Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:36 PM GMT

PDB ID	:	1GG4
Title	:	CRYSTAL STRUCTURE OF ESCHERICHIA COLI UDPMURNAC-TRIPEPTIDE D-ALANYL-D-ALANINE-ADDING ENZYME (MURF) AT 2.3 ANGSTROM RESOLUTION
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Deposited on	:	2000-07-12
Resolution	:	2.30 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:

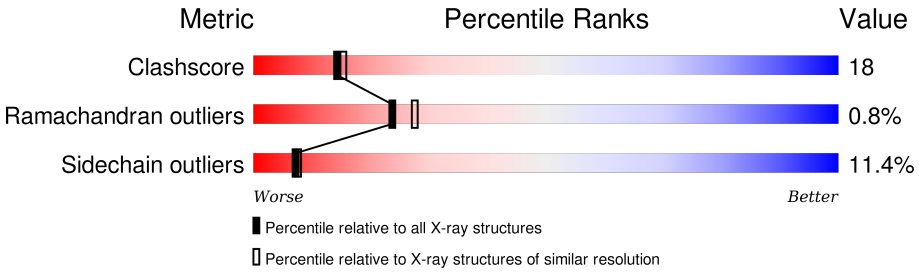
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	452	63% 29% 6% ·
1	B	452	61% 31% 6% ·

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6791 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 UDP-N-ACETYLMURAMOYLALANYL-D-GLUTAMYL-2, 6-DIAMINOPIMELATE-D-ALANYL-D-ALANYL LIGASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	Se	0	0	0
			3242	2036	567	627	3	9			
1	B	439	Total	C	N	O	S	Se	0	0	0
			3242	2036	567	627	3	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P11880
A	117	MSE	MET	MODIFIED RESIDUE	UNP P11880
A	143	MSE	MET	MODIFIED RESIDUE	UNP P11880
A	217	MSE	MET	MODIFIED RESIDUE	UNP P11880
A	294	MSE	MET	MODIFIED RESIDUE	UNP P11880
A	340	MSE	MET	MODIFIED RESIDUE	UNP P11880
A	350	MSE	MET	MODIFIED RESIDUE	UNP P11880
A	361	MSE	MET	MODIFIED RESIDUE	UNP P11880
A	439	MSE	MET	MODIFIED RESIDUE	UNP P11880
B	501	MSE	MET	MODIFIED RESIDUE	UNP P11880
B	617	MSE	MET	MODIFIED RESIDUE	UNP P11880
B	643	MSE	MET	MODIFIED RESIDUE	UNP P11880
B	717	MSE	MET	MODIFIED RESIDUE	UNP P11880
B	794	MSE	MET	MODIFIED RESIDUE	UNP P11880
B	840	MSE	MET	MODIFIED RESIDUE	UNP P11880
B	850	MSE	MET	MODIFIED RESIDUE	UNP P11880
B	861	MSE	MET	MODIFIED RESIDUE	UNP P11880
B	939	MSE	MET	MODIFIED RESIDUE	UNP P11880

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	175	Total	O	0	0
			175	175		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	132	Total	O	0	0
			132	132		

