
1:A:338:ALA:O	1:A:339:CYS:HB2	2.12	0.49
1:B:141:GLU:HG2	2:B:605:HOH:O	2.13	0.49
1:A:226:MSE:HE1	1:A:276:ALA:CB	2.43	0.49
1:B:271:TRP:HA	1:B:300:ALA:O	2.13	0.49
1:A:426:GLU:HG2	2:A:577:HOH:O	2.13	0.49
1:B:333:TRP:CH2	1:B:335:MSE:HE1	2.47	0.49
1:B:40:GLU:OE2	1:B:42:LYS:HE2	2.13	0.49
1:B:342:VAL:HG12	1:B:343:THR:HG23	1.95	0.48
1:B:113:GLU:OE1	1:B:513:ARG:NH1	2.45	0.48
1:A:506:ILE:HG13	1:A:507:SER:N	2.27	0.48
1:A:487:PRO:HA	1:A:490:ARG:HG3	1.94	0.48
1:A:202:ASN:HB3	1:A:339:CYS:SG	2.54	0.48
1:B:154:GLU:H	1:B:154:GLU:CD	2.16	0.48
1:A:302:GLY:O	1:A:303:ALA:HB3	2.14	0.48
1:A:52:ASN:OD1	1:A:55:GLU:HG3	2.14	0.48
1:A:338:ALA:C	1:A:340:PRO:HA	2.34	0.48
1:A:97:ARG:HG2	1:A:171:ASN:OD1	2.13	0.48
1:A:41:PRO:HD3	1:A:257:MSE:SE	2.64	0.48
1:A:62:LYS:O	1:A:165:GLY:HA3	2.13	0.48
1:B:338:ALA:O	1:B:339:CYS:HB2	2.14	0.47
1:B:331:GLN:HE22	1:B:356:GLN:HE21	1.60	0.47
1:B:451:GLU:OE2	1:B:513:ARG:NH1	2.47	0.47
1:A:303:ALA:O	1:A:304:TRP:HB2	2.13	0.47
1:B:456:LEU:HD12	1:B:456:LEU:HA	1.67	0.47
1:A:67:ILE:HD11	1:A:98:VAL:HG21	1.96	0.47
1:A:205:ALA:O	1:A:209:GLN:HG3	2.14	0.47
1:B:54:LEU:O	1:B:58:GLU:HG2	2.15	0.47
1:A:457:MSE:HE1	1:A:464:ASP:C	2.34	0.47
1:B:137:LYS:HB3	1:B:138:PRO:HD3	1.97	0.47
1:B:316:LYS:HE2	1:B:320:GLU:OE1	2.15	0.47
1:B:199:THR:H	1:B:202:ASN:HD22	1.62	0.47
1:A:370:LEU:HD22	1:A:382:GLY:HA2	1.94	0.47
1:B:154:GLU:OE2	1:B:154:GLU:N	2.47	0.47
1:A:264:LYS:HD3	1:A:265:TYR:CE1	2.50	0.47
1:A:237:VAL:HG12	1:A:247:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:PHE:CE1	1:B:59:VAL:HG11	2.49	0.47
1:A:197:MSE:HE2	1:A:395:TYR:O	2.14	0.47
1:A:6:LYS:HD3	1:B:295:TYR:CD2	2.50	0.47
1:A:206:ASN:HD21	1:A:341:MSE:HG2	1.80	0.47
1:B:174:VAL:O	1:B:176:PRO:HD3	2.15	0.47
1:B:514:GLU:HB2	2:B:660:HOH:O	2.16	0.46
1:B:255:GLN:HG2	1:B:256:GLU:H	1.80	0.46
1:B:500:GLU:O	1:B:504:GLU:HG3	2.16	0.46
1:A:157:SER:O	1:A:161:VAL:HG23	2.16	0.46
1:B:304:TRP:HA	2:B:620:HOH:O	2.15	0.46
1:B:385:VAL:HA	1:B:416:PHE:O	2.15	0.46
1:B:325:PRO:HG2	1:B:326:ARG:NH1	2.31	0.46
1:A:137:LYS:HB3	1:A:138:PRO:CD	2.32	0.46
1:A:227:PRO:HB2	1:A:230:HIS:CD2	2.51	0.46
1:B:478:VAL:HG13	1:B:516:GLU:CB	2.46	0.45
1:A:420:ASP:HB3	1:A:432:PHE:CE1	2.52	0.45
1:A:22:ARG:HG2	1:A:22:ARG:HH11	1.81	0.45
1:B:183:ILE:HG22	1:B:183:ILE:O	2.16	0.45
1:B:461:ALA:HB2	1:B:489:TYR:CD2	2.51	0.45
1:B:494:ASP:OD1	1:B:496:GLU:HB2	2.17	0.45
1:A:468:ILE:HG22	1:A:469:GLY:N	2.31	0.45
1:B:102:PRO:HG2	1:B:182:LEU:HD12	1.98	0.45
