



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:31 AM UTC

PDB ID : 2WO5 / pdb_00002wo5
Title : Structure of wild type E. coli N-acetylneuraminic acid lyase in space group P21 crystal form I
Authors : Campeotto, I.; Bolt, A.H.; Harman, T.A.; Trinh, C.H.; Dennis, C.A.; Phillips, S.E.V.; Pearson, A.R.; Nelson, A.; Berry, A.
Deposited on : 2009-07-21
Resolution : 2.20 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

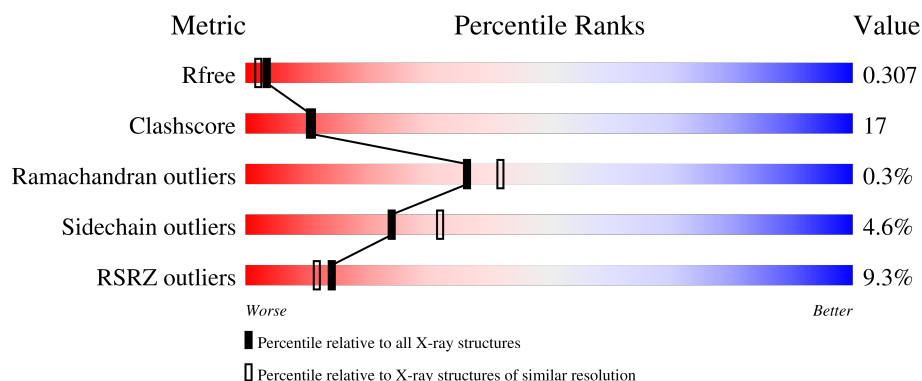
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	304	19% 62% 35% ..
1	B	304	8% 57% 36% ..
1	C	304	5% 63% 32% ..
1	D	304	5% 66% 28% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9335 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 N-ACETYLNEURAMINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	3	0
			2329	1483	397	438	11			
1	B	293	Total	C	N	O	S	0	4	0
			2285	1459	384	431	11			
1	C	295	Total	C	N	O	S	0	0	0
			2279	1452	386	431	10			
1	D	294	Total	C	N	O	S	0	1	0
			2273	1450	382	430	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP P0A6L4
A	-5	GLU	-	expression tag	UNP P0A6L4
A	-4	HIS	-	expression tag	UNP P0A6L4
A	-3	HIS	-	expression tag	UNP P0A6L4
A	-2	HIS	-	expression tag	UNP P0A6L4
A	-1	HIS	-	expression tag	UNP P0A6L4
A	0	HIS	-	expression tag	UNP P0A6L4
A	1	HIS	-	expression tag	UNP P0A6L4
B	-6	MET	-	expression tag	UNP P0A6L4
B	-5	GLU	-	expression tag	UNP P0A6L4
B	-4	HIS	-	expression tag	UNP P0A6L4
B	-3	HIS	-	expression tag	UNP P0A6L4
B	-2	HIS	-	expression tag	UNP P0A6L4
B	-1	HIS	-	expression tag	UNP P0A6L4
B	0	HIS	-	expression tag	UNP P0A6L4
B	1	HIS	-	expression tag	UNP P0A6L4
C	-6	MET	-	expression tag	UNP P0A6L4
C	-5	GLU	-	expression tag	UNP P0A6L4
C	-4	HIS	-	expression tag	UNP P0A6L4
C	-3	HIS	-	expression tag	UNP P0A6L4
C	-2	HIS	-	expression tag	UNP P0A6L4

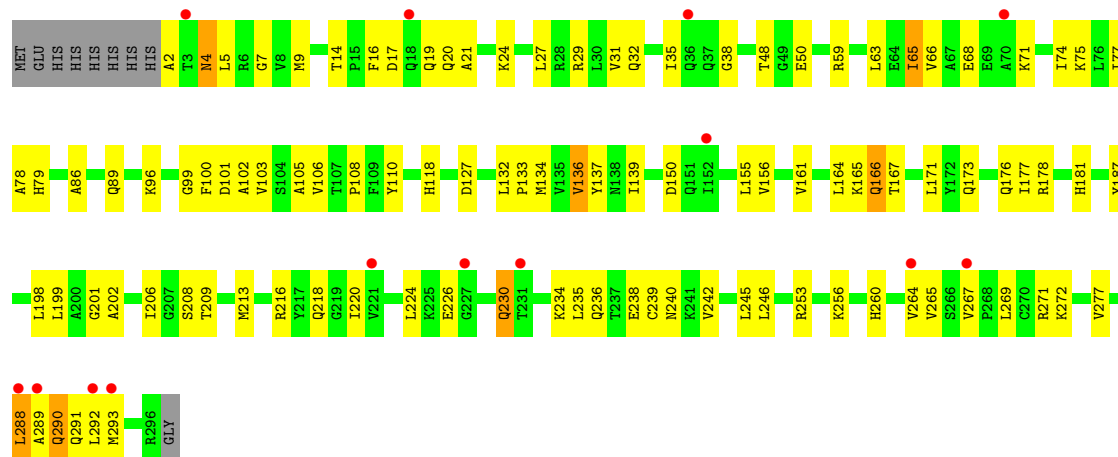
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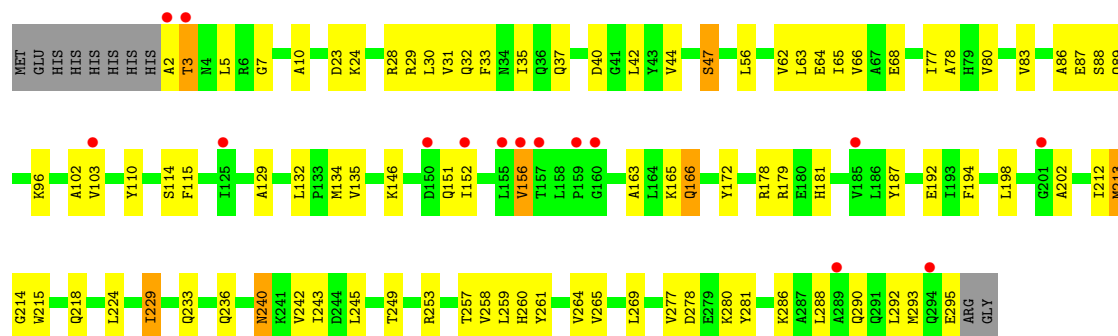
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	expression tag	UNP P0A6L4
C	0	HIS	-	expression tag	UNP P0A6L4
C	1	HIS	-	expression tag	UNP P0A6L4
D	-6	MET	-	expression tag	UNP P0A6L4
D	-5	GLU	-	expression tag	UNP P0A6L4
D	-4	HIS	-	expression tag	UNP P0A6L4
D	-3	HIS	-	expression tag	UNP P0A6L4
D	-2	HIS	-	expression tag	UNP P0A6L4
D	-1	HIS	-	expression tag	UNP P0A6L4
D	0	HIS	-	expression tag	UNP P0A6L4
