



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:35 AM EDT

PDB ID : 2G85 / pdb_00002g85
Title : Crystal structure of chorismate synthase from Mycobacterium tuberculosis at 2.22 angstroms of resolution
Authors : Dias, M.V.B.; dos Santos, B.B.; Ely, F.; Basso, L.A.; Santos, D.S.; de Azevedo Jr., W.F.
Deposited on : 2006-03-01
Resolution : 2.22 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

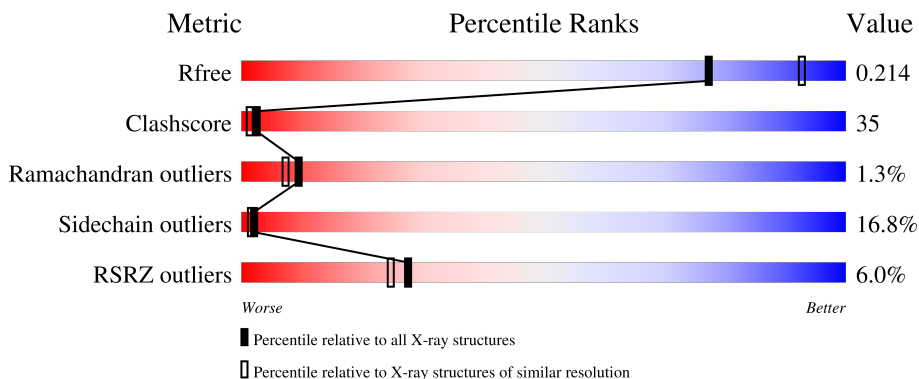
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	401	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3251 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	386	Total	C	N	O	S	0	0	0
			2829	1752	527	539	11			

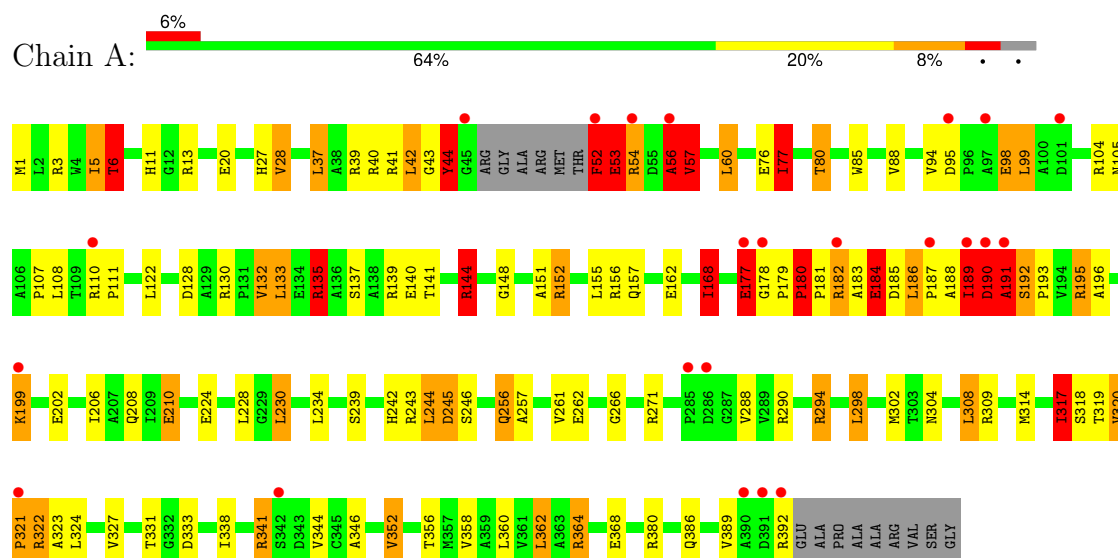
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	421	Total	O	0	1
			422	422		

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: Chorismate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	130.29Å 130.29Å 157.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.73 – 2.22 47.73 – 2.22	Depositor EDS
% Data completeness (in resolution range)	94.8 (47.73-2.22) 94.8 (47.73-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.173 , 0.214 0.174 , 0.214	Depositor DCC
R_{free} test set	1873 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3251	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 3.89% 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	1.00	5/2875 (0.2%)	1.43	40/3905 (1.0%)

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	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	GLY	N-CA	7.43	1.54	1.44
1	A	177	GLU	N-CA	7.08	1.54	1.46
1	A	177	GLU	CA-C	6.15	1.59	1.52
1	A	57	VAL	CA-CB	5.44	1.60	1.54
1	A	178	GLY	CA-C	5.23	1.59	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	GLU	N-CA-C	9.72	124.25	108.41
1	A	56	ALA	CA-C-N	9.38	134.44	120.75
1	A	56	ALA	C-N-CA	9.38	134.44	120.75
