



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:11 PM UTC

PDB ID : 3PS7 / pdb_00003ps7
Title : Biochemical studies and crystal structure determination of dihydrodipicolinate synthase from *Pseudomonas aeruginosa*
Authors : Kaur, N.; Gautam, A.; Kumar, S.; Singh, A.; Singh, N.; Sharma, S.; Sharma, R.; Tewari, R.; Singh, T.P.
Deposited on : 2010-12-01
Resolution : 2.85 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

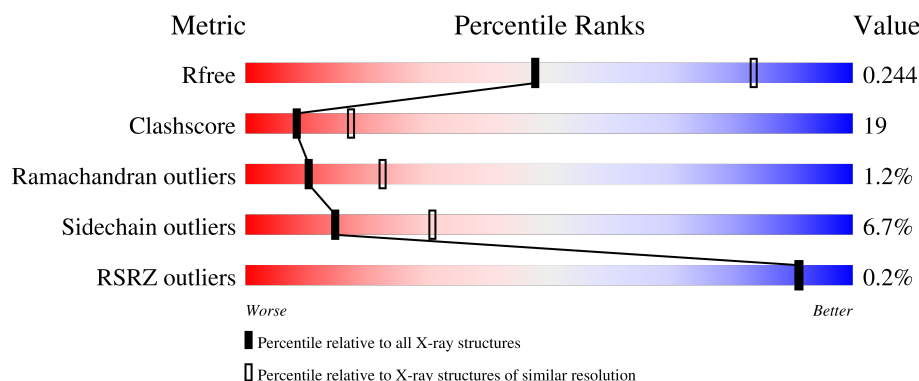
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	292	 61% 33% 6%
1	B	292	 56% 38% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4602 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.

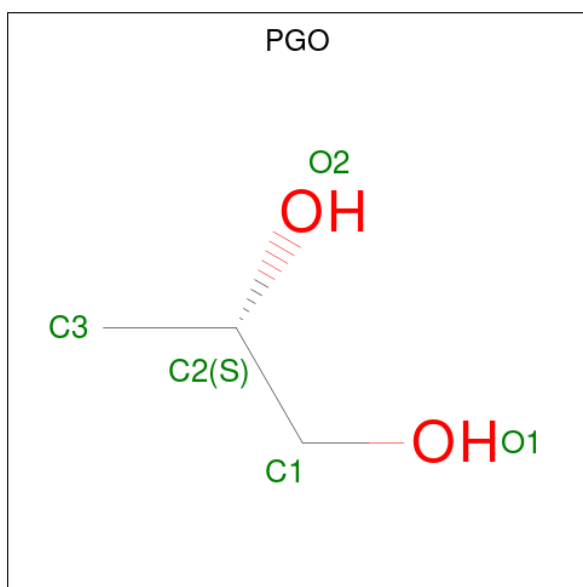
- Molecule 1 is a protein called Dihydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2200	1382	392	412	14			
1	B	292	Total	C	N	O	S	0	0	0
			2200	1382	392	412	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ASP	GLU	engineered mutation	UNP D1MH64
A	60	VAL	ILE	engineered mutation	UNP D1MH64
A	234	ASP	GLU	engineered mutation	UNP D1MH64
A	279	ASP	GLU	engineered mutation	UNP D1MH64
B	34	ASP	GLU	engineered mutation	UNP D1MH64
B	60	VAL	ILE	engineered mutation	UNP D1MH64
B	234	ASP	GLU	engineered mutation	UNP D1MH64
B	279	ASP	GLU	engineered mutation	UNP D1MH64

- Molecule 2 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			5	3	2		
2	A	1	Total	C	O	0	0
			5	3	2		
2	A	1	Total	C	O	0	0
			5	3	2		
2	B	1	Total	C	O	0	0
			5	3	2		
2	B	1	Total	C	O	0	0
			5	3	2		
2	B	1	Total	C	O	0	0
			5	3	2		
2	B	1	Total	C	O	0	0
			5	3	2		

