



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:56 AM UTC

PDB ID : 1I1Q / pdb_00001i1q
Title : STRUCTURE OF THE COOPERATIVE ALLOSTERIC ANTHRANILATE
SYNTHASE FROM SALMONELLA TYPHIMURIUM
Authors : Morollo, A.A.; Eck, M.J.
Deposited on : 2001-02-02
Resolution : 1.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

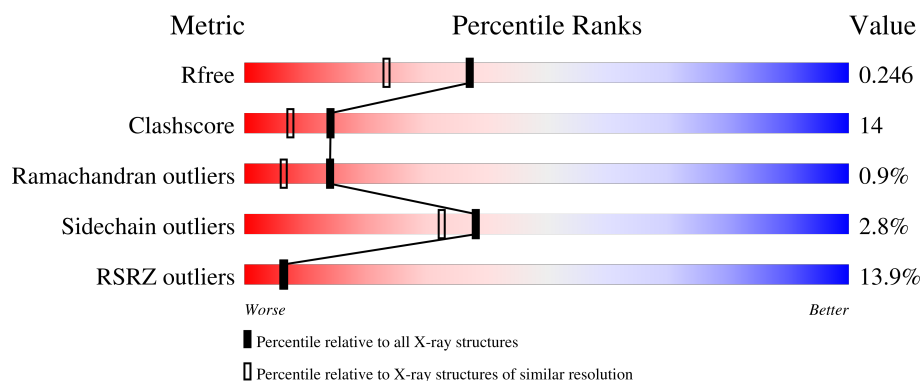
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	520	8% 79% 17% ••
2	B	192	29% 56% 38% •••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5490 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 ANTHRANILATE SYNTHASE COMPONENT I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3929	2464	696	747	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	ASN	ASP	SEE REMARK 999	UNP P00898
A	179	GLU	GLY	SEE REMARK 999	UNP P00898
A	440	ASP	GLU	SEE REMARK 999	UNP P00898
A	442	GLU	ASP	SEE REMARK 999	UNP P00898

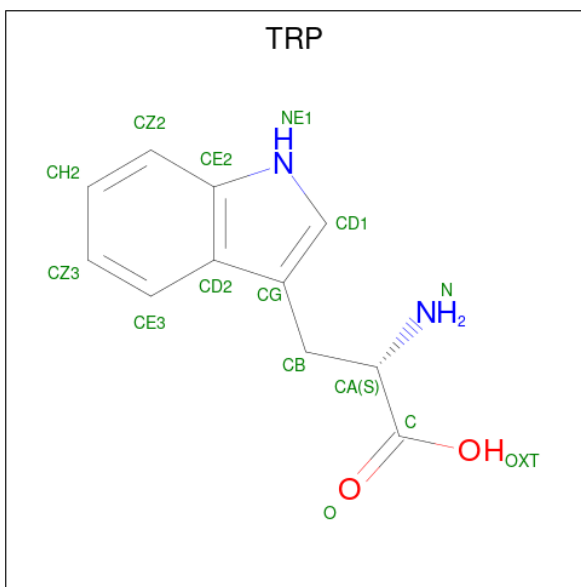
- Molecule 2 is a protein called ANTHRANILATE SYNTHASE COMPONENT II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	186	Total	C	N	O	S	0	0	0
			1420	898	257	256	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	109	THR	SER	SEE REMARK 999	UNP P00905