D	1	HIS	-	expression tag	UNP P0A6L4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	35	Total O 35 35	0	0
2	B	40	Total O 40 40	0	0
2	C	53	Total O 53 53	0	0
2	D	41	Total O 41 41	0	0



• Molecule 1: N-ACETYLNEURAMINATE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.80Å 142.17Å 84.18Å 90.00° 109.01° 90.00°	Depositor
Resolution (Å)	71.09 – 2.20 71.09 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.09-2.20) 99.8 (71.09-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0097	Depositor
R, R_{free}	0.211 , 0.272 (Not available) , 0.307	Depositor DCC
R_{free} test set	3186 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.628 for H,K,L 0.372 for -H,-K,H+L	Depositor
Outliers	0 of 61658 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9335	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.78	0/2381	0.98	6/3222 (0.2%)
1	B	0.81	1/2337 (0.0%)	1.02	3/3162 (0.1%)
1	C	0.90	0/2319	1.07	10/3139 (0.3%)
1	D	0.84	2/2316 (0.1%)	1.01	5/3135 (0.2%)
All	All	0.83	3/9353 (0.0%)	1.02	24/12658 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	240	ASN	C-O	-6.15	1.16	1.24
1	B	192	GLU	C-O	-5.17	1.17	1.24
1	D	47	SER	C-O	-5.14	1.18	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	GLN	N-CA-C	11.76	123.84	111.14
1	C	177	ILE	N-CA-C	-7.87	104.13	111.45
1	C	14	THR	CA-C-N	6.53	126.29	119.76
1	C	14	THR	C-N-CA	6.53	126.29	119.76
1	D	44	VAL	N-CA-C	6.23	116.90	108.17
1	B	192	GLU	N-CA-C	6.19	120.44	113.01
1	B	213	MET	N-CA-C	6.18	120.93	109.56
1	C	7	GLY	N-CA-C	6.05	119.59	110.75
1	D	7	GLY	N-CA-C	5.93	118.63	110.56
1	D	83	VAL	N-CA-C	-5.89	105.00	110.53
1	A	107	THR	CA-C-N	-5.84	113.67	119.92
1	A	107	THR	C-N-CA	-5.84	113.67	119.92
1	C	290	GLN	N-CA-C	-5.83	104.84	111.14
1	D	66	VAL	N-CA-C	5.80	115.99	110.42
1	C	288	LEU	N-CA-C	-5.79	105.05	111.36
1	B	250	GLY	N-CA-C	-5.52	100.09	113.18
1	C	181	HIS	CA-C-N	5.44	125.52	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	181	HIS	C-N-CA	5.44	125.52	119.32
1	A	7	GLY	N-CA-C	5.40	117.39	110.96
1	C	127	ASP	N-CA-C	5.28	116.84	111.14
1	A	68	GLU	N-CA-C	-5.20	105.04	111.33
1	A	296	ARG	N-CA-C	-5.13	105.86	112.68
1	D	47	SER	N-CA-CB	5.11	117.42	110.01
1	C	65	ILE	CB-CA-C	-5.05	105.43	112.04

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	2329	0	2348	78	0
1	B	2285	0	2317	95	0
1	C	2279	0	2300	77	0
1	D	2273	0	2296	69	0
2	A	35	0	0	2	0
2	B	40	0	0	1	0
2	C	53	0	0	0	0
2	D	41	0	0	1	0
All	All	9335	0	9261	310	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 17.