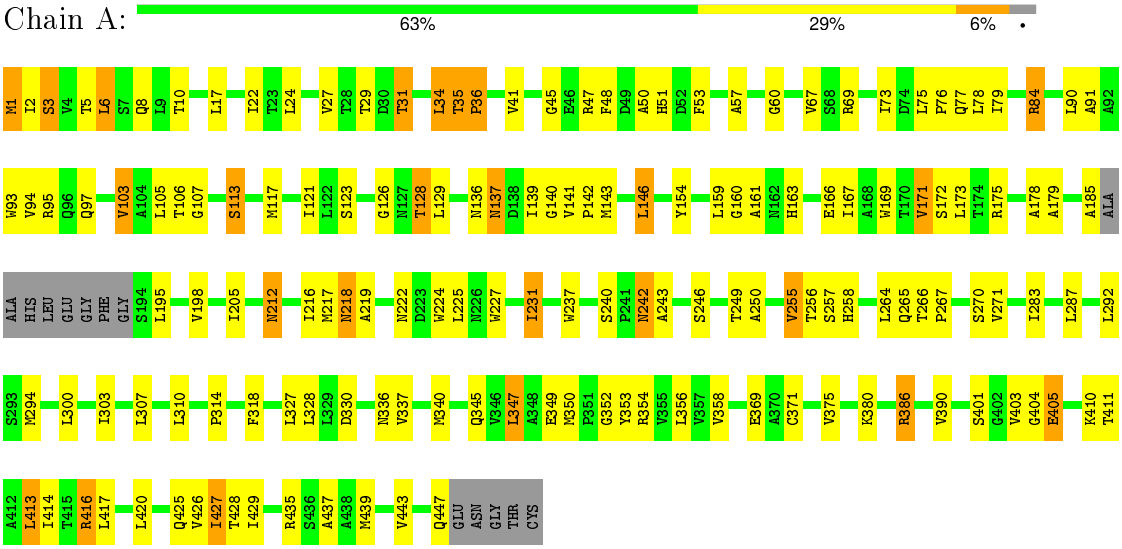
3 Residue-property plots (i)

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.

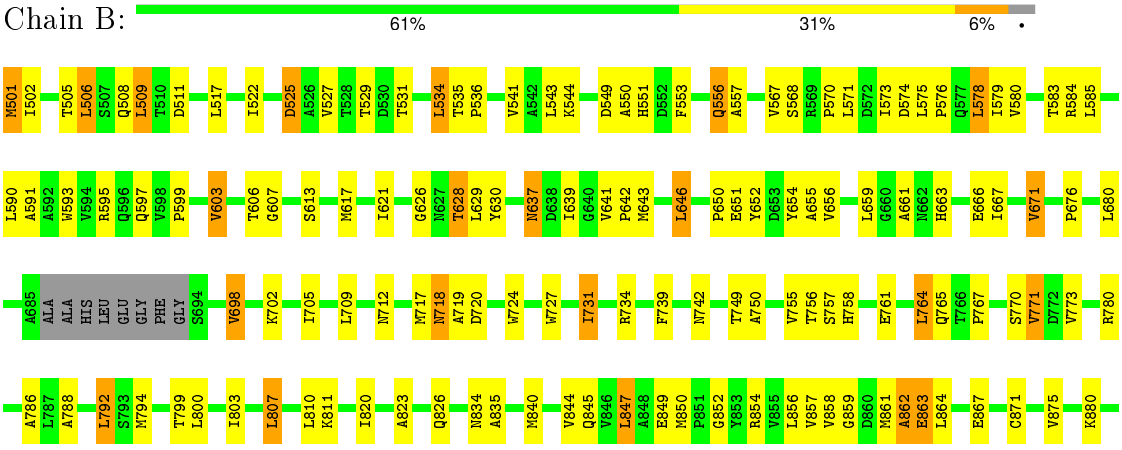
• Molecule 1: UDP-N-ACETYLMURAMOYLALANYL-D-GLUTAMYL-2,6-DIAMINOPIMELATE-D-ALANYL-D-ALANYL LIGASE

Chain A:



• Molecule 1: UDP-N-ACETYLMURAMOYLALANYL-D-GLUTAMYL-2,6-DIAMINOPIMELATE-D-ALANYL-D-ALANYL LIGASE

Chain B:




R886
V887
L888
S889
V890
S901
G902
V903
G904
E905
H906
F907
T911
A912
L913
R916
L917
L920
V926
I927
T928
I929
K932
G933
S934
R935
S936
A937
A938
M939
E940
V943
R944
Q947
GLU
ASN
GLY
THR
CYS

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 61	Depositor
Cell constants a, b, c, α, β, γ	74.20Å 74.20Å 429.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	0.8 (8.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.203 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6791	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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	0.47	0/3280	0.73	1/4451 (0.0%)
1	B	0.48	0/3280	0.73	0/4451
All	All	0.48	0/6560	0.73	1/8902 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	45	GLY	N-CA-C	-5.02	100.54	113.10

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	3242	0	3294	109	0
1	B	3242	0	3291	128	0
2	A	175	0	0	3	0
2	B	132	0	0	5	0
All	All	6791	0	6585	237	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 18.

