



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:17 AM UTC

PDB ID : 4LJ2 / pdb_00004lj2
Title : Crystal structure of chorismate synthase from *Acinetobacter baumannii* at 3.15Å resolution
Authors : Chaudhary, A.; Singh, N.; Kaushik, S.; Tyagi, T.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2013-07-04
Resolution : 3.15 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

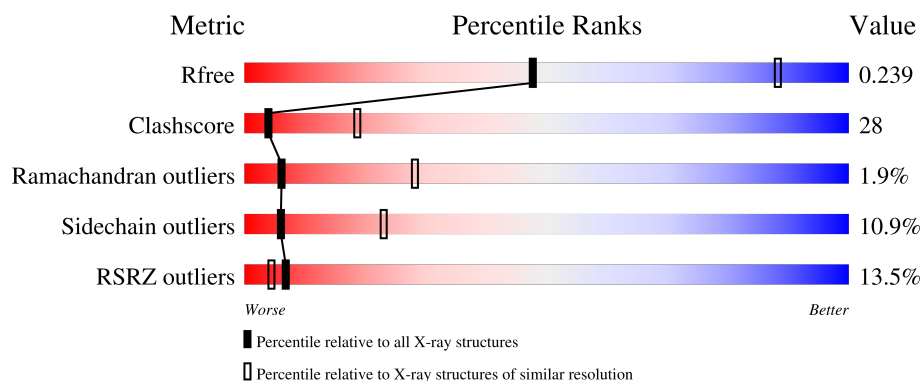
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	363	12% 42% 34% 12% • 11%
1	B	363	12% 44% 34% 10% • 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4840 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.

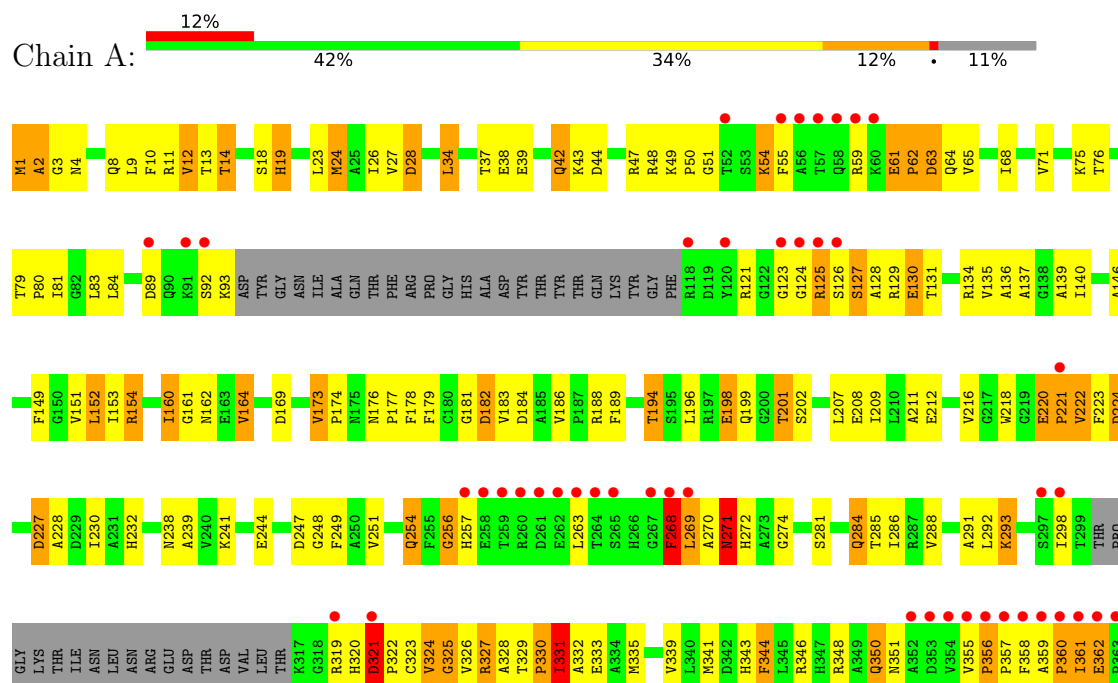
- Molecule 1 is a protein called Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2413	1510	437	455	11			
1	B	324	Total	C	N	O	S	0	0	0
			2427	1518	439	459	11			

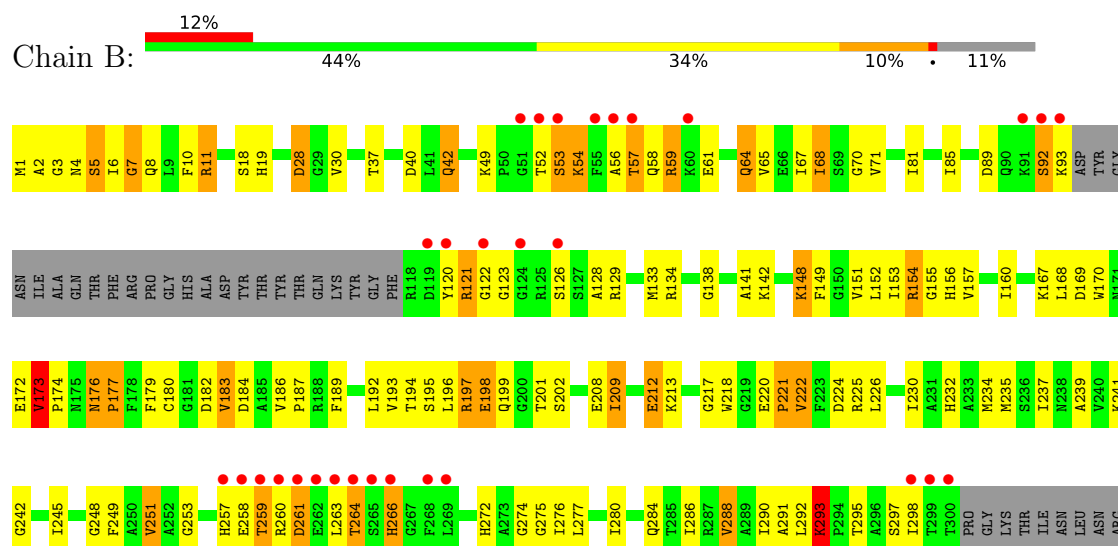
3 Residue-property plots

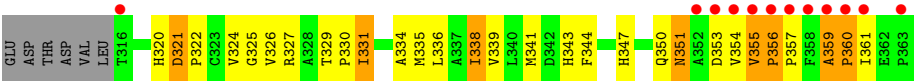
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Chorismate synthase



• Molecule 1: Chorismate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.77Å 72.61Å 89.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.54 – 3.15 46.54 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.54-3.15) 99.7 (46.54-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.252 0.223 , 0.239	Depositor DCC
R_{free} test set	654 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4840	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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	1.21	17/2455 (0.7%)	1.44	41/3316 (1.2%)
1	B	1.14	17/2469 (0.7%)	1.30	33/3336 (1.0%)
All	All	1.17	34/4924 (0.7%)	1.37	74/6652 (1.1%)

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
1	A	0	3
1	B	0	1
All	All	0	4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	347	HIS	CG-ND1	-7.77	1.29	1.38
1	B	7	GLY	C-O	-7.42	1.15	1.24
1	B	343	HIS	CG-ND1	-7.11	1.30	1.38
1	A	343	HIS	CG-ND1	-6.98	1.30	1.38
1	A	218	TRP	NE1-CE2	-6.78	1.29	1.37
1	A	325	GLY	C-O	-6.78	1.16	1.24
1	A	332	ALA	C-O	-6.69	1.16	1.24
1	A	298	ILE	N-CA	6.65	1.54	1.46
