



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:59 PM UTC

PDB ID : 2AW5 / pdb_00002aw5
Title : Crystal structure of a human malic enzyme
Authors : Papagrigoriou, E.; Berridge, G.; Smee, C.; Bray, J.; Arrowsmith, C.; Edwards, A.; Weigelt, J.; Sundstrom, M.; Oppermann, U.; Gileadi, O.; von Delft, F.; Structural Genomics Consortium (SGC)
Deposited on : 2005-08-31
Resolution : 2.50 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
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

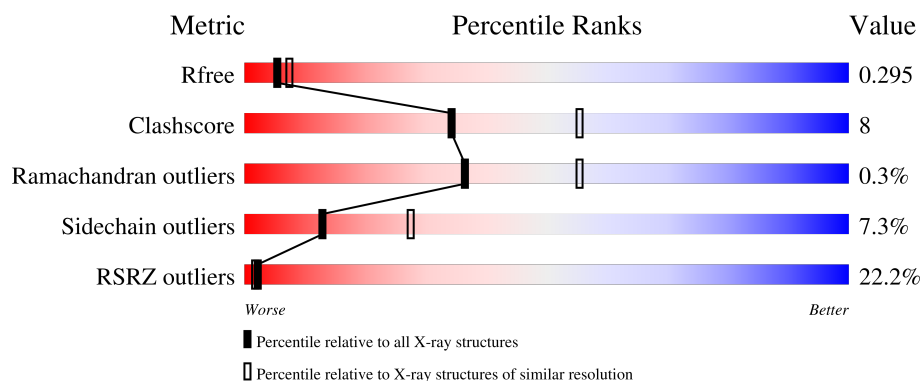
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	575	
1	B	575	
1	C	575	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11920 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 NADP-dependent malic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4004	2567	675	744	18			
1	B	536	Total	C	N	O	S	0	0	0
			3919	2500	670	730	19			
1	C	533	Total	C	N	O	S	0	0	0
			3997	2556	675	748	18			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	cloning artifact	UNP P48163
A	-9	HIS	-	cloning artifact	UNP P48163
A	-8	HIS	-	cloning artifact	UNP P48163
A	-7	HIS	-	cloning artifact	UNP P48163
A	-6	HIS	-	cloning artifact	UNP P48163
A	-5	HIS	-	cloning artifact	UNP P48163
A	-4	HIS	-	cloning artifact	UNP P48163
A	-3	SER	-	cloning artifact	UNP P48163
A	-2	SER	-	cloning artifact	UNP P48163
A	-1	GLY	-	cloning artifact	UNP P48163
A	0	VAL	-	cloning artifact	UNP P48163
A	1	ASP	-	cloning artifact	UNP P48163
A	2	LEU	-	cloning artifact	UNP P48163
A	3	GLY	-	cloning artifact	UNP P48163
A	4	THR	-	cloning artifact	UNP P48163
A	5	GLU	-	cloning artifact	UNP P48163
A	6	ASN	-	cloning artifact	UNP P48163
A	7	LEU	-	cloning artifact	UNP P48163
A	8	TYR	-	cloning artifact	UNP P48163
A	9	PHE	-	cloning artifact	UNP P48163
A	10	GLN	-	cloning artifact	UNP P48163
A	11	SER	-	cloning artifact	UNP P48163
A	12	MET	-	cloning artifact	UNP P48163

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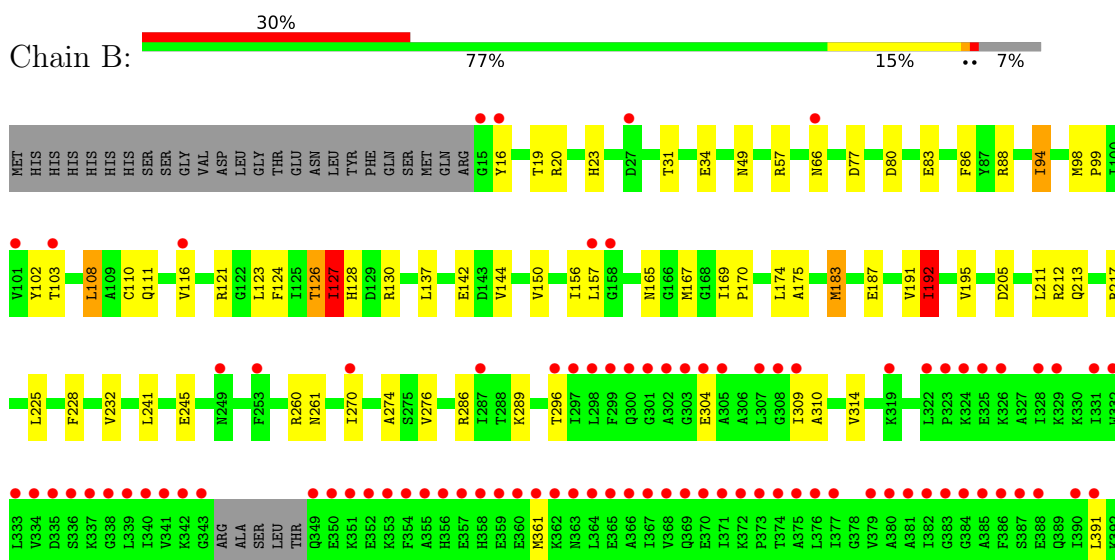
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	cloning artifact	UNP P48163
B	-9	HIS	-	cloning artifact	UNP P48163
B	-8	HIS	-	cloning artifact	UNP P48163
B	-7	HIS	-	cloning artifact	UNP P48163
B	-6	HIS	-	cloning artifact	UNP P48163
B	-5	HIS	-	cloning artifact	UNP P48163
B	-4	HIS	-	cloning artifact	UNP P48163
B	-3	SER	-	cloning artifact	UNP P48163
B	-2	SER	-	cloning artifact	UNP P48163
B	-1	GLY	-	cloning artifact	UNP P48163
B	0	VAL	-	cloning artifact	UNP P48163
B	1	ASP	-	cloning artifact	UNP P48163
B	2	LEU	-	cloning artifact	UNP P48163
B	3	GLY	-	cloning artifact	UNP P48163
B	4	THR	-	cloning artifact	UNP P48163
B	5	GLU	-	cloning artifact	UNP P48163
B	6	ASN	-	cloning artifact	UNP P48163
B	7	LEU	-	cloning artifact	UNP P48163
B	8	TYR	-	cloning artifact	UNP P48163