All (237) 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:B:852:GLY:HA3	1:B:926:VAL:HG12	1.53	0.90
1:B:767:PRO:HD2	1:B:794:MSE:HE1	1.58	0.86
1:A:50:ALA:HA	1:A:53:PHE:HD1	1.41	0.85
1:A:51:HIS:CE1	1:A:67:VAL:HG23	2.12	0.83
1:B:867:GLU:HG3	1:B:871:CYS:SG	2.20	0.82
1:A:106:THR:HG22	1:A:107:GLY:H	1.47	0.79
1:A:256:THR:HG22	1:A:258:HIS:H	1.47	0.77
1:B:859:GLY:HA3	1:B:939:MSE:HE3	1.67	0.77
1:A:161:ALA:HB2	1:A:167:ILE:HG13	1.68	0.76
1:A:113:SER:HB2	1:A:117:MSE:HE3	1.64	0.76
1:A:347:LEU:HD22	1:A:354:ARG:HB3	1.67	0.76
1:A:106:THR:HG23	1:A:159:LEU:O	1.87	0.75
1:A:6:LEU:HD22	1:A:22:ILE:HB	1.69	0.75
1:B:606:THR:HG23	1:B:659:LEU:O	1.87	0.74
1:A:50:ALA:HA	1:A:53:PHE:CD1	2.23	0.74
1:A:390:VAL:HG23	1:A:413:LEU:HD12	1.71	0.73
1:A:167:ILE:O	1:A:171:VAL:HG22	1.92	0.70
1:A:340:MSE:HG3	1:A:375:VAL:HG11	1.73	0.69
1:B:840:MSE:HG3	1:B:875:VAL:HG11	1.73	0.69
1:A:267:PRO:HD2	1:A:294:MSE:HE1	1.73	0.69
1:B:862:ALA:HB2	1:B:934:SER:HB2	1.76	0.68
1:B:826:GLN:HE21	1:B:927:ILE:HD11	1.59	0.67
1:A:390:VAL:CG2	1:A:413:LEU:HD12	2.25	0.67
1:B:826:GLN:NE2	1:B:927:ILE:HD11	2.09	0.67
1:B:850:MSE:HB3	1:B:928:THR:HG21	1.76	0.66
1:B:698:VAL:O	1:B:702:LYS:HG2	1.96	0.66
1:B:850:MSE:O	1:B:854:ARG:HD3	1.96	0.66
1:B:903:VAL:HG22	1:B:904:GLY:H	1.60	0.66
1:B:643:MSE:HE2	2:B:1186:HOH:O	1.96	0.65
1:B:591:ALA:HA	1:B:646:LEU:HD13	1.79	0.65
1:A:128:THR:HB	1:A:154:TYR:HB2	1.79	0.65
1:B:727:TRP:O	1:B:731:ILE:HG23	1.97	0.65
1:A:106:THR:HG21	1:A:167:ILE:HD11	1.79	0.64
1:B:606:THR:HG22	1:B:607:GLY:H	1.63	0.64
1:B:861:MSE:HE3	1:B:863:GLU:HG2	1.79	0.64
1:B:890:VAL:HG21	1:B:913:LEU:HD12	1.80	0.63
1:B:551:HIS:ND1	1:B:567:VAL:HG23	2.14	0.63
1:A:5:THR:OG1	1:A:8:GLN:HG3	1.99	0.63
1:A:227:TRP:O	1:A:231:ILE:HG23	1.99	0.62
1:A:352:GLY:HA3	1:A:426:VAL:HG12	1.81	0.62
1:A:137:ASN:ND2	1:A:140:GLY:H	1.96	0.62
1:B:556:GLN:HA	1:B:556:GLN:HE21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LYS:O	1:A:414:ILE:HG13	1.99	0.62
1:A:417:LEU:HD21	1:A:429:ILE:HD13	1.80	0.62
1:A:2:ILE:HD11	1:A:93:TRP:CZ3	2.35	0.62
1:B:637:ASN:H	1:B:637:ASN:HD22	1.48	0.61
1:A:350:MSE:HG3	1:A:428:THR:HG21	1.83	0.60