- Molecule 3 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		

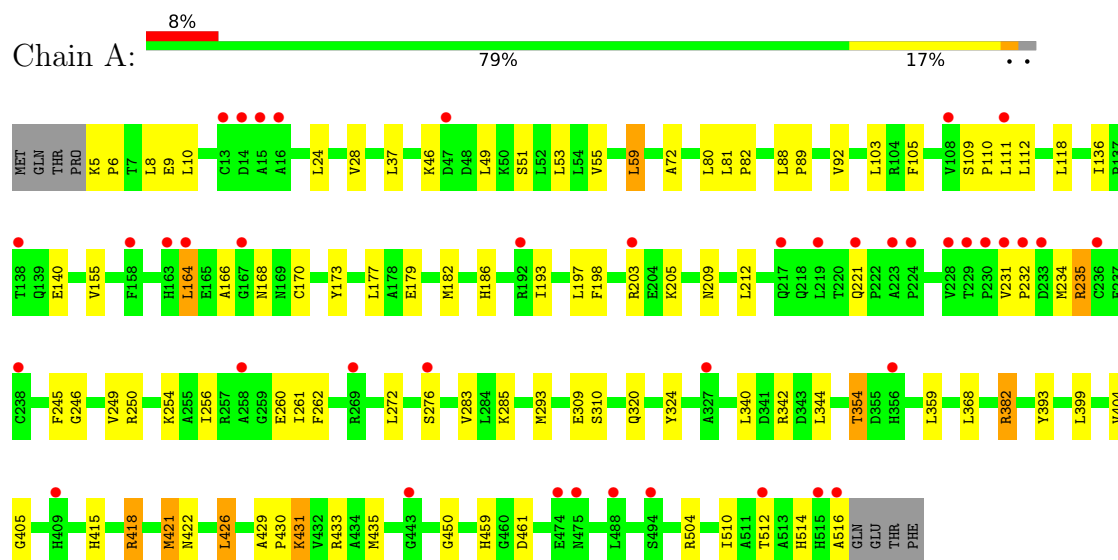
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	17	Total	O	0	0
			17	17		

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: ANTHRANILATE SYNTHASE COMPONENT I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.00Å 101.70Å 67.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.66 – 1.90 24.66 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.5 (24.66-1.90) 94.5 (24.66-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.246 0.218 , 0.246	Depositor DCC
R_{free} test set	3060 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5490	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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	0.37	0/4003	0.90	8/5440 (0.1%)
2	B	0.33	0/1450	0.88	6/1969 (0.3%)
All	All	0.36	0/5453	0.90	14/7409 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	GLU	N-CA-C	-6.70	103.78	112.68
1	A	105	PHE	CA-C-N	6.10	124.05	119.66
1	A	105	PHE	C-N-CA	6.10	124.05	119.66
2	B	37	GLN	N-CA-C	-5.95	104.86	111.71
2	B	124	ASN	CA-C-N	-5.92	113.09	120.79
2	B	124	ASN	C-N-CA	-5.92	113.09	120.79
1	A	431	LYS	N-CA-C	5.87	117.37	110.97
1	A	415	HIS	N-CA-C	-5.77	105.08	111.36
2	B	117	ALA	CB-CA-C	-5.38	110.36	116.54
2	B	176	THR	N-CA-C	5.35	117.53	111.11
1	A	399	LEU	N-CA-C	-5.29	100.11	108.73
2	B	126	LEU	N-CA-C	5.13	116.37	109.24
1	A	324	TYR	N-CA-C	5.01	118.23	108.21
1	A	177	LEU	N-CA-C	-5.00	101.01	108.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3929	0	3914	79	0
2	B	1420	0	1422	76	0
3	A	15	0	9	0	0
4	A	109	0	0	2	0
4	B	17	0	0	0	0
All	All	5490	0	5345	152	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 14.