All (310) 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:168:SER:C	1:B:190:TYR:HE2	1.58	1.10
1:B:168:SER:CA	1:B:190:TYR:HE2	1.68	1.06
1:B:168:SER:C	1:B:190:TYR:CE2	2.36	1.03
1:C:20:GLN:HE22	1:C:272:LYS:H	1.12	0.92
1:C:79:HIS:HE1	1:C:106:VAL:H	1.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:VAL:O	1:A:255:LEU:HD12	1.70	0.90
1:C:166:GLN:HA	1:C:166:GLN:HE21	1.36	0.88
1:B:169:GLY:N	1:B:190:TYR:CE2	2.43	0.86
1:B:168:SER:CA	1:B:190:TYR:CE2	2.58	0.86
1:B:188:ASN:ND2	1:B:190:TYR:O	2.13	0.81
1:C:108:PRO:HD2	1:C:118:HIS:CD2	2.17	0.79
1:D:10:ALA:HB3	1:D:42:LEU:HD23	1.65	0.79
1:A:8:VAL:HG12	1:A:39:ILE:HD11	1.65	0.78
1:A:213[B]:MET:HE1	1:A:239:CYS:HA	1.68	0.75
1:D:2:ALA:HB1	1:D:5:LEU:HD12	1.67	0.74
1:A:8:VAL:HG12	1:A:39:ILE:CD1	2.17	0.74
1:B:209:THR:O	1:B:212:ILE:HG12	1.87	0.74
1:C:20:GLN:HE22	1:C:272:LYS:N	1.86	0.74
1:C:20:GLN:NE2	1:C:272:LYS:H	1.85	0.74
1:B:32:GLN:HA	1:B:32:GLN:NE2	2.02	0.73
1:B:237:THR:HG22	1:D:179:ARG:HD3	1.71	0.73
1:A:218[A]:GLN:OE1	1:A:218[A]:GLN:HA	1.89	0.72
1:C:108:PRO:HD2	1:C:118:HIS:HD2	1.53	0.71
1:B:159:PRO:O	2:B:2025:HOH:O	2.06	0.71
1:C:230:GLN:H	1:C:230:GLN:HE21	1.37	0.71
1:C:289:ALA:O	1:C:293:MET:HG3	1.90	0.71
1:B:70:ALA:HB3	1:B:76:LEU:HD11	1.72	0.70
1:C:48:THR:HG21	1:C:208:SER:HB3	1.74	0.70
1:B:242:VAL:O	1:B:245:LEU:N	2.26	0.69
1:D:178:ARG:NH1	1:D:181:HIS:O	2.27	0.68
1:A:171:LEU:HD12	1:C:171:LEU:HD12	1.74	0.67
1:C:79:HIS:CE1	1:C:106:VAL:H	2.08	0.67
1:C:86:ALA:HA	1:C:89:GLN:HE21	1.58	0.67
1:D:236:GLN:HE21	1:D:240:ASN:ND2	1.92	0.66
1:A:156:VAL:HA	1:A:161:VAL:HG11	1.77	0.66
1:A:229:ILE:HD12	1:C:224:LEU:O	1.96	0.65
1:B:245:LEU:O	1:B:249:THR:HG23	1.96	0.65
1:A:10:ALA:HB3	1:A:42:LEU:HD22	1.78	0.65
1:C:173:GLN:HA	1:C:176:GLN:HE21	1.62	0.65
1:C:253:ARG:HG3	1:C:277:VAL:HG22	1.78	0.65
1:C:139:ILE:HG23	1:C:139:ILE:O	1.97	0.65
1:B:28:ARG:NH1	1:B:69:GLU:OE2	2.28	0.64
1:D:24:LYS:HD3	1:D:65:ILE:HD11	1.79	0.64
1:C:136:VAL:HG12	1:C:164:LEU:HD13	1.80	0.63
1:D:10:ALA:HB3	1:D:42:LEU:CD2	2.29	0.63
1:B:5:LEU:O	1:B:9:MET:HE2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:SER:N	1:B:190:TYR:HE2	1.96	0.62
1:D:135:VAL:HG22	1:D:163:ALA:HB3	1.80	0.62
1:A:45:GLY:O	1:A:79:HIS:HD2	1.83	0.62
1:C:267:VAL:HG11	1:C:269:LEU:HD12	1.80	0.62
1:C:230:GLN:H	1:C:230:GLN:NE2	1.99	0.61
1:A:35:ILE:HG22	1:A:74:ILE:HD13	1.83	0.61
1:B:168:SER:N	1:B:190:TYR:CE2	2.69	0.60
1:D:28:ARG:O	1:D:32:GLN:HG2	2.01	0.60
1:B:85:THR:O	1:B:89:GLN:HG3	2.01	0.60
1:C:32:GLN:HA	1:C:35:ILE:HD12	1.84	0.60
1:C:136:VAL:HG12	1:C:164:LEU:CD1	2.32	0.59
1:C:27:LEU:HD23	1:C:65:ILE:HD12	1.83	0.59
1:A:27:LEU:O	1:A:31:VAL:HG23	2.03	0.59
1:A:17:ASP:OD2	1:A:21:ALA:HB3	2.03	0.59
1:A:29:ARG:HB3	1:A:264:VAL:HG13	1.85	0.59
1:B:150:ASP:HA	1:B:153:ASN:HD22	1.68	0.58
1:C:290:GLN:HA	1:C:293:MET:HE2	1.84	0.58
1:B:26:SER:O	1:B:27:LEU:C	2.45	0.58
1:B:11:ALA:HA	1:B:43:TYR:HB3	1.86	0.58
1:B:31:VAL:HG11	1:B:69:GLU:HB2	1.86	0.58
