Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:38 PM GMT

PDB ID	:	1GLV
Title	:	THREE-DIMENSIONAL STRUCTURE OF THE GLUTATHIONE SYNTHETASE FROM ESCHERICHIA COLI B AT 2.0 ANGSTROMS RESOLUTION
Authors	:	Yamaguchi, H.; Kato, H.; Tanaka, T.; Katsube, Y.
Deposited on	:	1993-03-12
Resolution	:	2.70 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 (i)) were used in the production of this report:

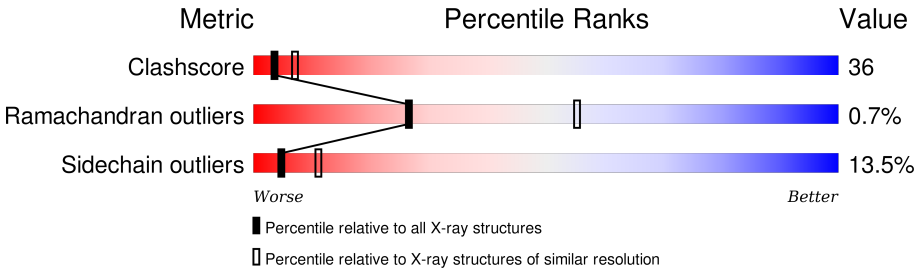
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	303	43% 41% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2407 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 GLUTATHIONE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	1	0
			2389	1523	402	450	14			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	DELETION	UNP P04425
A	?	-	PRO	DELETION	UNP P04425
A	?	-	GLN	DELETION	UNP P04425
A	?	-	GLY	DELETION	UNP P04425
A	?	-	GLY	DELETION	UNP P04425
A	?	-	GLU	DELETION	UNP P04425
A	?	-	THR	DELETION	UNP P04425
A	?	-	ARG	DELETION	UNP P04425
A	?	-	GLY	DELETION	UNP P04425
A	?	-	ASN	DELETION	UNP P04425
A	?	-	LEU	DELETION	UNP P04425
A	?	-	ALA	DELETION	UNP P04425
A	?	-	ALA	DELETION	UNP P04425
A	228	GLY	ARG	CONFLICT	UNP P04425

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		

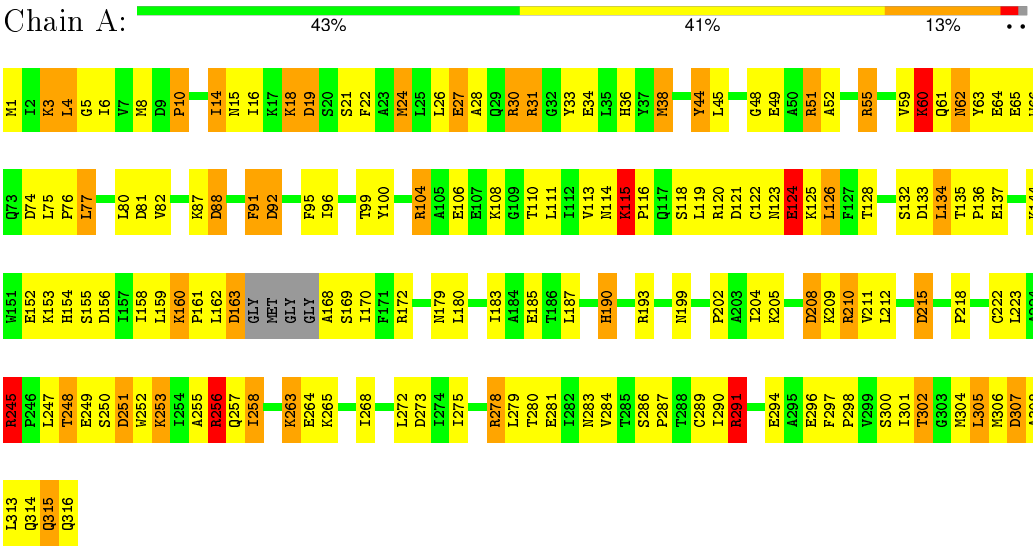
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: GLUTATHIONE SYNTHASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	87.70Å 87.70Å 169.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2407	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