All (152) 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:19:GLN:HE22	2:B:171:GLU:HA	1.31	0.95
2:B:53:LEU:HD22	2:B:66:MET:HE2	1.53	0.90
1:A:164:LEU:H	1:A:164:LEU:HD13	1.42	0.83
1:A:504:ARG:HH21	1:A:504:ARG:HB2	1.46	0.79
2:B:8:ASN:HD21	2:B:66:MET:HE1	1.47	0.79
1:A:232:PRO:HA	1:A:516:ALA:HB3	1.65	0.78
1:A:10:LEU:HD12	1:A:140:GLU:HG3	1.68	0.73
2:B:19:GLN:NE2	2:B:171:GLU:HA	2.02	0.73
1:A:89:PRO:O	1:A:92:VAL:HG22	1.89	0.73
1:A:235:ARG:HB2	1:A:235:ARG:NH1	2.04	0.73
2:B:47:LYS:C	2:B:49:PRO:HD3	2.16	0.71
1:A:5:LYS:HB3	1:A:6:PRO:HD3	1.73	0.70
1:A:382:ARG:C	1:A:382:ARG:HD2	2.16	0.70
2:B:124:ASN:HB2	2:B:125:PRO:CD	2.21	0.70
1:A:504:ARG:HB2	1:A:504:ARG:NH2	2.06	0.69
1:A:168:ASN:ND2	1:A:170:CYS:HB2	2.07	0.69
1:A:235:ARG:HB2	1:A:235:ARG:HH11	1.58	0.69
2:B:32:ASN:HD22	2:B:32:ASN:C	2.00	0.69
2:B:132:HIS:ND1	2:B:133:SER:N	2.41	0.69
1:A:59:LEU:HD12	1:A:72:ALA:HA	1.73	0.68
2:B:158:HIS:HB3	2:B:163:VAL:HG22	1.76	0.67
1:A:320:GLN:OE1	1:A:404:VAL:HG11	1.95	0.67
2:B:66:MET:HB3	2:B:67:PRO:HD3	1.76	0.67
1:A:276:SER:H	1:A:514:HIS:HE1	1.43	0.66
2:B:35:PRO:O	2:B:36:ALA:CB	2.44	0.66
2:B:6:LEU:HD23	2:B:66:MET:HE3	1.78	0.65
2:B:162:ARG:CZ	2:B:192:LYS:HD2	2.27	0.64
2:B:124:ASN:N	2:B:124:ASN:HD22	1.96	0.64
2:B:113:HIS:CD2	2:B:119:PHE:HB3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:ALA:HB3	2:B:155:ALA:HB3	1.81	0.63
1:A:55:VAL:HG21	1:A:182:MET:HE2	1.82	0.62
2:B:47:LYS:O	2:B:49:PRO:HD3	2.01	0.60
1:A:46:LYS:HE3	1:A:393:TYR:OH	2.01	0.60
1:A:309:GLU:HG3	1:A:310:SER:N	2.18	0.58
2:B:53:LEU:HD11	2:B:70:LEU:HD21	1.85	0.58
1:A:51:SER:OG	1:A:186:HIS:HE1	1.87	0.58
2:B:8:ASN:HD21	2:B:66:MET:CE	2.15	0.57
2:B:191:GLN:O	2:B:192:LYS:HB2	2.04	0.57
1:A:459:HIS:HD2	1:A:461:ASP:OD2	1.87	0.57
1:A:168:ASN:HD21	1:A:170:CYS:HB2	1.69	0.56
1:A:232:PRO:CA	1:A:516:ALA:HB3	2.36	0.56
1:A:155:VAL:HG21	1:A:435:MET:HE1	1.87	0.55
1:A:8:LEU:HD23	1:A:9:GLU:N	2.20	0.55
1:A:246:GLY:O	1:A:250:ARG:HG3	2.06	0.55
1:A:404:VAL:HG12	1:A:405:GLY:N	2.22	0.55
2:B:139:VAL:HG13	2:B:143:LEU:HD23	1.89	0.55
1:A:250:ARG:O	1:A:254:LYS:HD3	2.06	0.55
2:B:65:CYS:O	2:B:69:LEU:HB2	2.07	0.54
1:A:276:SER:H	1:A:514:HIS:CE1	2.25	0.54
2:B:87:GLN:OE1	2:B:97:VAL:HG21	2.08	0.54
1:A:422:ASN:HA	4:A:1056:HOH:O	2.06	0.54
1:A:272:LEU:CD1	1:A:510:ILE:HG21	2.37	0.54