1:B:493:VAL:HG23	1:B:493:VAL:O	2.17	0.45
1:A:233:GLU:O	1:A:237:VAL:HG13	2.17	0.45
1:B:336:THR:HA	1:B:340:PRO:HB3	1.99	0.45
1:B:350:LEU:O	1:B:353:SER:HB3	2.17	0.45
1:A:85:SER:HA	1:A:249:VAL:HG11	1.99	0.45
1:A:67:ILE:CG2	1:A:161:VAL:HG11	2.47	0.44
1:A:44:PRO:O	1:A:129:HIS:HE1	2.00	0.44
1:A:306:VAL:HG22	1:A:307:ALA:N	2.32	0.44
1:B:275:PRO:HG3	1:B:304:TRP:HZ2	1.83	0.44
1:A:468:ILE:HD12	1:A:482:PHE:HE1	1.81	0.44
1:B:364:GLU:HG2	1:B:415:PHE:HE1	1.83	0.44
1:A:337:GLU:N	1:A:337:GLU:OE1	2.48	0.44
1:A:277:LEU:HD11	1:A:314:LEU:HD22	1.99	0.44
1:B:468:ILE:HG22	1:B:469:GLY:N	2.32	0.43
1:A:365:LEU:HD23	1:A:366:LYS:N	2.33	0.43
1:B:255:GLN:HG2	1:B:256:GLU:N	2.33	0.43
1:B:303:ALA:HB1	1:B:304:TRP:CE3	2.53	0.43
1:B:67:ILE:HG12	1:B:72:VAL:HG21	2.00	0.43
1:A:333:TRP:CH2	1:A:335:MSE:HE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASN:HD22	1:A:288:ASN:HA	1.65	0.43
1:A:459:HIS:HB3	1:A:462:VAL:HG23	2.01	0.43
1:A:273:VAL:HG23	1:A:275:PRO:HD2	1.99	0.43
1:A:506:ILE:HG13	1:A:507:SER:H	1.84	0.43
1:B:468:ILE:HG22	1:B:469:GLY:H	1.84	0.43
1:B:503:ARG:HG2	2:B:660:HOH:O	2.19	0.42
1:B:478:VAL:HG13	1:B:516:GLU:HB2	2.00	0.42
1:A:453:GLU:CG	1:A:467:VAL:HG12	2.49	0.42
1:A:197:MSE:HE2	1:A:395:TYR:C	2.40	0.42
1:A:274:PRO:HB2	1:A:275:PRO:HD3	2.01	0.42
1:A:470:LYS:NZ	1:A:517:PHE:HD1	2.13	0.42
1:B:339:CYS:N	1:B:340:PRO:CA	2.77	0.42
1:A:150:VAL:O	1:A:157:SER:HA	2.20	0.42
1:A:120:ASP:CG	1:A:398:ARG:HH22	2.23	0.42
1:A:230:HIS:HB2	2:A:604:HOH:O	2.20	0.42
1:B:318:ALA:HA	1:B:322:CYS:HB2	2.00	0.42
1:B:302:GLY:O	1:B:303:ALA:HB3	2.20	0.42
1:B:281:VAL:HG13	1:B:317:LEU:CD1	2.50	0.42
1:A:59:VAL:HG23	1:A:60:THR:N	2.35	0.41
1:A:420:ASP:HB3	1:A:432:PHE:HE1	1.84	0.41
1:B:43:PHE:HZ	1:B:252:MSE:HE3	1.85	0.41
1:B:66:GLY:O	1:B:70:LYS:HG2	2.21	0.41
1:B:486:LYS:HE2	1:B:488:GLU:OE1	2.20	0.41
1:A:458:LYS:HE2	2:A:624:HOH:O	2.21	0.41
1:B:22:ARG:HH22	1:B:208:LEU:CD1	2.33	0.41
1:B:281:VAL:HG13	1:B:317:LEU:HD12	2.02	0.41
1:A:484:VAL:HG13	1:A:522:PRO:HA	2.03	0.41
1:A:102:PRO:HD2	1:A:181:ALA:O	2.21	0.41
1:B:206:ASN:HA	1:B:209:GLN:OE1	2.21	0.41
1:A:115:GLU:HB2	1:A:139:VAL:CG2	2.51	0.40
1:B:51:MSE:HA	1:B:55:GLU:OE1	2.20	0.40
1:B:348:LEU:HB2	2:B:587:HOH:O	2.21	0.40
1:A:226:MSE:HE3	1:A:272:ALA:HB1	2.03	0.40
1:B:255:GLN:HG3	1:B:283:THR:OG1	2.22	0.40
1:A:433:GLN:O	1:A:434:ASP:HB2	2.22	0.40
1:A:37:ILE:HG21	1:A:265:TYR:CE2	2.56	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	487/549 (89%)	462 (95%)	21 (4%)	4 (1%)	24	15
