



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:25 PM UTC

PDB ID : 4O9P / pdb_00004o9p
Title : Crystal structure of Thermus thermophilis transhydrogenase 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

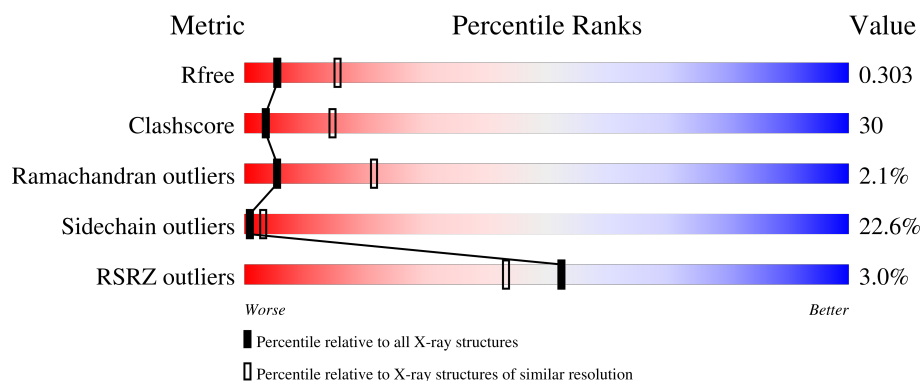
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4% 43% 37% 12% 6%
1	C	100	4% 39% 39% 8% 11%
2	B	283	2% 49% 33% 10% 7%
2	D	283	2% 48% 31% 11% 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			

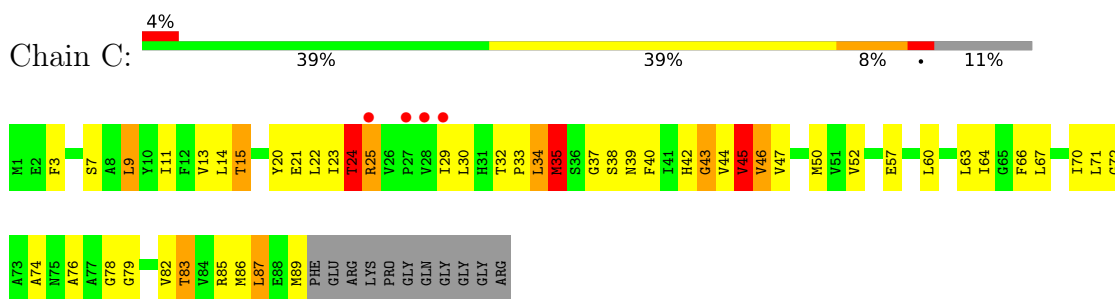
There are 16 discrepancies between the modelled and reference sequences:

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

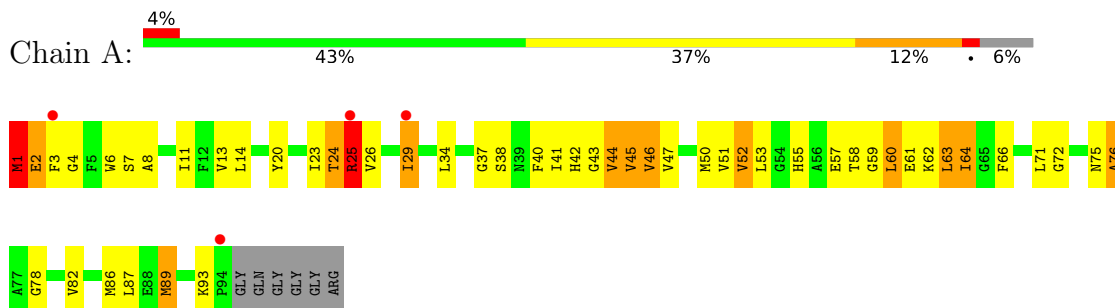
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