B	9	PHE	-	cloning artifact	UNP P48163
B	10	GLN	-	cloning artifact	UNP P48163
B	11	SER	-	cloning artifact	UNP P48163
B	12	MET	-	cloning artifact	UNP P48163
C	-10	MET	-	cloning artifact	UNP P48163
C	-9	HIS	-	cloning artifact	UNP P48163
C	-8	HIS	-	cloning artifact	UNP P48163
C	-7	HIS	-	cloning artifact	UNP P48163
C	-6	HIS	-	cloning artifact	UNP P48163
C	-5	HIS	-	cloning artifact	UNP P48163
C	-4	HIS	-	cloning artifact	UNP P48163
C	-3	SER	-	cloning artifact	UNP P48163
C	-2	SER	-	cloning artifact	UNP P48163
C	-1	GLY	-	cloning artifact	UNP P48163
C	0	VAL	-	cloning artifact	UNP P48163
C	1	ASP	-	cloning artifact	UNP P48163
C	2	LEU	-	cloning artifact	UNP P48163
C	3	GLY	-	cloning artifact	UNP P48163
C	4	THR	-	cloning artifact	UNP P48163
C	5	GLU	-	cloning artifact	UNP P48163
C	6	ASN	-	cloning artifact	UNP P48163
C	7	LEU	-	cloning artifact	UNP P48163
C	8	TYR	-	cloning artifact	UNP P48163

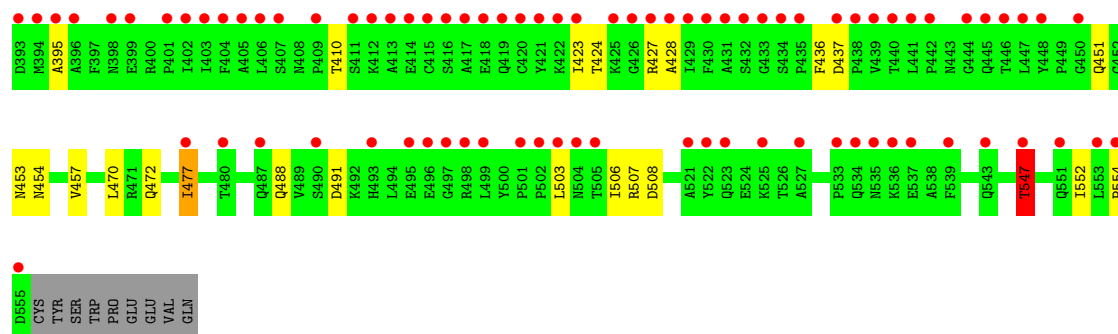
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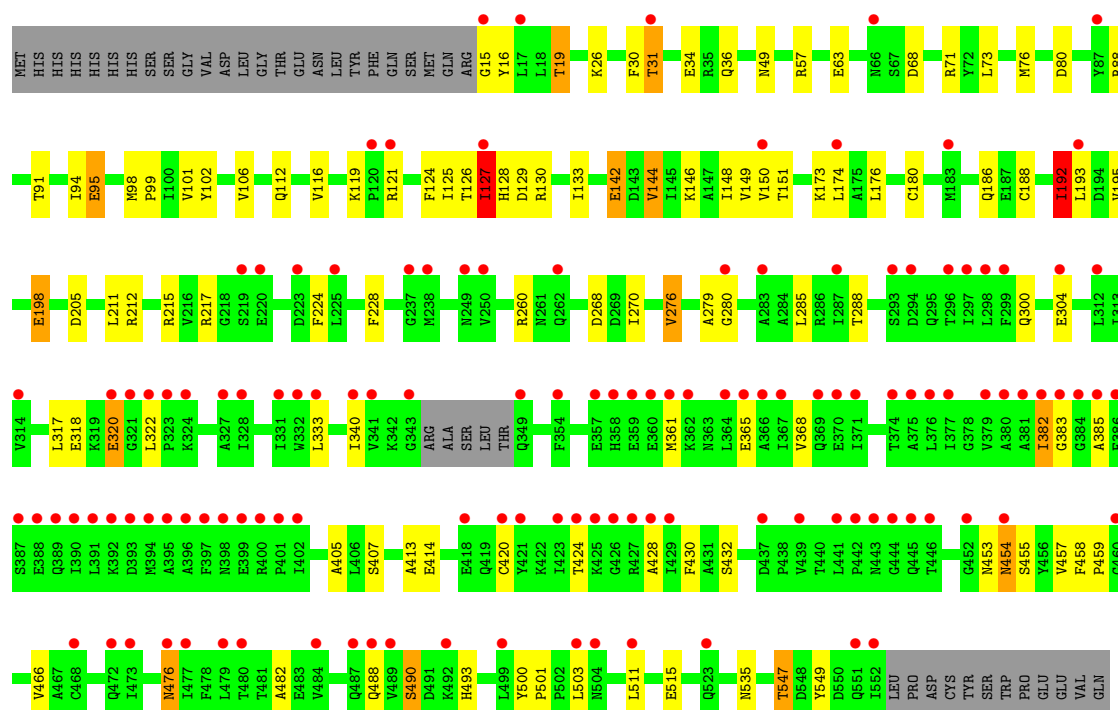
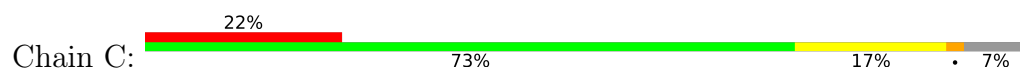
Chain	Residue	Modelled	Actual	Comment	Reference
C	9	PHE	-	cloning artifact	UNP P48163
C	10	GLN	-	cloning artifact	UNP P48163
C	11	SER	-	cloning artifact	UNP P48163
C	12	MET	-	cloning artifact	UNP P48163

- Molecule 1: NADP-dependent malic enzyme





● Molecule 1: NADP-dependent malic enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.50Å 136.96Å 117.84Å 90.00° 121.75° 90.00°	Depositor
Resolution (Å)	37.30 – 2.50 37.30 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.30-2.50) 97.7 (37.30-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.256 0.251 , 0.295	Depositor DCC
R_{free} test set	3520 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11920	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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	0.80	1/4080 (0.0%)	0.95	9/5546 (0.2%)
1	B	0.78	1/3993 (0.0%)	0.91	6/5440 (0.1%)
1	C	0.76	0/4074	0.94	6/5541 (0.1%)
All	All	0.78	2/12147 (0.0%)	0.94	21/16527 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	VAL	CA-CB	5.56	1.60	1.53
1	B	554	PRO	C-N	5.36	1.40	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	PRO	O-C-N	9.08	125.48	121.31
1	A	501	PRO	CA-C-O	-8.52	114.77	120.90
1	B	127	ILE	CB-CA-C	-7.55	101.95	112.14
1	A	276	VAL	CB-CA-C	-6.83	102.80	112.22
1	C	276	VAL	CB-CA-C	-6.75	101.70	112.16
1	C	127	ILE	CB-CA-C	-6.52	103.50	112.04
1	B	127	ILE	N-CA-CB	6.41	119.25	110.54
1	A	127	ILE	N-CA-CB	6.27	119.06	110.54
1	C	454	ASN	N-CA-C	5.63	118.95	111.75
1	C	127	ILE	N-CA-CB	5.55	117.41	110.47
1	B	547	THR	N-CA-C	-5.43	106.43	113.16
1	C	501	PRO	O-C-N	5.43	123.70	121.15
1	B	506	ILE	CB-CA-C	-5.26	104.00	112.16
1	C	192	ILE	N-CA-CB	5.25	119.26	110.86
1	A	265	THR	N-CA-C	5.21	116.43	108.52
