



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:27 AM UTC

PDB ID : 1QDL / pdb_00001qdl
Title : THE CRYSTAL STRUCTURE OF ANTHRANILATE SYNTHASE FROM
SULFOLOBUS SOLFATARICUS
Authors : Knoechel, T.; Ivens, A.; Hester, G.; Gonzalez, A.; Bauerle, R.; Wilmanns, M.;
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Deposited on : 1999-05-20
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

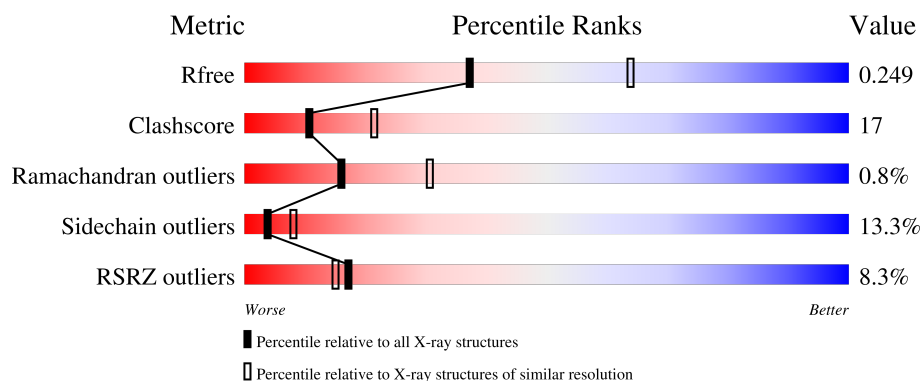
1 Overall quality at a glance

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	422	11% 54% 36% 9%
2	B	195	3% 63% 32% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5003 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 PROTEIN (ANTHRANILATE SYNTHASE (TRPE-SUBUNIT)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	1
			3324	2150	544	619	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	ALA	ARG	conflict	UNP Q06128

- Molecule 2 is a protein called PROTEIN (ANTHRANILATE SYNTHASE (TRPG-SUBUNIT)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1549	999	264	283	3			

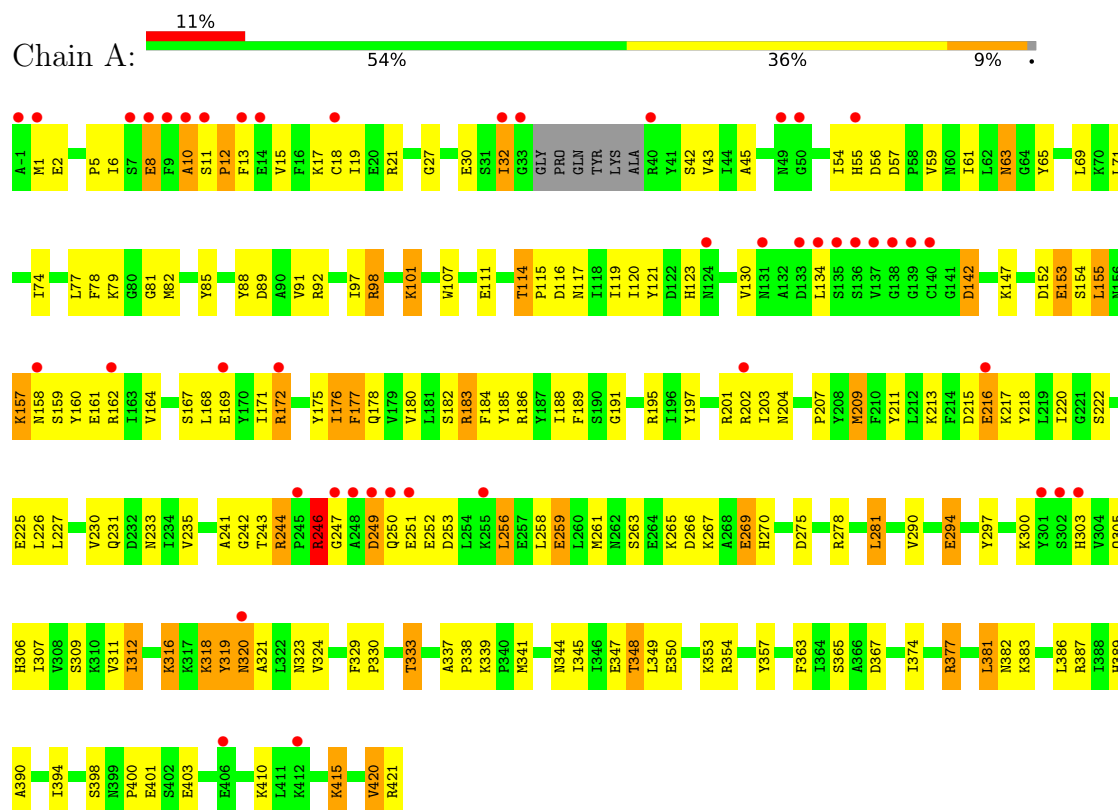
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	40	Total	O	0	0
			40	40		