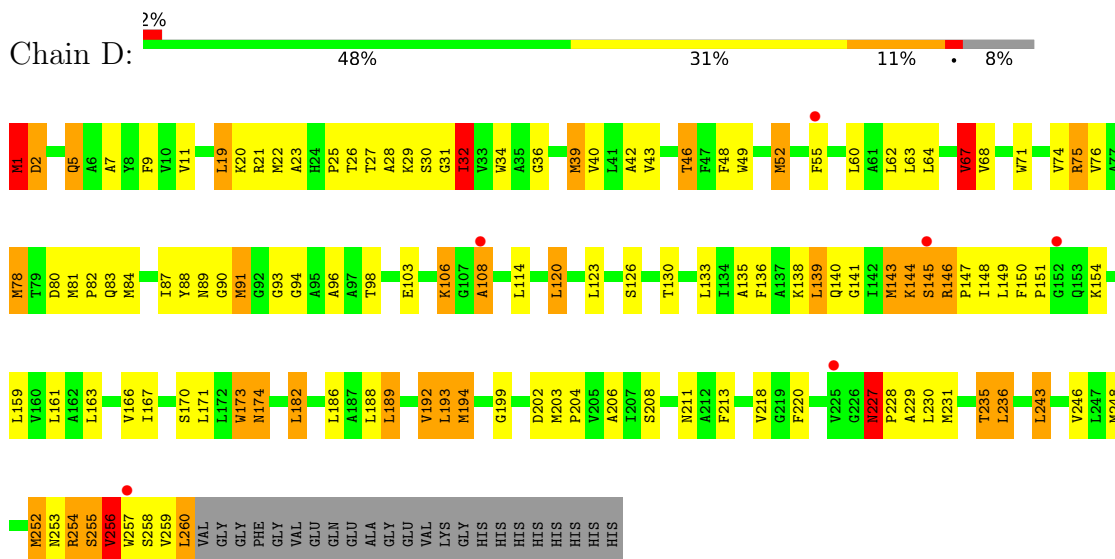
- Molecule 1: NAD(P) transhydrogenase subunit alpha 2



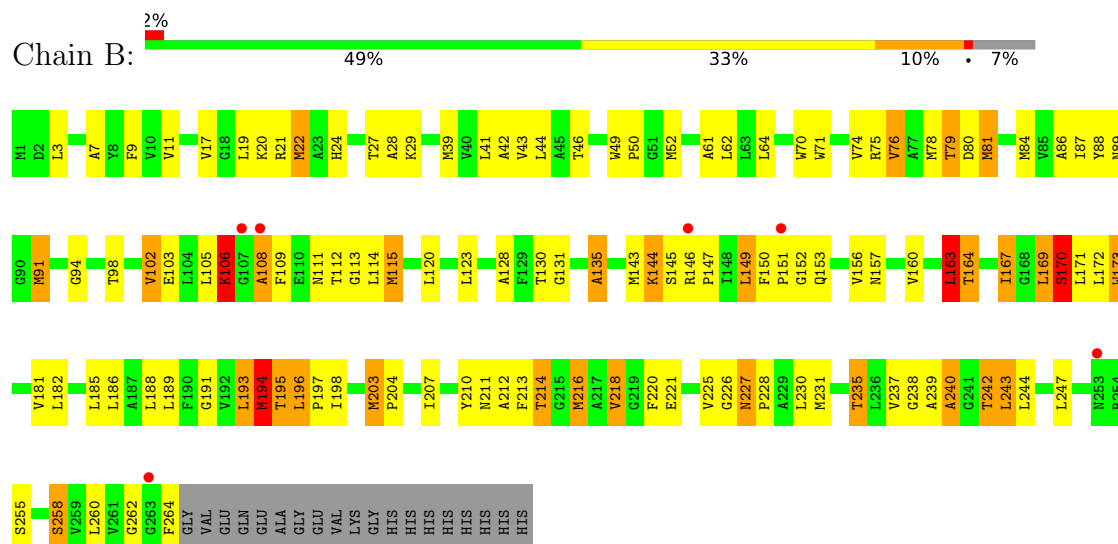
- Molecule 1: NAD(P) transhydrogenase subunit alpha 2