1	B	552	ILE	N-CA-C	-5.20	106.06	111.58
1	A	340	ILE	CB-CA-C	5.17	117.22	110.96
1	A	127	ILE	CB-CA-C	-5.12	105.23	112.14
1	A	547	THR	N-CA-C	-5.11	107.00	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ASP	CB-CA-C	-5.07	110.71	116.54
1	B	192	ILE	CB-CA-C	-5.04	103.14	110.81

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	4004	0	3879	61	0
1	B	3919	0	3687	55	0
1	C	3997	0	3832	63	0
All	All	11920	0	11398	176	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 8.

All (176) 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:C:124:PHE:CD2	1:C:192:ILE:HD11	1.90	1.06
1:B:150:VAL:HG21	1:B:228:PHE:CZ	2.13	0.83
1:B:124:PHE:CD2	1:B:192:ILE:HD11	2.20	0.77
1:B:16:TYR:O	1:B:19:THR:HB	1.87	0.74
1:A:150:VAL:HG22	1:A:191:VAL:HB	1.69	0.73
1:B:150:VAL:HG22	1:B:191:VAL:HB	1.73	0.70
1:A:358:HIS:CE1	1:A:361:MET:HE2	2.30	0.67
1:B:31:THR:HG23	1:B:34:GLU:H	1.59	0.67
1:B:286:ARG:O	1:B:289:LYS:NZ	2.28	0.66
1:B:274:ALA:HA	1:B:309:ILE:HG22	1.76	0.66
1:A:150:VAL:HG21	1:A:228:PHE:CZ	2.33	0.64
1:C:124:PHE:CD2	1:C:192:ILE:CD1	2.74	0.63
1:C:126:THR:HG22	1:C:128:HIS:N	2.14	0.63
1:A:88:ARG:HD3	1:A:547:THR:HG21	1.80	0.62
1:C:126:THR:HG22	1:C:128:HIS:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ASN:HD22	1:B:454:ASN:N	1.98	0.62
1:C:285:LEU:HA	1:C:288:THR:HG22	1.81	0.61
1:A:340:ILE:HD12	1:A:355:ALA:HA	1.84	0.59
1:A:156:ILE:HD12	1:A:169:ILE:HG13	1.85	0.59
1:B:150:VAL:HG21	1:B:228:PHE:HZ	1.64	0.58
1:B:205:ASP:O	1:B:212:ARG:NH2	2.36	0.58
1:C:270:ILE:HG22	1:C:304:GLU:C	2.27	0.58
1:A:102:TYR:OH	1:A:245:GLU:OE1	2.22	0.58
1:B:477:ILE:C	1:B:477:ILE:HD12	2.28	0.58
1:C:333:LEU:HB2	1:C:340:ILE:HG12	1.84	0.58
1:B:124:PHE:CD2	1:B:192:ILE:CD1	2.87	0.57
1:C:49:ASN:ND2	1:C:57:ARG:HH12	2.03	0.57
1:C:285:LEU:HA	1:C:288:THR:CG2	2.35	0.57
1:C:150:VAL:HG21	1:C:228:PHE:CZ	2.40	0.56
1:B:102:TYR:CD2	1:B:103:THR:HG22	2.40	0.56
1:A:118:ARG:HH11	1:A:118:ARG:CG	2.18	0.56
1:A:286:ARG:NH2	1:A:489:VAL:O	2.36	0.56
1:C:124:PHE:CE2	1:C:192:ILE:HD11	2.41	0.56
1:B:144:VAL:HG23	1:B:187:GLU:HG2	1.88	0.55
1:B:167:MET:HE2	1:B:192:ILE:HD11	1.89	0.55
1:C:150:VAL:HG12	1:C:151:THR:N	2.21	0.55
1:C:26:LYS:HE2	1:C:549:TYR:HB3	1.89	0.55
1:C:276:VAL:HG13	1:C:457:VAL:HG23	1.89	0.55
1:A:148:ILE:HG22	1:A:150:VAL:HG23	1.89	0.55
1:C:16:TYR:O	1:C:19:THR:HB	2.06	0.55
1:A:88:ARG:HD3	1:A:547:THR:CG2	2.37	0.54
1:A:476:ASN:O	1:A:480:THR:HG23	2.07	0.54
1:C:126:THR:HG23	1:C:211:LEU:HD11	1.90	0.54
1:A:453:ASN:HD22	1:A:455:SER:H	1.56	0.54
1:C:174:LEU:HD22	1:C:188:CYS:HB3	1.89	0.53
1:C:31:THR:HG22	1:C:34:GLU:H	1.73	0.53
1:A:461:VAL:HG13	1:A:477:ILE:HD11	1.89	0.53
1:B:391:LEU:HB2	1:B:423:ILE:HG21	1.90	0.53
1:C:205:ASP:O	1:C:212:ARG:NH2	2.41	0.53
1:C:511:LEU:O	1:C:515:GLU:HG3	2.08	0.53
1:A:126:THR:HG22	1:A:128:HIS:N	2.24	0.53
1:A:148:ILE:CG2	1:A:150:VAL:HG23	2.40	0.52
