Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:14 PM GMT

PDB ID	:	4O9P
Title	:	Crystal structure of Thermus thermophilis transhydrogeanse domain II dimer SeMet derivative
Authors	:	Leung, J.H.; Yamaguchi, M.; Moeller, A.; Schurig-Briccio, L.A.; Gennis, R.B.; Potter, C.S.; Carragher, B.; Stout, C.D.
Deposited on	:	2014-01-02
Resolution	:	2.89 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:

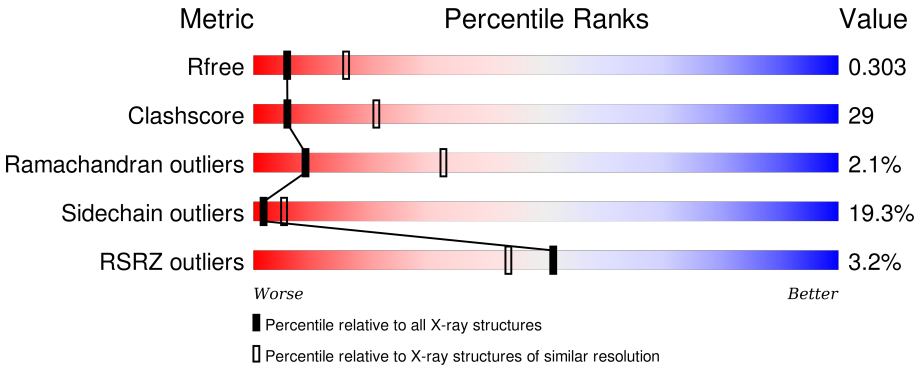
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.89 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 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	100	45% 36% 12% • 6%
1	C	100	2% 42% 36% 11% 11%
2	B	283	2% 51% 34% 8% • 7%
2	D	283	4% 51% 32% 8% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5191 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 NAD(P) transhydrogenase subunit alpha 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	89	Total	C	N	O	Se	0	0	0
			666	444	105	112	5			
1	A	94	Total	C	N	O	Se	0	0	0
			713	475	114	119	5			

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	260	Total	C	N	O	Se	0	0	0
			1893	1262	302	313	16			
2	B	264	Total	C	N	O	Se	0	0	0
			1919	1280	306	317	16			

There are 16 discrepancies between the modelled and reference sequences:

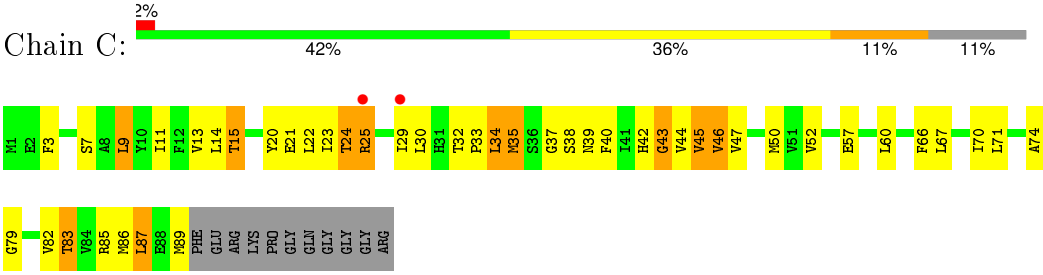
Chain	Residue	Modelled	Actual	Comment	Reference
D	276	HIS	-	EXPRESSION TAG	UNP Q72GS0
D	277	HIS	-	EXPRESSION TAG	UNP Q72GS0
D	278	HIS	-	EXPRESSION TAG	UNP Q72GS0
D	279	HIS	-	EXPRESSION TAG	UNP Q72GS0
D	280	HIS	-	EXPRESSION TAG	UNP Q72GS0
D	281	HIS	-	EXPRESSION TAG	UNP Q72GS0
D	282	HIS	-	EXPRESSION TAG	UNP Q72GS0
D	283	HIS	-	EXPRESSION TAG	UNP Q72GS0
B	276	HIS	-	EXPRESSION TAG	UNP Q72GS0
B	277	HIS	-	EXPRESSION TAG	UNP Q72GS0
B	278	HIS	-	EXPRESSION TAG	UNP Q72GS0
B	279	HIS	-	EXPRESSION TAG	UNP Q72GS0
B	280	HIS	-	EXPRESSION TAG	UNP Q72GS0
B	281	HIS	-	EXPRESSION TAG	UNP Q72GS0
B	282	HIS	-	EXPRESSION TAG	UNP Q72GS0
B	283	HIS	-	EXPRESSION TAG	UNP Q72GS0

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.

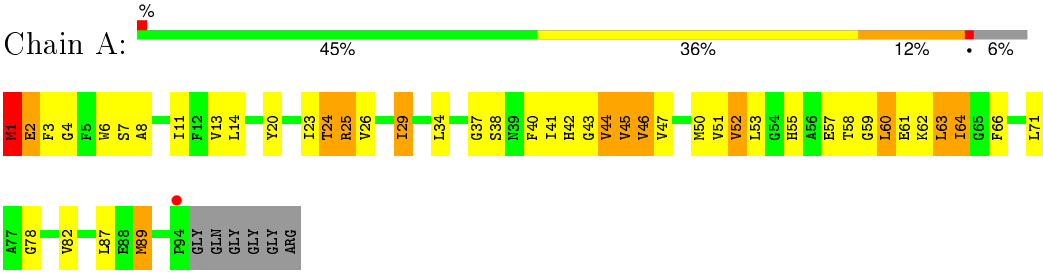
- Molecule 1: NAD(P) transhydrogenase subunit alpha 2