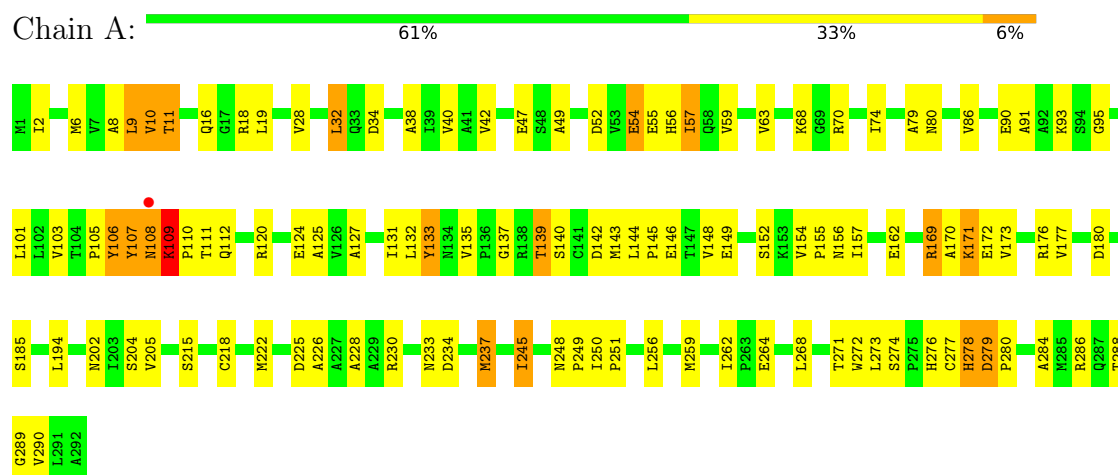
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total	O	0	0
			88	88		
3	B	79	Total	O	0	0
			79	79		

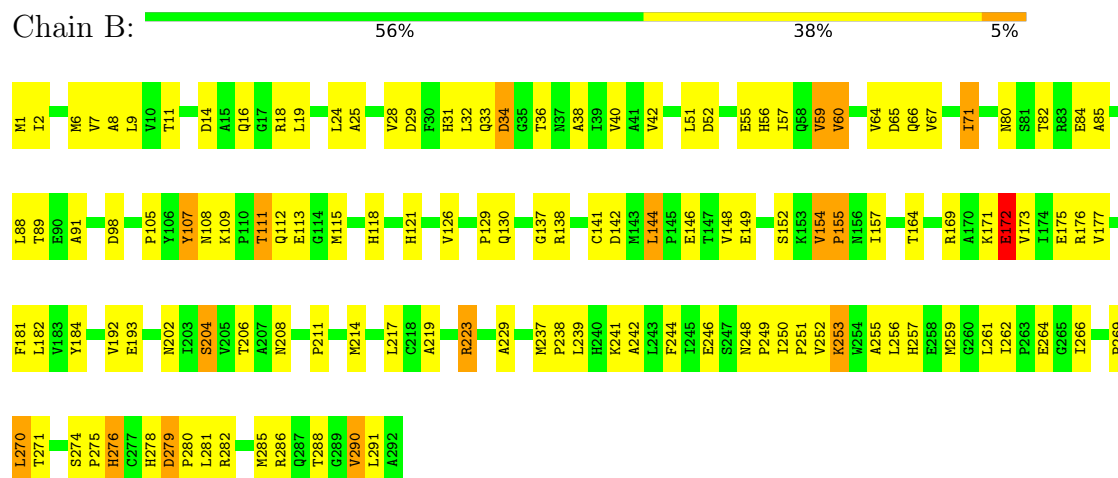
3 Residue-property plots

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: Dihydrodipicolinate synthase



• Molecule 1: Dihydrodipicolinate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.07Å 81.59Å 123.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.57 – 2.85 52.57 – 2.85	Depositor EDS
% Data completeness (in resolution range)	94.6 (52.57-2.85) 94.8 (52.57-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.205 , 0.242 0.204 , 0.244	Depositor DCC
R_{free} test set	681 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4602	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PGO