1:C:48:THR:CG2	1:C:208:SER:HB3	2.33	0.58
1:D:253:ARG:HG3	1:D:277:VAL:CG2	2.33	0.58
1:A:192:GLU:HG2	1:A:193:ILE:HG23	1.86	0.58
1:C:216:ARG:O	1:C:220:ILE:HG13	2.03	0.58
1:D:213[B]:MET:CE	1:D:242:VAL:HG11	2.34	0.58
1:A:198:LEU:HD23	1:A:202:ALA:HB3	1.86	0.57
1:D:166:GLN:HA	1:D:166:GLN:HE21	1.68	0.57
1:A:71:LYS:O	2:A:2010:HOH:O	2.18	0.57
1:B:190:TYR:HB2	1:B:193:ILE:HG12	1.87	0.57
1:A:31:VAL:O	1:A:35:ILE:HG23	2.05	0.57
1:B:166:GLN:HE21	1:B:166:GLN:HA	1.70	0.57
1:D:253:ARG:HG3	1:D:277:VAL:HG23	1.86	0.57
1:A:198:LEU:HA	1:A:202:ALA:HB3	1.87	0.56
1:A:195:ALA:N	1:A:236:GLN:OE1	2.21	0.56
1:A:234:LYS:O	1:A:238:GLU:HG2	2.06	0.56
1:D:115:PHE:CE1	1:D:151:GLN:HB3	2.41	0.56
1:D:245:LEU:HD23	1:D:288:LEU:HD22	1.88	0.56
1:B:152:ILE:O	1:B:156:VAL:HG13	2.06	0.55
1:A:41:GLY:O	1:A:42:LEU:HD23	2.06	0.55
1:A:79:HIS:HE1	1:A:106:VAL:H	1.54	0.55
1:C:178:ARG:NE	1:C:201:GLY:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:MET:HE3	1:C:239:CYS:SG	2.47	0.55
1:B:156:VAL:HG12	1:B:164:LEU:HD13	1.87	0.55
1:A:142:LEU:HD22	1:D:110:TYR:O	2.07	0.55
1:C:96:LYS:HD3	1:C:132:LEU:CD1	2.37	0.54
1:C:19:GLN:O	1:C:20:GLN:HB2	2.07	0.54
1:C:27:LEU:HD23	1:C:65:ILE:CD1	2.36	0.54
1:C:106:VAL:HA	1:C:137:TYR:HB3	1.89	0.54
1:B:178:ARG:NH1	1:B:184:LEU:O	2.33	0.54
1:A:67:ALA:O	1:A:68:GLU:C	2.51	0.54
1:B:85:THR:OG1	1:B:121:HIS:ND1	2.31	0.53
1:A:288:LEU:HG	1:A:292:LEU:HD12	1.90	0.53
1:B:56:LEU:HD11	1:B:87:GLU:HG2	1.89	0.53
1:C:20:GLN:NE2	1:C:271:ARG:HA	2.24	0.53
1:C:96:LYS:HD3	1:C:132:LEU:HD11	1.89	0.53
1:D:213[A]:MET:HE1	1:D:242:VAL:HB	1.91	0.52
1:A:166:GLN:HE21	1:A:166:GLN:HA	1.73	0.52
1:B:168:SER:HA	1:B:190:TYR:CE2	2.41	0.52
1:D:212:ILE:O	1:D:292:LEU:HD13	2.10	0.52
1:A:65:ILE:O	1:A:65:ILE:CG2	2.57	0.52
1:C:136:VAL:CG1	1:C:164:LEU:HD13	2.38	0.52
1:C:290:GLN:O	1:C:291:GLN:C	2.53	0.52
1:D:64:GLU:O	1:D:68:GLU:HG3	2.09	0.52
1:A:65:ILE:O	1:A:65:ILE:HG22	2.10	0.52
1:A:192:GLU:HA	1:A:240:ASN:HD21	1.74	0.52
1:B:32:GLN:HA	1:B:32:GLN:HE21	1.71	0.52
1:A:240:ASN:HA	1:A:243:ILE:HB	1.90	0.51
1:B:253:ARG:HG3	1:B:277:VAL:HG22	1.91	0.51
1:D:194:PHE:CE2	1:D:198:LEU:HD11	2.45	0.51
1:A:24:LYS:O	1:A:28:ARG:HG3	2.10	0.51
1:B:4:ASN:OD1	1:B:4:ASN:N	2.43	0.51
1:B:165:LYS:HG3	1:B:206:ILE:HD12	1.92	0.51
1:C:165:LYS:HA	1:C:187:TYR:HB2	1.93	0.51
1:D:86:ALA:HA	1:D:89:GLN:HB2	1.93	0.51
1:A:137:TYR:CD1	1:A:137:TYR:C	2.89	0.51
1:A:251:VAL:O	1:A:255:LEU:CD1	2.54	0.51
1:A:108:PRO:HD2	1:A:118:HIS:CD2	2.46	0.50
1:A:213[A]:MET:HE3	1:A:239:CYS:SG	2.50	0.50
1:C:38:GLY:O	1:C:218:GLN:NE2	2.38	0.50
1:C:230:GLN:NE2	1:C:230:GLN:N	2.58	0.50
1:A:192:GLU:HA	1:A:240:ASN:ND2	2.27	0.50
1:A:290:GLN:HA	1:A:293:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ALA:HB1	1:B:228:ASP:O	2.12	0.50
1:A:149:LEU:HD13	1:A:176:GLN:NE2	2.26	0.50
1:B:155:LEU:HD23	1:B:158:LEU:HD11	1.92	0.50
1:D:249:THR:HG22	1:D:281:TYR:CG	2.47	0.50
1:C:48:THR:HG21	1:C:208:SER:CB	2.39	0.50
1:B:236:GLN:HE21	1:B:240:ASN:ND2	2.10	0.50