1	A	331	ILE	C-O	-6.38	1.17	1.24
1	B	68	ILE	C-O	-6.15	1.17	1.24
1	B	347	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	343	HIS	CD2-NE2	-6.01	1.31	1.37
1	B	4	ASN	C-O	-5.98	1.16	1.24
1	A	13	THR	C-O	-5.87	1.17	1.24
1	B	335	MET	C-O	-5.87	1.17	1.24
1	B	220	GLU	C-O	-5.85	1.19	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	ILE	CA-CB	-5.82	1.47	1.54
1	B	272	HIS	CG-ND1	-5.73	1.31	1.38
1	A	199	GLN	C-O	-5.71	1.16	1.24
1	B	343	HIS	CD2-NE2	-5.67	1.31	1.37
1	B	11	ARG	C-O	-5.63	1.16	1.24
1	A	12	VAL	C-O	-5.59	1.18	1.24
1	A	330	PRO	C-O	-5.48	1.17	1.24
1	A	288	VAL	C-O	-5.45	1.18	1.24
1	B	347	HIS	CA-C	-5.26	1.46	1.52
1	A	182	ASP	C-O	-5.26	1.18	1.24
1	B	11	ARG	CA-C	-5.20	1.46	1.52
1	B	320	HIS	CA-C	-5.18	1.46	1.52
1	A	14	THR	C-O	-5.17	1.17	1.23
1	A	224	ASP	C-O	-5.09	1.17	1.24
1	A	198	GLU	C-O	-5.04	1.17	1.24
1	A	3	GLY	C-O	-5.03	1.17	1.23
1	B	221	PRO	CA-C	-5.03	1.46	1.52
1	B	321	ASP	N-CA	-5.00	1.42	1.46

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	ILE	N-CA-C	14.58	123.14	111.62
1	A	321	ASP	CA-C-N	13.16	133.66	119.05
1	A	321	ASP	C-N-CA	13.16	133.66	119.05
1	A	324	VAL	N-CA-C	-12.26	100.77	112.29
1	A	128	ALA	N-CA-C	-11.28	99.47	113.01
1	A	272	HIS	N-CA-C	-11.01	99.88	113.97
1	A	42	GLN	OE1-CD-NE2	-9.97	112.63	122.60
1	A	351	ASN	N-CA-C	9.36	124.29	109.50
1	A	54	LYS	N-CA-C	9.07	121.24	111.36
1	B	64	GLN	N-CA-C	8.86	122.85	108.41
1	B	221	PRO	CA-C-O	-8.08	110.92	122.31
1	B	259	THR	N-CA-C	-8.06	102.49	111.28
1	A	270	ALA	N-CA-C	-7.97	95.53	108.52
1	B	128	ALA	N-CA-C	7.87	119.94	111.36
1	A	28	ASP	N-CA-C	7.81	122.36	109.95
1	B	224	ASP	N-CA-C	7.62	121.05	112.97
1	B	217	GLY	N-CA-C	7.62	123.75	114.69
1	A	268	PHE	N-CA-C	7.52	119.56	111.36
1	A	263	LEU	N-CA-C	7.23	119.24	111.36
1	A	121	ARG	N-CA-C	7.11	119.91	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ILE	N-CA-C	-7.01	97.39	107.77
1	B	28	ASP	N-CA-C	6.92	120.79	109.72
1	A	319	ARG	N-CA-C	-6.81	97.26	108.76
1	A	271	ASN	N-CA-C	6.64	119.85	109.96
1	A	64	GLN	N-CA-C	6.62	120.66	110.20
1	A	2	ALA	N-CA-C	6.57	118.52	108.07
1	A	42	GLN	CG-CD-NE2	6.51	126.16	116.40
1	A	298	ILE	CB-CA-C	-6.50	101.99	110.84