- Molecule 2: NAD(P) transhydrogenase subunit beta



● Molecule 2: NAD(P) transhydrogenase subunit beta



4 Data and refinement statistics

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 97.93 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.6 (97.93-2.89) 93.7 (97.93-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	0/726	1.28	8/978 (0.8%)
1	C	0.74	0/677	1.21	2/913 (0.2%)
2	B	0.95	1/1946 (0.1%)	1.32	15/2626 (0.6%)
2	D	0.81	0/1919	1.24	14/2590 (0.5%)
All	All	0.87	1/5268 (0.0%)	1.27	39/7107 (0.5%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	203	MSE	CA-C	-5.16	1.46	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	196	LEU	CA-C-N	-9.76	109.24	121.04
2	B	196	LEU	C-N-CA	-9.76	109.24	121.04
2	B	150	PHE	N-CA-C	9.69	116.94	108.22
2	D	173	TRP	N-CA-C	-8.49	96.97	110.14
2	B	227	ASN	N-CA-C	7.82	122.77	108.69
2	D	145	SER	N-CA-C	7.69	122.13	109.06
2	D	28	ALA	N-CA-C	7.42	119.06	110.97
2	D	67	VAL	N-CA-C	7.42	118.21	110.72
1	A	2	GLU	CA-C-N	7.40	135.02	121.70
1	A	2	GLU	C-N-CA	7.40	135.02	121.70
1	A	89	MSE	CG-SE-CE	-6.70	84.18	98.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	MSE	CG-SE-CE	6.52	113.27	98.92
2	D	143	MSE	N-CA-C	-6.39	106.06	114.31
2	B	216	MSE	CG-SE-CE	6.38	112.96	98.92
2	B	106	LYS	N-CA-C	-6.30	105.55	113.18
2	B	194	MSE	CB-CA-C	-6.30	100.13	110.85
2	B	81	MSE	CA-C-N	-5.98	112.75	118.97
2	B	81	MSE	C-N-CA	-5.98	112.75	118.97
1	C	35	MSE	CG-SE-CE	5.96	112.05	98.92
2	D	192	VAL	CB-CA-C	-5.84	104.50	111.97
2	D	32	ILE	N-CA-CB	5.82	118.46	110.54
2	B	260	LEU	N-CA-C	5.76	117.64	111.36
1	A	25	ARG	N-CA-C	5.69	119.41	111.90
2	D	213	PHE	N-CA-C	5.65	117.89	111.11
1	A	76	ALA	N-CA-C	5.47	116.93	110.97
2	B	102	VAL	N-CA-C	5.22	116.69	111.00
2	B	135	ALA	N-CA-C	-5.20	105.26	111.03
2	D	227	ASN	CA-C-N	5.19	124.98	119.28
2	D	227	ASN	C-N-CA	5.19	124.98	119.28
2	D	255	SER	N-CA-C	5.17	119.07	109.56
2	D	1	MSE	CG-SE-CE	5.12	110.18	98.92
2	D	2	ASP	N-CA-C	5.11	115.03	108.34
2	D	174	ASN	N-CA-C	5.07	121.61	110.80
2	B	163	LEU	CA-C-N	5.05	127.01	120.44
2	B	163	LEU	C-N-CA	5.05	127.01	120.44
1	C	45	VAL	CB-CA-C	-5.05	103.01	111.29
2	B	203	MSE	CB-CA-C	-5.04	102.27	111.64
1	A	2	GLU	CA-C-O	-5.03	116.34	121.87
1	A	86	MSE	N-CA-CB	-5.01	102.74	110.16

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	77	0
2	B	1919	0	2030	115	0
2	D	1893	0	2006	151	0
All	All	5191	0	5466	316	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 30.