1:B:171:LEU:HD21	1:B:193:ILE:HD12	1.94	0.50
1:D:80:VAL:O	1:D:88:SER:HA	2.11	0.49
1:A:2:ALA:O	1:A:185:VAL:HG21	2.12	0.49
1:D:192:GLU:HB3	1:D:243:ILE:HD13	1.94	0.49
1:B:288:LEU:HD12	1:B:288:LEU:O	2.13	0.49
1:B:192:GLU:HG3	1:D:172:TYR:CG	2.47	0.49
1:D:253:ARG:CG	1:D:277:VAL:HG23	2.43	0.49
1:D:77:ILE:HG23	1:D:102:ALA:HB3	1.94	0.49
1:B:92:ALA:O	1:B:93:ALA:C	2.55	0.48
1:C:78:ALA:HB2	1:C:100:PHE:CD2	2.48	0.48
1:A:253:ARG:HG3	1:A:277:VAL:HG22	1.94	0.48
1:B:137:TYR:CD1	1:B:137:TYR:C	2.90	0.48
1:C:165:LYS:HE3	1:C:206:ILE:HB	1.94	0.48
1:B:34:ASN:CB	1:B:42:LEU:HD21	2.43	0.48
1:B:173:GLN:O	1:B:177:ILE:HG13	2.13	0.48
1:C:77:ILE:HG12	1:C:102:ALA:HB3	1.94	0.48
1:B:101:ASP:O	1:B:133:PRO:HD2	2.14	0.48
1:D:290:GLN:HA	1:D:293:MET:HE3	1.93	0.48
1:B:237:THR:CG2	1:D:179:ARG:HD3	2.40	0.48
1:D:29:ARG:HD2	1:D:264:VAL:O	2.14	0.48
1:A:12:LEU:HD13	1:A:42:LEU:HD13	1.94	0.48
1:A:13:LEU:HD23	1:A:48:THR:HG22	1.94	0.48
1:A:228:ASP:OD2	1:A:231:THR:HG22	2.13	0.48
1:B:42:LEU:CD1	1:B:74:ILE:HD11	2.43	0.48
1:B:278:ASP:OD1	1:B:279:GLU:N	2.47	0.48
1:A:32:GLN:O	1:A:33:PHE:C	2.56	0.48
1:A:78:ALA:HB2	1:A:100:PHE:CD2	2.49	0.48
1:B:64:GLU:O	1:B:65:ILE:C	2.57	0.48
1:A:10:ALA:HB3	1:A:42:LEU:CD2	2.43	0.47
1:C:235:LEU:O	1:C:236:GLN:C	2.57	0.47
1:D:192:GLU:HA	1:D:240:ASN:HD21	1.79	0.47
1:B:249:THR:OG1	1:B:250:GLY:O	2.29	0.47
1:D:40:ASP:CG	1:D:218:GLN:HE22	2.22	0.47
1:D:236:GLN:HE21	1:D:240:ASN:HD21	1.62	0.47
1:B:32:GLN:NE2	1:B:32:GLN:CA	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:VAL:HG21	1:C:66:VAL:HG22	1.97	0.47
1:D:165:LYS:HA	1:D:187:TYR:HB2	1.97	0.47
1:A:45:GLY:O	1:A:51:ALA:HB2	2.15	0.47
1:B:79:HIS:HE1	1:B:106:VAL:H	1.61	0.47
1:A:48:THR:HG21	1:A:208:SER:CB	2.45	0.47
1:C:17:ASP:OD2	1:C:21:ALA:HB3	2.14	0.47
1:A:213[B]:MET:CE	1:A:239:CYS:HA	2.43	0.47
1:B:236:GLN:HE21	1:B:240:ASN:HD21	1.61	0.47
1:A:126:ILE:O	1:A:129:ALA:HB3	2.15	0.47
1:B:231:THR:O	1:B:232:ALA:C	2.57	0.47
1:C:267:VAL:CG1	1:C:269:LEU:HD12	2.44	0.47
1:D:261:TYR:CD2	1:D:286:LYS:HA	2.50	0.47
1:B:78:ALA:O	1:B:103:VAL:HA	2.15	0.46
1:D:198:LEU:HD23	1:D:202:ALA:O	2.16	0.46
1:B:22[B]:LEU:HD23	1:B:23:ASP:N	2.29	0.46
1:A:258:VAL:HG12	1:A:259:LEU:N	2.30	0.46
1:C:166:GLN:HE21	1:C:166:GLN:CA	2.13	0.46
1:B:180:GLU:HG3	1:B:181:HIS:CE1	2.51	0.46
1:D:31:VAL:O	1:D:35:ILE:HG13	2.16	0.46
1:A:258:VAL:O	1:A:261:TYR:N	2.44	0.46
1:B:42:LEU:HD12	1:B:74:ILE:HD11	1.98	0.45
1:B:258:VAL:HG23	1:B:285:LEU:CD2	2.45	0.45
1:D:277:VAL:CG1	1:D:278:ASP:N	2.78	0.45
1:A:12:LEU:HD13	1:A:42:LEU:CD1	2.47	0.45
1:A:80:VAL:HB	1:A:91:LEU:HB2	1.97	0.45
1:B:79:HIS:CE1	1:B:106:VAL:H	2.34	0.45
1:B:175:GLU:OE1	1:B:179:ARG:NH2	2.49	0.45
1:D:56:LEU:HD11	1:D:87:GLU:HG2	1.97	0.45
1:B:80:VAL:HB	1:B:91:LEU:HB2	1.97	0.45
1:C:79:HIS:CE1	1:C:105:ALA:HA	2.52	0.45
1:A:146:LYS:NZ	2:A:2020:HOH:O	2.42	0.45
1:C:9:MET:O	1:C:206:ILE:HA	2.17	0.45
1:A:245:LEU:HD13	1:A:248:LYS:NZ	2.32	0.45
1:B:229:ILE:HD11	1:D:224:LEU:HD22	1.99	0.45