Chain C:



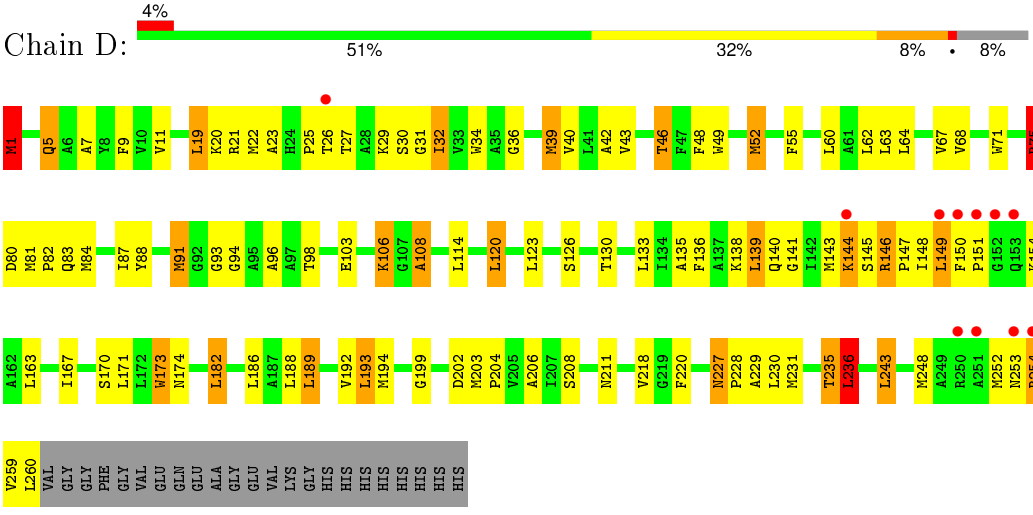
- Molecule 1: NAD(P) transhydrogenase subunit alpha 2

Chain A:



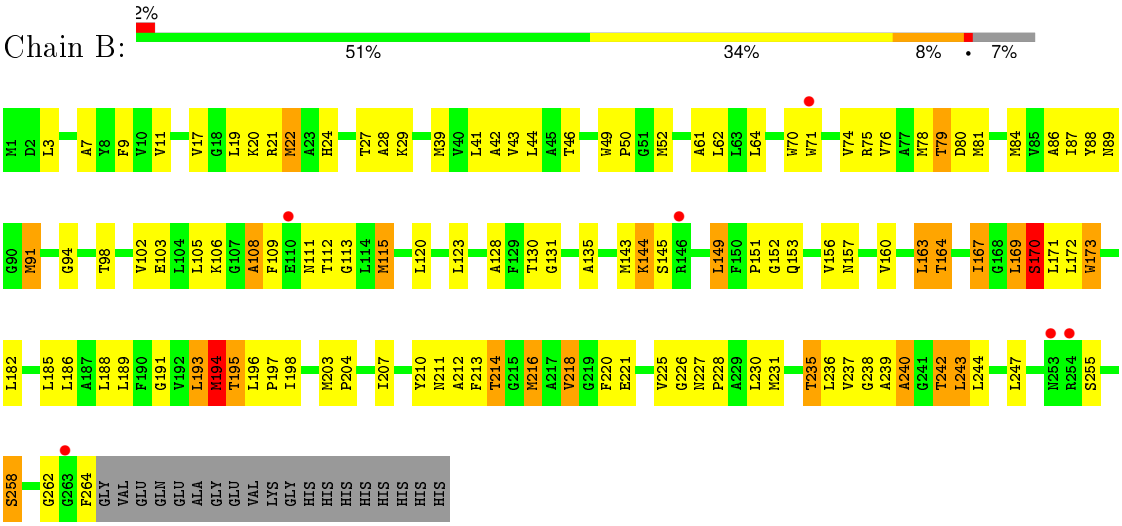
- Molecule 2: NAD(P) transhydrogenase subunit beta

Chain D:



- Molecule 2: NAD(P) transhydrogenase subunit beta

Chain B:


2%
51%
34%
8%
7%
M1 D2 L3 A7 Y8 F9 V10 V11 V17 G18 L19 K20 R21 M22 A23 H24 T27 A28 K29 M39 V40 L41 A42 V43 L44 A45 T46 W49 P50 G51 M52 A61 L62 L63 L64 W70 W71 V74 R75 V76 A77 M78 T79 D80 M81 M84 V85 A86 I87 Y88 N89
G90 M91 G94 T98 V102 E103 L104 L105 K106 G107 A108 F109 E110 N111 T112 G113 L114 M115 L120 L123 A128 F129 T130 G131 A135 M143 K144 S145 R146 L149 F150 P151 G152 Q153 V156 N157 V160 L163 T164 I167 G168 L169 S170 L171 L172 W173
L182 L185 L186 A187 L188 L189 F190 G191 V192 L193 M194 T195 L196 P197 I198 M203 P204 I207 Y210 N211 A212 F213 T214 G215 M216 A217 V218 G219 F220 E221 V225 G226 N227 P228 A229 L230 M231 T235 L236 V237 G238 A239 A240 G241 T242 L243 L244 L247 N253 R254 S255
S258 G262 G263 F264 GLY VAL GLU GLN GLU ALA GLY GLU VAL LYS GLY HIS HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.57Å 86.87Å 99.16Å 90.00° 94.91° 90.00°	Depositor
Resolution (Å)	97.93 – 2.89 37.84 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.6 (97.93-2.89) 93.8 (37.84-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.222 , 0.288 0.235 , 0.303	Depositor DCC
R_{free} test set	1159 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 22605 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	5191	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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	0.67	0/726	0.96	3/978 (0.3%)
1	C	0.54	0/677	0.85	1/913 (0.1%)
2	B	0.68	0/1946	0.92	3/2626 (0.1%)
2	D	0.62	0/1919	0.86	5/2590 (0.2%)
All	All	0.64	0/5268	0.90	12/7107 (0.2%)