1	B	331	ILE	N-CA-C	-6.36	104.65	110.82
1	B	177	PRO	N-CA-C	-6.35	99.40	112.47
1	A	361	ILE	N-CA-C	6.33	117.54	107.98
1	A	348	ARG	N-CA-C	-6.28	104.36	111.07
1	A	319	ARG	CA-C-N	-6.09	114.41	123.00
1	A	319	ARG	C-N-CA	-6.09	114.41	123.00
1	A	321	ASP	N-CA-C	6.08	121.91	113.45
1	A	361	ILE	CB-CA-C	-6.07	104.67	111.23
1	A	61	GLU	N-CA-C	6.07	121.78	113.16
1	B	19	HIS	N-CA-C	-5.85	105.04	111.82
1	A	126	SER	N-CA-C	-5.84	99.00	108.52
1	B	198	GLU	CB-CA-C	-5.80	101.77	110.88
1	A	89	ASP	N-CA-C	5.80	119.33	112.72
1	B	183	VAL	CB-CA-C	-5.77	104.35	112.14
1	B	49	LYS	CA-C-N	5.76	127.04	119.84
1	B	49	LYS	C-N-CA	5.76	127.04	119.84
1	A	10	PHE	N-CA-C	-5.73	96.33	107.62
1	A	89	ASP	CB-CA-C	-5.70	101.53	110.94
1	B	355	VAL	C-N-CD	-5.66	101.78	125.00
1	B	92	SER	CB-CA-C	-5.65	110.07	116.63
1	A	254	GLN	N-CA-C	5.65	118.03	110.35
1	A	3	GLY	N-CA-C	-5.62	99.86	113.18
1	B	30	VAL	CA-C-N	5.56	126.11	120.38
1	B	30	VAL	C-N-CA	5.56	126.11	120.38
1	B	338	ILE	CB-CA-C	-5.55	104.59	111.70
1	B	173	VAL	CB-CA-C	-5.49	108.53	114.35
1	A	344	PHE	N-CA-C	-5.48	104.94	111.03
1	B	122	GLY	N-CA-C	5.43	119.14	112.14
1	B	293	LYS	N-CA-C	5.40	117.60	110.36
1	B	197	ARG	CA-C-N	5.36	127.41	120.44
1	B	197	ARG	C-N-CA	5.36	127.41	120.44
1	B	221	PRO	CA-C-N	5.35	131.33	121.70
1	B	221	PRO	C-N-CA	5.35	131.33	121.70
1	A	19	HIS	N-CA-C	-5.34	106.77	113.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	GLY	N-CA-C	-5.28	104.80	111.72
1	B	180	CYS	N-CA-C	5.27	118.08	110.28
1	A	125	ARG	N-CA-C	5.24	117.45	108.90
1	A	146	ALA	N-CA-C	-5.22	105.03	111.40
1	B	133	MET	N-CA-C	5.17	116.91	111.28
1	B	351	ASN	N-CA-C	5.11	116.74	108.41
1	A	59	ARG	N-CA-C	5.10	118.39	110.17
1	B	226	LEU	N-CA-C	-5.08	105.74	111.28
1	A	8	GLN	N-CA-C	5.08	119.43	112.68
1	A	34	LEU	N-CA-C	-5.07	101.43	109.59
1	B	53	SER	CB-CA-C	-5.06	110.76	116.63
1	A	61	GLU	C-N-CD	-5.01	109.58	120.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	GLY	Peptide
1	A	269	LEU	Peptide
1	A	321	ASP	Peptide
1	B	59	ARG	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	2413	0	2422	155	0
1	B	2427	0	2436	140	0
All	All	4840	0	4858	272	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 28.