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	0.96	5/2239 (0.2%)	1.18	22/3043 (0.7%)
1	B	0.89	2/2239 (0.1%)	1.17	22/3043 (0.7%)
All	All	0.93	7/4478 (0.2%)	1.18	44/6086 (0.7%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	MET	C-O	-8.83	1.16	1.24
1	A	133	TYR	C-N	7.92	1.44	1.33
1	A	107	TYR	C-O	-6.24	1.16	1.24
1	B	108	ASN	CA-C	-6.01	1.44	1.52
1	A	108	ASN	CB-CG	-5.89	1.37	1.52
1	A	106	TYR	C-O	-5.79	1.16	1.23
1	B	107	TYR	C-O	-5.78	1.16	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	VAL	CB-CA-C	-8.54	101.73	111.55
1	B	60	VAL	N-CA-C	-8.05	102.41	110.62
1	A	11	THR	CA-C-N	7.63	127.69	119.90
1	A	11	THR	C-N-CA	7.63	127.69	119.90
1	A	139	THR	N-CA-C	6.92	118.90	111.36
1	B	11	THR	CA-C-N	6.89	126.88	119.78
1	B	11	THR	C-N-CA	6.89	126.88	119.78
1	B	204	SER	N-CA-C	6.84	120.61	110.48
1	A	109	LYS	N-CA-C	6.80	124.84	109.81
1	B	172	GLU	N-CA-C	-6.69	104.14	112.90
1	A	157	ILE	N-CA-C	-6.67	98.02	107.75
1	A	125	ALA	N-CA-C	6.61	118.56	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ASN	N-CA-CB	-6.52	100.51	110.16
1	A	63	VAL	N-CA-C	-6.45	105.45	111.45
1	B	111	THR	N-CA-C	-6.26	101.51	110.59
1	B	108	ASN	N-CA-CB	6.23	119.81	110.65
1	B	64	VAL	CA-C-N	6.05	128.66	120.38
1	B	64	VAL	C-N-CA	6.05	128.66	120.38
1	B	155	PRO	N-CA-C	5.86	124.54	112.47
1	A	290	VAL	N-CA-C	-5.85	107.05	113.43
1	B	155	PRO	CA-C-N	-5.82	113.42	123.25
1	B	155	PRO	C-N-CA	-5.82	113.42	123.25
1	B	264	GLU	N-CA-C	-5.81	101.45	110.10
1	B	9	LEU	N-CA-C	5.80	118.86	110.28
1	B	253	LYS	N-CA-C	-5.75	104.93	111.14
1	A	79	ALA	N-CA-C	-5.70	101.08	109.81
1	A	154	VAL	CA-C-N	5.66	126.91	119.84
1	A	154	VAL	C-N-CA	5.66	126.91	119.84
1	A	205	VAL	N-CA-C	-5.66	107.32	111.90
1	B	85	ALA	N-CA-C	-5.65	105.03	111.07
1	A	259	MET	N-CA-C	-5.57	106.49	113.28
1	B	154	VAL	CA-C-N	5.56	126.78	119.84
1	B	154	VAL	C-N-CA	5.56	126.78	119.84
1	A	274	SER	CA-C-N	5.53	125.62	119.32
1	A	274	SER	C-N-CA	5.53	125.62	119.32
1	B	223	ARG	N-CA-C	-5.52	106.71	113.50
1	A	34	ASP	N-CA-C	5.46	119.42	112.87
1	B	144	LEU	CA-C-N	5.39	125.21	119.28
1	B	144	LEU	C-N-CA	5.39	125.21	119.28
1	A	111	THR	N-CA-C	-5.38	103.59	110.53
1	A	8	ALA	N-CA-C	-5.18	98.58	108.17
1	A	215	SER	N-CA-C	-5.14	105.59	111.14
1	A	289	GLY	N-CA-C	5.08	124.32	114.16
1	A	278	HIS	N-CA-C	5.03	116.57	111.14

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	2200	0	2235	82	0
1	B	2200	0	2235	99	0
2	A	15	0	24	2	0
2	B	20	0	32	4	0
3	A	88	0	0	1	0
3	B	79	0	0	0	0
All	All	4602	0	4526	171	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 19.