1:B:862:ALA:H	1:B:934:SER:HB3	1.67	0.60
1:A:425:GLN:HG3	1:A:426:VAL:HG23	1.83	0.60
1:A:67:VAL:HG22	1:A:69:ARG:H	1.66	0.60
1:A:225:LEU:HB2	2:A:1009:HOH:O	2.02	0.60
1:B:501:MSE:HE1	1:B:590:LEU:HD11	1.83	0.59
1:A:47:ARG:O	1:A:48:PHE:CD1	2.55	0.59
1:B:756:THR:HG22	1:B:758:HIS:H	1.67	0.59
1:A:113:SER:HB2	1:A:117:MSE:CE	2.32	0.59
1:A:255:VAL:HG11	1:A:349:GLU:HB3	1.85	0.59
1:A:10:THR:HG21	1:A:17:LEU:HB2	1.85	0.58
1:A:141:VAL:HB	1:A:142:PRO:HD3	1.86	0.58
1:A:126:GLY:O	1:A:128:THR:HG22	2.03	0.58
1:B:940:GLU:O	1:B:944:ARG:HG2	2.04	0.58
1:B:641:VAL:HB	1:B:642:PRO:HD3	1.86	0.58
1:B:862:ALA:N	1:B:934:SER:HB3	2.18	0.57
1:A:22:ILE:HD11	1:A:76:PRO:HG2	1.86	0.57
1:B:543:LEU:HD13	1:B:639:ILE:HD12	1.86	0.57
1:B:534:LEU:HD21	1:B:557:ALA:HA	1.86	0.57
1:B:613:SER:HB2	1:B:617:MSE:HE3	1.86	0.57
1:A:137:ASN:HD22	1:A:137:ASN:H	1.52	0.57
1:B:639:ILE:O	1:B:643:MSE:HG3	2.03	0.57
1:A:91:ALA:HA	1:A:146:LEU:HD13	1.85	0.57
1:B:767:PRO:HD2	1:B:794:MSE:CE	2.34	0.56
1:B:886:ARG:HD3	1:B:920:LEU:HD11	1.87	0.56
1:B:501:MSE:SE	1:B:502:ILE:H	2.38	0.56
1:B:506:LEU:HD22	1:B:522:ILE:HB	1.86	0.56
1:A:106:THR:HG21	1:A:167:ILE:CD1	2.36	0.56
1:A:265:GLN:HG2	1:A:270:SER:OG	2.06	0.56
1:B:857:VAL:HG21	1:B:917:LEU:HD11	1.88	0.56
1:B:509:LEU:HB3	1:B:578:LEU:HD11	1.88	0.56
1:A:35:THR:HG22	1:A:36:PRO:HD2	1.86	0.56
1:B:591:ALA:HA	1:B:646:LEU:CD1	2.36	0.55
1:B:840:MSE:SE	1:B:932:LYS:HD3	2.55	0.55
1:B:799:THR:HB	2:B:1205:HOH:O	2.06	0.55
1:B:551:HIS:CE1	1:B:567:VAL:HG23	2.42	0.55
1:A:350:MSE:CG	1:A:428:THR:HG21	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:HIS:O	1:B:666:GLU:HG3	2.07	0.55
1:A:212:ASN:H	1:A:212:ASN:HD22	1.55	0.54
1:A:403:VAL:HG22	1:A:404:GLY:N	2.22	0.54
1:B:847:LEU:O	1:B:854:ARG:HD2	2.08	0.54
1:A:31:THR:O	1:A:34:LEU:HD22	2.07	0.54
1:B:606:THR:HG21	1:B:667:ILE:HD11	1.90	0.54
1:B:629:LEU:O	1:B:655:ALA:HA	2.07	0.54
1:B:579:ILE:HD12	1:B:579:ILE:N	2.22	0.54
1:B:917:LEU:HD21	1:B:929:ILE:HD13	1.90	0.54
1:B:820:ILE:HD13	1:B:947:GLN:NE2	2.22	0.54
1:B:529:THR:HG22	1:B:541:VAL:HB	1.90	0.53
1:A:347:LEU:O	1:A:354:ARG:HD2	2.09	0.53
1:A:22:ILE:CD1	1:A:76:PRO:HG2	2.38	0.53
1:B:863:GLU:O	1:B:864:LEU:HD12	2.08	0.53