1	A	191	ALA	N-CA-C	-8.28	93.16	110.80
1	A	54	ARG	N-CA-C	8.07	121.51	108.76
1	A	195	ARG	NE-CZ-NH2	-7.60	112.36	119.20
1	A	317	ILE	CB-CA-C	-7.42	99.13	111.29
1	A	245	ASP	N-CA-CB	-7.08	98.52	110.49
1	A	179	PRO	N-CA-C	7.02	119.27	110.70
1	A	28	VAL	CB-CA-C	-6.98	98.62	111.18
1	A	309	ARG	NE-CZ-NH2	-6.79	113.08	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ILE	CA-C-N	-6.56	109.01	121.54
1	A	189	ILE	C-N-CA	-6.56	109.01	121.54
1	A	168	ILE	CG1-CB-CG2	-6.52	91.13	110.70
1	A	364	ARG	NE-CZ-NH1	-6.44	115.06	121.50
1	A	57	VAL	CB-CA-C	-6.33	102.55	111.28
1	A	6	THR	N-CA-CB	-6.22	100.01	110.83
1	A	135	ARG	NE-CZ-NH2	6.06	124.65	119.20
1	A	99	LEU	N-CA-C	-6.04	106.55	114.04
1	A	144	ARG	CD-NE-CZ	6.02	132.82	124.40
1	A	364	ARG	NE-CZ-NH2	6.02	124.61	119.20
1	A	321	PRO	N-CA-C	5.95	124.72	112.47
1	A	144	ARG	NE-CZ-NH2	-5.93	113.86	119.20
1	A	132	VAL	N-CA-C	5.92	116.10	110.53
1	A	180	PRO	CA-C-N	5.83	127.22	120.98
1	A	180	PRO	C-N-CA	5.83	127.22	120.98
1	A	152	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	A	192	SER	N-CA-C	5.65	119.67	109.44
1	A	13	ARG	N-CA-C	5.57	117.03	111.07
1	A	77	ILE	CA-CB-CG2	5.49	119.84	110.50
1	A	144	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	A	190	ASP	CA-C-N	-5.44	111.15	121.54
1	A	190	ASP	C-N-CA	-5.44	111.15	121.54
1	A	177	GLU	CA-C-O	-5.43	114.48	120.30
1	A	320	VAL	CA-C-N	5.38	126.57	119.84
1	A	320	VAL	C-N-CA	5.38	126.57	119.84
1	A	271	ARG	N-CA-C	-5.17	106.99	113.72
1	A	6	THR	OG1-CB-CG2	5.16	119.62	109.30
1	A	135	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	184	GLU	CB-CA-C	-5.01	100.58	110.11

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	PRO	Peptide
1	A	189	ILE	Peptide
1	A	190	ASP	Peptide
1	A	52	PHE	Peptide
1	A	56	ALA	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	2829	0	2833	196	4
2	A	422	0	0	85	12
All	All	3251	0	2833	196	13

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 35.