2:B:129:ALA:HB2	2:B:174:LEU:HB2	1.89	0.54
1:A:272:LEU:HD12	1:A:272:LEU:O	2.07	0.54
1:A:285:LYS:HA	1:A:293:MET:HE1	1.90	0.53
1:A:46:LYS:HE3	1:A:393:TYR:HH	1.72	0.53
2:B:145:ILE:HD12	2:B:145:ILE:N	2.23	0.53
2:B:132:HIS:O	2:B:133:SER:CB	2.56	0.53
2:B:32:ASN:O	2:B:64:GLY:HA3	2.09	0.53
1:A:429:ALA:HA	1:A:430:PRO:C	2.34	0.53
2:B:104:LEU:HB3	2:B:107:LYS:HD2	1.89	0.53
2:B:109:THR:OG1	2:B:130:ARG:HD3	2.09	0.52
1:A:340:LEU:HD21	1:A:342:ARG:HH21	1.75	0.52
2:B:32:ASN:C	2:B:32:ASN:ND2	2.65	0.52
1:A:136:ILE:HD12	1:A:136:ILE:N	2.25	0.52
2:B:36:ALA:HB2	2:B:65:CYS:HB2	1.91	0.52
2:B:132:HIS:O	2:B:133:SER:HB3	2.09	0.51
1:A:118:LEU:HD12	1:A:418:ARG:HD2	1.90	0.51
2:B:162:ARG:HD2	2:B:192:LYS:HB2	1.92	0.51
1:A:272:LEU:HD13	1:A:510:ILE:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:HIS:HB3	2:B:171:GLU:OE2	2.10	0.51
2:B:110:SER:HB3	2:B:125:PRO:HB2	1.92	0.51
1:A:235:ARG:HH11	1:A:235:ARG:CB	2.23	0.50
1:A:81:LEU:HB2	1:A:82:PRO:HD3	1.93	0.50
2:B:53:LEU:HB3	2:B:66:MET:CE	2.42	0.50
2:B:162:ARG:HD2	2:B:191:GLN:O	2.12	0.50
2:B:45:THR:HG22	2:B:45:THR:O	2.11	0.50
1:A:272:LEU:HD11	1:A:510:ILE:HD13	1.93	0.49
2:B:94:GLY:O	2:B:140:PRO:CG	2.60	0.49
2:B:103:ILE:HD12	2:B:103:ILE:N	2.27	0.49
2:B:139:VAL:HB	2:B:145:ILE:HD11	1.95	0.49
1:A:8:LEU:HD23	1:A:8:LEU:C	2.39	0.48
1:A:88:LEU:HB3	1:A:92:VAL:CG2	2.44	0.48
2:B:35:PRO:O	2:B:36:ALA:HB2	2.13	0.48
2:B:162:ARG:NE	2:B:192:LYS:HD2	2.28	0.48
1:A:10:LEU:HD12	1:A:140:GLU:CG	2.41	0.48
1:A:359:LEU:HB2	4:A:1070:HOH:O	2.12	0.48
2:B:4:LEU:C	2:B:4:LEU:HD23	2.39	0.48
2:B:86:HIS:O	2:B:90:VAL:HG23	2.13	0.48
2:B:124:ASN:N	2:B:124:ASN:ND2	2.62	0.48
1:A:197:LEU:HD11	1:A:205:LYS:CB	2.44	0.47
2:B:29:ILE:HD12	2:B:29:ILE:N	2.30	0.47
1:A:103:LEU:HD22	1:A:103:LEU:N	2.30	0.47
1:A:354:THR:O	1:A:354:THR:CG2	2.63	0.47
1:A:256:ILE:HG12	1:A:261:ILE:HG13	1.96	0.46
1:A:197:LEU:HD11	1:A:205:LYS:HB2	1.96	0.46
1:A:164:LEU:H	1:A:164:LEU:CD1	2.19	0.46
2:B:124:ASN:HB2	2:B:125:PRO:HD3	1.94	0.46
1:A:109:SER:HB3	1:A:112:LEU:HD11	1.98	0.46
2:B:59:VAL:HG13	2:B:60:PRO:HD2	1.97	0.45
2:B:132:HIS:CG	2:B:133:SER:N	2.84	0.45
1:A:203:ARG:HH11	1:A:203:ARG:HG2	1.82	0.45
1:A:426:LEU:HD23	1:A:450:GLY:HA2	1.99	0.45
2:B:74:ARG:HG3	2:B:74:ARG:O	2.16	0.45
2:B:53:LEU:CD2	2:B:66:MET:HE2	2.35	0.44
2:B:186:LEU:O	2:B:190:GLN:HG3	2.17	0.44