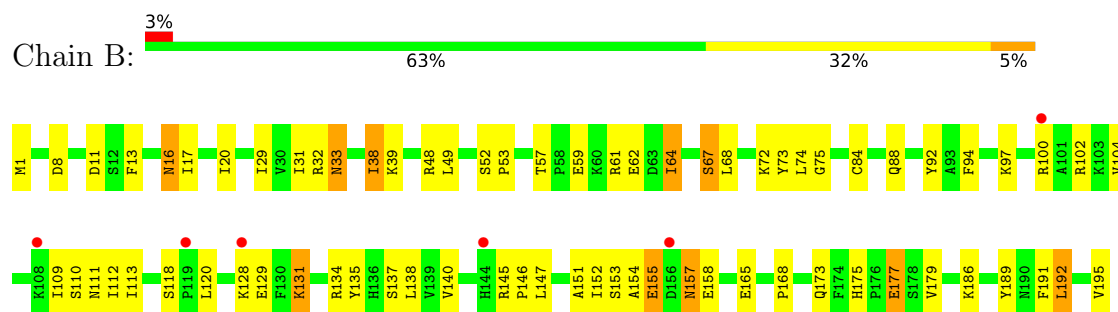
3 Residue-property plots

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: PROTEIN (ANTHRANILATE SYNTHASE (TRPE-SUBUNIT))



• Molecule 2: PROTEIN (ANTHRANILATE SYNTHASE (TRPG-SUBUNIT))



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	162.00Å 162.00Å 212.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.50) 99.7 (30.00-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 2.51Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.226 , 0.254 0.217 , 0.249	Depositor DCC
R_{free} test set	2887 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5003	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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	0.53	1/3404 (0.0%)	1.03	23/4605 (0.5%)
2	B	0.47	0/1583	0.97	6/2145 (0.3%)
All	All	0.51	1/4987 (0.0%)	1.01	29/6750 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	ILE	C-N	-5.73	1.25	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ALA	N-CA-C	-8.00	102.16	112.23
1	A	177	PHE	N-CA-C	-7.44	103.82	113.12
1	A	116	ASP	N-CA-C	-7.07	103.64	112.90
1	A	1	MET	N-CA-C	7.00	121.27	110.20
2	B	16	ASN	N-CA-C	-6.79	103.67	112.23
1	A	354	ARG	N-CA-C	6.78	119.51	111.71
1	A	188	ILE	N-CA-C	-6.02	101.08	109.45
1	A	250	GLN	N-CA-C	-5.93	105.75	112.87
1	A	203	ILE	N-CA-C	5.92	116.56	110.82
1	A	319	TYR	N-CA-C	5.75	118.59	110.14
1	A	377	ARG	N-CA-C	-5.74	103.47	111.39
2	B	118	SER	CA-C-N	5.72	125.74	119.90
2	B	118	SER	C-N-CA	5.72	125.74	119.90
1	A	259	GLU	N-CA-C	-5.70	105.15	111.36
2	B	67	SER	N-CA-C	5.51	118.00	111.33
1	A	281	LEU	N-CA-C	-5.36	105.60	111.82
2	B	52	SER	N-CA-C	5.25	117.62	110.01
1	A	204	ASN	CA-C-N	-5.23	114.85	120.03
1	A	204	ASN	C-N-CA	-5.23	114.85	120.03
1	A	101	LYS	N-CA-C	5.20	117.33	110.36
2	B	104	VAL	N-CA-C	5.19	115.24	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	PHE	N-CA-C	5.17	116.67	108.96
1	A	191	GLY	N-CA-C	5.16	118.28	111.52
1	A	353	LYS	N-CA-C	-5.10	102.74	110.28
1	A	114	THR	CA-C-N	5.09	125.37	119.93
1	A	114	THR	C-N-CA	5.09	125.37	119.93
1	A	10	ALA	N-CA-C	-5.07	99.99	110.80
1	A	233	ASN	N-CA-C	5.07	119.41	113.23
1	A	227	LEU	N-CA-C	-5.04	105.44	111.03