All (272) 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:A:355:VAL:HB	1:A:356:PRO:HD2	1.25	1.13
1:B:173:VAL:HG22	1:B:174:PRO:HD3	1.37	1.04
1:A:358:PHE:CE2	1:A:361:ILE:HD11	1.94	1.02
1:A:331:ILE:HG13	1:A:331:ILE:O	1.60	1.01
1:A:251:VAL:HG11	1:B:293:LYS:HB3	1.44	0.99
1:A:359:ALA:HB1	1:A:360:PRO:HD2	1.41	0.99
1:A:355:VAL:HB	1:A:356:PRO:CD	1.95	0.96
1:A:18:SER:HB2	1:A:125:ARG:HB3	1.51	0.92
1:A:355:VAL:CB	1:A:356:PRO:HD2	1.99	0.91
1:A:18:SER:HB2	1:A:125:ARG:CB	2.03	0.88
1:B:195:SER:O	1:B:198:GLU:HB2	1.74	0.88
1:B:321:ASP:HB3	1:B:324:VAL:HG13	1.55	0.86
1:B:68:ILE:O	1:B:68:ILE:HG22	1.77	0.84
1:A:251:VAL:CG1	1:B:293:LYS:HB3	2.09	0.83
1:A:327:ARG:O	1:A:330:PRO:HD2	1.78	0.83
1:B:359:ALA:N	1:B:360:PRO:CD	2.43	0.81
1:B:248:GLY:O	1:B:251:VAL:HB	1.82	0.80
1:A:54:LYS:HE3	1:A:177:PRO:HB3	1.63	0.80
1:A:271:ASN:HD21	1:A:284:GLN:CD	1.91	0.79
1:A:358:PHE:CE2	1:A:361:ILE:CD1	2.65	0.79
1:B:359:ALA:N	1:B:360:PRO:HD3	1.97	0.79
1:A:331:ILE:O	1:A:331:ILE:CG1	2.29	0.79
1:B:57:THR:O	1:B:57:THR:CG2	2.30	0.79
1:A:293:LYS:HA	1:B:251:VAL:HG13	1.65	0.79
1:A:232:HIS:HB2	1:B:232:HIS:HB2	1.65	0.78
1:A:221:PRO:O	1:B:2:ALA:HA	1.84	0.78
1:B:58:GLN:HG3	1:B:59:ARG:N	1.99	0.78
1:B:173:VAL:HG22	1:B:174:PRO:CD	2.14	0.77
1:B:334:ALA:O	1:B:338:ILE:HG12	1.84	0.77
1:A:269:LEU:HD13	1:A:284:GLN:NE2	2.01	0.75
1:A:251:VAL:CG1	1:B:293:LYS:CB	2.64	0.75
1:B:89:ASP:OD1	1:B:129:ARG:NH2	2.20	0.74
1:A:201:THR:HG22	1:A:202:SER:H	1.51	0.74
1:B:70:GLY:HA3	1:B:81:ILE:HD13	1.70	0.74
1:A:127:SER:HB2	1:A:130:GLU:HG2	1.71	0.73
1:A:92:SER:O	1:A:93:LYS:HB2	1.88	0.73
1:A:1:MET:O	1:A:2:ALA:HB2	1.89	0.73
1:A:268:PHE:N	1:A:268:PHE:CD1	2.54	0.72
1:A:324:VAL:HG13	1:A:324:VAL:O	1.90	0.72
1:B:57:THR:O	1:B:57:THR:HG22	1.89	0.71
1:A:127:SER:HA	1:A:129:ARG:HG3	1.74	0.70
1:A:362:GLU:O	1:A:362:GLU:HG2	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ILE:HD12	1:B:336:LEU:HD12	1.72	0.70
1:B:126:SER:OG	1:B:129:ARG:HG3	1.92	0.70
1:A:131:THR:O	1:A:131:THR:HG22	1.92	0.70
1:A:196:LEU:HD22	1:A:201:THR:HB	1.74	0.70
1:A:251:VAL:CG1	1:B:293:LYS:HA	2.23	0.69
1:B:359:ALA:H	1:B:360:PRO:HD3	1.56	0.69
1:A:182:ASP:OD1	1:A:182:ASP:C	2.30	0.69
1:A:251:VAL:HG11	1:B:293:LYS:CB	2.21	0.68
1:A:92:SER:O	1:A:93:LYS:CB	2.43	0.67
1:A:251:VAL:CG1	1:B:293:LYS:CA	2.73	0.66
1:B:53:SER:O	1:B:54:LYS:HB2	1.93	0.66
1:B:68:ILE:O	1:B:68:ILE:CG2	2.43	0.66
1:A:359:ALA:HB1	1:A:360:PRO:CD	2.24	0.66
1:B:170:TRP:O	1:B:173:VAL:HG13	1.96	0.66
1:B:183:VAL:HG13	1:B:184:ASP:N	2.11	0.65
1:A:269:LEU:CD1	1:A:284:GLN:NE2	2.61	0.64
1:A:328:ALA:O	1:A:331:ILE:HG23	1.97	0.64
1:A:227:ASP:OD1	1:A:227:ASP:N	2.29	0.64
1:B:173:VAL:CG2	1:B:174:PRO:HD3	2.23	0.64
1:A:268:PHE:N	1:A:268:PHE:HD1	1.95	0.64
1:A:131:THR:HG23	1:A:331:ILE:CD1	2.28	0.63
1:A:251:VAL:HG12	1:B:293:LYS:HA	1.81	0.63
1:A:152:LEU:O	1:A:153:ILE:HD13	1.98	0.63
1:B:350:GLN:C	1:B:351:ASN:HD22	2.06	0.63
1:A:269:LEU:HG	1:A:269:LEU:O	1.99	0.63
1:B:152:LEU:HD13	1:B:154:ARG:HD2	1.82	0.61
1:A:131:THR:HG23	1:A:331:ILE:HD12	1.81	0.61