1:B:850:MSE:CB	1:B:928:THR:HG21	2.38	0.53
1:A:136:ASN:HB2	1:A:160:GLY:N	2.24	0.53
1:A:179:ALA:HB1	1:A:205:ILE:HG12	1.90	0.52
1:B:890:VAL:CG2	1:B:913:LEU:HD12	2.38	0.52
1:A:218:ASN:HD22	1:A:219:ALA:N	2.07	0.52
1:A:212:ASN:H	1:A:212:ASN:ND2	2.08	0.52
1:B:856:LEU:HG	1:B:858:VAL:HG13	1.91	0.52
1:B:771:VAL:HG22	1:B:800:LEU:HD22	1.92	0.52
1:B:756:THR:HG22	1:B:757:SER:N	2.24	0.51
1:A:403:VAL:HG22	1:A:404:GLY:H	1.75	0.51
1:A:350:MSE:CB	1:A:428:THR:HG21	2.41	0.51
1:B:927:ILE:H	1:B:927:ILE:HD12	1.74	0.51
1:A:90:LEU:O	1:A:94:VAL:HG23	2.11	0.51
1:A:103:VAL:HG22	1:A:178:ALA:HB3	1.93	0.51
1:B:888:LEU:HD11	1:B:920:LEU:HD12	1.94	0.50
1:B:755:VAL:HG12	2:B:1140:HOH:O	2.11	0.50
1:B:629:LEU:HD12	1:B:652:TYR:CE2	2.47	0.50
1:A:380:LYS:HB2	1:A:401:SER:HA	1.93	0.50
1:B:861:MSE:C	1:B:863:GLU:H	2.15	0.50
1:B:717:MSE:HE1	1:B:724:TRP:CE3	2.47	0.49
1:B:835:ALA:HB2	1:B:932:LYS:HG2	1.94	0.49
1:B:501:MSE:HE2	1:B:527:VAL:HG11	1.94	0.49
1:B:709:LEU:O	1:B:734:ARG:NH1	2.46	0.49
1:A:1:MSE:HE2	1:A:27:VAL:CG1	2.43	0.49
1:A:328:LEU:HD21	1:A:443:VAL:HG13	1.95	0.49
1:A:137:ASN:HD22	1:A:137:ASN:N	2.11	0.49
1:A:47:ARG:HG2	2:A:1079:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:TRP:CZ2	1:A:173:LEU:HD21	2.48	0.49
1:A:350:MSE:HB3	1:A:428:THR:HG21	1.93	0.49
1:B:573:ILE:O	1:B:575:LEU:N	2.46	0.49
1:B:551:HIS:HD1	1:B:567:VAL:HG23	1.77	0.48
1:B:847:LEU:O	1:B:850:MSE:HB2	2.13	0.48
1:A:3:SER:HA	1:A:24:LEU:O	2.12	0.48
1:B:847:LEU:HD22	1:B:854:ARG:HB3	1.96	0.48
1:B:661:ALA:HB2	1:B:667:ILE:CD1	2.43	0.48
1:A:139:ILE:O	1:A:143:MSE:HG3	2.13	0.48
1:B:626:GLY:O	1:B:628:THR:HG22	2.13	0.48
1:A:386:ARG:HH11	1:A:386:ARG:HB2	1.79	0.48
1:A:106:THR:OG1	1:A:205:ILE:HD12	2.13	0.48
1:B:764:LEU:O	1:B:770:SER:HA	2.14	0.47
1:A:34:LEU:HD23	1:A:60:GLY:HA3	1.96	0.47
1:B:765:GLN:HG2	1:B:770:SER:OG	2.15	0.47
1:B:861:MSE:HE3	1:B:863:GLU:CG	2.44	0.47
1:B:810:LEU:O	1:B:811:LYS:NZ	2.47	0.47
1:B:603:VAL:HG22	1:B:792:LEU:HD22	1.96	0.47
1:B:621:ILE:HD11	1:B:807:LEU:HD13	1.96	0.47
1:A:371:CYS:O	1:A:375:VAL:HG23	2.15	0.47
1:A:340:MSE:HG3	1:A:375:VAL:CG1	2.43	0.47
1:A:1:MSE:HE2	1:A:27:VAL:HG11	1.97	0.47