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	3324	0	3299	120	0
2	B	1549	0	1574	44	0
3	A	90	0	0	2	0
3	B	40	0	0	1	0
All	All	5003	0	4873	163	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 (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ARG:HD2	2:B:192:LEU:HD22	1.52	0.90
1:A:381:LEU:HD22	1:A:386:LEU:HG	1.55	0.85
1:A:249:ASP:OD2	1:A:251:GLU:HB2	1.78	0.82
1:A:42:SER:HB2	1:A:121:TYR:HB2	1.62	0.80
2:B:146:PRO:O	2:B:165:GLU:HG3	1.84	0.78
1:A:420:VAL:HG12	1:A:421:ARG:HG2	1.64	0.77
2:B:145:ARG:HD2	2:B:165:GLU:OE2	1.89	0.72
2:B:128:LYS:HG3	2:B:129:GLU:HG2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASP:HB2	1:A:61:ILE:HD11	1.72	0.71
1:A:77:LEU:HD11	1:A:231:GLN:HG3	1.75	0.68
1:A:387:ARG:HH11	1:A:389:HIS:HD2	1.39	0.68
1:A:85:TYR:CE2	1:A:111:GLU:HB2	2.29	0.68
1:A:341:MET:HE3	1:A:345:ILE:HG13	1.77	0.67
1:A:415:LYS:HG2	1:A:420:VAL:HG11	1.77	0.67
1:A:154:SER:O	1:A:155:LEU:HB2	1.96	0.66
1:A:222:SER:O	1:A:377:ARG:HD2	1.96	0.65
1:A:159:SER:O	1:A:162:ARG:HG2	1.98	0.63
1:A:45:ALA:HB1	1:A:115:PRO:HB3	1.82	0.62
1:A:10:ALA:HB3	1:A:15:VAL:HG22	1.82	0.61
1:A:381:LEU:N	1:A:381:LEU:HD23	2.14	0.61
1:A:81:GLY:O	1:A:114:THR:HG23	2.01	0.61
1:A:11:SER:O	1:A:15:VAL:HG23	2.00	0.61
1:A:270:HIS:HE1	1:A:309:SER:OG	1.84	0.60
2:B:75:GLY:O	2:B:168:PRO:HD2	2.02	0.60
1:A:263:SER:O	1:A:267:LYS:HG3	2.01	0.60
1:A:175:TYR:O	1:A:341:MET:HG2	2.01	0.59
2:B:110:SER:HB2	2:B:134:ARG:HD3	1.84	0.59
2:B:38:ILE:HG22	3:B:210:HOH:O	2.02	0.58
1:A:318:LYS:HD2	1:A:319:TYR:CZ	2.39	0.57
1:A:15:VAL:O	1:A:19:ILE:HG12	2.05	0.57
2:B:64:ILE:HB	2:B:67:SER:HB2	1.86	0.57
1:A:10:ALA:HB3	1:A:15:VAL:CG2	2.35	0.56
1:A:101:LYS:HD3	1:A:347:GLU:O	2.05	0.56
2:B:53:PRO:HB3	2:B:84:CYS:HB3	1.87	0.56
1:A:13:PHE:HD1	1:A:201:ARG:HH11	1.54	0.56
1:A:32:ILE:H	1:A:207:PRO:HA	1.71	0.56
1:A:249:ASP:C	1:A:251:GLU:H	2.15	0.56
1:A:98:ARG:HG3	1:A:344:ASN:OD1	2.07	0.55
2:B:153:SER:HB3	2:B:158:GLU:H	1.71	0.55
1:A:176:ILE:HA	1:A:338:PRO:HD2	1.89	0.55
2:B:38:ILE:HD11	2:B:74:LEU:HD13	1.89	0.55
2:B:146:PRO:HA	2:B:165:GLU:OE2	2.06	0.55
2:B:111:ASN:HD21	2:B:131:LYS:HE3	1.71	0.54
1:A:154:SER:HB2	1:A:184:PHE:CZ	2.43	0.54
1:A:256:LEU:HD12	1:A:259:GLU:OE2	2.08	0.54
1:A:77:LEU:CD1	1:A:231:GLN:HG3	2.38	0.53
1:A:241:ALA:HB1	1:A:269:GLU:HG2	1.90	0.53
1:A:294:GLU:HB3	1:A:297:TYR:CD2	2.43	0.53
1:A:365:SER:HB3	1:A:367:ASP:OD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LEU:CD1	2:B:74:LEU:N	2.72	0.53
1:A:225:GLU:HB3	1:A:374:ILE:HD12	1.90	0.53
2:B:153:SER:O	2:B:157:ASN:HA	2.09	0.53