1:B:55:SER:OG	1:B:58:GLU:HG3	2.16	0.45
1:B:35:ILE:HG12	1:B:74:ILE:HD13	1.99	0.45
1:B:48:THR:HA	1:B:252:PHE:CZ	2.52	0.45
1:C:236:GLN:HE21	1:C:240:ASN:HD21	1.66	0.44
1:A:4:ASN:OD1	1:A:5:LEU:N	2.50	0.44
1:A:48:THR:HA	1:A:252:PHE:CE1	2.53	0.44
1:A:231:THR:HA	1:A:234:LYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:CZ	1:B:91:LEU:CD1	2.95	0.44
1:B:80:VAL:HG11	1:B:92:ALA:HA	1.99	0.44
1:B:213:MET:HB2	1:B:216:ARG:HB2	1.99	0.44
1:B:215:TRP:HA	1:B:218:GLN:HB2	2.00	0.44
1:C:198:LEU:O	1:C:199:LEU:C	2.61	0.44
1:C:155:LEU:O	1:C:161:VAL:HG21	2.17	0.44
1:C:178:ARG:HG2	1:C:201:GLY:HA3	1.99	0.44
1:C:235:LEU:O	1:C:238:GLU:N	2.51	0.44
1:D:78:ALA:O	1:D:80:VAL:HG13	2.17	0.44
1:D:129:ALA:O	1:D:132:LEU:HD13	2.18	0.44
1:D:213[A]:MET:HA	1:D:215:TRP:CZ3	2.52	0.44
1:A:5:LEU:HB3	1:A:187:TYR:OH	2.18	0.44
1:A:20:GLN:OE1	1:A:271:ARG:HA	2.17	0.44
1:B:37:GLN:NE2	1:B:214:GLY:H	2.15	0.44
1:B:70:ALA:HB1	1:B:76:LEU:HD21	1.99	0.44
1:B:227:GLY:HA2	1:D:229:ILE:HD12	2.00	0.44
1:C:16:PHE:HA	1:C:21:ALA:O	2.18	0.44
1:C:156:VAL:HA	1:C:161:VAL:HG11	2.00	0.44
1:C:198:LEU:HD23	1:C:202:ALA:O	2.17	0.44
1:C:260:HIS:HA	1:C:265:VAL:O	2.18	0.44
1:D:269:LEU:HD23	1:D:269:LEU:HA	1.78	0.44
1:C:59:ARG:O	1:C:63:LEU:HG	2.18	0.43
1:D:213[B]:MET:HE1	1:D:242:VAL:CB	2.48	0.43
1:D:260:HIS:HD2	1:D:265:VAL:O	2.00	0.43
1:B:27:LEU:HD23	1:B:65:ILE:HG21	1.99	0.43
1:B:171:LEU:CD1	1:B:196:SER:HB3	2.48	0.43
1:C:2:ALA:HB1	1:C:5:LEU:HD12	2.00	0.43
1:D:23:ASP:OD1	1:D:23:ASP:C	2.60	0.43
1:C:101:ASP:O	1:C:133:PRO:HD2	2.18	0.43
1:D:213[B]:MET:HE1	1:D:242:VAL:HB	2.00	0.43
1:A:242:VAL:HG13	1:A:288:LEU:HD21	2.00	0.43
1:D:33:PHE:O	1:D:37:GLN:HB2	2.19	0.43
1:B:192:GLU:HG3	1:D:172:TYR:CD2	2.54	0.43
1:A:5:LEU:HB3	1:A:187:TYR:HH	1.84	0.43
1:C:139:ILE:HD12	1:C:167:THR:HG21	2.01	0.43
1:D:96:LYS:HD3	1:D:132:LEU:HD13	1.99	0.43
1:B:35:ILE:CG1	1:B:74:ILE:HD13	2.49	0.43
1:D:2:ALA:HB1	1:D:5:LEU:CD1	2.41	0.43
1:B:258:VAL:HG23	1:B:285:LEU:HD23	2.01	0.43
1:C:292:LEU:HA	1:C:292:LEU:HD23	1.86	0.43
1:D:87:GLU:OE1	2:D:2016:HOH:O	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:VAL:HG23	1:C:134:MET:HE2	2.01	0.42
1:A:215:TRP:O	1:A:216:ARG:C	2.62	0.42
1:B:235:LEU:O	1:B:236:GLN:C	2.62	0.42
1:B:257:THR:O	1:B:260:HIS:HB3	2.19	0.42
1:C:4:ASN:OD1	1:C:4:ASN:N	2.47	0.42
1:D:242:VAL:HG13	1:D:288:LEU:HD21	2.01	0.42
1:D:5:LEU:O	1:D:187:TYR:OH	2.37	0.42
1:A:210:TYR:N	1:A:210:TYR:CD1	2.87	0.42
1:B:164:LEU:HD23	1:B:166:GLN:HB2	2.02	0.42
1:D:152:ILE:O	1:D:156:VAL:HG13	2.19	0.42
1:D:257:THR:O	1:D:258:VAL:C	2.61	0.42
1:C:29:ARG:HB3	1:C:264:VAL:HG13	2.00	0.42
1:A:46:GLY:HA2	1:A:79:HIS:CD2	2.54	0.42
1:B:156:VAL:CG1	1:B:164:LEU:HD13	2.50	0.42
1:D:236:GLN:NE2	1:D:240:ASN:HD21	2.17	0.42
1:A:209:THR:HG21	1:A:243:ILE:HG12	2.02	0.42
1:A:249:THR:HG21	1:A:285:LEU:HD21	2.01	0.42
1:C:213:MET:O	1:C:213:MET:CG	2.68	0.42
1:A:140:PRO:O	1:A:141:ALA:C	2.62	0.42
1:B:137:TYR:C	1:B:137:TYR:HD1	2.28	0.42