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	1.12	0/2435	2.08	68/3294 (2.1%)

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	1

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	VAL	C-N-CA	23.27	179.86	121.70
1	A	51	ARG	NE-CZ-NH1	-18.59	111.00	120.30
1	A	278	ARG	NE-CZ-NH1	14.18	127.39	120.30
1	A	120	ARG	NE-CZ-NH1	13.60	127.10	120.30
1	A	51	ARG	NE-CZ-NH2	12.05	126.33	120.30
1	A	215	ASP	CB-CG-OD1	11.92	129.03	118.30
1	A	278	ARG	NE-CZ-NH2	-11.87	114.36	120.30
1	A	124	GLU	CA-CB-CG	11.30	138.26	113.40
1	A	121	ASP	CB-CG-OD1	10.99	128.19	118.30
1	A	210	ARG	NE-CZ-NH2	10.75	125.67	120.30
1	A	291	ARG	NE-CZ-NH1	10.65	125.62	120.30
1	A	100	TYR	CB-CG-CD1	10.46	127.28	121.00
1	A	51	ARG	CD-NE-CZ	-10.09	109.48	123.60
1	A	104	ARG	NE-CZ-NH1	-9.97	115.31	120.30
1	A	121	ASP	CB-CG-OD2	-9.88	109.41	118.30
1	A	30	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	A	104	ARG	NE-CZ-NH2	9.31	124.95	120.30
1	A	251	ASP	CB-CG-OD1	8.98	126.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	225	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	A	251	ASP	CB-CG-OD2	-8.62	110.54	118.30
1	A	281	GLU	CA-CB-CG	8.43	131.96	113.40
1	A	100	TYR	CB-CG-CD2	-8.32	116.01	121.00
1	A	31	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	307	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	A	24	MET	CA-CB-CG	-7.36	100.80	113.30
1	A	27	GLU	CG-CD-OE1	7.25	132.80	118.30
1	A	60	LYS	O-C-N	7.25	134.30	122.70
1	A	19	ASP	CB-CG-OD2	6.81	124.43	118.30
1	A	113	VAL	CB-CA-C	6.76	124.25	111.40
1	A	190	HIS	CA-CB-CG	-6.67	102.27	113.60
1	A	44	TYR	CB-CG-CD1	-6.58	117.05	121.00
1	A	281	GLU	CG-CD-OE2	6.53	131.36	118.30
1	A	125	LYS	CB-CA-C	-6.40	97.60	110.40
1	A	88	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	27	GLU	OE1-CD-OE2	-6.18	115.88	123.30
1	A	60	LYS	CA-CB-CG	6.09	126.79	113.40
1	A	152	GLU	OE1-CD-OE2	6.03	130.54	123.30
1	A	81	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	249	GLU	CA-CB-CG	5.92	126.43	113.40
1	A	122	CYS	CA-CB-SG	-5.79	103.59	114.00
1	A	30	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	302	THR	CA-CB-CG2	5.75	120.45	112.40
1	A	256	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	A	55	ARG	CA-CB-CG	5.71	125.97	113.40
1	A	243	GLU	OE1-CD-OE2	-5.71	116.44	123.30
1	A	72	GLU	CA-CB-CG	5.70	125.94	113.40
1	A	300	SER	N-CA-CB	5.62	118.93	110.50
1	A	3	LYS	O-C-N	5.59	131.64	122.70
1	A	264	GLU	CG-CD-OE1	-5.56	107.18	118.30
1	A	92	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	291	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	208	ASP	CB-CA-C	5.49	121.38	110.40
1	A	115	LYS	CB-CA-C	5.39	121.18	110.40
1	A	243	GLU	CG-CD-OE1	5.31	128.93	118.30
1	A	3	LYS	N-CA-CB	5.27	120.09	110.60
1	A	49	GLU	CG-CD-OE2	-5.27	107.76	118.30
1	A	80	LEU	CB-CA-C	5.24	120.15	110.20
1	A	114	ASN	CB-CA-C	5.20	120.80	110.40
1	A	115	LYS	CA-CB-CG	5.15	124.73	113.40
1	A	91	PHE	C-N-CA	5.07	134.38	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	281	GLU	N-CA-CB	5.06	119.71	110.60
1	A	81	ASP	O-C-N	5.03	130.75	122.70
1	A	273	ASP	O-C-N	5.03	130.75	122.70
1	A	134	LEU	CA-CB-CG	5.01	126.83	115.30
1	A	100	TYR	CA-CB-CG	5.01	122.92	113.40
1	A	245	ARG	CD-NE-CZ	5.01	130.61	123.60
1	A	281	GLU	CG-CD-OE1	-5.00	108.29	118.30
1	A	69	PHE	CB-CA-C	5.00	120.41	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	30	ARG	Sidechain