1:A:249:ASP:N	1:A:249:ASP:OD1	2.43	0.52
1:A:111:GLU:OE2	1:A:217:LYS:HE3	2.09	0.52
1:A:157:LYS:NZ	1:A:401:GLU:HG3	2.25	0.52
1:A:43:VAL:HG13	1:A:120:ILE:CD1	2.40	0.52
2:B:48:ARG:CD	2:B:192:LEU:HD22	2.31	0.52
2:B:59:GLU:HG2	2:B:92:TYR:CE1	2.45	0.52
2:B:64:ILE:CD1	2:B:68:LEU:HD12	2.40	0.52
1:A:218:TYR:HB2	1:A:381:LEU:HG	1.91	0.51
1:A:153:GLU:HB2	1:A:185:TYR:CD2	2.46	0.51
1:A:164:VAL:HG11	1:A:400:PRO:HA	1.93	0.51
1:A:249:ASP:C	1:A:251:GLU:N	2.65	0.50
2:B:74:LEU:N	2:B:74:LEU:HD12	2.26	0.50
1:A:247:GLY:HA3	1:A:253:ASP:CA	2.41	0.50
1:A:337:ALA:HA	1:A:338:PRO:C	2.36	0.50
1:A:275:ASP:OD1	1:A:278:ARG:NH1	2.45	0.50
1:A:256:LEU:HB3	1:A:305:GLN:HE21	1.77	0.49
2:B:17:ILE:CG1	2:B:177:GLU:HG2	2.42	0.49
1:A:11:SER:HB2	1:A:12:PRO:HD2	1.94	0.49
1:A:318:LYS:HG2	3:A:432:HOH:O	2.10	0.49
1:A:17:LYS:O	1:A:21:ARG:HG3	2.12	0.49
1:A:119:ILE:HG12	1:A:130:VAL:HG13	1.94	0.49
1:A:230:VAL:HG22	1:A:235:VAL:HG22	1.96	0.48
1:A:316:LYS:HB2	1:A:319:TYR:CD1	2.49	0.48
1:A:180:VAL:HG21	1:A:333:THR:O	2.13	0.48
1:A:243:THR:HG23	1:A:306:HIS:CE1	2.48	0.48
1:A:5:PRO:HG2	1:A:8:GLU:HB2	1.95	0.48
1:A:263:SER:HB3	1:A:266:ASP:HB2	1.95	0.48
1:A:74:ILE:HD11	1:A:79:LYS:HA	1.95	0.48
1:A:89:ASP:O	1:A:92:ARG:HG3	2.14	0.48
1:A:243:THR:O	1:A:244:ARG:HD3	2.14	0.48
1:A:241:ALA:O	1:A:307:ILE:HB	2.14	0.48
1:A:330:PRO:HD2	1:A:339:LYS:HD3	1.96	0.47
1:A:142:ASP:N	1:A:142:ASP:OD1	2.48	0.47
1:A:211:TYR:CD1	1:A:220:ILE:HG12	2.50	0.47
1:A:213:LYS:HG3	1:A:218:TYR:CE2	2.50	0.47
1:A:294:GLU:HB3	1:A:297:TYR:CE2	2.50	0.47
2:B:145:ARG:HB3	2:B:165:GLU:OE2	2.14	0.47
2:B:155:GLU:H	2:B:155:GLU:CD	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:THR:HG22	1:A:349:LEU:HD23	1.96	0.47
2:B:189:TYR:C	2:B:189:TYR:CD2	2.92	0.47
1:A:88:TYR:HA	1:A:329:PHE:CZ	2.51	0.46
2:B:64:ILE:HD11	2:B:68:LEU:HD12	1.97	0.46
1:A:320:ASN:O	1:A:324:VAL:HG23	2.15	0.46
2:B:53:PRO:HB3	2:B:84:CYS:CB	2.46	0.46
1:A:258:LEU:HA	1:A:261:MET:HB2	1.97	0.46
2:B:175:HIS:HB3	2:B:177:GLU:OE2	2.16	0.45
1:A:182:SER:HB2	1:A:390:ALA:O	2.16	0.45
1:A:175:TYR:O	1:A:176:ILE:HG23	2.17	0.45
1:A:357:TYR:CD1	1:A:389:HIS:HB3	2.51	0.45
1:A:101:LYS:HE2	1:A:350:GLU:O	2.17	0.45
1:A:256:LEU:O	1:A:259:GLU:HB2	2.15	0.45
2:B:64:ILE:H	2:B:64:ILE:HG13	1.66	0.45
1:A:247:GLY:HA3	1:A:253:ASP:CB	2.47	0.45
1:A:186:ARG:HG2	1:A:387:ARG:HB2	1.99	0.45
2:B:111:ASN:ND2	2:B:131:LYS:HG3	2.32	0.45
1:A:177:PHE:CZ	2:B:135:TYR:HB3	2.52	0.44
1:A:386:LEU:C	1:A:386:LEU:HD23	2.42	0.44
1:A:91:VAL:HG13	1:A:97:ILE:HD13	2.00	0.44
1:A:247:GLY:HA3	1:A:253:ASP:HB2	1.99	0.44