1:A:245:PHE:O	1:A:249:VAL:HG23	2.16	0.44
2:B:43:LEU:C	2:B:45:THR:H	2.24	0.44
1:A:260:GLU:OE1	1:A:433:ARG:NH1	2.50	0.44
1:A:340:LEU:CD2	1:A:342:ARG:HH21	2.30	0.44
1:A:168:ASN:HD22	1:A:170:CYS:H	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:GLY:O	2:B:140:PRO:HG2	2.17	0.44
1:A:24:LEU:O	1:A:28:VAL:HG22	2.18	0.44
1:A:231:VAL:O	1:A:234:MET:HB2	2.17	0.44
2:B:34:ILE:CG2	2:B:35:PRO:HD2	2.48	0.44
1:A:109:SER:HB3	1:A:112:LEU:CD1	2.48	0.44
1:A:231:VAL:N	1:A:232:PRO:HD3	2.33	0.43
2:B:124:ASN:CB	2:B:125:PRO:CD	2.94	0.43
2:B:53:LEU:HB3	2:B:66:MET:HE2	2.01	0.43
2:B:81:GLY:O	2:B:165:GLY:HA2	2.18	0.43
2:B:149:PHE:O	2:B:150:ASN:HB2	2.18	0.43
2:B:39:LEU:O	2:B:42:ARG:HB3	2.18	0.43
1:A:368:LEU:CD1	2:B:11:SER:HB3	2.49	0.42
1:A:37:LEU:HD13	1:A:53:LEU:HG	2.00	0.42
1:A:92:VAL:O	1:A:92:VAL:HG23	2.19	0.42
1:A:504:ARG:HH21	1:A:504:ARG:CB	2.25	0.42
2:B:124:ASN:HD22	2:B:124:ASN:H	1.65	0.42
1:A:80:LEU:HD21	1:A:198:PHE:HB3	2.00	0.42
2:B:83:CYS:O	2:B:86:HIS:HB3	2.20	0.42
2:B:104:LEU:CB	2:B:107:LYS:HD2	2.48	0.42
2:B:113:HIS:HD2	2:B:119:PHE:HB3	1.83	0.42
1:A:262:PHE:CE2	2:B:131:TYR:HB3	2.55	0.42
2:B:124:ASN:ND2	2:B:124:ASN:H	2.16	0.42
2:B:103:ILE:O	2:B:104:LEU:HD22	2.20	0.42
1:A:155:VAL:HG23	1:A:421:MET:HG2	2.01	0.42
1:A:320:GLN:HG3	1:A:404:VAL:CG1	2.50	0.42
2:B:73:LEU:HD22	2:B:76:LYS:HE2	2.02	0.42
1:A:272:LEU:HD11	1:A:510:ILE:CD1	2.50	0.41
1:A:221:GLN:H	1:A:221:GLN:HG2	1.62	0.41
2:B:126:LEU:HA	2:B:127:PRO:HD3	1.92	0.41
2:B:113:HIS:HE1	2:B:123:ALA:O	2.04	0.41
1:A:309:GLU:CG	1:A:310:SER:N	2.83	0.41
1:A:53:LEU:HD22	1:A:182:MET:HE3	2.03	0.41
2:B:96:TYR:HB3	2:B:138:ASN:HD22	1.85	0.41
2:B:158:HIS:HD2	2:B:160:ALA:H	1.68	0.41
1:A:182:MET:HG2	1:A:193:ILE:HG12	2.03	0.41
1:A:283:VAL:HG11	1:A:512:THR:OG1	2.21	0.41
1:A:431:LYS:HG2	1:A:435:MET:HE2	2.03	0.41
1:A:55:VAL:CG2	1:A:182:MET:HE2	2.50	0.40
1:A:110:PRO:C	1:A:111:LEU:HD12	2.46	0.40
2:B:139:VAL:HA	2:B:140:PRO:HD3	1.96	0.40
1:A:368:LEU:HD11	2:B:11:SER:CB	2.52	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	510/520 (98%)	492 (96%)	16 (3%)	2 (0%)	30	22
2	B	180/192 (94%)	160 (89%)	16 (9%)	4 (2%)	5	1
All	All	690/712 (97%)	652 (94%)	32 (5%)	6 (1%)	14	6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	36	ALA
2	B	132	HIS
1	A	166	ALA
2	B	124	ASN
1	A	421	MET
2	B	151	GLY