1:A:416:SER:HG	1:A:419:GLN:H	1.56	0.52
1:B:23:HIS:HD1	1:B:83:GLU:CD	2.17	0.52
1:B:127:ILE:HG13	1:B:195:VAL:HA	1.90	0.52
1:A:270:ILE:HG22	1:A:304:GLU:C	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ILE:HD11	1:C:224:PHE:CE1	2.44	0.52
1:A:142:GLU:HG2	1:A:186:GLN:O	2.08	0.52
1:B:124:PHE:HA	1:B:192:ILE:HD12	1.90	0.52
1:A:465:VAL:HG13	1:A:470:LEU:HB2	1.91	0.52
1:A:49:ASN:ND2	1:A:57:ARG:HH12	2.08	0.52
1:A:167:MET:O	1:A:170:PRO:HD2	2.09	0.52
1:B:169:ILE:HB	1:B:170:PRO:HD3	1.92	0.51
1:C:68:ASP:HA	1:C:71:ARG:HD2	1.93	0.51
1:C:198:GLU:OE1	1:C:215:ARG:HG3	2.11	0.51
1:B:276:VAL:HG13	1:B:457:VAL:HG23	1.91	0.51
1:A:31:THR:HG22	1:A:34:GLU:CG	2.40	0.51
1:A:461:VAL:O	1:A:465:VAL:HG23	2.11	0.51
1:B:80:ASP:HB2	1:B:121:ARG:HH21	1.77	0.50
1:B:126:THR:HG22	1:B:128:HIS:N	2.26	0.50
1:B:261:ASN:O	1:B:472:GLN:NE2	2.43	0.50
1:C:150:VAL:CG1	1:C:151:THR:N	2.75	0.50
1:C:317:LEU:O	1:C:320:GLU:HG3	2.11	0.50
1:A:143:ASP:OD1	1:A:143:ASP:N	2.40	0.49
1:B:98:MET:CE	1:B:503:LEU:HD21	2.42	0.49
1:B:102:TYR:OH	1:B:245:GLU:OE1	2.30	0.49
1:C:127:ILE:HG13	1:C:195:VAL:HA	1.94	0.49
1:A:149:VAL:HG23	1:A:174:LEU:HD21	1.93	0.49
1:B:110:CYS:O	1:B:165:ASN:HB3	2.13	0.49
1:A:127:ILE:HG13	1:A:195:VAL:HA	1.95	0.49
1:A:395:ALA:HB2	1:A:424:THR:HG22	1.95	0.49
1:B:83:GLU:O	1:B:86:PHE:HB3	2.13	0.49
1:B:451:GLN:NE2	1:B:453:ASN:OD1	2.46	0.48
1:C:49:ASN:HD22	1:C:57:ARG:HH12	1.61	0.48
1:C:73:LEU:HD21	1:C:116:VAL:HG21	1.94	0.48
1:C:318:GLU:HA	1:C:322:LEU:O	2.14	0.48
1:A:270:ILE:CG2	1:A:304:GLU:HB3	2.43	0.48
1:B:126:THR:HG23	1:B:211:LEU:HD11	1.95	0.48
1:B:156:ILE:O	1:B:157:LEU:C	2.55	0.48
1:B:183:MET:HE3	1:B:183:MET:HA	1.96	0.48
1:C:176:LEU:O	1:C:180:CYS:HB2	2.14	0.48
1:A:112:GLN:HE21	1:A:115:LEU:HD12	1.78	0.48
1:C:98:MET:O	1:C:102:TYR:HB3	2.13	0.48
1:C:146:LYS:HD3	1:C:466:VAL:CG1	2.43	0.48
1:C:80:ASP:OD1	1:C:119:LYS:HD2	2.13	0.48
1:C:126:THR:HB	1:C:129:ASP:OD2	2.13	0.48
1:B:309:ILE:HG13	1:B:310:ALA:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:GLY:HA3	1:C:500:TYR:OH	2.13	0.48
1:A:18:LEU:HD21	1:A:24:LEU:HB3	1.96	0.47
1:B:49:ASN:ND2	1:B:57:ARG:HH12	2.12	0.47
1:C:125:ILE:O	1:C:193:LEU:HA	2.15	0.47
1:C:268:ASP:CG	1:C:454:ASN:HD22	2.22	0.47
1:C:407:SER:OG	1:C:414:GLU:OE2	2.31	0.47
1:C:405:ALA:O	1:C:432:SER:HA	2.15	0.47
1:B:453:ASN:HD22	1:B:453:ASN:C	2.23	0.46
1:A:16:TYR:O	1:A:19:THR:HB	2.15	0.46
1:A:412:LYS:HE2	1:B:491:ASP:OD1	2.16	0.46
1:A:162:LEU:O	1:A:165:ASN:HB2	2.16	0.46
1:C:95:GLU:HG3	1:C:503:LEU:HB2	1.97	0.46
1:B:20:ARG:NH2	1:C:80:ASP:OD2	2.48	0.45
1:C:149:VAL:HG23	1:C:174:LEU:HD21	1.97	0.45
1:B:241:LEU:C	1:B:241:LEU:HD23	2.42	0.45
1:A:150:VAL:HG21	1:A:228:PHE:HZ	1.80	0.45
1:C:535:ASN:C	1:C:535:ASN:OD1	2.58	0.45
1:A:260:ARG:NH1	1:A:271:GLN:HE22	2.15	0.45
1:C:26:LYS:HD2	1:C:30:PHE:CD2	2.52	0.45
1:B:410:THR:HG23	1:B:436:PHE:CZ	2.52	0.44