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	2389	0	2406	172	0
2	A	18	0	0	1	0
All	All	2407	0	2406	172	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 36.

All (172) 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:38:MET:CE	1:A:77:LEU:HD11	1.80	1.11
1:A:252:TRP:O	1:A:256:ARG:HB2	1.53	1.09
1:A:48:GLY:O	1:A:104:ARG:NH1	1.87	1.08
1:A:208:ASP:O	1:A:225:ARG:HG2	1.51	1.08
1:A:168:ALA:HB1	1:A:170:ILE:HD12	1.28	1.07
1:A:316:GLN:HG2	1:A:316:GLN:O	1.50	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HD11	1:A:63:TYR:CE1	2.01	0.96
1:A:16:ILE:HD11	1:A:63:TYR:CD1	1.99	0.96
1:A:38:MET:HE3	1:A:77:LEU:HD11	1.48	0.92
1:A:137:GLU:HB2	1:A:199:ASN:OD1	1.67	0.92
1:A:61:GLN:HE22	1:A:291:ARG:HH22	1.11	0.91
1:A:168:ALA:HB1	1:A:170:ILE:CD1	2.00	0.91
1:A:38:MET:HE1	1:A:77:LEU:HD11	1.53	0.91
1:A:91:PHE:CE1	1:A:95:PHE:CD1	2.60	0.90
1:A:4:LEU:C	1:A:4:LEU:HD12	1.93	0.89
1:A:159:LEU:HD23	1:A:183:ILE:HG21	1.55	0.87
1:A:51:ARG:NH1	1:A:74:ASP:OD1	2.08	0.87
1:A:159:LEU:HD23	1:A:183:ILE:CG2	2.06	0.85
1:A:95:PHE:O	1:A:99:THR:HG23	1.77	0.85
1:A:75:LEU:HB2	1:A:76:PRO:HD2	1.59	0.84
1:A:91:PHE:HE1	1:A:95:PHE:CD1	1.97	0.82
1:A:225:ARG:HH11	1:A:225:ARG:HB3	1.45	0.82
1:A:44:TYR:OH	1:A:51:ARG:NH1	2.13	0.81
1:A:210:ARG:CG	1:A:225:ARG:HD3	2.11	0.80
1:A:91:PHE:CE2	1:A:96:ILE:HD11	2.17	0.79
1:A:244:PRO:HB2	1:A:297:PHE:HE2	1.48	0.79
1:A:156:ASP:OD2	1:A:172:ARG:NH2	2.17	0.77
1:A:315:GLN:HG3	1:A:316:GLN:H	1.48	0.76
1:A:215:ASP:O	1:A:263:LYS:HG3	1.88	0.73
1:A:297:PHE:HB3	1:A:298:PRO:HD2	1.70	0.73
1:A:248:THR:CG2	1:A:250:SER:H	2.01	0.73
1:A:204:ILE:HD12	1:A:275:ILE:CD1	2.19	0.72
1:A:268:ILE:HD11	1:A:312:ARG:HD2	1.72	0.71
1:A:202:PRO:O	1:A:205:LYS:HG2	1.90	0.71
1:A:61:GLN:HE22	1:A:291:ARG:NH2	1.87	0.71
1:A:225:ARG:NH1	1:A:225:ARG:HB3	2.06	0.70
1:A:91:PHE:CE1	1:A:95:PHE:HD1	2.09	0.70
1:A:210:ARG:HG2	1:A:225:ARG:HD3	1.73	0.70
1:A:4:LEU:HD13	1:A:5:GLY:O	1.91	0.69
1:A:4:LEU:C	1:A:4:LEU:CD1	2.61	0.69
1:A:204:ILE:HD12	1:A:275:ILE:HD11	1.75	0.68
1:A:202:PRO:O	1:A:205:LYS:CG	2.41	0.68
1:A:210:ARG:NE	1:A:225:ARG:HE	1.92	0.68
1:A:248:THR:HG23	1:A:250:SER:H	1.60	0.67