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
2	B	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	75	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	89	MSE	CG-SE-CE	-6.69	84.18	98.90
1	A	1	MSE	CG-SE-CE	6.53	113.27	98.90
2	B	216	MSE	CG-SE-CE	6.39	112.96	98.90
2	D	149	LEU	CA-CB-CG	6.01	129.12	115.30
1	C	35	MSE	CG-SE-CE	5.97	112.05	98.90
2	D	236	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	2	GLU	C-N-CA	5.33	135.02	121.70
2	B	236	LEU	CA-CB-CG	5.22	127.30	115.30
2	D	173	TRP	N-CA-C	-5.20	96.97	111.00
2	B	194	MSE	CB-CA-C	-5.13	100.13	110.40
2	D	1	MSE	CG-SE-CE	5.13	110.18	98.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	226	GLY	Peptide

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	713	0	739	56	0
1	C	666	0	691	76	0
2	B	1919	0	2030	111	0
2	D	1893	0	2006	148	0
All	All	5191	0	5466	308	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 29.

All (308) 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)
2:B:135:ALA:CB	2:B:203:MSE:HE2	1.53	1.37
1:C:87:LEU:HD23	2:D:32:ILE:CD1	1.83	1.09
2:D:71:TRP:HE1	2:D:75:ARG:HD2	0.95	1.08
1:C:82:VAL:HB	2:D:81:MSE:HE1	1.32	1.08
2:B:135:ALA:CB	2:B:203:MSE:CE	2.30	1.08
1:C:50:MSE:HE2	2:D:62:LEU:HD21	1.38	1.04
2:B:135:ALA:HB1	2:B:203:MSE:HE2	1.07	1.04
2:B:135:ALA:HB1	2:B:203:MSE:CE	1.88	1.03
1:C:71:LEU:HD23	2:D:91:MSE:HE3	1.39	1.03
2:D:71:TRP:NE1	2:D:75:ARG:HD2	1.72	1.01
1:C:82:VAL:HB	2:D:81:MSE:CE	1.88	1.01
1:C:82:VAL:CB	2:D:81:MSE:HE1	1.91	1.01
1:C:87:LEU:HD23	2:D:32:ILE:HD12	1.40	1.00
1:C:76:ALA:HB2	2:D:39:MSE:HE2	1.41	0.98
1:C:76:ALA:HB2	2:D:39:MSE:CE	1.93	0.97
1:C:79:GLY:O	1:C:83:THR:HG22	1.66	0.96
1:C:76:ALA:CB	2:D:39:MSE:HE2	1.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:ILE:H	2:D:32:ILE:HD13	1.33	0.93
2:D:71:TRP:HE1	2:D:75:ARG:CD	1.81	0.93
1:A:60:LEU:O	1:A:64:ILE:HG22	1.68	0.93
2:D:27:THR:O	2:D:30:SER:HB3	1.68	0.93
1:C:76:ALA:CB	2:D:39:MSE:CE	2.48	0.91
2:B:160:VAL:HG11	2:B:189:LEU:HD12	1.52	0.90
2:B:238:GLY:O	2:B:242:THR:HG23	1.74	0.88
1:A:1:MSE:O	1:A:8:ALA:CB	2.22	0.88
1:A:76:ALA:HB1	2:B:39:MSE:HE2	1.55	0.87
2:D:189:LEU:HD22	2:D:193:LEU:HD23	1.58	0.86
2:D:163:LEU:O	2:D:167:ILE:HD12	1.75	0.86
1:C:43:GLY:O	1:C:46:VAL:HG23	1.76	0.85
1:A:50:MSE:HE1	2:B:43:VAL:HG13	1.58	0.85
2:B:231:MSE:O	2:B:235:THR:HG23	1.77	0.84
2:B:24:HIS:HB2	2:B:27:THR:HG22	1.59	0.84
2:B:135:ALA:HB2	2:B:203:MSE:CE	2.05	0.84
2:D:147:PRO:HD3	2:D:199:GLY:HA2	1.58	0.83
1:A:1:MSE:O	1:A:8:ALA:HB1	1.78	0.83
2:D:255:SER:O	2:D:257:TRP:N	2.11	0.83
1:A:23:ILE:O	1:A:26:VAL:HG12	1.78	0.82
1:C:87:LEU:HD23	2:D:32:ILE:HD11	1.60	0.82
2:D:78:MSE:HA	2:D:78:MSE:HE2	1.61	0.82
1:C:87:LEU:CD2	2:D:32:ILE:HD12	2.08	0.82
2:D:32:ILE:H	2:D:32:ILE:CD1	1.92	0.81
2:D:227:ASN:C	2:D:227:ASN:HD22	1.84	0.80
1:A:64:ILE:HD13	2:B:102:VAL:HG23	1.63	0.80
2:D:167:ILE:O	2:D:170:SER:OG	2.00	0.79
2:D:32:ILE:N	2:D:32:ILE:HD13	1.99	0.77