1:B:61:GLU:CD	1:B:61:GLU:H	2.04	0.61
1:B:67:ILE:HG21	1:B:71:VAL:HG22	1.83	0.61
1:A:329:THR:O	1:A:333:GLU:HG3	1.99	0.60
1:B:324:VAL:HG12	1:B:327:ARG:HH12	1.67	0.60
1:A:127:SER:C	1:A:129:ARG:N	2.57	0.60
1:B:7:GLY:O	1:B:11:ARG:HG3	2.01	0.60
1:A:220:GLU:O	1:A:224:ASP:C	2.45	0.59
1:A:42:GLN:OE1	1:A:65:VAL:HG12	2.02	0.59
1:A:19:HIS:HB3	1:A:124:GLY:HA2	1.83	0.59
1:A:127:SER:C	1:A:129:ARG:H	2.07	0.59
1:A:212:GLU:HA	1:A:285:THR:HG22	1.84	0.59
1:A:131:THR:HG22	1:A:135:VAL:HG23	1.84	0.58
1:A:274:GLY:O	1:A:286:ILE:HA	2.04	0.58
1:B:274:GLY:O	1:B:286:ILE:HA	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD13	1:A:292:LEU:CD1	2.34	0.58
1:A:211:ALA:HB3	1:A:286:ILE:HB	1.85	0.57
1:B:239:ALA:O	1:B:292:LEU:HA	2.03	0.57
1:B:192:LEU:O	1:B:196:LEU:HG	2.04	0.57
1:A:152:LEU:HD13	1:A:154:ARG:CZ	2.36	0.56
1:B:138:GLY:HA2	1:B:338:ILE:HD13	1.88	0.56
1:B:361:ILE:HD12	1:B:361:ILE:O	2.06	0.56
1:A:359:ALA:CB	1:A:360:PRO:HD2	2.26	0.55
1:A:51:GLY:HA3	1:A:54:LYS:HB2	1.89	0.55
1:A:269:LEU:HD13	1:A:284:GLN:HE21	1.72	0.55
1:A:134:ARG:HD2	1:A:335:MET:HE1	1.89	0.55
1:B:153:ILE:HD12	1:B:153:ILE:N	2.22	0.55
1:B:141:ALA:HB1	1:B:341:MET:HB2	1.87	0.55
1:B:18:SER:HA	1:B:129:ARG:HD2	1.90	0.54
1:A:251:VAL:HG13	1:B:293:LYS:CB	2.37	0.54
1:A:54:LYS:CE	1:A:177:PRO:HB3	2.34	0.54
1:A:68:ILE:HD13	1:A:84:LEU:HB3	1.89	0.54
1:A:136:ALA:O	1:A:140:ILE:HD12	2.07	0.54
1:A:320:HIS:O	1:A:322:PRO:HD3	2.07	0.54
1:A:350:GLN:HG2	1:B:1:MET:SD	2.48	0.54
1:B:230:ILE:HD12	1:B:336:LEU:CD1	2.38	0.54
1:A:12:VAL:HG22	1:A:27:VAL:HG13	1.89	0.53
1:A:182:ASP:OD1	1:A:184:ASP:N	2.41	0.53
1:B:230:ILE:CD1	1:B:336:LEU:HD12	2.37	0.53
1:B:70:GLY:CA	1:B:81:ILE:HD13	2.39	0.53
1:B:261:ASP:HB3	1:B:263:LEU:HG	1.91	0.53
1:B:276:ILE:N	1:B:276:ILE:HD12	2.24	0.53
1:A:18:SER:HB2	1:A:125:ARG:HB2	1.85	0.52
1:B:295:THR:HG21	1:B:324:VAL:HG21	1.90	0.52
1:B:321:ASP:HB2	1:B:322:PRO:CA	2.39	0.52
1:A:221:PRO:HA	1:A:222:VAL:C	2.34	0.52
1:A:207:LEU:HD13	1:A:292:LEU:HD13	1.91	0.52
1:B:61:GLU:HG2	1:B:61:GLU:O	2.09	0.52
1:A:43:LYS:O	1:A:47:ARG:HG3	2.09	0.52
1:A:81:ILE:HD12	1:A:81:ILE:N	2.24	0.52
1:B:186:VAL:HB	1:B:187:PRO:CD	2.39	0.52
1:B:245:ILE:CD1	1:B:288:VAL:HB	2.40	0.52
1:A:209:ILE:HD12	1:A:209:ILE:N	2.24	0.52
1:B:170:TRP:HA	1:B:173:VAL:CG1	2.38	0.52
1:A:160:ILE:HD11	1:A:189:PHE:CD2	2.44	0.52
1:A:19:HIS:H	1:A:19:HIS:CD2	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ALA:O	1:B:57:THR:HB	2.09	0.52
1:A:18:SER:CB	1:A:125:ARG:HB2	2.40	0.51
1:B:183:VAL:CG1	1:B:184:ASP:N	2.73	0.51
1:A:238:ASN:HA	1:B:225:ARG:HH12	1.76	0.51
1:B:67:ILE:HG21	1:B:71:VAL:CG2	2.41	0.51
1:A:291:ALA:HB2	1:B:249:PHE:CD1	2.46	0.51
1:A:293:LYS:HA	1:B:251:VAL:CG1	2.39	0.51
1:A:216:VAL:HG23	1:A:281:SER:O	2.11	0.50
1:B:324:VAL:HG12	1:B:327:ARG:NH1	2.25	0.50
1:A:131:THR:O	1:A:131:THR:CG2	2.58	0.50
1:A:241:LYS:HE3	1:B:245:ILE:O	2.11	0.50
1:A:61:GLU:HB2	1:A:62:PRO:O	2.11	0.50
1:B:218:TRP:CH2	1:B:344:PHE:HB2	2.46	0.50
1:B:259:THR:HG21	1:B:263:LEU:HB2	1.94	0.50
1:B:351:ASN:HD22	1:B:351:ASN:N	2.09	0.50
1:A:331:ILE:HD11	1:A:335:MET:HE3	1.94	0.50