1:B:803:ILE:O	1:B:807:LEU:HB2	2.14	0.47
1:A:336:ASN:HB3	2:A:1295:HOH:O	2.15	0.47
1:B:771:VAL:CG1	1:B:800:LEU:HB3	2.45	0.47
1:B:628:THR:HB	1:B:654:TYR:HB2	1.96	0.47
1:B:505:THR:OG1	1:B:508:GLN:HG3	2.15	0.47
1:B:603:VAL:CG2	1:B:792:LEU:HD22	2.44	0.46
1:B:661:ALA:HB2	1:B:667:ILE:HG13	1.98	0.46
1:A:75:LEU:O	1:A:77:GLN:HG3	2.15	0.46
1:B:756:THR:CG2	1:B:757:SER:N	2.79	0.46
1:A:216:ILE:HA	1:A:237:TRP:O	2.16	0.46
1:A:34:LEU:HD21	1:A:57:ALA:HA	1.97	0.46
1:A:172:SER:O	1:A:175:ARG:HG2	2.16	0.46
1:B:543:LEU:CD1	1:B:639:ILE:HD12	2.46	0.45
1:B:702:LYS:NZ	2:B:1249:HOH:O	2.48	0.45
1:A:283:ILE:O	1:A:287:LEU:HG	2.16	0.45
1:A:318:PHE:HB3	1:A:330:ASP:HB3	1.97	0.45
1:A:84:ARG:CD	1:A:139:ILE:HD11	2.47	0.45
1:A:73:ILE:O	1:A:75:LEU:N	2.49	0.45
1:B:606:THR:OG1	1:B:705:ILE:HD12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:THR:CG2	1:A:257:SER:N	2.80	0.45
1:B:903:VAL:HG22	1:B:904:GLY:N	2.30	0.45
1:B:718:ASN:ND2	1:B:720:ASP:H	2.15	0.45
1:B:599:PRO:HD2	1:B:650:PRO:HA	1.97	0.44
1:A:121:ILE:HG23	1:A:303:ILE:HA	1.99	0.44
1:A:79:ILE:N	1:A:79:ILE:HD12	2.33	0.44
1:B:840:MSE:HG3	1:B:875:VAL:CG1	2.44	0.44
1:B:856:LEU:HG	1:B:858:VAL:CG1	2.47	0.44
1:B:630:TYR:HA	1:B:656:VAL:O	2.17	0.44
1:B:550:ALA:HA	1:B:553:PHE:CD1	2.52	0.44
1:A:185:ALA:O	1:A:195:LEU:HD13	2.17	0.44
1:A:159:LEU:CD1	1:A:171:VAL:HG13	2.48	0.44
1:A:10:THR:CG2	1:A:17:LEU:HB2	2.48	0.44
1:B:943:VAL:O	1:B:947:GLN:HG2	2.17	0.44
1:A:242:ASN:HD22	1:A:242:ASN:N	2.15	0.44
1:B:731:ILE:HD11	2:B:1044:HOH:O	2.18	0.44
1:B:786:ALA:HB1	1:B:807:LEU:HD21	2.00	0.44
1:B:680:LEU:HD11	1:B:788:ALA:HB1	2.00	0.44
1:A:271:VAL:CG1	1:A:300:LEU:HB3	2.48	0.43
1:A:242:ASN:HD22	1:A:242:ASN:H	1.67	0.43
1:B:937:ALA:HB1	1:B:939:MSE:HE3	2.01	0.43
1:A:217:MSE:HE1	1:A:224:TRP:CE3	2.53	0.43
1:B:667:ILE:O	1:B:671:VAL:HG22	2.18	0.43
1:A:29:THR:HG22	1:A:41:VAL:HB	2.01	0.43
1:A:266:THR:OG1	1:A:300:LEU:HD21	2.19	0.43
1:A:163:HIS:ND1	1:A:166:GLU:OE2	2.52	0.43
1:B:905:GLU:HG3	1:B:907:PHE:CZ	2.54	0.43
1:B:593:TRP:O	1:B:597:GLN:HG2	2.18	0.43
1:B:568:SER:HA	1:B:580:VAL:O	2.19	0.43
1:A:405:GLU:OE2	1:A:416:ARG:NH1	2.51	0.43