All (196) 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:186:LEU:H	1:A:186:LEU:CD1	1.07	1.43
1:A:188:ALA:HB2	2:A:751:HOH:O	1.27	1.33
1:A:189:ILE:O	1:A:190:ASP:C	1.74	1.28
1:A:386:GLN:HG3	2:A:705:HOH:O	1.26	1.27
1:A:290:ARG:NH1	2:A:479:HOH:O	1.65	1.26
1:A:40:ARG:NH1	1:A:141:THR:OG1	1.73	1.22
1:A:188:ALA:HB1	2:A:752:HOH:O	1.09	1.21
1:A:380:ARG:HD3	2:A:530:HOH:O	1.34	1.20
1:A:53:GLU:CG	1:A:80:THR:HG21	1.74	1.18
1:A:168:ILE:HB	2:A:428:HOH:O	1.43	1.17
1:A:56:ALA:O	2:A:599:HOH:O	1.62	1.16
1:A:317:ILE:HG21	2:A:749:HOH:O	0.99	1.15
1:A:186:LEU:HD12	1:A:186:LEU:N	1.13	1.15
1:A:57:VAL:HA	2:A:764:HOH:O	1.47	1.11
1:A:53:GLU:HG2	1:A:80:THR:HG21	1.34	1.08
1:A:189:ILE:HD12	1:A:195:ARG:HD2	1.32	1.08
1:A:189:ILE:O	1:A:191:ALA:N	1.88	1.07
1:A:168:ILE:CB	2:A:428:HOH:O	1.98	1.04
1:A:188:ALA:CB	2:A:751:HOH:O	1.90	1.03
1:A:187:PRO:CD	2:A:485:HOH:O	2.06	1.03
1:A:40:ARG:NE	2:A:702:HOH:O	1.88	1.00
1:A:52:PHE:CD2	1:A:52:PHE:N	2.27	0.97
1:A:53:GLU:HG3	1:A:80:THR:HG21	1.47	0.97
1:A:6:THR:HG21	1:A:140:GLU:OE1	1.66	0.94
1:A:187:PRO:HD3	2:A:485:HOH:O	1.62	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:CG1	2:A:682:HOH:O	2.16	0.92
1:A:27:HIS:H	1:A:157:GLN:HE22	1.13	0.92
1:A:256:GLN:H	1:A:256:GLN:HE21	0.94	0.91
1:A:189:ILE:CD1	1:A:195:ARG:HH11	1.83	0.90
1:A:188:ALA:CB	2:A:752:HOH:O	1.82	0.89
1:A:314:MET:HE2	1:A:317:ILE:HG12	1.55	0.89
1:A:52:PHE:N	1:A:52:PHE:HD2	1.68	0.88
1:A:182:ARG:HD3	1:A:182:ARG:H	1.39	0.88
1:A:40:ARG:NH2	2:A:702:HOH:O	2.00	0.87
1:A:185:ASP:C	1:A:186:LEU:HD12	2.02	0.84
1:A:189:ILE:HG12	2:A:682:HOH:O	1.75	0.84
1:A:368:GLU:HG3	2:A:794:HOH:O	1.76	0.83
1:A:256:GLN:HE21	1:A:256:GLN:N	1.75	0.83
1:A:368:GLU:OE1	2:A:754:HOH:O	1.95	0.82
1:A:317:ILE:HD11	1:A:346:ALA:HB3	1.59	0.82
1:A:199:LYS:H	1:A:199:LYS:HZ2	1.28	0.82
1:A:189:ILE:CD1	1:A:195:ARG:HD2	2.08	0.81
1:A:189:ILE:HD12	1:A:195:ARG:CD	2.10	0.79
1:A:53:GLU:HG2	1:A:80:THR:CG2	2.14	0.78
1:A:107:PRO:HA	2:A:809:HOH:O	1.84	0.78
1:A:44:TYR:HD1	1:A:44:TYR:C	1.92	0.78
1:A:181:PRO:HD2	1:A:184:GLU:OE2	1.84	0.77
1:A:6:THR:HG22	1:A:135:ARG:HH22	1.50	0.76
1:A:182:ARG:HD2	2:A:762:HOH:O	1.86	0.75