1:A:376:LEU:HG	1:A:386:PHE:CZ	2.52	0.44
1:B:123:LEU:HD11	1:B:137:LEU:HA	1.99	0.44
1:C:424:THR:HG21	1:C:428:ALA:HB2	2.00	0.44
1:C:382:ILE:HG12	1:C:385:ALA:HB2	1.99	0.44
1:B:395:ALA:HB1	1:B:427:ARG:HH22	1.83	0.44
1:C:490:SER:HB3	1:C:493:HIS:CE1	2.53	0.44
1:A:167:MET:HE2	1:A:192:ILE:HG22	2.00	0.44
1:B:124:PHE:HA	1:B:192:ILE:CD1	2.48	0.44
1:B:174:LEU:O	1:B:175:ALA:C	2.61	0.44
1:C:144:VAL:O	1:C:144:VAL:HG23	2.17	0.44
1:C:276:VAL:HG11	1:C:453:ASN:O	2.18	0.43
1:A:314:VAL:HG21	1:A:328:ILE:HD13	2.00	0.43
1:C:458:PHE:N	1:C:459:PRO:CD	2.81	0.43
1:A:68:ASP:HA	1:A:71:ARG:HD2	2.00	0.43
1:C:279:ALA:HB2	1:C:482:ALA:HA	2.01	0.43
1:A:441:LEU:HB3	1:A:442:PRO:HD2	2.01	0.43
1:B:167:MET:O	1:B:170:PRO:HD2	2.19	0.43
1:A:399:GLU:C	1:A:400:ARG:HG2	2.44	0.43
1:A:521:ALA:HA	1:A:526:THR:OG1	2.19	0.43
1:A:110:CYS:O	1:A:165:ASN:HB3	2.18	0.43
1:C:383:GLY:HA2	1:C:413:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:THR:HG21	1:A:428:ALA:HB2	1.99	0.43
1:A:49:ASN:HD22	1:A:57:ARG:HH12	1.66	0.43
1:B:98:MET:N	1:B:99:PRO:CD	2.82	0.42
1:A:169:ILE:HB	1:A:170:PRO:HD3	2.01	0.42
1:A:511:LEU:O	1:A:515:GLU:HG3	2.19	0.42
1:A:261:ASN:HA	1:A:472:GLN:HG2	2.01	0.42
1:A:293:SER:OG	1:A:320:GLU:OE1	2.31	0.42
1:B:424:THR:HG21	1:B:428:ALA:HB2	2.01	0.42
1:A:384:GLY:HA3	1:B:289:LYS:HB3	2.02	0.42
1:B:477:ILE:HD12	1:B:477:ILE:O	2.20	0.42
1:C:127:ILE:HD11	1:C:211:LEU:HD13	2.01	0.42
1:C:142:GLU:OE2	1:C:186:GLN:NE2	2.53	0.42
1:A:118:ARG:CG	1:A:118:ARG:NH1	2.80	0.42
1:B:310:ALA:O	1:B:314:VAL:HG23	2.20	0.42
1:A:198:GLU:HG2	1:A:215:ARG:HG3	2.01	0.42
1:C:420:CYS:HG	1:C:430:PHE:HD1	1.61	0.42
1:A:333:LEU:O	1:A:339:LEU:HD12	2.20	0.41
1:A:455:SER:HA	1:A:458:PHE:CE2	2.55	0.41
1:C:102:TYR:CG	1:C:176:LEU:HD11	2.56	0.41
1:C:365:GLU:O	1:C:368:VAL:HG22	2.21	0.41
1:B:127:ILE:CG1	1:B:195:VAL:HA	2.50	0.41
1:A:18:LEU:HD21	1:A:24:LEU:CB	2.51	0.41
1:A:51:GLN:HE22	1:A:547:THR:HG23	1.84	0.41
1:A:174:LEU:HD13	1:A:188:CYS:HB3	2.02	0.41
1:B:88:ARG:HD3	1:B:547:THR:HG23	2.03	0.41
1:C:15:GLY:O	1:C:16:TYR:C	2.62	0.41
1:C:476:ASN:HD22	1:C:476:ASN:N	2.19	0.41
1:C:98:MET:N	1:C:99:PRO:CD	2.84	0.41
1:C:148:ILE:HG22	1:C:150:VAL:HG23	2.02	0.41
1:A:318:GLU:HA	1:A:322:LEU:O	2.22	0.40
1:B:286:ARG:O	1:B:289:LYS:CE	2.69	0.40
1:C:88:ARG:HD3	1:C:547:THR:HG21	2.04	0.40
1:A:31:THR:HG22	1:A:34:GLU:HG3	2.02	0.40
1:A:31:THR:CG2	1:A:34:GLU:H	2.34	0.40
1:B:94:ILE:HD13	1:B:98:MET:HB2	2.04	0.40
1:B:108:LEU:HA	1:B:111:GLN:HE21	1.86	0.40
1:B:144:VAL:HG23	1:B:144:VAL:O	2.22	0.40
1:C:76:MET:O	1:C:121:ARG:NH2	2.54	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	525/575 (91%)	508 (97%)	14 (3%)	3 (1%)	21	38
1	B	532/575 (92%)	517 (97%)	14 (3%)	1 (0%)	43	63
1	C	529/575 (92%)	502 (95%)	27 (5%)	0	100	100
All	All	1586/1725 (92%)	1527 (96%)	55 (4%)	4 (0%)	36	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	GLU