5.3.2 Protein sidechains [i](#)

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	422/432 (98%)	410 (97%)	12 (3%)	38	32
2	B	150/153 (98%)	146 (97%)	4 (3%)	39	34
All	All	572/585 (98%)	556 (97%)	16 (3%)	38	32

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	59	LEU
1	A	164	LEU
1	A	173	TYR
1	A	209	ASN
1	A	212	LEU
1	A	235	ARG
1	A	344	LEU
1	A	354	THR
1	A	382	ARG
1	A	418	ARG
1	A	426	LEU
2	B	32	ASN
2	B	104	LEU
2	B	124	ASN
2	B	182	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	169	ASN
1	A	186	HIS
1	A	206	GLN
1	A	240	GLN
1	A	299	ASN
1	A	409	HIS
1	A	459	HIS
1	A	514	HIS
2	B	8	ASN
2	B	19	GLN
2	B	86	HIS
2	B	113	HIS
2	B	116	GLN
2	B	124	ASN
2	B	138	ASN
2	B	177	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TRP	A	1001	-	15,16,16	2.31	1 (6%)	18,22,22	1.01	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRP	A	1001	-	-	0/8/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	TRP	OXT-C	-8.61	1.03	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	1001	TRP	OXT-C-O	-3.83	115.40	124.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	512/520 (98%)	0.57	41 (8%) 18 19	21, 37, 63, 80	0
2	B	186/192 (96%)	1.68	56 (30%) 1 1	27, 56, 82, 91	0
All	All	698/712 (98%)	0.86	97 (13%) 6 6	21, 42, 72, 91	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	516	ALA	6.8
2	B	104	LEU	5.7
2	B	36	ALA	5.0
2	B	133	SER	5.0
2	B	124	ASN	4.7
2	B	142	GLY	4.6
2	B	105	HIS	4.6
2	B	192	LYS	4.4
2	B	103	ILE	4.4
2	B	131	TYR	4.4
1	A	164	LEU	4.2
2	B	106	GLY	4.1
2	B	89	ILE	4.0
2	B	59	VAL	3.9
2	B	151	GLY	3.7
2	B	40	ILE	3.7
2	B	44	ALA	3.6
2	B	125	PRO	3.6
2	B	145	ILE	3.5
2	B	63	ALA	3.5
2	B	35	PRO	3.4
1	A	515	HIS	3.3
2	B	67	PRO	3.3
1	A	163	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	258	ALA	3.3
2	B	97	VAL	3.3
2	B	132	HIS	3.2
2	B	38	THR	3.2
1	A	13	CYS	3.1
2	B	137	SER	3.1
1	A	14	ASP	3.0
1	A	16	ALA	3.0
1	A	409	HIS	2.9
2	B	43	LEU	2.9
2	B	39	LEU	2.9
1	A	228	VAL	2.9
1	A	158	PHE	2.8
2	B	92	ALA	2.8
1	A	231	VAL	2.8
1	A	232	PRO	2.7
2	B	148	HIS	2.7
2	B	141	ALA	2.6
2	B	108	ALA	2.6
1	A	229	THR	2.6
2	B	111	ILE	2.6
2	B	160	ALA	2.5
1	A	224	PRO	2.5
1	A	238	CYS	2.5
2	B	85	GLY	2.5
1	A	138	THR	2.5
2	B	57	PRO	2.5
2	B	150	ASN	2.5
1	A	494	SER	2.5
1	A	15	ALA	2.5
2	B	70	LEU	2.4
2	B	75	GLY	2.4
2	B	95	GLY	2.4
2	B	93	TYR	2.4
1	A	512	THR	2.4
1	A	327	ALA	2.4
1	A	236	CYS	2.4
1	A	488	LEU	2.3
1	A	474	GLU	2.3
1	A	221	GLN	2.3
2	B	60	PRO	2.3
2	B	139	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	158	HIS	2.3
1	A	219	LEU	2.3
2	B	96	TYR	2.3
2	B	56	GLY	2.3
2	B	115	GLY	2.3
1	A	276	SER	2.3
1	A	443	GLY	2.2
2	B	163	VAL	2.2
2	B	58	GLY	2.2
2	B	94	GLY	2.2
1	A	192	ARG	2.2
2	B	69	LEU	2.2
1	A	223	ALA	2.2
2	B	88	ALA	2.2
1	A	108	VAL	2.2
1	A	233	ASP	2.1
1	A	230	PRO	2.1
2	B	143	LEU	2.1
2	B	182	LEU	2.1
1	A	356	HIS	2.1
1	A	475	ASN	2.1
1	A	47	ASP	2.1
1	A	269	ARG	2.1
2	B	99	GLN	2.1
1	A	111	LEU	2.1
1	A	167	GLY	2.0
2	B	167	GLN	2.0
2	B	65	CYS	2.0
2	B	46	MET	2.0
1	A	217	GLN	2.0
1	A	203	ARG	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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TRP	A	1001	15/15	0.97	0.04	20,23,26,28	0

6.5 Other polymers

There are no such residues in this entry.