All (171) 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:42:VAL:HG11	1:A:56:HIS:CD2	1.81	1.15
1:A:42:VAL:HG11	1:A:56:HIS:HD2	0.95	1.11
1:A:103:VAL:HA	1:A:133:TYR:HB3	1.53	0.87
1:A:9:LEU:HD23	1:A:10:VAL:O	1.82	0.80
1:B:36:THR:O	1:B:71:ILE:HD11	1.81	0.79
1:B:256:LEU:HB3	1:B:262:ILE:HG12	1.64	0.79
1:A:40:VAL:HG22	1:A:74:ILE:HB	1.68	0.75
1:A:42:VAL:CG1	1:A:56:HIS:HD2	1.89	0.75
1:B:6:MET:HG2	1:B:38:ALA:HB3	1.70	0.74
1:A:132:LEU:HD13	1:A:143:MET:HE1	1.69	0.74
1:A:225:ASP:HB3	1:A:228:ALA:HB3	1.67	0.74
1:B:24:LEU:HD21	1:B:59:VAL:HG13	1.70	0.74
1:B:237:MET:HG3	1:B:241:LYS:HE3	1.70	0.73
1:B:252:VAL:O	1:B:256:LEU:HD23	1.90	0.72
1:A:143:MET:HE3	1:A:148:VAL:HG22	1.73	0.71
1:B:255:ALA:HB1	1:B:285:MET:HE3	1.74	0.70
1:B:149:GLU:HG3	1:B:176:ARG:HB3	1.74	0.68
1:A:19:LEU:HD12	1:A:19:LEU:H	1.60	0.67
1:B:111:THR:HG22	1:B:113:GLU:H	1.58	0.66
1:B:52:ASP:HB3	1:B:55:GLU:HG3	1.77	0.66
1:B:31:HIS:HD2	1:B:211:PRO:HB3	1.61	0.66
1:B:173:VAL:O	1:B:177:VAL:HG22	1.95	0.65
1:B:172:GLU:O	1:B:176:ARG:HG3	1.96	0.65
1:A:106:TYR:C	1:A:108:ASN:H	2.04	0.65
1:A:169:ARG:O	1:A:173:VAL:HG23	1.96	0.64
1:A:139:THR:O	1:A:140:SER:HB2	1.97	0.64
1:A:277:CYS:C	1:A:280:PRO:HD2	2.23	0.64
1:B:285:MET:HB3	1:B:290:VAL:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:HG21	1:A:74:ILE:HD11	1.80	0.64
1:B:249:PRO:HD2	1:B:270:LEU:HD21	1.79	0.63
1:B:154:VAL:HB	1:B:157:ILE:HD12	1.81	0.63
1:A:6:MET:HG2	1:A:38:ALA:HB3	1.81	0.62
1:B:8:ALA:HA	1:B:40:VAL:HB	1.82	0.62
1:B:279:ASP:OD1	1:B:280:PRO:HD3	2.00	0.61
1:B:286:ARG:HA	1:B:291:LEU:O	2.01	0.60
1:A:202:ASN:ND2	1:A:204:SER:HB2	2.17	0.60
1:A:250:ILE:HB	1:A:251:PRO:HD3	1.84	0.59
1:A:170:ALA:C	1:A:172:GLU:H	2.08	0.59
1:B:274:SER:OG	1:B:276:HIS:HB2	2.02	0.59
1:B:202:ASN:ND2	1:B:204:SER:HB2	2.18	0.59
1:A:226:ALA:O	1:A:230:ARG:HG3	2.02	0.59
1:B:142:ASP:CG	1:B:169:ARG:HH12	2.11	0.59
1:A:28:VAL:O	1:A:32:LEU:HB2	2.03	0.59
1:B:31:HIS:CD2	1:B:211:PRO:HB3	2.39	0.58
1:B:217:LEU:C	1:B:217:LEU:HD23	2.29	0.57
1:B:248:ASN:OD1	1:B:249:PRO:HA	2.05	0.56
1:B:255:ALA:HB1	1:B:285:MET:CE	2.35	0.56
1:A:185:SER:HB2	1:A:194:LEU:HD22	1.87	0.56
1:A:218:CYS:O	1:A:222:MET:HG3	2.05	0.56
1:B:28:VAL:HB	1:B:66:GLN:NE2	2.21	0.56