1:A:181:PRO:HG2	2:A:728:HOH:O	1.85	0.74
1:A:107:PRO:CA	2:A:809:HOH:O	2.35	0.74
1:A:148:GLY:O	1:A:152:ARG:HG3	1.87	0.74
1:A:39:ARG:HA	1:A:42:LEU:HD22	1.69	0.74
1:A:40:ARG:CZ	2:A:702:HOH:O	2.20	0.73
1:A:44:TYR:C	1:A:44:TYR:CD1	2.65	0.73
1:A:189:ILE:HD13	1:A:195:ARG:HH11	1.52	0.73
1:A:177:GLU:HA	2:A:427:HOH:O	1.88	0.72
1:A:27:HIS:HD2	2:A:796:HOH:O	1.72	0.71
1:A:182:ARG:CD	2:A:762:HOH:O	2.36	0.71
1:A:182:ARG:HD3	1:A:182:ARG:N	2.04	0.70
1:A:186:LEU:HB2	1:A:187:PRO:HD3	1.73	0.70
1:A:39:ARG:HH11	1:A:189:ILE:HD11	1.57	0.70
1:A:41:ARG:HD3	2:A:610:HOH:O	1.93	0.69
1:A:168:ILE:HG13	2:A:428:HOH:O	1.92	0.69
1:A:368:GLU:HG3	2:A:735:HOH:O	1.92	0.68
1:A:56:ALA:HB2	2:A:814:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:HIS:CD2	2:A:745:HOH:O	2.46	0.67
1:A:181:PRO:O	1:A:184:GLU:HG2	1.94	0.67
1:A:183:ALA:HB3	2:A:429:HOH:O	1.93	0.67
1:A:77:ILE:HD11	2:A:732:HOH:O	1.96	0.66
1:A:6:THR:HG23	1:A:135:ARG:HH12	1.61	0.66
1:A:168:ILE:CG1	2:A:428:HOH:O	2.29	0.65
1:A:290:ARG:NE	2:A:410:HOH:O	1.95	0.64
1:A:152:ARG:NH2	2:A:453:HOH:O	2.31	0.64
1:A:243:ARG:NH1	2:A:723:HOH:O	2.30	0.64
1:A:5:ILE:HG22	2:A:731:HOH:O	1.97	0.63
1:A:189:ILE:HD11	1:A:195:ARG:HH11	1.62	0.63
1:A:56:ALA:C	2:A:764:HOH:O	2.41	0.62
1:A:57:VAL:CA	2:A:764:HOH:O	2.24	0.62
1:A:27:HIS:HB2	2:A:420:HOH:O	1.99	0.62
1:A:41:ARG:NH1	1:A:52:PHE:HB3	2.15	0.61
1:A:230:LEU:HB2	2:A:409:HOH:O	2.01	0.61
1:A:27:HIS:N	1:A:157:GLN:HE22	1.94	0.60
1:A:168:ILE:CD1	1:A:224:GLU:HB2	2.32	0.60
1:A:317:ILE:HD11	1:A:346:ALA:CB	2.29	0.60
1:A:88:VAL:HG13	1:A:105:ASN:HD22	1.67	0.60
1:A:185:ASP:O	1:A:189:ILE:HB	2.02	0.60
1:A:206:ILE:O	1:A:210:GLU:HG2	2.03	0.58
1:A:43:GLY:C	2:A:727:HOH:O	2.46	0.58
1:A:189:ILE:HA	1:A:195:ARG:HD2	1.86	0.58
1:A:256:GLN:H	1:A:256:GLN:NE2	1.80	0.58
1:A:44:TYR:HD1	1:A:44:TYR:O	1.87	0.57
1:A:54:ARG:HB2	2:A:592:HOH:O	2.04	0.57
1:A:20:GLU:CD	2:A:706:HOH:O	2.47	0.56
1:A:184:GLU:O	1:A:187:PRO:HD2	2.05	0.56
1:A:189:ILE:HG21	2:A:733:HOH:O	2.05	0.56
1:A:189:ILE:HG21	2:A:682:HOH:O	2.06	0.55
1:A:186:LEU:H	1:A:186:LEU:HD12	0.40	0.55
1:A:290:ARG:NH2	2:A:410:HOH:O	2.38	0.55
1:A:257:ALA:HB2	1:A:317:ILE:HG23	1.87	0.55