1	B	486/549 (88%)	470 (97%)	15 (3%)	1 (0%)	52	51
All	All	973/1098 (89%)	932 (96%)	36 (4%)	5 (0%)	34	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	VAL
1	A	339	CYS
1	B	339	CYS
1	A	460	GLU
1	A	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	430/453 (95%)	423 (98%)	7 (2%)	70	76
1	B	430/453 (95%)	418 (97%)	12 (3%)	51	52
All	All	860/906 (95%)	841 (98%)	19 (2%)	60	63

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS

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Mol	Chain	Res	Type
1	A	130	SER
1	A	340	PRO
1	A	354	THR
1	A	392	PHE
1	A	460	GLU
1	A	517	PHE
1	B	2	GLU
1	B	131	MSE
1	B	252	MSE
1	B	340	PRO
1	B	348	LEU
1	B	392	PHE
1	B	410	GLU
1	B	456	LEU
1	B	458	LYS
1	B	496	GLU
1	B	503	ARG
1	B	517	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	200	HIS
1	A	202	ASN
1	A	206	ASN
1	A	230	HIS
1	A	282	ASN
1	A	288	ASN
1	A	324	ASN
1	A	329	HIS
1	B	116	HIS
1	B	119	ASN
1	B	200	HIS
1	B	202	ASN
1	B	206	ASN
1	B	324	ASN
1	B	329	HIS
1	B	331	GLN
1	B	402	ASN
1	B	431	HIS

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	479/549 (87%)	0.52	42 (8%)	12	18	14, 33, 64, 77	0
1	B	477/549 (86%)	0.07	20 (4%)	40	50	13, 25, 61, 72	0
All	All	956/1098 (87%)	0.29	62 (6%)	22	31	13, 29, 63, 77	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	GLY	13.2
1	A	468	ILE	7.2
1	A	190	THR	6.9
1	B	517	PHE	6.3
1	B	521	LEU	5.7
1	A	466	ALA	4.6
1	A	116	HIS	4.3
1	A	188	GLY	4.1
1	A	167	GLU	4.1
1	A	470	LYS	4.0
1	A	189	THR	3.9
1	A	517	PHE	3.9
1	A	522	PRO	3.9
1	B	304	TRP	3.7
1	A	462	VAL	3.7
1	A	513	ARG	3.5
1	A	455	LEU	3.5
1	B	490	ARG	3.3
1	B	482	PHE	3.3
1	A	370	LEU	3.3
1	A	141	GLU	3.2
1	B	478	VAL	3.2
1	A	459	HIS	3.2
1	A	139	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	470	LYS	3.1
1	B	471	PRO	3.1
1	B	487	PRO	3.0
1	A	518	VAL	3.0
1	B	522	PRO	3.0
1	A	165	GLY	3.0
1	A	112	PHE	2.9
1	B	484	VAL	2.9
1	A	187	GLY	2.8
1	A	467	VAL	2.8
1	A	400	LYS	2.7
1	A	168	ASP	2.7
1	B	288	ASN	2.7
1	B	496	GLU	2.7
1	B	498	ILE	2.6
1	A	155	VAL	2.5
1	A	136	PHE	2.5
1	A	450	PHE	2.5
1	A	436	VAL	2.5
1	B	499	ILE	2.5
1	B	503	ARG	2.5
1	A	454	ALA	2.5
1	B	461	ALA	2.4
1	A	479	PRO	2.4
1	A	111	SER	2.4
1	A	399	GLU	2.4
1	B	437	LYS	2.4
1	A	403	GLN	2.3
1	A	166	SER	2.3
1	A	487	PRO	2.3
1	A	471	PRO	2.2
1	B	485	LEU	2.2
1	A	163	ASP	2.2
1	A	458	LYS	2.2
1	A	460	GLU	2.2
1	A	495	GLU	2.2
1	A	372	ASP	2.0
1	B	493	VAL	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.