All (316) 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
1:C:71:LEU:HD23	2:D:91:MSE:HE3	1.39	1.03
2:B:135:ALA:HB1	2:B:203:MSE:CE	1.88	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
2:D:32:ILE:HD13	2:D:32:ILE:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:227:ASN:C	2:D:227:ASN:HD22	1.84	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
2:D:255:SER:O	2:D:257:TRP:N	2.11	0.83
1:A:1:MSE:O	1:A:8:ALA:HB1	1.78	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:CD1	2:D:32:ILE:H	1.92	0.81
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:HD13	2:D:32:ILE:N	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
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
1:C:13:VAL:HG21	2:B:9:PHE:HZ	1.58	0.69
2:D:63:LEU:O	2:D:67:VAL:HG13	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ILE:O	1:A:44:VAL:HG22	1.94	0.68
2:B:144:LYS:H	2:B:144:LYS:HE3	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:D:231:MSE:O	2:D:235:THR:CG2	2.46	0.64
2:B:157:ASN:OD1	2:B:193:LEU:HD13	1.98	0.64
2:B:157:ASN:OD1	2:B:193:LEU:CD1	2.46	0.64
1:C:15:THR:HG22	1:A:14:LEU:HD13	1.79	0.64
2:B:210:TYR:O	2:B:214:THR:HG23	1.97	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
2:D:227:ASN:ND2	2:D:229:ALA:H	1.96	0.63
1:A:50:MSE:HE2	2:B:62:LEU:HD21	1.79	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
1:A:47:VAL:O	1:A:51:VAL:HG23	1.99	0.63
2:B:89:ASN:HD21	2:B:211:ASN:HA	1.61	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:1:MSE:HA	1:A:6:TRP:HE1	1.66	0.61
2:D:106:LYS:HD2	2:D:108:ALA:H	1.65	0.61
1:C:35:MSE:HE3	2:D:248:MSE:SE	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:TYR:CE1	2:D:243:LEU:HG	2.35	0.60
2:B:49:TRP:CD1	2:B:50:PRO:HD2	2.37	0.60
2:B:169:LEU:O	2:B:171:LEU:N	2.34	0.60
2:D:188:LEU:O	2:D:192:VAL:HG23	2.01	0.60
1:A:46:VAL:HG13	1:A:72:GLY:C	2.26	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
1:C:13:VAL:HG21	2:B:9:PHE:CZ	2.37	0.58
2:B:189:LEU:HD13	2:B:193:LEU:HG	1.85	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:D:148:ILE:O	2:D:148:ILE:HG22	2.04	0.57
2:B:103:GLU:OE2	2:B:108:ALA:HB3	2.04	0.57
1:A:24:THR:HG22	2:B:243:LEU:HD11	1.86	0.57
2:D:19:LEU:HD12	2:D:236:LEU:CD1	2.33	0.57
2:D:39:MSE:O	2:D:43:VAL:HG23	2.05	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
1:C:42:HIS:O	1:C:44:VAL:N	2.39	0.56
1:C:42:HIS:C	1:C:44:VAL:N	2.64	0.56
2:D:81:MSE:N	2:D:82:PRO:HD2	2.20	0.56
1:A:23:ILE:HG13	2:B:240:ALA:HB1	1.88	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: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
1:C:30:LEU:HD23	1:C:33:PRO:HG2	1.89	0.54
2:B:212:ALA:HB1	2:B:242:THR:HG22	1.89	0.54
2:D:94:GLY:O	2:D:98:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:TRP:CD1	2:B:75:ARG:HH21	2.26	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
1:C:42:HIS:C	1:C:44:VAL:H	2.16	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:D:106:LYS:HE3	2:D:108:ALA:C	2.34	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
2:D:120:LEU:HD13	2:D:220:PHE:CE2	2.46	0.51
1:A:23:ILE:CG1	2:B:240:ALA:HB1	2.41	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
2:D:203:MSE:O	2:D:204:PRO:C	2.54	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:227:ASN:C	2:D:227:ASN:ND2	2.58	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
1:C:66:PHE:CE1	1:C:70:ILE:HD11	2.47	0.50
2:B:135:ALA:HA	2:B:203:MSE:HE2	1.93	0.50
2:D:22:MSE:CG	2:D:31:GLY:HA3	2.42	0.49
1:C:35:MSE:CE	2:D:208:SER:HB2	2.40	0.49
1:C:82:VAL:CG1	2:D:81:MSE:HE1	2.42	0.49