2:B:191:GLY:O	2:B:195:THR:HG22	1.83	0.77
2:B:135:ALA:CA	2:B:203:MSE:HE2	2.14	0.77
2:D:231:MSE:O	2:D:235:THR:HG23	1.84	0.77
2:D:20:LYS:O	2:D:23:ALA:HB3	1.87	0.75
2:D:42:ALA:O	2:D:46:THR:HG23	1.87	0.75
1:A:64:ILE:HD13	2:B:102:VAL:CG2	2.17	0.75
2:B:131:GLY:HA2	2:B:195:THR:HG21	1.67	0.74
1:A:76:ALA:CB	2:B:39:MSE:HE2	2.17	0.74
2:B:128:ALA:HB1	2:B:214:THR:HG22	1.69	0.74
1:A:46:VAL:HB	1:A:50:MSE:HE3	1.70	0.73
1:A:55:HIS:O	2:B:106:LYS:HE3	1.88	0.73
2:B:128:ALA:CB	2:B:214:THR:HG22	2.20	0.72
2:D:138:LYS:HG2	2:D:145:SER:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:MSE:HA	2:D:78:MSE:CE	2.21	0.71
1:C:50:MSE:HE1	2:D:43:VAL:HG13	1.72	0.70
2:D:106:LYS:HE3	2:D:108:ALA:O	1.92	0.70
1:A:64:ILE:CD1	2:B:102:VAL:HG23	2.21	0.69
2:B:89:ASN:ND2	2:B:211:ASN:HA	2.08	0.69
2:D:63:LEU:O	2:D:67:VAL:HG13	1.93	0.69
1:C:13:VAL:HG21	2:B:9:PHE:HZ	1.58	0.69
1:A:42:HIS:HD1	1:A:75:ASN:HD21	1.41	0.69
2:B:103:GLU:HG2	2:B:109:PHE:CZ	2.26	0.69
2:D:5:GLN:HE21	2:D:5:GLN:HA	1.56	0.69
1:C:35:MSE:HE2	2:D:208:SER:HB2	1.74	0.68
1:C:11:ILE:O	1:C:15:THR:HG23	1.94	0.68
2:D:170:SER:O	2:D:173:TRP:O	2.10	0.68
1:A:41:ILE:O	1:A:44:VAL:HG22	1.94	0.68
2:B:144:LYS:HE3	2:B:144:LYS:H	1.58	0.67
2:D:218:VAL:HG13	2:D:230:LEU:HD13	1.77	0.67
2:D:138:LYS:HE3	2:D:145:SER:CB	2.25	0.66
1:A:38:SER:HB2	2:B:237:VAL:HG13	1.76	0.66
1:A:57:GLU:O	1:A:59:GLY:N	2.27	0.66
2:B:191:GLY:O	2:B:195:THR:CG2	2.44	0.66
2:B:135:ALA:HB2	2:B:203:MSE:HE1	1.76	0.65
2:D:167:ILE:HG12	2:D:182:LEU:HD13	1.78	0.65
1:C:85:ARG:NH1	2:D:78:MSE:HE3	2.11	0.65
2:B:94:GLY:O	2:B:98:THR:HG23	1.97	0.64
2:D:7:ALA:O	2:D:11:VAL:HG23	1.97	0.64
2:B:258:SER:O	2:B:262:GLY:HA3	1.98	0.64
2:B:157:ASN:OD1	2:B:193:LEU:HD13	1.98	0.64
2:D:231:MSE:O	2:D:235:THR:CG2	2.46	0.64
2:B:157:ASN:OD1	2:B:193:LEU:CD1	2.46	0.64
2:B:210:TYR:O	2:B:214:THR:HG23	1.97	0.64
1:C:15:THR:HG22	1:A:14:LEU:HD13	1.79	0.64
2:B:86:ALA:HB2	2:B:207:ILE:HD13	1.79	0.63
2:B:194:MSE:O	2:B:197:PRO:HD2	1.99	0.63
1:A:50:MSE:HE2	2:B:62:LEU:HD21	1.79	0.63
2:D:227:ASN:ND2	2:D:229:ALA:H	1.96	0.63
1:C:45:VAL:HG13	2:D:218:VAL:HG22	1.79	0.63
2:B:87:ILE:O	2:B:91:MSE:HG2	1.99	0.63
2:B:163:LEU:O	2:B:167:ILE:HG22	1.98	0.63
2:D:103:GLU:O	2:D:106:LYS:HE2	1.99	0.63
2:D:106:LYS:HD2	2:D:108:ALA:N	2.13	0.63
2:D:138:LYS:CE	2:D:145:SER:HB3	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:ASN:HD21	2:B:211:ASN:HA	1.61	0.63
1:A:47:VAL:O	1:A:51:VAL:HG23	1.99	0.63
1:C:76:ALA:CB	2:D:39:MSE:HE3	2.28	0.62
2:D:36:GLY:O	2:D:40:VAL:HG23	1.99	0.62
1:A:45:VAL:HG13	2:B:218:VAL:HB	1.82	0.62
1:C:47:VAL:HG13	2:D:46:THR:HG21	1.82	0.61
1:C:82:VAL:CA	2:D:81:MSE:HE1	2.30	0.61
1:C:76:ALA:HB1	2:D:39:MSE:CE	2.28	0.61
2:D:147:PRO:HD3	2:D:199:GLY:CA	2.28	0.61
2:B:109:PHE:CB	2:B:115:MSE:HG3	2.29	0.61
2:D:106:LYS:HD2	2:D:108:ALA:H	1.65	0.61
2:D:1:MSE:HA	1:A:6:TRP:HE1	1.66	0.61
1:C:35:MSE:HE3	2:D:248:MSE:SE	2.50	0.60