1:C:242:VAL:HG22	1:C:288:LEU:HD11	2.02	0.42
1:A:16:PHE:HA	1:A:21:ALA:O	2.19	0.42
1:A:175:GLU:HA	1:A:200:ALA:O	2.19	0.42
1:B:62:VAL:O	1:B:63:LEU:C	2.62	0.42
1:B:39:ILE:HG23	1:B:41:GLY:H	1.84	0.41
1:B:106:VAL:O	1:B:107:THR:C	2.63	0.41
1:D:37:GLN:NE2	1:D:214:GLY:H	2.17	0.41
1:B:115:PHE:CE1	1:B:151:GLN:HB3	2.55	0.41
1:C:71:LYS:HE3	1:C:99:GLY:HA3	2.03	0.41
1:C:139:ILE:CD1	1:C:167:THR:HG21	2.49	0.41
1:A:4:ASN:C	1:A:6:ARG:H	2.28	0.41
1:D:213[B]:MET:HE1	1:D:242:VAL:HG11	2.03	0.41
1:A:4:ASN:C	1:A:6:ARG:N	2.79	0.41
1:D:257:THR:O	1:D:260:HIS:HB3	2.20	0.41
1:B:51:ALA:HA	1:B:54:GLN:HE21	1.86	0.41
1:D:215:TRP:CZ2	1:D:292:LEU:HD22	2.55	0.41
1:B:282:LEU:N	1:B:283:PRO:CD	2.84	0.41
1:D:62:VAL:O	1:D:63:LEU:C	2.63	0.41
1:D:103:VAL:O	1:D:134:MET:HA	2.21	0.41
1:A:63:LEU:HD22	1:A:100:PHE:CZ	2.56	0.41
1:D:290:GLN:HA	1:D:293:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:LEU:O	1:C:9:MET:HE2	2.20	0.41
1:C:24:LYS:HD3	1:C:65:ILE:HD11	2.03	0.41
1:C:50:GLU:OE2	1:C:256:LYS:NZ	2.41	0.41
1:C:245:LEU:O	1:C:245:LEU:HD12	2.21	0.41
1:C:253:ARG:CG	1:C:277:VAL:HG22	2.50	0.41
1:D:198:LEU:HA	1:D:202:ALA:O	2.21	0.41
1:A:178:ARG:O	1:A:179:ARG:C	2.62	0.40
1:B:171:LEU:HD21	1:B:193:ILE:CD1	2.52	0.40
1:B:198:LEU:HA	1:B:202:ALA:O	2.20	0.40
1:D:30:LEU:HD13	1:D:259:LEU:HD13	2.03	0.40
1:D:96:LYS:HD2	1:D:132:LEU:HD11	2.03	0.40
1:A:198:LEU:HD11	1:A:221:VAL:HG22	2.03	0.40
1:B:85:THR:O	1:B:86:ALA:C	2.64	0.40
1:C:209:THR:HG22	1:C:246:LEU:CD1	2.52	0.40
1:B:257:THR:O	1:B:260:HIS:N	2.54	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	300/304 (99%)	270 (90%)	29 (10%)	1 (0%)	36	42
1	B	295/304 (97%)	269 (91%)	26 (9%)	0	100	100
1	C	293/304 (96%)	276 (94%)	16 (6%)	1 (0%)	36	42
1	D	293/304 (96%)	271 (92%)	19 (6%)	3 (1%)	12	11
All	All	1181/1216 (97%)	1086 (92%)	90 (8%)	5 (0%)	36	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3	THR
1	A	5	LEU
1	C	110	TYR
1	D	213[A]	MET
1	D	213[B]	MET

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	249/251 (99%)	237 (95%)	12 (5%)	23	30
1	B	246/251 (98%)	232 (94%)	14 (6%)	18	23
1	C	243/251 (97%)	233 (96%)	10 (4%)	27	37
1	D	243/251 (97%)	233 (96%)	10 (4%)	27	37
All	All	981/1004 (98%)	935 (95%)	46 (5%)	24	31

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	MET
1	A	42	LEU
1	A	47	SER
1	A	132	LEU
1	A	166	GLN
1	A	168	SER
1	A	183[A]	ASP
1	A	183[B]	ASP
1	A	210	TYR
1	A	234	LYS
1	A	269	LEU
1	A	292	LEU
1	B	4	ASN
1	B	39	ILE
1	B	47	SER
1	B	66	VAL
1	B	126	ILE

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Mol	Chain	Res	Type
1	B	132	LEU
1	B	152	ILE
1	B	156	VAL
1	B	166	GLN
1	B	168	SER
1	B	213	MET
1	B	237	THR
1	B	258	VAL
1	B	286	LYS
1	C	4	ASN
1	C	68	GLU
1	C	74	ILE
1	C	75	LYS
1	C	136	VAL
1	C	150	ASP
1	C	166	GLN
1	C	226	GLU
1	C	230	GLN
1	C	234	LYS
1	D	3	THR
1	D	47	SER
1	D	114	SER
1	D	146	LYS
1	D	156	VAL
1	D	166	GLN
1	D	229	ILE
1	D	233	GLN
1	D	280	LYS
1	D	295	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	79	HIS