1:A:11:ARG:HG2	1:A:28:ASP:HB2	1.93	0.50
1:A:321:ASP:HB3	1:A:324:VAL:HB	1.93	0.50
1:B:10:PHE:HA	1:B:28:ASP:O	2.12	0.50
1:B:354:VAL:HG12	1:B:355:VAL:O	2.12	0.50
1:A:238:ASN:O	1:A:239:ALA:HB3	2.12	0.49
1:B:154:ARG:NH1	1:B:212:GLU:OE2	2.45	0.49
1:A:183:VAL:HG13	1:A:184:ASP:N	2.25	0.49
1:B:148:LYS:HG2	1:B:149:PHE:CE2	2.47	0.49
1:B:295:THR:HG21	1:B:324:VAL:CG2	2.41	0.49
1:B:59:ARG:HG3	1:B:59:ARG:O	2.11	0.49
1:B:120:TYR:HD1	1:B:121:ARG:HG3	1.77	0.49
1:A:1:MET:O	1:A:2:ALA:CB	2.54	0.49
1:B:170:TRP:C	1:B:173:VAL:HG13	2.37	0.49
1:B:353:ASP:OD2	1:B:353:ASP:N	2.44	0.49
1:A:153:ILE:HD13	1:A:211:ALA:HA	1.92	0.49
1:B:173:VAL:CG2	1:B:174:PRO:CD	2.86	0.49
1:B:276:ILE:HD11	1:B:286:ILE:HG23	1.94	0.49
1:A:355:VAL:O	1:A:356:PRO:C	2.55	0.49
1:B:234:MET:O	1:B:237:ILE:HD12	2.13	0.49
1:B:160:ILE:HD12	1:B:189:PHE:CD2	2.48	0.49
1:A:328:ALA:O	1:A:331:ILE:CG2	2.61	0.48
1:A:4:ASN:HB2	1:A:14:THR:O	2.12	0.48
1:A:71:VAL:HG12	1:A:76:THR:HA	1.95	0.48
1:A:222:VAL:HG11	1:B:134:ARG:CZ	2.43	0.48
1:A:271:ASN:ND2	1:A:284:GLN:CD	2.67	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLY:O	1:A:251:VAL:HG23	2.12	0.48
1:B:153:ILE:HG23	1:B:336:LEU:HD23	1.95	0.48
1:B:277:LEU:O	1:B:280:ILE:HG13	2.14	0.48
1:A:173:VAL:HG22	1:A:174:PRO:HD3	1.95	0.48
1:A:49:LYS:HD3	1:A:55:PHE:HZ	1.79	0.47
1:B:57:THR:O	1:B:57:THR:HG23	2.12	0.47
1:B:54:LYS:HA	1:B:54:LYS:HD3	1.65	0.47
1:B:155:GLY:HA2	1:B:209:ILE:HA	1.96	0.47
1:A:62:PRO:HB2	1:A:63:ASP:H	1.39	0.47
1:B:275:GLY:C	1:B:276:ILE:HD12	2.40	0.47
1:A:131:THR:HG22	1:A:135:VAL:CG2	2.45	0.47
1:A:152:LEU:HD22	1:A:154:ARG:CD	2.45	0.47
1:A:161:GLY:O	1:B:253:GLY:HA2	2.14	0.47
1:A:223:PHE:HB2	1:B:3:GLY:O	2.15	0.47
1:B:149:PHE:HB2	1:B:151:VAL:HG23	1.97	0.47
1:A:23:LEU:HD11	1:A:129:ARG:HB3	1.97	0.47
1:B:169:ASP:O	1:B:172:GLU:HB3	2.15	0.47
1:B:167:LYS:HE2	1:B:182:ASP:OD1	2.15	0.47
1:A:176:ASN:HB2	1:A:177:PRO:HD2	1.96	0.46
1:A:9:LEU:HD12	1:A:346:ARG:HA	1.98	0.46
1:A:38:GLU:OE1	1:A:38:GLU:N	2.48	0.46
1:A:152:LEU:HD22	1:A:154:ARG:HD2	1.97	0.46
1:B:170:TRP:HA	1:B:173:VAL:HG13	1.96	0.46
1:A:173:VAL:HG12	1:A:181:GLY:HA2	1.98	0.46
1:A:256:GLY:O	1:A:257:HIS:CG	2.68	0.46
1:B:172:GLU:O	1:B:176:ASN:ND2	2.48	0.46
1:B:70:GLY:C	1:B:81:ILE:HD13	2.40	0.46
1:B:292:LEU:HD22	1:B:325:GLY:HA2	1.98	0.46
1:B:280:ILE:C	1:B:280:ILE:HD12	2.40	0.45
1:A:230:ILE:HA	1:A:339:VAL:HG21	1.99	0.45
1:B:37:THR:O	1:B:40:ASP:HB2	2.17	0.45
1:A:131:THR:HG23	1:A:331:ILE:HD13	1.98	0.45
1:B:257:HIS:O	1:B:257:HIS:ND1	2.40	0.45
1:B:5:SER:OG	1:B:6:ILE:N	2.48	0.45
1:A:153:ILE:CD1	1:A:211:ALA:HA	2.46	0.45
1:B:263:LEU:O	1:B:264:THR:C	2.58	0.45
1:B:324:VAL:O	1:B:325:GLY:C	2.58	0.45
1:B:138:GLY:HA2	1:B:338:ILE:CD1	2.46	0.45
1:A:355:VAL:O	1:A:356:PRO:O	2.35	0.44
1:B:156:HIS:CE1	1:B:168:LEU:HD13	2.52	0.44
1:B:321:ASP:CB	1:B:324:VAL:HG13	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:HA	1:B:242:GLY:HA2	2.00	0.44
1:B:222:VAL:H	1:B:222:VAL:HG23	1.36	0.44
1:A:50:PRO:O	1:A:54:LYS:HE2	2.18	0.44
1:A:61:GLU:N	1:A:62:PRO:HA	2.32	0.44