1:C:20:TYR:CE1	2:D:243:LEU:HG	2.35	0.60
2:B:169:LEU:O	2:B:171:LEU:N	2.34	0.60
2:B:49:TRP:CD1	2:B:50:PRO:HD2	2.37	0.60
2:D:188:LEU:O	2:D:192:VAL:HG23	2.01	0.60
2:D:202:ASP:HB3	2:D:259:VAL:HG13	1.84	0.60
2:D:218:VAL:HG13	2:D:230:LEU:CD1	2.31	0.60
1:C:82:VAL:HB	2:D:81:MSE:HE3	1.79	0.59
1:C:42:HIS:HE1	2:D:211:ASN:OD1	1.85	0.59
2:B:221:GLU:O	2:B:225:VAL:HG22	2.03	0.59
1:C:14:LEU:CD1	1:A:11:ILE:HG23	2.33	0.59
1:C:35:MSE:HE2	2:D:208:SER:N	2.18	0.58
2:B:189:LEU:HD13	2:B:193:LEU:HG	1.85	0.58
1:C:13:VAL:HG21	2:B:9:PHE:CZ	2.37	0.58
2:D:138:LYS:CE	2:D:145:SER:CB	2.81	0.58
2:B:49:TRP:HB3	2:B:52:MSE:CG	2.34	0.58
1:C:23:ILE:CD1	1:C:34:LEU:HD11	2.34	0.58
2:B:79:THR:HG22	2:B:80:ASP:OD1	2.04	0.58
2:D:138:LYS:HE3	2:D:145:SER:HB3	1.85	0.57
2:B:111:ASN:ND2	2:B:113:GLY:H	2.02	0.57
2:B:109:PHE:HB2	2:B:115:MSE:HG3	1.86	0.57
2:B:103:GLU:OE2	2:B:108:ALA:HB3	2.04	0.57
2:D:148:ILE:O	2:D:148:ILE:HG22	2.04	0.57
1:A:24:THR:HG22	2:B:243:LEU:HD11	1.86	0.57
2:D:39:MSE:O	2:D:43:VAL:HG23	2.05	0.57
2:D:19:LEU:HD12	2:D:236:LEU:CD1	2.33	0.57
1:C:50:MSE:CE	2:D:62:LEU:HD21	2.26	0.56
2:D:138:LYS:HG2	2:D:145:SER:CB	2.35	0.56
2:D:81:MSE:N	2:D:82:PRO:HD2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ILE:HG13	2:B:240:ALA:HB1	1.88	0.56
1:C:42:HIS:O	1:C:44:VAL:N	2.39	0.56
2:D:218:VAL:CG1	2:D:230:LEU:HD13	2.36	0.56
1:A:59:GLY:HA2	1:A:62:LYS:HB2	1.87	0.55
2:B:238:GLY:O	2:B:242:THR:CG2	2.52	0.55
1:A:46:VAL:HG13	1:A:72:GLY:C	2.26	0.55
2:D:103:GLU:OE1	2:D:106:LYS:NZ	2.36	0.55
1:C:7:SER:HB3	1:A:7:SER:HB3	1.89	0.55
1:C:74:ALA:HB3	2:D:91:MSE:HE2	1.89	0.55
2:B:160:VAL:O	2:B:164:THR:OG1	2.25	0.54
2:B:212:ALA:HB1	2:B:242:THR:HG22	1.89	0.54
1:C:30:LEU:HD23	1:C:33:PRO:HG2	1.89	0.54
2:D:94:GLY:O	2:D:98:THR:HG23	2.07	0.54
1:A:50:MSE:CE	2:B:43:VAL:HG13	2.35	0.54
1:C:76:ALA:HB1	2:D:39:MSE:HE2	1.83	0.54
2:B:255:SER:O	2:B:258:SER:OG	2.25	0.53
2:D:106:LYS:CE	2:D:108:ALA:O	2.56	0.53
1:C:74:ALA:CB	2:D:91:MSE:HE2	2.39	0.53
2:D:138:LYS:HE2	2:D:145:SER:HB3	1.91	0.52
2:B:76:VAL:HG13	2:B:80:ASP:HB2	1.91	0.52
1:A:78:GLY:O	1:A:82:VAL:HG23	2.09	0.52
2:B:203:MSE:O	2:B:207:ILE:HG13	2.09	0.52
2:D:19:LEU:HD12	2:D:236:LEU:HD13	1.91	0.52
2:D:87:ILE:O	2:D:91:MSE:HG2	2.10	0.51
2:D:135:ALA:HB1	2:D:203:MSE:HE2	1.91	0.51
1:A:40:PHE:CZ	2:B:39:MSE:HG3	2.46	0.51
1:C:42:HIS:C	1:C:44:VAL:N	2.64	0.51
1:A:23:ILE:CG1	2:B:240:ALA:HB1	2.41	0.51
2:D:120:LEU:HD13	2:D:220:PHE:CE2	2.46	0.51
1:C:23:ILE:HD12	1:C:34:LEU:HD11	1.91	0.51
2:D:203:MSE:HE3	2:D:206:ALA:HB3	1.92	0.51
1:C:30:LEU:HD12	2:D:25:PRO:HD3	1.92	0.50
1:C:43:GLY:O	1:C:46:VAL:CG2	2.54	0.50
2:B:17:VAL:O	2:B:21:ARG:HG3	2.11	0.50
1:C:78:GLY:HA3	2:D:88:TYR:CE1	2.46	0.50
2:D:167:ILE:HD13	2:D:186:LEU:HD12	1.92	0.50
2:D:135:ALA:O	2:D:139:LEU:HD12	2.12	0.50
1:C:14:LEU:HD11	1:A:11:ILE:HG23	1.92	0.50
2:B:135:ALA:HA	2:B:203:MSE:HE2	1.93	0.50