1:A:315:GLN:O	1:A:316:GLN:HB3	1.95	0.67
1:A:118:SER:OG	1:A:265:LYS:O	2.06	0.67
1:A:134:LEU:HD21	1:A:257:GLN:OE1	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:GLN:CG	1:A:316:GLN:H	2.09	0.66
1:A:62:ASN:HD22	1:A:62:ASN:C	1.99	0.66
1:A:144:LYS:HZ1	1:A:185:GLU:CD	1.99	0.65
1:A:45:LEU:HD11	1:A:104:ARG:HG3	1.78	0.65
1:A:135:THR:HB	1:A:136:PRO:HD2	1.79	0.65
1:A:210:ARG:HE	1:A:225:ARG:HE	1.44	0.65
1:A:4:LEU:HA	1:A:82:VAL:O	1.98	0.64
1:A:27:GLU:OE2	1:A:31:ARG:NE	2.24	0.64
1:A:275:ILE:HG13	1:A:280:THR:HG21	1.80	0.63
1:A:38:MET:CE	1:A:52:ALA:CB	2.76	0.63
1:A:306:MET:O	1:A:310:GLU:HG3	2.00	0.62
1:A:210:ARG:HG3	1:A:225:ARG:HD3	1.80	0.62
1:A:38:MET:HE2	1:A:52:ALA:CB	2.30	0.61
1:A:148:LYS:HG2	1:A:180:LEU:CD2	2.31	0.61
1:A:38:MET:HE3	1:A:52:ALA:HB3	1.82	0.61
1:A:283:ASN:OD1	1:A:287:PRO:HD3	2.00	0.60
1:A:153:LYS:HG2	1:A:154:HIS:CD2	2.37	0.60
1:A:21:SER:O	1:A:24:MET:HB2	2.02	0.59
1:A:4:LEU:HD12	1:A:4:LEU:O	2.01	0.59
1:A:91:PHE:CD2	1:A:96:ILE:HD11	2.37	0.59
1:A:218:PRO:HG2	1:A:252:TRP:CZ3	2.38	0.59
1:A:248:THR:HG22	1:A:251:ASP:H	1.67	0.59
1:A:75:LEU:O	1:A:75:LEU:HD12	2.03	0.58
1:A:315:GLN:HG3	1:A:316:GLN:N	2.18	0.58
1:A:87:LYS:NZ	1:A:88:ASP:O	2.36	0.58
1:A:275:ILE:O	1:A:275:ILE:HG22	2.03	0.58
1:A:75:LEU:HB2	1:A:76:PRO:CD	2.33	0.58
1:A:75:LEU:C	1:A:75:LEU:HD12	2.25	0.57
1:A:91:PHE:CE2	1:A:96:ILE:CD1	2.86	0.57
1:A:6:ILE:HG12	1:A:8:MET:CE	2.34	0.57
1:A:91:PHE:CD1	1:A:95:PHE:CD1	2.92	0.57
1:A:247:LEU:HB3	1:A:251:ASP:HB2	1.86	0.56
1:A:248:THR:HB	1:A:251:ASP:OD2	2.05	0.56
1:A:159:LEU:HD23	1:A:183:ILE:HG22	1.86	0.56
1:A:62:ASN:ND2	1:A:64:GLU:H	2.03	0.56
1:A:310:GLU:O	1:A:314:GLN:NE2	2.37	0.56
1:A:6:ILE:HG12	1:A:8:MET:HE3	1.86	0.56
1:A:294:GLU:OE2	1:A:301:ILE:N	2.36	0.55
1:A:248:THR:HG22	1:A:250:SER:H	1.72	0.55
1:A:14:ILE:HD12	1:A:14:ILE:C	2.26	0.55
1:A:16:ILE:CD1	1:A:63:TYR:CE1	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:HIS:O	1:A:156:ASP:N	2.34	0.54
1:A:283:ASN:C	1:A:283:ASN:OD1	2.45	0.54
1:A:38:MET:HE3	1:A:77:LEU:CD1	2.30	0.53
1:A:248:THR:HG22	1:A:250:SER:N	2.23	0.53
1:A:305:LEU:O	1:A:308:ALA:HB3	2.08	0.53
1:A:91:PHE:HE1	1:A:95:PHE:HD1	1.48	0.53