1:B:761:GLU:HA	1:B:773:VAL:O	2.19	0.43
1:B:880:LYS:HD3	1:B:901:SER:O	2.19	0.43
1:A:106:THR:HG22	1:A:107:GLY:N	2.24	0.43
1:B:755:VAL:HG11	1:B:849:GLU:HB3	2.00	0.43
1:A:340:MSE:CG	1:A:375:VAL:HG11	2.46	0.42
1:B:840:MSE:O	1:B:844:VAL:HG23	2.19	0.42
1:B:749:THR:CG2	1:B:750:ALA:N	2.82	0.42
1:B:606:THR:HG21	1:B:667:ILE:CD1	2.50	0.42
1:A:123:SER:HA	1:A:128:THR:HG23	2.02	0.42
1:B:712:ASN:H	1:B:712:ASN:ND2	2.18	0.42
1:B:861:MSE:HE1	1:B:871:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:TYR:O	1:A:427:ILE:HG22	2.19	0.42
1:B:556:GLN:HA	1:B:556:GLN:NE2	2.32	0.42
1:A:93:TRP:O	1:A:97:GLN:HG2	2.20	0.42
1:B:659:LEU:CD1	1:B:671:VAL:HG13	2.50	0.42
1:A:437:ALA:O	1:A:439:MSE:HE2	2.19	0.42
1:A:350:MSE:O	1:A:354:ARG:HD3	2.20	0.41
1:A:218:ASN:O	1:A:222:ASN:ND2	2.52	0.41
1:A:443:VAL:O	1:A:447:GLN:HG2	2.20	0.41
1:B:718:ASN:HD22	1:B:719:ALA:N	2.19	0.41
1:B:502:ILE:HD11	1:B:593:TRP:CZ3	2.55	0.41
1:A:243:ALA:HB3	1:A:246:SER:HB2	2.03	0.41
1:B:937:ALA:O	1:B:939:MSE:HE2	2.19	0.41
1:B:823:ALA:H	1:B:826:GLN:HB2	1.85	0.41
1:A:137:ASN:ND2	1:A:137:ASN:H	2.16	0.41
1:A:356:LEU:HG	1:A:358:VAL:HG13	2.01	0.41
1:A:267:PRO:HD2	1:A:294:MSE:CE	2.45	0.41
1:B:570:PRO:O	1:B:571:LEU:HD23	2.20	0.41
1:B:522:ILE:HD12	1:B:576:PRO:HG2	2.02	0.41
1:A:410:LYS:HE2	1:A:439:MSE:CE	2.50	0.41
1:A:249:THR:CG2	1:A:250:ALA:N	2.83	0.41
1:B:739:PHE:CZ	1:B:788:ALA:HB2	2.56	0.41
1:A:117:MSE:HG2	1:A:310:LEU:HD11	2.03	0.41
1:B:551:HIS:CE1	1:B:568:SER:H	2.39	0.41
1:B:676:PRO:O	1:B:709:LEU:HD23	2.21	0.41
1:B:840:MSE:CG	1:B:875:VAL:HG11	2.47	0.40
1:B:501:MSE:HB3	1:B:525:ASP:O	2.20	0.40
1:B:550:ALA:HA	1:B:553:PHE:HD1	1.86	0.40
1:B:544:LYS:HA	1:B:549:ASP:HA	2.03	0.40
1:B:771:VAL:HG13	1:B:800:LEU:HB3	2.03	0.40
1:B:659:LEU:HD11	1:B:671:VAL:HG13	2.04	0.40
1:A:257:SER:O	1:A:327:LEU:HD22	2.22	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	435/452 (96%)	407 (94%)	26 (6%)	2 (0%)	34 41
1	B	435/452 (96%)	408 (94%)	22 (5%)	5 (1%)	17 18
All	All	870/904 (96%)	815 (94%)	48 (6%)	7 (1%)	24 27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	525	ASP
1	B	863	GLU
1	B	574	ASP
1	B	862	ALA
1	B	536	PRO
1	A	36	PRO
1	A	240	SER