1	A	128	HIS
1	B	304	GLU
1	A	19	THR

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	401/492 (82%)	370 (92%)	31 (8%)	12	25
1	B	372/492 (76%)	346 (93%)	26 (7%)	14	29
1	C	397/492 (81%)	369 (93%)	28 (7%)	13	29
All	All	1170/1476 (79%)	1085 (93%)	85 (7%)	13	27

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	19	THR
1	A	31	THR
1	A	63	GLU
1	A	94	ILE
1	A	115	LEU
1	A	116	VAL
1	A	118	ARG
1	A	126	THR
1	A	127	ILE
1	A	142	GLU
1	A	144	VAL
1	A	200	GLU
1	A	217	ARG
1	A	219	SER
1	A	225	LEU
1	A	254	ARG
1	A	260	ARG
1	A	270	ILE
1	A	276	VAL
1	A	297	ILE
1	A	300	GLN
1	A	336	SER
1	A	340	ILE
1	A	361	MET
1	A	410	THR
1	A	453	ASN
1	A	477	ILE
1	A	480	THR
1	A	488	GLN
1	A	547	THR
1	B	66	ASN
1	B	77	ASP
1	B	94	ILE
1	B	108	LEU
1	B	116	VAL
1	B	126	THR
1	B	127	ILE
1	B	130	ARG
1	B	142	GLU
1	B	183	MET
1	B	192	ILE
1	B	213	GLN

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Mol	Chain	Res	Type
1	B	217	ARG
1	B	225	LEU
1	B	232	VAL
1	B	260	ARG
1	B	270	ILE
1	B	296	THR
1	B	361	MET
1	B	437	ASP
1	B	470	LEU
1	B	477	ILE
1	B	488	GLN
1	B	507	ARG
1	B	508	ASP
1	B	547	THR
1	C	19	THR
1	C	31	THR
1	C	36	GLN
1	C	63	GLU
1	C	91	THR
1	C	94	ILE
1	C	95	GLU
1	C	101	VAL
1	C	106	VAL
1	C	112	GLN
1	C	127	ILE
1	C	130	ARG
1	C	142	GLU
1	C	144	VAL
1	C	173	LYS
1	C	192	ILE
1	C	198	GLU
1	C	217	ARG
1	C	260	ARG
1	C	300	GLN
1	C	320	GLU
1	C	361	MET
1	C	382	ILE
1	C	455	SER
1	C	476	ASN
1	C	488	GLN
1	C	490	SER
1	C	547	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	23	HIS
1	A	49	ASN
1	A	51	GLN
1	A	61	ASN
1	A	111	GLN
1	A	112	GLN
1	A	186	GLN
1	A	243	GLN
1	A	300	GLN
1	A	443	ASN
1	A	453	ASN
1	A	488	GLN
1	B	49	ASN
1	B	61	ASN
1	B	111	GLN
1	B	239	ASN
1	B	262	GLN
1	B	419	GLN
1	B	451	GLN
1	B	453	ASN
1	B	488	GLN
1	C	36	GLN
1	C	49	ASN
1	C	186	GLN
1	C	213	GLN
1	C	369	GLN
1	C	443	ASN
1	C	476	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	531/575 (92%)	1.00	56 (10%)	11 10	25, 60, 79, 87	0
1	B	536/575 (93%)	1.60	170 (31%)	1 1	25, 63, 84, 95	0
1	C	533/575 (92%)	1.46	129 (24%)	2 1	25, 63, 79, 93	0
All	All	1600/1725 (92%)	1.36	355 (22%)	2 2	25, 62, 81, 95	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	444	GLY	7.2
1	C	552	ILE	7.0
1	B	445	GLN	6.8
1	B	441	LEU	6.5
1	B	380	ALA	5.7
1	B	555	ASP	5.4
1	B	446	THR	5.2
1	B	358	HIS	5.0
1	C	370	GLU	5.0
1	B	299	PHE	4.9
1	C	442	PRO	4.9
1	B	341	VAL	4.9
1	B	382	ILE	4.8
1	B	355	ALA	4.8
1	B	298	LEU	4.7
1	B	300	GLN	4.6
1	B	384	GLY	4.6
1	B	417	ALA	4.6
1	B	350	GLU	4.5
1	B	365	GLU	4.5
1	B	413	ALA	4.5
1	B	420	CYS	4.5
1	B	305	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	354	PHE	4.5
1	B	442	PRO	4.4
1	B	381	ALA	4.4
1	B	416	SER	4.4
1	B	360	GLU	4.4
1	B	308	GLY	4.3
1	B	439	VAL	4.3
1	B	411	SER	4.3
1	C	150	VAL	4.2
1	C	391	LEU	4.2
1	A	341	VAL	4.1
1	C	395	ALA	4.1
1	C	332	TRP	4.1
1	B	367	ILE	4.1