1:B:258:GLU:OE1	1:B:260:ARG:CZ	2.65	0.44
1:A:320:HIS:O	1:A:322:PRO:CD	2.66	0.44
1:B:212:GLU:O	1:B:213:LYS:HB2	2.17	0.44
1:B:354:VAL:O	1:B:356:PRO:HD3	2.17	0.44
1:A:24:MET:HA	1:A:83:LEU:O	2.18	0.44
1:A:173:VAL:HG12	1:A:181:GLY:CA	2.48	0.44
1:B:157:VAL:HG21	1:B:326:VAL:HG12	2.00	0.43
1:B:321:ASP:HB2	1:B:322:PRO:HA	1.99	0.43
1:A:129:ARG:C	1:A:131:THR:N	2.73	0.43
1:A:358:PHE:CZ	1:A:361:ILE:HD12	2.53	0.43
1:B:329:THR:HB	1:B:330:PRO:HD3	2.00	0.43
1:A:48:ARG:O	1:A:50:PRO:HD3	2.18	0.43
1:B:65:VAL:HA	1:B:85:ILE:HG13	2.01	0.43
1:B:321:ASP:HB2	1:B:322:PRO:C	2.44	0.43
1:A:362:GLU:O	1:A:362:GLU:CG	2.63	0.43
1:A:341:MET:O	1:A:344:PHE:HB3	2.18	0.43
1:A:68:ILE:CD1	1:A:84:LEU:HB3	2.49	0.43
1:A:149:PHE:HB2	1:A:151:VAL:HG23	2.01	0.43
1:A:323:CYS:C	1:A:325:GLY:H	2.26	0.43
1:B:42:GLN:OE1	1:B:64:GLN:HA	2.19	0.43
1:B:92:SER:C	1:B:93:LYS:HG3	2.43	0.42
1:B:176:ASN:C	1:B:177:PRO:O	2.57	0.42
1:B:266:HIS:HD2	1:B:266:HIS:O	2.02	0.42
1:B:292:LEU:CD2	1:B:325:GLY:HA2	2.50	0.42
1:A:137:ALA:HA	1:A:140:ILE:CD1	2.49	0.42
1:A:194:THR:O	1:A:198:GLU:HG2	2.19	0.42
1:B:173:VAL:CG2	1:B:174:PRO:N	2.81	0.42
1:B:202:SER:HA	1:B:322:PRO:O	2.20	0.42
1:A:18:SER:CB	1:A:125:ARG:CB	2.86	0.42
1:A:134:ARG:HD2	1:A:335:MET:CE	2.48	0.42
1:A:136:ALA:O	1:A:139:ALA:HB3	2.20	0.42
1:B:331:ILE:HD12	1:B:331:ILE:N	2.34	0.42
1:A:178:PHE:O	1:A:179:PHE:C	2.59	0.42
1:B:120:TYR:HA	1:B:121:ARG:HA	1.73	0.42
1:B:258:GLU:HB2	1:B:260:ARG:HG3	2.02	0.42
1:B:290:ILE:HD12	1:B:292:LEU:HD11	2.01	0.42
1:A:344:PHE:CD1	1:A:344:PHE:C	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:VAL:N	1:B:174:PRO:CD	2.83	0.41
1:A:162:ASN:OD1	1:A:162:ASN:C	2.63	0.41
1:B:53:SER:HB3	1:B:54:LYS:H	1.68	0.41
1:A:34:LEU:C	1:A:75:LYS:HG2	2.45	0.41
1:A:79:THR:HB	1:A:80:PRO:HD2	2.02	0.41
1:B:52:THR:O	1:B:53:SER:HB2	2.20	0.41
1:A:182:ASP:O	1:A:186:VAL:HG23	2.21	0.41
1:A:228:ALA:HA	1:B:235:MET:HB3	2.01	0.41
1:B:208:GLU:C	1:B:209:ILE:HD13	2.45	0.41
1:A:153:ILE:C	1:A:154:ARG:HG3	2.45	0.41
1:A:238:ASN:HA	1:B:225:ARG:NH1	2.34	0.41
1:A:247:ASP:OD1	1:A:254:GLN:NE2	2.49	0.41
1:A:256:GLY:O	1:A:257:HIS:ND1	2.53	0.41
1:A:249:PHE:CD1	1:B:291:ALA:HB2	2.55	0.41
1:A:129:ARG:O	1:A:130:GLU:C	2.63	0.41
1:A:137:ALA:HA	1:A:140:ILE:HD13	2.01	0.41
1:B:241:LYS:HA	1:B:241:LYS:HD2	1.77	0.41
1:A:284:GLN:H	1:A:284:GLN:HG2	1.56	0.41
1:B:230:ILE:CD1	1:B:339:VAL:HB	2.51	0.41
1:A:164:VAL:O	1:A:188:ARG:NH2	2.54	0.40
1:B:286:ILE:HD12	1:B:286:ILE:N	2.36	0.40
1:A:358:PHE:CZ	1:A:361:ILE:CD1	3.03	0.40
1:A:134:ARG:CB	1:A:335:MET:HE1	2.51	0.40
1:A:208:GLU:C	1:A:209:ILE:HD12	2.46	0.40
1:B:196:LEU:O	1:B:197:ARG:C	2.65	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	316/363 (87%)	288 (91%)	22 (7%)	6 (2%)	6	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	318/363 (88%)	283 (89%)	29 (9%)	6 (2%)	6	28
All	All	634/726 (87%)	571 (90%)	51 (8%)	12 (2%)	6	28

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	PRO
1	A	221	PRO
1	B	357	PRO
1	B	360	PRO
1	A	123	GLY
1	A	356	PRO
1	B	123	GLY
1	B	179	PHE
1	A	357	PRO