1:C:66:PHE:CE1	1:C:70:ILE:HD11	2.47	0.50
2:D:22:MSE:CG	2:D:31:GLY:HA3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:VAL:CG1	2:D:81:MSE:HE1	2.42	0.49
1:C:35:MSE:CE	2:D:208:SER:HB2	2.40	0.49
2:D:42:ALA:O	2:D:46:THR:CG2	2.57	0.49
2:D:227:ASN:HD22	2:D:228:PRO:N	2.10	0.49
1:C:3:PHE:CE2	2:D:228:PRO:HG3	2.48	0.49
2:D:1:MSE:HG2	1:A:6:TRP:CZ2	2.47	0.49
2:B:21:ARG:O	2:B:27:THR:HG23	2.12	0.49
2:B:102:VAL:O	2:B:106:LYS:HB2	2.12	0.48
2:D:167:ILE:CD1	2:D:186:LEU:HD12	2.43	0.48
1:C:42:HIS:O	1:C:45:VAL:HG22	2.13	0.48
1:C:25:ARG:HH21	1:A:25:ARG:HD3	1.78	0.48
2:D:227:ASN:HD22	2:D:229:ALA:H	1.60	0.48
2:D:9:PHE:HZ	1:A:13:VAL:HG21	1.78	0.48
1:C:35:MSE:HE2	2:D:208:SER:H	1.78	0.48
2:B:144:LYS:CE	2:B:144:LYS:H	2.24	0.48
1:A:23:ILE:HD12	1:A:34:LEU:HD21	1.95	0.48
1:C:42:HIS:C	1:C:44:VAL:H	2.16	0.48
2:B:130:THR:HG23	2:B:188:LEU:HD22	1.96	0.48
2:B:195:THR:HA	2:B:198:ILE:HD12	1.95	0.48
2:B:167:ILE:HG13	2:B:182:LEU:HD23	1.96	0.48
1:A:76:ALA:CB	2:B:39:MSE:CE	2.90	0.47
1:C:40:PHE:CZ	2:D:39:MSE:HG2	2.50	0.47
2:D:93:GLY:O	2:D:96:ALA:HB3	2.15	0.47
1:C:85:ARG:NH1	2:D:78:MSE:CE	2.76	0.47
1:A:66:PHE:CE1	2:B:61:ALA:HB2	2.49	0.47
2:D:106:LYS:HE3	2:D:108:ALA:C	2.34	0.47
1:A:63:LEU:O	1:A:66:PHE:HB3	2.15	0.47
2:B:130:THR:OG1	2:B:191:GLY:HA3	2.14	0.47
2:B:216:MSE:HE2	2:B:220:PHE:CE1	2.50	0.47
1:A:37:GLY:HA3	2:B:22:MSE:SE	2.63	0.47
2:D:64:LEU:O	2:D:68:VAL:HG23	2.15	0.47
2:D:83:GLN:HB2	2:D:136:PHE:CD1	2.49	0.47
1:C:21:GLU:O	1:C:24:THR:OG1	2.23	0.46
2:B:152:GLY:O	2:B:156:VAL:HG23	2.15	0.46
2:D:227:ASN:C	2:D:227:ASN:ND2	2.58	0.46
1:C:9:LEU:O	1:C:13:VAL:HG23	2.15	0.46
2:B:203:MSE:N	2:B:204:PRO:CD	2.78	0.46
2:B:167:ILE:HG21	2:B:186:LEU:HD13	1.97	0.46
2:B:153:GLN:CG	2:B:264:PHE:HE2	2.29	0.46
1:C:76:ALA:HB1	2:D:39:MSE:HE3	1.95	0.46
1:C:30:LEU:O	1:C:34:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:MSE:O	2:D:204:PRO:C	2.54	0.46
1:C:22:LEU:HD22	2:D:20:LYS:HB2	1.97	0.46
2:B:70:TRP:O	2:B:74:VAL:HG23	2.15	0.46
1:A:37:GLY:O	1:A:41:ILE:HG13	2.16	0.45
2:B:227:ASN:HA	2:B:228:PRO:HD3	1.84	0.45
1:A:2:GLU:HA	1:A:4:GLY:N	2.31	0.45
2:B:149:LEU:HA	2:B:153:GLN:NE2	2.31	0.45
2:D:141:GLY:O	2:D:144:LYS:HB3	2.16	0.45
1:C:15:THR:HG22	1:A:14:LEU:CD1	2.46	0.45
1:C:37:GLY:HA3	2:D:22:MSE:HE1	1.98	0.45
1:A:64:ILE:CD1	2:B:102:VAL:CG2	2.88	0.45
2:B:22:MSE:HA	2:B:28:ALA:HA	1.98	0.45
2:B:49:TRP:HB3	2:B:52:MSE:HG2	1.98	0.45
2:D:22:MSE:HG3	2:D:31:GLY:HA3	1.99	0.45
2:D:143:MSE:O	2:D:144:LYS:O	2.35	0.45
1:A:89:MSE:HE3	1:A:89:MSE:HB3	1.80	0.45
1:C:43:GLY:O	2:D:39:MSE:HE1	2.16	0.45
1:C:35:MSE:HE2	2:D:208:SER:CB	2.44	0.44
2:D:48:PHE:O	2:D:49:TRP:C	2.55	0.44
2:D:154:LYS:HB3	2:D:154:LYS:HE2	1.79	0.44
1:C:78:GLY:O	1:C:82:VAL:HG22	2.18	0.44
2:B:71:TRP:O	2:B:75:ARG:HG2	2.18	0.44
2:B:143:MSE:O	2:B:144:LYS:C	2.56	0.44
2:D:194:MSE:O	2:D:194:MSE:HG2	2.17	0.44
2:B:157:ASN:OD1	2:B:193:LEU:HD12	2.15	0.44
1:C:78:GLY:HA3	2:D:88:TYR:CZ	2.53	0.44