1:A:41:ARG:CZ	1:A:52:PHE:HB3	2.37	0.55
1:A:130:ARG:HA	1:A:133:LEU:HD13	1.89	0.55
1:A:187:PRO:HG2	2:A:486:HOH:O	2.06	0.55
1:A:317:ILE:CG2	2:A:749:HOH:O	1.85	0.55
1:A:52:PHE:HB2	1:A:53:GLU:C	2.33	0.54
1:A:338:ILE:HG23	2:A:700:HOH:O	2.06	0.54
1:A:168:ILE:HD11	1:A:224:GLU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:TYR:N	2:A:727:HOH:O	2.41	0.54
1:A:77:ILE:HD11	1:A:139:ARG:HH22	1.72	0.54
1:A:41:ARG:HG3	1:A:52:PHE:HA	1.91	0.53
1:A:80:THR:HB	2:A:769:HOH:O	2.09	0.53
1:A:189:ILE:HD11	1:A:195:ARG:NH1	2.24	0.53
1:A:294:ARG:HD3	2:A:478:HOH:O	2.09	0.53
1:A:380:ARG:NH2	2:A:763:HOH:O	2.30	0.53
1:A:144:ARG:NH2	2:A:407:HOH:O	2.42	0.52
1:A:3:ARG:NH1	2:A:744:HOH:O	2.15	0.52
1:A:140:GLU:OE2	1:A:144:ARG:HD2	2.08	0.52
1:A:6:THR:CG2	1:A:135:ARG:HH22	2.21	0.52
1:A:60:LEU:HD22	1:A:76:GLU:HB2	1.90	0.52
1:A:318:SER:HA	1:A:341:ARG:HG3	1.91	0.52
1:A:57:VAL:N	2:A:764:HOH:O	2.36	0.52
1:A:187:PRO:CG	2:A:485:HOH:O	2.48	0.52
1:A:352:VAL:HG23	2:A:405:HOH:O	2.09	0.51
1:A:141:THR:HA	1:A:144:ARG:HD3	1.93	0.51
1:A:239:SER:HB3	1:A:242:HIS:CD2	2.45	0.51
1:A:56:ALA:HB1	2:A:605:HOH:O	2.11	0.51
1:A:189:ILE:O	1:A:190:ASP:O	2.23	0.51
1:A:107:PRO:CB	2:A:809:HOH:O	2.58	0.50
1:A:182:ARG:HD2	2:A:788:HOH:O	2.11	0.50
1:A:128:ASP:CG	2:A:809:HOH:O	2.55	0.50
1:A:189:ILE:CD1	1:A:195:ARG:NH1	2.64	0.50
1:A:320:VAL:HG13	1:A:323:ALA:HB3	1.94	0.50
1:A:386:GLN:NE2	2:A:705:HOH:O	2.37	0.50
1:A:189:ILE:CB	2:A:682:HOH:O	2.54	0.50
1:A:94:VAL:CG1	1:A:99:LEU:HG	2.42	0.50
1:A:1:MET:CE	1:A:3:ARG:NH2	2.75	0.49
1:A:183:ALA:CB	2:A:429:HOH:O	2.55	0.49
1:A:184:GLU:C	1:A:187:PRO:HD2	2.37	0.48
1:A:242:HIS:HD2	2:A:745:HOH:O	1.92	0.48
1:A:208:GLN:HG2	2:A:480:HOH:O	2.12	0.48
1:A:156:ARG:HD3	1:A:162:GLU:OE2	2.14	0.48
1:A:196:ALA:HB3	1:A:202:GLU:HB2	1.95	0.48
1:A:111:PRO:HD2	1:A:327:VAL:O	2.14	0.48
1:A:88:VAL:HG21	1:A:104:ARG:HB3	1.96	0.47
1:A:262:GLU:HB2	1:A:266:GLY:HA3	1.96	0.47
1:A:60:LEU:CD2	1:A:76:GLU:HB2	2.44	0.47
1:A:331:THR:OG1	1:A:333:ASP:HB2	2.13	0.47
1:A:44:TYR:CD1	1:A:44:TYR:O	2.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PRO:HB2	1:A:182:ARG:HH11	1.80	0.47
1:A:364:ARG:HD2	2:A:406:HOH:O	2.14	0.47