1	B	356	PRO
1	A	360	PRO
1	B	359	ALA

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	251/286 (88%)	223 (89%)	28 (11%)	6	22
1	B	253/286 (88%)	226 (89%)	27 (11%)	6	24
All	All	504/572 (88%)	449 (89%)	55 (11%)	6	23

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	24	MET
1	A	37	THR
1	A	39	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	44	ASP
1	A	63	ASP
1	A	127	SER
1	A	130	GLU
1	A	152	LEU
1	A	154	ARG
1	A	160	ILE
1	A	164	VAL
1	A	169	ASP
1	A	173	VAL
1	A	194	THR
1	A	201	THR
1	A	220	GLU
1	A	222	VAL
1	A	227	ASP
1	A	268	PHE
1	A	271	ASN
1	A	284	GLN
1	A	293	LYS
1	A	326	VAL
1	A	327	ARG
1	A	331	ILE
1	A	350	GLN
1	A	362	GLU
1	B	5	SER
1	B	8	GLN
1	B	42	GLN
1	B	54	LYS
1	B	57	THR
1	B	121	ARG
1	B	142	LYS
1	B	148	LYS
1	B	154	ARG
1	B	173	VAL
1	B	176	ASN
1	B	193	VAL
1	B	194	THR
1	B	199	GLN
1	B	201	THR
1	B	209	ILE
1	B	212	GLU
1	B	221	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	222	VAL
1	B	251	VAL
1	B	261	ASP
1	B	264	THR
1	B	266	HIS
1	B	284	GLN
1	B	288	VAL
1	B	293	LYS
1	B	297	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	175	ASN
1	A	232	HIS
1	A	271	ASN
1	A	284	GLN
1	B	42	GLN
1	B	90	GLN
1	B	175	ASN
1	B	176	ASN
1	B	266	HIS
1	B	351	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	322/363 (88%)	0.28	45 (13%) 6 4	2, 15, 100, 100	0
1	B	324/363 (89%)	0.33	42 (12%) 7 5	3, 21, 100, 100	0
All	All	646/726 (88%)	0.30	87 (13%) 7 4	2, 17, 100, 100	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	SER	5.8
1	A	361	ILE	5.5
1	B	355	VAL	5.1
1	A	362	GLU	5.0
1	A	259	THR	4.8
1	A	57	THR	4.7
1	A	263	LEU	4.4
1	A	355	VAL	4.4
1	B	52	THR	4.1
1	A	92	SER	4.1
1	B	359	ALA	4.0
1	B	126	SER	4.0
1	B	263	LEU	3.9
1	A	363	PRO	3.8
1	A	298	ILE	3.8
1	A	262	GLU	3.7
1	A	360	PRO	3.7
1	A	55	PHE	3.6
1	A	354	VAL	3.6
1	B	120	TYR	3.6
1	B	299	THR	3.6
1	B	300	THR	3.6
1	A	321	ASP	3.6
1	A	357	PRO	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	55	PHE	3.5
1	B	363	PRO	3.5
1	B	361	ILE	3.4
1	B	261	ASP	3.4
1	B	354	VAL	3.3
1	A	297	SER	3.3
1	B	51	GLY	3.2
1	B	56	ALA	3.2
1	A	258	GLU	3.2
1	A	56	ALA	3.2
1	A	126	SER	3.2
1	A	265	SER	3.1
1	B	93	LYS	3.1
1	B	268	PHE	3.1
1	B	57	THR	3.1
1	B	264	THR	3.1
1	B	360	PRO	3.1
1	B	258	GLU	3.0
1	B	356	PRO	3.0
1	A	125	ARG	3.0
1	A	260	ARG	3.0
1	A	356	PRO	3.0
1	B	259	THR	3.0
1	B	260	ARG	3.0
1	B	53	SER	3.0
1	A	123	GLY	3.0
1	B	262	GLU	2.9
1	B	119	ASP	2.9
1	A	358	PHE	2.9
1	B	358	PHE	2.9
1	A	264	THR	2.8
1	A	269	LEU	2.8
1	A	352	ALA	2.8
1	A	91	LYS	2.8
1	A	221	PRO	2.7
1	B	357	PRO	2.6
1	B	266	HIS	2.6
1	A	89	ASP	2.6
1	B	316	THR	2.6
1	A	267	GLY	2.6
1	B	269	LEU	2.6
1	A	59	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	353	ASP	2.5
1	B	124	GLY	2.5
1	B	265	SER	2.5
1	B	353	ASP	2.5
1	A	120	TYR	2.5
1	B	257	HIS	2.5
1	A	359	ALA	2.4
1	A	319	ARG	2.4
1	A	261	ASP	2.4
1	B	298	ILE	2.4
1	A	118	ARG	2.3
1	B	122	GLY	2.2
1	A	58	GLN	2.2
1	A	60	LYS	2.1
1	A	52	THR	2.1
1	A	257	HIS	2.1
1	A	268	PHE	2.1
1	B	91	LYS	2.0
1	B	352	ALA	2.0
1	A	124	GLY	2.0
1	B	60	LYS	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.