2:D:42:ALA:O	2:D:46:THR:CG2	2.57	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:D:48:PHE:O	2:D:49:TRP:C	2.55	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:B:143:MSE:O	2:B:144:LYS:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ARG:HH21	1:A:25:ARG:HD3	1.78	0.48
1:C:42:HIS:O	1:C:45:VAL:HG22	2.13	0.48
2:D:167:ILE:CD1	2:D:186:LEU:HD12	2.43	0.48
2:D:9:PHE:HZ	1:A:13:VAL:HG21	1.78	0.48
2:D:227:ASN:HD22	2:D:229:ALA:H	1.60	0.48
1:C:35:MSE:HE2	2:D:208:SER:H	1.78	0.48
2:B:144:LYS:H	2:B:144:LYS:CE	2.24	0.48
1:A:23:ILE:HD12	1:A:34:LEU:HD21	1.95	0.48
2:B:130:THR:HG23	2:B:188:LEU:HD22	1.96	0.48
2:B:123:LEU:HD23	2:B:123:LEU:C	2.39	0.48
2:B:167:ILE:HG13	2:B:182:LEU:HD23	1.96	0.48
2:B:195:THR:HA	2:B:198:ILE:HD12	1.95	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
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
2:D:64:LEU:O	2:D:68:VAL:HG23	2.15	0.47
1:A:37:GLY:HA3	2:B:22:MSE:SE	2.63	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:D:227:ASN:HD22	2:D:228:PRO:N	2.10	0.46
2:B:152:GLY:O	2:B:156:VAL:HG23	2.15	0.46
1:C:9:LEU:O	1:C:13:VAL:HG23	2.15	0.46
2:B:153:GLN:CG	2:B:264:PHE:HE2	2.29	0.46
2:B:167:ILE:HG21	2:B:186:LEU:HD13	1.97	0.46
2:B:203:MSE:N	2:B:204:PRO:CD	2.78	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
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:2:GLU:HA	1:A:4:GLY:N	2.31	0.45
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
2:D:63:LEU:C	2:D:63:LEU:HD23	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:103:GLU:OE1	2:D:106:LYS:NZ	2.36	0.45
1:C:43:GLY:O	2:D:39:MSE:HE1	2.16	0.45
2:B:169:LEU:O	2:B:170:SER:C	2.59	0.44
1:C:35:MSE:HE2	2:D:208:SER:CB	2.44	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:D:163:LEU:C	2:D:167:ILE:HD12	2.42	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
1:C:32:THR:N	1:C:33:PRO:HD2	2.33	0.43
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
2:D:252:MSE:HE2	2:D:254:ARG:HG3	2.00	0.43
2:D:252:MSE:O	2:D:253:ASN:HB2	2.18	0.43
1:A:41:ILE:O	1:A:44:VAL:CG2	2.65	0.43
1:C:42:HIS:CE1	2:D:211:ASN:OD1	2.70	0.43
2:D:21:ARG:HH12	2:D:27:THR:HG22	1.82	0.43
2:D:91:MSE:HE3	2:D:91:MSE:HB3	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:HE2	2:B:91:MSE:HB3	1.86	0.43
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
1:C:39:ASN:HA	1:C:42:HIS:CE1	2.53	0.42
2:B:24:HIS:HB2	2:B:27:THR:CG2	2.41	0.42
2:B:170:SER:HA	2:B:173:TRP:CZ3	2.54	0.42
2:B:182:LEU:O	2:B:186:LEU:HD12	2.19	0.42
2:D:254:ARG:HE	2:D:254:ARG:HB3	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:GLU:OE2	2:B:108:ALA:CB	2.66	0.42
2:B:169:LEU:C	2:B:171:LEU:N	2.77	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:B:106:LYS:C	2:B:108:ALA:H	2.27	0.42
2:D:2:ASP:OD1	2:D:2:ASP:C	2.62	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:C:46:VAL:HG22	1:C:72:GLY:C	2.45	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:D:89:ASN:O	2:D:90:GLY:C	2.63	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:22:MSE:HG2	2:D:31:GLY:HA3	2.01	0.41
1:A:41:ILE:C	1:A:43:GLY:N	2.75	0.41
2:B:7:ALA:O	2:B:11:VAL:HG23	2.20	0.41
2:B:22:MSE:HB3	2:B:22:MSE:HE3	1.58	0.41
1:C:85:ARG:CZ	2:D:78:MSE:CE	2.99	0.41
1:A:1:MSE:O	1:A:8:ALA:HB2	2.14	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:HA	2:D:114:LEU:HD23	1.77	0.40
2:B:29:LYS:H	2:B:29:LYS:HG2	1.56	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
1:A:23:ILE:O	1:A:26:VAL:CG1	2.60	0.40
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
2:B:146:ARG:O	2:B:147:PRO:C	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	3	13
1	C	87/100 (87%)	82 (94%)	3 (3%)	2 (2%)	5	19
2	B	262/283 (93%)	232 (88%)	24 (9%)	6 (2%)	5	19
2	D	258/283 (91%)	236 (92%)	18 (7%)	4 (2%)	7	27
All	All	699/766 (91%)	632 (90%)	52 (7%)	15 (2%)	5	21