1:A:42:LEU:HG	1:A:190:ASP:H	1.79	0.47
1:A:11:HIS:HB3	1:A:85:TRP:CD2	2.50	0.46
1:A:39:ARG:CA	1:A:42:LEU:HD22	2.42	0.46
1:A:182:ARG:HD3	2:A:762:HOH:O	2.12	0.46
1:A:188:ALA:O	1:A:195:ARG:HA	2.16	0.46
1:A:189:ILE:HG22	2:A:654:HOH:O	2.15	0.46
1:A:185:ASP:CA	1:A:186:LEU:HD12	2.46	0.46
1:A:156:ARG:NH2	1:A:162:GLU:OE1	2.49	0.46
1:A:181:PRO:HB2	1:A:182:ARG:NH1	2.31	0.46
1:A:168:ILE:HG21	1:A:168:ILE:HD12	1.16	0.45
1:A:364:ARG:CD	2:A:406:HOH:O	2.64	0.45
1:A:95:ASP:HB3	1:A:98:GLU:HG2	1.97	0.45
1:A:56:ALA:O	2:A:764:HOH:O	2.20	0.45
1:A:94:VAL:HG12	1:A:99:LEU:HG	1.97	0.45
1:A:245:ASP:HB3	1:A:246:SER:H	1.48	0.45
1:A:181:PRO:CB	1:A:182:ARG:HH11	2.31	0.44
1:A:151:ALA:HB2	1:A:360:LEU:HD23	1.99	0.44
1:A:239:SER:CB	1:A:242:HIS:CD2	3.00	0.44
1:A:108:LEU:N	2:A:809:HOH:O	2.50	0.44
1:A:37:LEU:HB3	1:A:52:PHE:HE1	1.83	0.43
1:A:192:SER:HA	1:A:193:PRO:HD3	1.89	0.43
1:A:56:ALA:N	2:A:814:HOH:O	2.52	0.43
1:A:319:THR:HG23	1:A:324:LEU:HD12	1.99	0.43
1:A:298:LEU:HA	1:A:302:MET:O	2.19	0.43
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.83	0.43
1:A:380:ARG:NH1	2:A:763:HOH:O	2.41	0.43
1:A:37:LEU:HB3	1:A:52:PHE:CE1	2.54	0.42
1:A:308:LEU:HD12	1:A:362:LEU:HD21	2.02	0.42
1:A:177:GLU:H	1:A:177:GLU:HG2	1.51	0.42
1:A:317:ILE:H	1:A:317:ILE:HG13	1.47	0.42
1:A:190:ASP:HA	1:A:192:SER:O	2.20	0.42
1:A:110:ARG:HH11	1:A:338:ILE:CD1	2.33	0.41
1:A:181:PRO:HA	1:A:228:LEU:HD11	2.02	0.41
1:A:186:LEU:CD1	1:A:186:LEU:N	1.91	0.41
1:A:180:PRO:CB	1:A:184:GLU:HG3	2.50	0.41
1:A:56:ALA:CB	2:A:814:HOH:O	2.59	0.41
1:A:20:GLU:HG2	2:A:433:HOH:O	2.21	0.41
1:A:230:LEU:HD11	1:A:362:LEU:HG	2.01	0.41
1:A:304:ASN:C	1:A:304:ASN:OD1	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ARG:HD2	2:A:432:HOH:O	2.20	0.41
1:A:185:ASP:O	1:A:189:ILE:N	2.45	0.41
1:A:168:ILE:HG23	1:A:168:ILE:HD13	0.95	0.41
1:A:210:GLU:HG3	2:A:775:HOH:O	2.20	0.40
1:A:380:ARG:CD	2:A:530:HOH:O	2.19	0.40
1:A:41:ARG:NH1	2:A:608:HOH:O	2.53	0.40
1:A:358:VAL:HG12	1:A:362:LEU:HD22	2.04	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:NH2	1:A:110:ARG:NH2[12_545]	1.31	0.89
2:A:710:HOH:O	2:A:723:HOH:O[4_655]	1.51	0.69