2:B:112:ILE:O	2:B:129:GLU:HA	2.18	0.44
1:A:57:ASP:O	1:A:61:ILE:HG12	2.17	0.44
1:A:13:PHE:CE1	1:A:197:TYR:HD2	2.35	0.44
1:A:27:GLY:HA2	1:A:211:TYR:O	2.17	0.44
1:A:168:LEU:O	1:A:172:ARG:HD3	2.18	0.44
1:A:216:GLU:H	1:A:216:GLU:HG3	1.39	0.43
2:B:191:PHE:HA	2:B:195:VAL:CG2	2.48	0.43
1:A:54:ILE:HG23	1:A:61:ILE:HG13	1.99	0.43
2:B:16:ASN:O	2:B:20:ILE:HG13	2.18	0.43
1:A:160:TYR:CG	1:A:183:ARG:HD2	2.53	0.43
1:A:242:GLY:O	1:A:306:HIS:HA	2.18	0.43
2:B:73:TYR:N	2:B:73:TYR:CD1	2.85	0.43
1:A:121:TYR:HB3	1:A:123:HIS:CE1	2.53	0.43
2:B:94:PHE:HB2	2:B:147:LEU:CD1	2.49	0.43
1:A:30:GLU:HB2	1:A:209:MET:HB2	2.01	0.43
1:A:153:GLU:HB2	1:A:185:TYR:HD2	1.84	0.43
1:A:78:PHE:HD1	1:A:363:PHE:CD1	2.37	0.42
1:A:91:VAL:HG21	1:A:330:PRO:HD3	2.01	0.42
1:A:85:TYR:CD1	1:A:85:TYR:C	2.97	0.42
2:B:113:ILE:HD11	2:B:154:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HG12	1:A:19:ILE:H	1.72	0.42
1:A:246:ARG:HD2	1:A:246:ARG:HA	1.53	0.42
2:B:33:ASN:HB2	2:B:64:ILE:O	2.20	0.42
2:B:94:PHE:HB2	2:B:147:LEU:HD11	2.02	0.42
2:B:112:ILE:HG22	2:B:151:ALA:HB1	2.01	0.42
1:A:107:TRP:CZ2	1:A:382:ASN:HB2	2.55	0.42
1:A:246:ARG:O	1:A:256:LEU:HD23	2.20	0.42
1:A:281:LEU:HD22	1:A:311:VAL:HG12	2.01	0.42
1:A:320:ASN:HB2	1:A:323:ASN:OD1	2.19	0.42
1:A:59:VAL:O	1:A:63:ASN:HB2	2.20	0.42
1:A:65:TYR:O	1:A:69:LEU:HG	2.20	0.42
2:B:88:GLN:NE2	2:B:173:GLN:HE22	2.17	0.42
1:A:61:ILE:HG12	1:A:61:ILE:H	1.73	0.41
2:B:100:ARG:HG2	2:B:138:LEU:HD23	2.02	0.41
1:A:74:ILE:O	1:A:79:LYS:HD3	2.20	0.41
1:A:316:LYS:HB2	1:A:319:TYR:HD1	1.84	0.41
1:A:157:LYS:O	1:A:161:GLU:HG3	2.21	0.41
1:A:55:HIS:HB2	3:A:434:HOH:O	2.19	0.41
2:B:17:ILE:HG13	2:B:177:GLU:HG2	2.01	0.41
1:A:152:ASP:OD2	1:A:186:ARG:HB2	2.21	0.41
1:A:167:SER:O	1:A:171:ILE:HG13	2.20	0.41
1:A:290:VAL:HA	1:A:312:ILE:O	2.20	0.41
2:B:8:ASP:O	2:B:32:ARG:HA	2.21	0.41
1:A:178:GLN:HA	1:A:394:ILE:O	2.21	0.41
1:A:252:GLU:O	1:A:256:LEU:HD22	2.21	0.41
1:A:300:LYS:NZ	1:A:305:GLN:OE1	2.54	0.41
1:A:381:LEU:HD22	1:A:386:LEU:CG	2.39	0.41
2:B:17:ILE:HG12	2:B:177:GLU:HG2	2.02	0.41
2:B:11:ASP:OD1	2:B:13:PHE:HB2	2.21	0.40
1:A:182:SER:OG	1:A:389:HIS:HE1	2.04	0.40
1:A:43:VAL:HG13	1:A:120:ILE:HD13	2.03	0.40
1:A:381:LEU:N	1:A:381:LEU:CD2	2.84	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	412/422 (98%)	386 (94%)	22 (5%)	4 (1%)	12	24
2	B	193/195 (99%)	186 (96%)	6 (3%)	1 (0%)	24	43
All	All	605/617 (98%)	572 (94%)	28 (5%)	5 (1%)	16	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	ARG
1	A	155	LEU
2	B	33	ASN
1	A	215	ASP
1	A	12	PRO