1	A	343	GLY	4.1
1	B	385	ALA	4.0
1	B	386	PHE	4.0
1	B	447	LEU	4.0
1	B	448	TYR	4.0
1	A	350	GLU	3.9
1	B	343	GLY	3.9
1	B	435	PRO	3.9
1	B	421	TYR	3.9
1	B	349	GLN	3.9
1	B	418	GLU	3.9
1	C	349	GLN	3.9
1	C	397	PHE	3.9
1	A	349	GLN	3.9
1	C	388	GLU	3.9
1	C	341	VAL	3.9
1	C	423	ILE	3.8
1	B	433	GLY	3.8
1	B	440	THR	3.8
1	B	328	ILE	3.8
1	B	377	ILE	3.8
1	B	357	GLU	3.8
1	A	327	ALA	3.8
1	B	404	PHE	3.8
1	B	304	GLU	3.8
1	B	391	LEU	3.8
1	B	342	LYS	3.7
1	B	553	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	551	GLN	3.7
1	C	425	LYS	3.7
1	C	381	ALA	3.7
1	B	430	PHE	3.7
1	C	220	GLU	3.7
1	B	333	LEU	3.7
1	B	535	ASN	3.7
1	B	396	ALA	3.7
1	B	415	CYS	3.7
1	B	337	LYS	3.7
1	B	332	TRP	3.6
1	C	250	VAL	3.6
1	B	414	GLU	3.6
1	C	445	GLN	3.6
1	B	394	MET	3.6
1	C	390	ILE	3.6
1	B	450	GLY	3.6
1	C	444	GLY	3.6
1	B	334	VAL	3.5
1	C	380	ALA	3.5
1	C	443	ASN	3.5
1	B	101	VAL	3.5
1	A	355	ALA	3.5
1	B	15	GLY	3.4
1	B	393	ASP	3.4
1	B	502	PRO	3.4
1	C	382	ILE	3.4
1	B	496	GLU	3.4
1	B	368	VAL	3.3
1	C	15	GLY	3.3
1	C	365	GLU	3.3
1	C	389	GLN	3.3
1	C	401	PRO	3.3
1	C	66	ASN	3.3
1	C	399	GLU	3.3
1	B	402	ILE	3.3
1	C	127	ILE	3.3
1	B	375	ALA	3.3
1	C	396	ALA	3.3
1	B	373	PRO	3.2
1	C	441	LEU	3.2
1	B	390	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	375	ALA	3.2
1	B	322	LEU	3.2
1	C	343	GLY	3.2
1	B	431	ALA	3.2
1	B	369	GLN	3.2
1	C	324	LYS	3.2
1	C	361	MET	3.2
1	B	301	GLY	3.2
1	B	407	SER	3.2
1	B	426	GLY	3.2
1	C	328	ILE	3.2
1	C	504	ASN	3.1
1	B	287	ILE	3.1
1	C	387	SER	3.1
1	A	340	ILE	3.1
1	C	427	ARG	3.1
1	B	302	ALA	3.1
1	B	428	ALA	3.1
1	B	422	LYS	3.1
1	B	533	PRO	3.1
1	B	364	LEU	3.1
1	C	219	SER	3.1
1	C	331	ILE	3.1
1	A	381	ALA	3.1
1	C	386	PHE	3.1
1	C	473	ILE	3.1
1	B	419	GLN	3.0
1	C	393	ASP	3.0
1	B	403	ILE	3.0
1	C	283	ALA	3.0
1	A	550	ASP	3.0
1	C	523	GLN	3.0
1	B	395	ALA	3.0
1	A	15	GLY	3.0
1	B	296	THR	3.0
1	C	428	ALA	3.0
1	A	16	TYR	3.0
1	B	307	LEU	3.0
1	B	412	LYS	3.0
1	B	297	ILE	2.9
1	B	352	GLU	2.9
1	C	322	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	539	PHE	2.9
1	C	364	LEU	2.9
1	C	376	LEU	2.9
1	B	16	TYR	2.9
1	B	359	GLU	2.9
1	C	383	GLY	2.9
1	B	356	HIS	2.9
1	B	366	ALA	2.9
1	C	487	GLN	2.9
1	B	371	ILE	2.8
1	B	493	HIS	2.8
1	B	554	PRO	2.8
1	B	398	ASN	2.8
1	B	432	SER	2.8
1	A	339	LEU	2.8
1	B	309	ILE	2.8
1	C	296	THR	2.8
1	B	335	ASP	2.8
1	A	249	ASN	2.8
1	B	434	SER	2.8
1	B	323	PRO	2.8
1	A	360	GLU	2.8
1	B	388	GLU	2.8
1	A	433	GLY	2.7
1	B	336	SER	2.7
1	B	406	LEU	2.7
1	C	327	ALA	2.7
1	C	394	MET	2.7
1	C	297	ILE	2.7
1	B	438	PRO	2.7
1	B	339	LEU	2.7
1	B	505	THR	2.7
1	C	31	THR	2.7
1	C	371	ILE	2.7
1	B	319	LYS	2.7
1	B	504	ASN	2.7
1	B	157	LEU	2.7
1	B	361	MET	2.7
1	A	380	ALA	2.7
1	C	551	GLN	2.7
1	B	338	GLY	2.6
1	A	94	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	401	PRO	2.6
1	C	468	CYS	2.6
1	C	400	ARG	2.6
1	C	454	ASN	2.6
1	B	495	GLU	2.6
1	C	293	SER	2.6
1	A	302	ALA	2.6