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
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%)	60 (82%)	13 (18%)	2	6
1	C	68/70 (97%)	48 (71%)	20 (29%)	0	1
2	B	189/188 (100%)	150 (79%)	39 (21%)	1	4
2	D	187/188 (100%)	142 (76%)	45 (24%)	1	2
All	All	517/516 (100%)	400 (77%)	117 (23%)	1	3

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	9	LEU
1	C	15	THR
1	C	24	THR
1	C	25	ARG
1	C	29	ILE
1	C	34	LEU
1	C	35	MSE
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	63	LEU
1	C	64	ILE
1	C	67	LEU
1	C	83	THR
1	C	86	MSE
1	C	87	LEU
1	C	89	MSE
2	D	1	MSE
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

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Mol	Chain	Res	Type
2	D	67	VAL
2	D	74	VAL
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	166	VAL
2	D	171	LEU
2	D	182	LEU
2	D	189	LEU
2	D	193	LEU
2	D	194	MSE
2	D	227	ASN
2	D	235	THR
2	D	236	LEU
2	D	243	LEU
2	D	246	VAL
2	D	252	MSE
2	D	254	ARG
2	D	256	VAL
2	D	258	SER
2	D	260	LEU
1	A	1	MSE
1	A	24	THR
1	A	25	ARG
1	A	29	ILE
1	A	44	VAL
1	A	45	VAL
1	A	46	VAL
1	A	52	VAL

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Mol	Chain	Res	Type
1	A	60	LEU
1	A	63	LEU
1	A	64	ILE
1	A	87	LEU
1	A	93	LYS
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	76	VAL
2	B	79	THR
2	B	84	MSE
2	B	91	MSE
2	B	105	LEU
2	B	106	LYS
2	B	114	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	181	VAL
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

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Mol	Chain	Res	Type
2	B	244	LEU
2	B	258	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	42	HIS
2	D	5	GLN
2	D	153	GLN
2	D	227	ASN
1	A	75	ASN
2	B	24	HIS
2	B	89	ASN
2	B	111	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 oligosaccharides 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, 95th 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%)	-0.11	4 (4%) 38 30	17, 27, 62, 87	0
1	C	84/100 (84%)	0.31	4 (4%) 35 28	21, 35, 60, 78	0
2	B	248/283 (87%)	0.02	6 (2%) 59 50	14, 29, 54, 71	0
2	D	244/283 (86%)	0.21	6 (2%) 58 48	21, 38, 72, 100	0
All	All	665/766 (86%)	0.11	20 (3%) 52 43	14, 33, 64, 100	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	29	ILE	7.4
1	A	25	ARG	4.1
1	A	94	PRO	3.6
1	C	28	VAL	3.5
2	B	146	ARG	3.5
1	C	27	PRO	3.3
2	B	263	GLY	3.2
2	D	108	ALA	3.1
2	D	257	TRP	3.0
1	C	25	ARG	2.8
2	D	145	SER	2.7
1	A	29	ILE	2.6
2	B	107	GLY	2.5
2	B	253	ASN	2.5
2	B	108	ALA	2.4
2	D	55	PHE	2.3
1	A	3	PHE	2.2
2	D	152	GLY	2.1
2	D	225	VAL	2.1
2	B	151	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.