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	356/360 (99%)	311 (87%)	45 (13%)	4	9
2	B	169/169 (100%)	144 (85%)	25 (15%)	3	6
All	All	525/529 (99%)	455 (87%)	70 (13%)	4	8

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	6	ILE
1	A	8	GLU
1	A	18	CYS
1	A	63	ASN
1	A	71	LEU
1	A	82	MET

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Mol	Chain	Res	Type
1	A	98	ARG
1	A	117	ASN
1	A	134	LEU
1	A	142	ASP
1	A	147	LYS
1	A	153	GLU
1	A	157	LYS
1	A	158	ASN
1	A	169	GLU
1	A	172	ARG
1	A	176	ILE
1	A	183	ARG
1	A	195	ARG
1	A	202	ARG
1	A	209	MET
1	A	216	GLU
1	A	226	LEU
1	A	244	ARG
1	A	246	ARG
1	A	249	ASP
1	A	256	LEU
1	A	265	LYS
1	A	269	GLU
1	A	294	GLU
1	A	303	HIS
1	A	312	ILE
1	A	316	LYS
1	A	318	LYS
1	A	320	ASN
1	A	333	THR
1	A	348	THR
1	A	381	LEU
1	A	383	LYS
1	A	398	SER
1	A	403	GLU
1	A	410	LYS
1	A	415	LYS
1	A	420	VAL
2	B	1	MET
2	B	29	ILE
2	B	31	ILE
2	B	38	ILE