2:A:472:HOH:O	2:A:709:HOH:O[4_655]	1.60	0.60
1:A:322:ARG:N	2:A:759:HOH:O[12_545]	1.63	0.57
2:A:537:HOH:O	2:A:704:HOH:O[8_556]	1.95	0.25
1:A:243:ARG:NH1	2:A:710:HOH:O[4_655]	1.99	0.21
1:A:20:GLU:OE1	2:A:746:HOH:O[8_556]	2.02	0.18
2:A:737:HOH:O	2:A:755:HOH:O[8_556]	2.09	0.11
2:A:539:HOH:O	2:A:755:HOH:O[8_556]	2.12	0.08
2:A:535:HOH:O	2:A:755:HOH:O[8_556]	2.13	0.07
2:A:537:HOH:O	2:A:755:HOH:O[8_556]	2.15	0.05
2:A:466:HOH:O	2:A:763:HOH:O[11_656]	2.16	0.04
2:A:783:HOH:O	2:A:783:HOH:O[11_656]	2.16	0.04

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	382/401 (95%)	367 (96%)	10 (3%)	5 (1%)	9 7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	191	ALA
1	A	190	ASP
1	A	44	TYR
1	A	56	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	279/288 (97%)	232 (83%)	47 (17%)	2 1

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	THR
1	A	28	VAL
1	A	37	LEU
1	A	42	LEU
1	A	44	TYR
1	A	52	PHE
1	A	53	GLU
1	A	57	VAL
1	A	60	LEU
1	A	77	ILE
1	A	80	THR
1	A	98	GLU
1	A	122	LEU
1	A	132	VAL
1	A	133	LEU
1	A	135	ARG
1	A	137	SER
1	A	144	ARG
1	A	155	LEU

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Mol	Chain	Res	Type
1	A	168	ILE
1	A	177	GLU
1	A	182	ARG
1	A	184	GLU
1	A	186	LEU
1	A	189	ILE
1	A	199	LYS
1	A	210	GLU
1	A	230	LEU
1	A	234	LEU
1	A	244	LEU
1	A	256	GLN
1	A	261	VAL
1	A	288	VAL
1	A	294	ARG
1	A	298	LEU
1	A	308	LEU
1	A	317	ILE
1	A	321	PRO
1	A	322	ARG
1	A	341	ARG
1	A	344	VAL
1	A	352	VAL
1	A	356	THR
1	A	362	LEU
1	A	389	VAL
1	A	392	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	157	GLN
1	A	242	HIS
1	A	256	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	386/401 (96%)	-0.10	23 (5%)	27 25	19, 29, 55, 72	2 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	ASP	7.9
1	A	191	ALA	5.6
1	A	52	PHE	5.2
1	A	178	GLY	4.0
1	A	56	ALA	3.4
1	A	45	GLY	3.4
1	A	182	ARG	3.3
1	A	177	GLU	2.8
1	A	189	ILE	2.7
1	A	321	PRO	2.6
1	A	286	ASP	2.6
1	A	101	ASP	2.5
1	A	97	ALA	2.4
1	A	54	ARG	2.4
1	A	285	PRO	2.3
1	A	342	SER	2.3
1	A	390	ALA	2.3
1	A	391	ASP	2.3
1	A	392	ARG	2.2
1	A	110	ARG	2.2
1	A	199	LYS	2.1
1	A	187	PRO	2.0
1	A	95	ASP	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.