1	A	138	ASN
1	A	166	GLN
1	A	176	GLN
1	A	181	HIS
1	A	240	ASN
1	A	260	HIS
1	A	291	GLN

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Mol	Chain	Res	Type
1	B	4	ASN
1	B	32	GLN
1	B	36	GLN
1	B	54	GLN
1	B	61	GLN
1	B	79	HIS
1	B	90	GLN
1	B	138	ASN
1	B	153	ASN
1	B	166	GLN
1	B	181	HIS
1	B	240	ASN
1	B	291	GLN
1	C	20	GLN
1	C	79	HIS
1	C	89	GLN
1	C	118	HIS
1	C	138	ASN
1	C	151	GLN
1	C	166	GLN
1	C	176	GLN
1	C	230	GLN
1	C	240	ASN
1	C	260	HIS
1	D	37	GLN
1	D	54	GLN
1	D	79	HIS
1	D	138	ASN
1	D	166	GLN
1	D	176	GLN
1	D	230	GLN
1	D	240	ASN
1	D	260	HIS

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	299/304 (98%)	1.15	57 (19%) 3 2	17, 36, 51, 61	3 (1%)
1	B	293/304 (96%)	0.91	24 (8%) 17 15	16, 33, 45, 52	4 (1%)
1	C	295/304 (97%)	0.65	14 (4%) 36 33	14, 31, 43, 54	0
1	D	294/304 (96%)	0.59	15 (5%) 33 30	15, 30, 43, 49	1 (0%)
All	All	1181/1216 (97%)	0.83	110 (9%) 14 12	14, 32, 47, 61	8 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	7.5
1	B	190	TYR	5.7
1	A	264	VAL	4.3
1	A	292	LEU	4.2
1	A	268	PRO	4.2
1	A	22	LEU	4.0
1	B	212	ILE	3.9
1	A	70	ALA	3.6
1	A	212	ILE	3.5
1	A	35	ILE	3.4
1	A	1	HIS	3.4
1	A	242	VAL	3.4
1	D	201	GLY	3.4
1	A	149	LEU	3.3
1	A	261	TYR	3.3
1	A	254	GLY	3.2
1	A	285	LEU	3.2
1	B	139	ILE	3.1
1	A	230	GLN	3.1
1	B	137	TYR	3.1
1	A	5	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	25	ALA	3.0
1	B	231	THR	3.0
1	A	263	ASP	2.9
1	C	231	THR	2.9
1	B	141	ALA	2.9
1	A	4	ASN	2.9
1	A	74	ILE	2.8
1	C	289	ALA	2.8
1	A	293	MET	2.8
1	D	185	VAL	2.8
1	A	229	ILE	2.8
1	C	3	THR	2.8
1	A	36	GLN	2.7
1	A	267	VAL	2.7
1	C	227	GLY	2.7
1	D	2	ALA	2.7
1	B	219	GLY	2.7
1	B	229	ILE	2.7
1	A	27	LEU	2.7
1	A	235	LEU	2.7
1	A	24	LYS	2.6
1	C	36	GLN	2.6
1	A	223	ALA	2.6
1	D	152	ILE	2.6
1	C	18	GLN	2.6
1	C	288	LEU	2.6
1	B	156	VAL	2.6
1	D	150	ASP	2.5
1	A	39	ILE	2.5
1	B	185	VAL	2.5
1	C	264	VAL	2.5
1	D	160	GLY	2.5
1	B	242	VAL	2.4
1	D	156	VAL	2.4
1	A	30	LEU	2.4
1	B	261	TYR	2.4
1	A	-1	HIS	2.4
1	A	296	ARG	2.4
1	A	297	GLY	2.4
1	A	7	GLY	2.4
1	A	3	THR	2.4
1	D	103	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	260	HIS	2.3
1	A	37	GLN	2.3
1	D	125	ILE	2.3
1	A	31	VAL	2.3
1	A	289	ALA	2.3
1	D	289	ALA	2.3
1	A	277	VAL	2.3
1	C	293	MET	2.3
1	A	275	GLY	2.2
1	A	227	GLY	2.2
1	D	294	GLN	2.2
1	A	232	ALA	2.2
1	B	285	LEU	2.2
1	C	292	LEU	2.2
1	B	145	VAL	2.2
1	C	221	VAL	2.2
1	A	274	PHE	2.2
1	A	72	GLY	2.2
1	A	259	LEU	2.2
1	B	142	LEU	2.2
1	A	276	PRO	2.2
1	A	231	THR	2.2
1	B	93	ALA	2.2
1	D	157	THR	2.2
1	D	155	LEU	2.1
1	D	159	PRO	2.1
1	A	0	HIS	2.1
1	C	70	ALA	2.1
1	A	221	VAL	2.1
1	A	265	VAL	2.1
1	A	41	GLY	2.1
1	A	32	GLN	2.1
1	B	140	PRO	2.1
1	B	268	PRO	2.1
1	C	267	VAL	2.1
1	D	3	THR	2.1
1	A	213[A]	MET	2.1
1	A	69	GLU	2.1
1	A	142	LEU	2.1
1	B	264	VAL	2.1
1	A	201	GLY	2.1
1	B	143	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	136	VAL	2.0
1	B	144	GLY	2.0
1	A	283	PRO	2.0
1	B	283	PRO	2.0
1	C	152	ILE	2.0

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.