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Mol	Chain	Res	Type
2	B	39	LYS
2	B	49	LEU
2	B	57	THR
2	B	61	ARG
2	B	62	GLU
2	B	64	ILE
2	B	72	LYS
2	B	97	LYS
2	B	102	ARG
2	B	109	ILE
2	B	120	LEU
2	B	131	LYS
2	B	137	SER
2	B	140	VAL
2	B	152	ILE
2	B	155	GLU
2	B	157	ASN
2	B	177	GLU
2	B	179	VAL
2	B	186	LYS
2	B	192	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	156	ASN
1	A	270	HIS
1	A	320	ASN
1	A	389	HIS
2	B	111	ASN
2	B	173	GLN

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	416/422 (98%)	0.38	45 (10%) 11 9	28, 47, 88, 100	0
2	B	195/195 (100%)	0.12	6 (3%) 51 47	32, 48, 75, 90	0
All	All	611/617 (99%)	0.30	51 (8%) 17 15	28, 47, 84, 100	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	GLU	5.8
1	A	-1	ALA	5.7
1	A	10	ALA	4.9
1	A	137	VAL	4.9
1	A	40	ARG	4.6
1	A	248	ALA	4.4
1	A	301	TYR	4.2
1	A	303	HIS	4.1
1	A	302	SER	4.0
1	A	9	PHE	3.7
1	A	158	ASN	3.7
1	A	133	ASP	3.7
1	A	8	GLU	3.6
1	A	255	LYS	3.5
1	A	33	GLY	3.5
1	A	1	MET	3.4
1	A	247	GLY	3.4
1	A	138	GLY	3.3
1	A	136	SER	3.2
1	A	135	SER	3.2
1	A	162	ARG	3.1
2	B	156	ASP	3.0
1	A	124	ASN	3.0
1	A	249	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	50	GLY	2.9
1	A	139	GLY	2.9
1	A	172	ARG	2.9
1	A	134	LEU	2.9
2	B	144	HIS	2.8
2	B	108	LYS	2.8
1	A	14	GLU	2.7
1	A	18	CYS	2.7
1	A	250	GLN	2.6
1	A	13	PHE	2.6
1	A	245	PRO	2.5
2	B	128	LYS	2.5
1	A	32	ILE	2.5
2	B	100	ARG	2.4
2	B	119	PRO	2.4
1	A	320	ASN	2.4
1	A	406	GLU	2.4
1	A	412	LYS	2.2
1	A	7	SER	2.2
1	A	11	SER	2.2
1	A	216	GLU	2.2
1	A	49	ASN	2.1
1	A	140	CYS	2.1
1	A	131	ASN	2.1
1	A	202	ARG	2.1
1	A	55	HIS	2.0
1	A	169	GLU	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.