1:A:4:LEU:CD1	1:A:5:GLY:O	2.57	0.53
1:A:27:GLU:O	1:A:31:ARG:HG3	2.08	0.53
1:A:15:ASN:ND2	1:A:18:LYS:HG2	2.24	0.53
1:A:48:GLY:C	1:A:104:ARG:HH12	2.13	0.52
1:A:243:GLU:CD	1:A:245:ARG:HH11	2.13	0.52
1:A:62:ASN:HD22	1:A:64:GLU:H	1.57	0.52
1:A:258:ILE:HD11	1:A:279:LEU:HD22	1.91	0.52
1:A:144:LYS:NZ	1:A:185:GLU:CD	2.62	0.51
1:A:28:ALA:HB1	1:A:33:TYR:CD2	2.45	0.51
1:A:44:TYR:OH	1:A:74:ASP:OD2	2.26	0.50
1:A:62:ASN:ND2	1:A:65:GLU:H	2.09	0.50
1:A:302:THR:O	1:A:306:MET:HG2	2.12	0.50
1:A:268:ILE:CD1	1:A:312:ARG:HD2	2.40	0.50
1:A:38:MET:HE3	1:A:52:ALA:CB	2.40	0.50
1:A:208:ASP:O	1:A:225:ARG:CG	2.42	0.49
1:A:111:LEU:HD22	1:A:313:LEU:CD1	2.43	0.49
1:A:51:ARG:NH2	1:A:75:LEU:HA	2.27	0.49
1:A:179:ASN:O	1:A:180:LEU:C	2.51	0.49
1:A:248:THR:HG22	1:A:251:ASP:N	2.27	0.49
1:A:204:ILE:HB	1:A:275:ILE:HD12	1.94	0.49
1:A:92:ASP:O	1:A:96:ILE:HD12	2.13	0.48
1:A:128:THR:HB	1:A:135:THR:HG21	1.95	0.48
1:A:26:LEU:HD11	1:A:61:GLN:NE2	2.28	0.48
1:A:115:LYS:HA	1:A:116:PRO:HD3	1.71	0.48
1:A:19:ASP:OD2	1:A:21:SER:HB2	2.14	0.48
1:A:304:MET:O	1:A:307:ASP:HB2	2.13	0.48
1:A:161:PRO:HG3	1:A:187:LEU:CD2	2.44	0.48
1:A:123:ASN:HB3	1:A:126:LEU:HB2	1.94	0.48
1:A:75:LEU:CB	1:A:76:PRO:HD2	2.39	0.47
1:A:95:PHE:HE1	1:A:119:LEU:HD13	1.79	0.47
1:A:244:PRO:HB2	1:A:297:PHE:CE2	2.38	0.47
1:A:137:GLU:OE1	1:A:137:GLU:HA	2.14	0.47
1:A:209:LYS:NZ	1:A:251:ASP:OD1	2.31	0.47
1:A:222:CYS:O	1:A:244:PRO:HA	2.14	0.47
1:A:210:ARG:HG3	1:A:225:ARG:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLY:C	1:A:104:ARG:NH1	2.68	0.47
1:A:315:GLN:CG	1:A:316:GLN:N	2.76	0.47
1:A:134:LEU:CD1	1:A:258:ILE:HD11	2.45	0.46
1:A:211:VAL:O	1:A:272:LEU:N	2.45	0.46
1:A:258:ILE:CD1	1:A:279:LEU:HD22	2.45	0.46
1:A:18:LYS:HB3	1:A:18:LYS:HE3	1.66	0.46
1:A:51:ARG:HH12	1:A:74:ASP:CG	2.12	0.46
1:A:4:LEU:HB2	1:A:82:VAL:HG13	1.97	0.46
1:A:62:ASN:C	1:A:62:ASN:ND2	2.69	0.46
1:A:124:GLU:OE1	1:A:284:VAL:HG22	2.17	0.45
1:A:59:VAL:HA	1:A:66:TRP:O	2.15	0.45
1:A:60:LYS:HE2	1:A:65:GLU:O	2.16	0.45
1:A:244:PRO:HG2	1:A:296:GLU:HG3	1.98	0.45
1:A:158:ILE:HG23	1:A:170:ILE:HG23	1.98	0.45
1:A:91:PHE:HE1	1:A:95:PHE:CE1	2.33	0.45