1	C	421	TYR	2.6
1	C	238	MET	2.6
1	C	503	LEU	2.6
1	B	374	THR	2.6
1	C	366	ALA	2.6
1	B	497	GLY	2.6
1	C	287	ILE	2.6
1	C	298	LEU	2.6
1	A	332	TRP	2.6
1	C	121	ARG	2.6
1	C	429	ILE	2.6
1	B	499	LEU	2.6
1	C	304	GLU	2.6
1	B	487	GLN	2.6
1	C	385	ALA	2.6
1	C	357	GLU	2.5
1	C	359	GLU	2.5
1	A	18	LEU	2.5
1	B	503	LEU	2.5
1	A	443	ASN	2.5
1	B	551	GLN	2.5
1	C	369	GLN	2.5
1	B	490	SER	2.5
1	B	525	LYS	2.5
1	C	321	GLY	2.5
1	C	384	GLY	2.5
1	C	460	GLY	2.5
1	B	249	ASN	2.5
1	C	340	ILE	2.5
1	A	365	GLU	2.4
1	C	437	ASP	2.4
1	C	472	GLN	2.4
1	A	121	ARG	2.4
1	C	183	MET	2.4
1	C	367	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	354	PHE	2.4
1	C	489	VAL	2.4
1	B	325	GLU	2.4
1	B	329	LYS	2.4
1	A	383	GLY	2.4
1	A	429	ILE	2.4
1	C	402	ILE	2.4
1	B	353	LYS	2.4
1	B	547	THR	2.4
1	C	480	THR	2.4
1	A	506	ILE	2.4
1	B	534	GLN	2.4
1	A	31	THR	2.3
1	B	376	LEU	2.3
1	B	437	ASP	2.3
1	C	484	VAL	2.3
1	B	405	ALA	2.3
1	A	410	THR	2.3
1	C	193	LEU	2.3
1	A	436	PHE	2.3
1	C	379	VAL	2.3
1	C	320	GLU	2.3
1	A	66	ASN	2.3
1	B	427	ARG	2.3
1	A	36	GLN	2.3
1	B	270	ILE	2.3
1	B	351	LYS	2.3
1	A	370	GLU	2.3
1	C	418	GLU	2.3
1	C	420	CYS	2.3
1	C	87	TYR	2.3
1	B	409	PRO	2.3
1	C	374	THR	2.3
1	C	424	THR	2.3
1	A	356	HIS	2.3
1	A	382	ILE	2.3
1	C	377	ILE	2.3
1	B	362	LYS	2.3
1	B	425	LYS	2.3
1	B	536	LYS	2.3
1	C	120	PRO	2.3
1	C	323	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	363	ASN	2.2
1	B	480	THR	2.2
1	C	237	GLY	2.2
1	C	426	GLY	2.2
1	A	115	LEU	2.2
1	A	270	ILE	2.2
1	A	470	LEU	2.2
1	B	379	VAL	2.2
1	A	310	ALA	2.2
1	C	249	ASN	2.2
1	B	543	GLN	2.2
1	B	303	GLY	2.2
1	C	452	GLY	2.2
1	A	377	ILE	2.2
1	C	477	ILE	2.2
1	C	223	ASP	2.2
1	A	352	GLU	2.2
1	B	370	GLU	2.2
1	C	314	VAL	2.2
1	A	330	LYS	2.2
1	C	362	LYS	2.2
1	A	303	GLY	2.2
1	A	92	SER	2.2
1	B	326	LYS	2.2
1	B	372	LYS	2.2
1	C	492	LYS	2.2
1	C	262	GLN	2.2
1	C	333	LEU	2.2
1	B	429	ILE	2.2
1	B	477	ILE	2.2
1	B	116	VAL	2.1
1	B	521	ALA	2.1
1	C	225	LEU	2.1
1	B	331	ILE	2.1
1	B	423	ILE	2.1
1	B	522	TYR	2.1
1	B	399	GLU	2.1
1	C	488	GLN	2.1
1	B	527	ALA	2.1
1	A	230	GLU	2.1
1	C	294	ASP	2.1
1	A	361	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	439	VAL	2.1
1	C	439	VAL	2.1
1	C	398	ASN	2.1
1	B	158	GLY	2.1
1	C	312	LEU	2.1
1	A	507	ARG	2.1
1	B	498	ARG	2.1
1	A	351	LYS	2.1
1	A	358	HIS	2.1
1	A	157	LEU	2.1
1	C	17	LEU	2.1
1	C	479	LEU	2.1
1	C	499	LEU	2.1
1	B	383	GLY	2.1
1	C	360	GLU	2.1
1	B	340	ILE	2.1
1	B	324	LYS	2.1
1	C	392	LYS	2.1
1	B	27	ASP	2.1
1	B	387	SER	2.1
1	C	358	HIS	2.1
1	C	299	PHE	2.0
1	A	306	ALA	2.0
1	C	174	LEU	2.0
1	C	476	ASN	2.0
1	C	511	LEU	2.0
1	C	446	THR	2.0
1	B	523	GLN	2.0
1	B	253	PHE	2.0
1	A	391	LEU	2.0
1	B	537	GLU	2.0
1	A	261	ASN	2.0
1	B	66	ASN	2.0
1	C	280	GLY	2.0
1	B	103	THR	2.0
1	A	409	PRO	2.0
1	A	502	PRO	2.0
1	B	501	PRO	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 [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.