1:A:78:GLY:HA3	2:B:88:TYR:CE2	2.53	0.44
2:D:20:LYS:O	2:D:23:ALA:CB	2.63	0.43
2:D:103:GLU:O	2:D:106:LYS:HG3	2.18	0.43
1:A:41:ILE:O	1:A:44:VAL:CG2	2.65	0.43
1:C:32:THR:N	1:C:33:PRO:HD2	2.33	0.43
2:D:252:MSE:O	2:D:253:ASN:HB2	2.18	0.43
2:D:252:MSE:HE2	2:D:254:ARG:HG3	2.00	0.43
2:D:21:ARG:HH12	2:D:27:THR:HG22	1.82	0.43
1:C:42:HIS:CE1	2:D:211:ASN:OD1	2.70	0.43
2:D:91:MSE:HB3	2:D:91:MSE:HE3	1.95	0.43
2:B:42:ALA:O	2:B:46:THR:HG22	2.19	0.43
1:C:23:ILE:HD11	1:C:34:LEU:HD11	2.00	0.43
1:C:85:ARG:CZ	2:D:78:MSE:HE1	2.48	0.43
2:B:91:MSE:HB3	2:B:91:MSE:HE2	1.86	0.43
2:B:123:LEU:C	2:B:123:LEU:HD23	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:146:ARG:HG2	2:D:147:PRO:HD2	2.00	0.43
2:B:195:THR:HB	2:B:210:TYR:OH	2.19	0.43
2:D:189:LEU:HD22	2:D:193:LEU:CD2	2.38	0.43
2:B:112:THR:HA	2:B:115:MSE:HB2	2.01	0.43
2:B:24:HIS:HB2	2:B:27:THR:CG2	2.41	0.42
1:C:39:ASN:HA	1:C:42:HIS:CE1	2.53	0.42
2:B:182:LEU:O	2:B:186:LEU:HD12	2.19	0.42
2:B:170:SER:HA	2:B:173:TRP:CZ3	2.54	0.42
2:B:103:GLU:OE2	2:B:108:ALA:CB	2.66	0.42
2:D:254:ARG:HB3	2:D:254:ARG:HE	1.62	0.42
2:D:150:PHE:HB2	2:D:151:PRO:HD2	2.01	0.42
2:D:30:SER:O	2:D:34:TRP:HD1	2.03	0.42
1:A:42:HIS:O	1:A:45:VAL:HG22	2.20	0.42
2:B:78:MSE:HE1	2:B:81:MSE:HE2	2.00	0.42
2:D:189:LEU:CD2	2:D:193:LEU:HD23	2.39	0.42
2:B:210:TYR:O	2:B:214:THR:CG2	2.66	0.42
2:B:156:VAL:O	2:B:160:VAL:HG23	2.20	0.42
1:A:71:LEU:HD22	2:B:91:MSE:HB3	2.02	0.42
2:B:49:TRP:HB3	2:B:52:MSE:HG3	2.00	0.42
1:A:20:TYR:CE2	2:B:243:LEU:HG	2.55	0.41
1:C:82:VAL:HA	2:D:81:MSE:HE1	2.02	0.41
2:B:210:TYR:HA	2:B:213:PHE:HB2	2.02	0.41
1:A:52:VAL:HG12	1:A:53:LEU:N	2.35	0.41
1:C:71:LEU:HD23	2:D:91:MSE:CE	2.30	0.41
2:D:49:TRP:O	2:D:52:MSE:HB2	2.21	0.41
2:D:63:LEU:C	2:D:63:LEU:HD23	2.40	0.41
2:D:22:MSE:HG2	2:D:31:GLY:HA3	2.01	0.41
2:B:22:MSE:HE3	2:B:22:MSE:HB3	1.58	0.41
2:B:7:ALA:O	2:B:11:VAL:HG23	2.20	0.41
1:A:1:MSE:O	1:A:8:ALA:HB2	2.14	0.41
1:C:85:ARG:CZ	2:D:78:MSE:CE	2.99	0.41
1:A:42:HIS:NE2	2:B:89:ASN:ND2	2.69	0.41
2:D:21:ARG:NH1	2:D:27:THR:CG2	2.84	0.41
1:A:57:GLU:O	1:A:61:GLU:HB2	2.21	0.41
2:B:243:LEU:HD22	2:B:247:LEU:CD1	2.51	0.41
2:D:114:LEU:HD23	2:D:114:LEU:HA	1.77	0.40
2:B:29:LYS:H	2:B:29:LYS:HG2	1.56	0.40
1:A:23:ILE:O	1:A:26:VAL:CG1	2.60	0.40
2:D:120:LEU:HD23	2:D:120:LEU:HA	1.86	0.40
2:D:256:VAL:O	2:D:260:LEU:HG	2.21	0.40
2:B:169:LEU:O	2:B:170:SER:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:THR:HG23	2:D:188:LEU:HD23	2.02	0.40
2:D:136:PHE:CZ	2:D:140:GLN:HG2	2.57	0.40
2:D:21:ARG:NH1	2:D:27:THR:HG22	2.37	0.40
1:A:41:ILE:C	1:A:43:GLY:N	2.75	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	92/100 (92%)	82 (89%)	7 (8%)	3 (3%)	5 20
1	C	87/100 (87%)	82 (94%)	3 (3%)	2 (2%)	8 30
2	B	262/283 (93%)	232 (88%)	24 (9%)	6 (2%)	8 30
2	D	258/283 (91%)	236 (92%)	18 (7%)	4 (2%)	12 40
All	All	699/766 (91%)	632 (90%)	52 (7%)	15 (2%)	9 32