1:A:252:TRP:O	1:A:256:ARG:CB	2.44	0.44
1:A:22:PHE:CZ	1:A:66:TRP:HB2	2.53	0.44
1:A:218:PRO:HB3	1:A:255:ALA:HB1	1.99	0.44
1:A:74:ASP:OD1	1:A:74:ASP:C	2.56	0.44
1:A:34:GLU:OE2	1:A:36:HIS:NE2	2.36	0.44
1:A:150:PHE:O	1:A:154:HIS:HD2	2.01	0.43
1:A:144:LYS:O	1:A:148:LYS:HB2	2.18	0.43
1:A:290:ILE:O	1:A:294:GLU:HG3	2.18	0.43
1:A:223:LEU:HD22	1:A:289:CYS:SG	2.59	0.43
1:A:51:ARG:CZ	1:A:74:ASP:OD1	2.67	0.43
1:A:312:ARG:HH11	1:A:312:ARG:HD3	1.57	0.43
1:A:62:ASN:HD22	1:A:64:GLU:N	2.16	0.43
1:A:253:LYS:HE3	1:A:253:LYS:HB2	1.49	0.43
1:A:204:ILE:HB	1:A:275:ILE:CD1	2.49	0.43
1:A:52:ALA:O	1:A:74:ASP:HA	2.20	0.42
1:A:160:LYS:HA	1:A:161:PRO:HD3	1.78	0.42
1:A:297:PHE:HB3	1:A:298:PRO:CD	2.45	0.42
1:A:185:GLU:HG3	1:A:190:HIS:ND1	2.35	0.42
1:A:63:TYR:O	1:A:66:TRP:HZ3	2.03	0.41
1:A:134:LEU:HD12	1:A:258:ILE:HD11	2.01	0.41
1:A:154:HIS:O	1:A:155:SER:OG	2.38	0.41
1:A:316:GLN:CG	1:A:316:GLN:O	2.36	0.41
1:A:163:ASP:OD1	1:A:163:ASP:N	2.52	0.41
1:A:124:GLU:HB2	2:A:416:HOH:O	2.21	0.41
1:A:14:ILE:C	1:A:14:ILE:CD1	2.89	0.40
1:A:48:GLY:CA	1:A:104:ARG:HH12	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:THR:HB	1:A:136:PRO:CD	2.49	0.40
1:A:106:GLU:HA	1:A:110:THR:O	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	295/303 (97%)	267 (90%)	26 (9%)	2 (1%)	26 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	PRO
1	A	315	GLN

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	260/260 (100%)	224 (86%)	36 (14%)	4 10

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	MET
1	A	1[B]	MET
1	A	3	LYS
1	A	4	LEU
1	A	10	PRO
1	A	14	ILE
1	A	18	LYS
1	A	38	MET
1	A	55	ARG
1	A	60	LYS
1	A	62	ASN
1	A	77	LEU
1	A	108	LYS
1	A	115	LYS
1	A	124	GLU
1	A	126	LEU
1	A	132	SER
1	A	133	ASP
1	A	148	LYS
1	A	160	LYS
1	A	162	LEU
1	A	163	ASP
1	A	169	SER
1	A	193	ARG
1	A	212	LEU
1	A	225	ARG
1	A	245	ARG
1	A	248	THR
1	A	253	LYS
1	A	256	ARG
1	A	258	ILE
1	A	263	LYS
1	A	278	ARG
1	A	286	SER
1	A	291	ARG
1	A	305	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	62	ASN
1	A	154	HIS

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Mol	Chain	Res	Type
1	A	314	GLN

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.