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	341/340 (100%)	302 (89%)	39 (11%)	7 7
1	B	341/340 (100%)	302 (89%)	39 (11%)	7 7
All	All	682/680 (100%)	604 (89%)	78 (11%)	7 7

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	3	SER
1	A	6	LEU
1	A	31	THR
1	A	34	LEU
1	A	35	THR

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Mol	Chain	Res	Type
1	A	78	LEU
1	A	84	ARG
1	A	95	ARG
1	A	103	VAL
1	A	105	LEU
1	A	113	SER
1	A	128	THR
1	A	129	LEU
1	A	137	ASN
1	A	146	LEU
1	A	171	VAL
1	A	198	VAL
1	A	212	ASN
1	A	218	ASN
1	A	231	ILE
1	A	242	ASN
1	A	255	VAL
1	A	264	LEU
1	A	292	LEU
1	A	307	LEU
1	A	314	PRO
1	A	337	VAL
1	A	345	GLN
1	A	347	LEU
1	A	369	GLU
1	A	386	ARG
1	A	405	GLU
1	A	411	THR
1	A	413	LEU
1	A	416	ARG
1	A	420	LEU
1	A	427	ILE
1	A	435	ARG
1	B	501	MSE
1	B	506	LEU
1	B	509	LEU
1	B	511	ASP
1	B	517	LEU
1	B	531	THR
1	B	534	LEU
1	B	535	THR
1	B	556	GLN

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Mol	Chain	Res	Type
1	B	578	LEU
1	B	583	THR
1	B	584	ARG
1	B	585	LEU
1	B	595	ARG
1	B	603	VAL
1	B	628	THR
1	B	637	ASN
1	B	646	LEU
1	B	651	GLU
1	B	671	VAL
1	B	698	VAL
1	B	718	ASN
1	B	731	ILE
1	B	742	ASN
1	B	764	LEU
1	B	771	VAL
1	B	780	ARG
1	B	792	LEU
1	B	807	LEU
1	B	834	ASN
1	B	845	GLN
1	B	847	LEU
1	B	886	ARG
1	B	911	THR
1	B	913	LEU
1	B	916	ARG
1	B	917	LEU
1	B	927	ILE
1	B	935	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	137	ASN
1	A	164	GLN
1	A	212	ASN
1	A	218	ASN
1	A	242	ASN
1	A	447	GLN
1	B	556	GLN

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Mol	Chain	Res	Type
1	B	637	ASN
1	B	682	ASN
1	B	712	ASN
1	B	718	ASN
1	B	742	ASN
1	B	781	HIS
1	B	836	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

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.