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	144	LYS
2	D	174	ASN
1	A	3	PHE
1	A	58	THR
2	B	170	SER
1	C	43	GLY
1	C	24	THR
2	D	108	ALA
1	A	29	ILE
2	B	44	LEU
2	B	108	ALA

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Mol	Chain	Res	Type
2	B	151	PRO
2	B	239	ALA
2	B	240	ALA
2	D	256	VAL

5.3.2 Protein sidechains

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	73/70 (104%)	61 (84%)	12 (16%)	3 8
1	C	68/70 (97%)	52 (76%)	16 (24%)	1 2
2	B	189/188 (100%)	154 (82%)	35 (18%)	2 6
2	D	187/188 (100%)	150 (80%)	37 (20%)	1 5
All	All	517/516 (100%)	417 (81%)	100 (19%)	2 5

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	9	LEU
1	C	15	THR
1	C	25	ARG
1	C	29	ILE
1	C	34	LEU
1	C	38	SER
1	C	45	VAL
1	C	46	VAL
1	C	52	VAL
1	C	57	GLU
1	C	60	LEU
1	C	67	LEU
1	C	83	THR
1	C	86	MSE
1	C	87	LEU
1	C	89	MSE
2	D	1	MSE

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Mol	Chain	Res	Type
2	D	5	GLN
2	D	19	LEU
2	D	26	THR
2	D	29	LYS
2	D	32	ILE
2	D	39	MSE
2	D	46	THR
2	D	52	MSE
2	D	55	PHE
2	D	60	LEU
2	D	75	ARG
2	D	76	VAL
2	D	78	MSE
2	D	80	ASP
2	D	84	MSE
2	D	91	MSE
2	D	106	LYS
2	D	120	LEU
2	D	123	LEU
2	D	126	SER
2	D	133	LEU
2	D	139	LEU
2	D	146	ARG
2	D	149	LEU
2	D	159	LEU
2	D	161	LEU
2	D	171	LEU
2	D	182	LEU
2	D	189	LEU
2	D	193	LEU
2	D	227	ASN
2	D	235	THR
2	D	236	LEU
2	D	243	LEU
2	D	254	ARG
2	D	258	SER
1	A	1	MSE
1	A	24	THR
1	A	25	ARG
1	A	29	ILE
1	A	44	VAL
1	A	45	VAL

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Mol	Chain	Res	Type
1	A	46	VAL
1	A	52	VAL
1	A	60	LEU
1	A	63	LEU
1	A	64	ILE
1	A	87	LEU
2	B	3	LEU
2	B	19	LEU
2	B	20	LYS
2	B	22	MSE
2	B	41	LEU
2	B	64	LEU
2	B	79	THR
2	B	84	MSE
2	B	91	MSE
2	B	105	LEU
2	B	115	MSE
2	B	120	LEU
2	B	144	LYS
2	B	145	SER
2	B	149	LEU
2	B	163	LEU
2	B	164	THR
2	B	167	ILE
2	B	169	LEU
2	B	170	SER
2	B	172	LEU
2	B	173	TRP
2	B	185	LEU
2	B	193	LEU
2	B	194	MSE
2	B	195	THR
2	B	196	LEU
2	B	214	THR
2	B	218	VAL
2	B	230	LEU
2	B	235	THR
2	B	242	THR
2	B	243	LEU
2	B	244	LEU
2	B	258	SER

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

sidechains are listed below:

Mol	Chain	Res	Type
1	C	42	HIS
1	C	75	ASN
2	D	5	GLN
2	D	153	GLN
2	D	227	ASN
2	B	24	HIS
2	B	89	ASN
2	B	111	ASN
2	B	153	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

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	89/100 (89%)	-0.27	1 (1%)	82 80	17, 27, 62, 87	0
1	C	84/100 (84%)	0.05	2 (2%)	62 57	21, 35, 60, 78	0
2	B	248/283 (87%)	-0.16	6 (2%)	62 57	14, 29, 54, 71	0
2	D	244/283 (86%)	0.02	12 (4%)	33 27	21, 38, 72, 100	0
All	All	665/766 (86%)	-0.08	21 (3%)	51 43	14, 33, 64, 100	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	151	PRO	5.6
2	D	253	ASN	4.8
1	C	29	ILE	4.7
2	B	253	ASN	4.1
2	D	150	PHE	3.8
2	D	149	LEU	3.6
2	D	152	GLY	3.2
2	B	146	ARG	3.0
2	D	144	LYS	2.8
2	D	254	ARG	2.7
2	D	26	THR	2.7
2	D	250	ARG	2.7
2	B	110	GLU	2.6
2	D	251	ALA	2.6
2	D	257	TRP	2.5
2	B	263	GLY	2.1
2	B	254	ARG	2.1
1	A	94	PRO	2.1
2	B	71	TRP	2.0
1	C	25	ARG	2.0
2	D	153	GLN	2.0

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

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.