1:A:57:ILE:CG2	1:A:91:ALA:HB1	2.36	0.55
1:A:132:LEU:HD13	1:A:143:MET:CE	2.36	0.55
1:B:24:LEU:CD2	1:B:59:VAL:HG13	2.35	0.55
1:B:259:MET:HB2	1:B:261:LEU:HD12	1.88	0.55
1:A:256:LEU:HB3	1:A:262:ILE:HG12	1.89	0.55
1:B:89:THR:HG22	1:B:126:VAL:HG11	1.88	0.54
1:B:257:HIS:HD2	1:B:262:ILE:O	1.91	0.54
1:B:142:ASP:H	2:B:295:PGO:H11	1.73	0.54
1:A:49:ALA:HB1	1:B:80:ASN:ND2	2.22	0.54
1:A:52:ASP:HB2	1:A:55:GLU:H	1.72	0.54
1:A:105:PRO:HB2	1:A:110:PRO:HG2	1.90	0.53
1:A:42:VAL:HG12	1:A:42:VAL:O	2.08	0.53
1:A:135:VAL:O	1:A:135:VAL:HG13	2.09	0.53
1:B:239:LEU:HD22	1:B:288:THR:HG21	1.91	0.53
1:B:219:ALA:O	1:B:223:ARG:HG3	2.08	0.53
1:B:36:THR:HG22	1:B:38:ALA:H	1.74	0.53
1:A:93:LYS:C	1:A:95:GLY:H	2.18	0.52
1:B:144:LEU:O	1:B:148:VAL:HG23	2.09	0.52
1:B:121:HIS:C	1:B:121:HIS:CD2	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ALA:HA	1:B:66:GLN:OE1	2.10	0.52
1:A:52:ASP:HB2	1:A:55:GLU:HB2	1.91	0.52
1:A:170:ALA:C	1:A:172:GLU:N	2.68	0.52
1:A:137:GLY:O	1:B:109:LYS:CE	2.58	0.52
1:B:42:VAL:HG13	1:B:51:LEU:CD1	2.40	0.52
1:A:256:LEU:CB	1:A:262:ILE:HG12	2.40	0.51
1:A:284:ALA:O	1:A:288:THR:HG22	2.10	0.51
1:A:145:PRO:HG2	1:A:146:GLU:OE1	2.11	0.50
1:B:253:LYS:O	1:B:262:ILE:HD11	2.11	0.50
1:A:112:GLN:HG3	1:A:144:LEU:HD12	1.94	0.50
1:A:108:ASN:ND2	1:B:269:PRO:CG	2.75	0.50
1:A:142:ASP:OD2	1:A:169:ARG:NH2	2.45	0.50
1:B:206:THR:HG23	1:B:239:LEU:HD23	1.94	0.49
1:B:146:GLU:H	1:B:146:GLU:CD	2.21	0.49
1:B:111:THR:HG22	1:B:112:GLN:N	2.26	0.49
1:B:192:VAL:HG13	1:B:193:GLU:N	2.28	0.49
1:A:112:GLN:HB2	2:A:294:PGO:H33	1.95	0.48
1:A:264:GLU:HA	1:A:272:TRP:CH2	2.49	0.48
1:B:208:ASN:HB3	1:B:256:LEU:HD21	1.95	0.48
1:A:86:VAL:O	1:A:90:GLU:HB2	2.14	0.48
1:A:276:HIS:CD2	1:A:276:HIS:C	2.91	0.48
1:B:56:HIS:O	1:B:60:VAL:HG23	2.13	0.48
1:A:106:TYR:O	1:A:108:ASN:N	2.36	0.48
1:B:24:LEU:O	1:B:28:VAL:HG23	2.13	0.47
1:B:202:ASN:HD22	1:B:214:MET:HE2	1.80	0.47
1:A:32:LEU:HD21	1:A:70:ARG:NH1	2.29	0.47
1:B:244:PHE:C	1:B:246:GLU:N	2.73	0.47
1:A:47:GLU:HG3	3:A:336:HOH:O	2.14	0.47
1:A:137:GLY:O	1:B:109:LYS:HE3	2.14	0.47
1:B:141:CYS:HA	2:B:295:PGO:H11	1.95	0.47
1:B:237:MET:N	1:B:238:PRO:CD	2.78	0.47
1:B:1:MET:SD	2:B:294:PGO:H31	2.54	0.46
1:A:149:GLU:O	1:A:152:SER:OG	2.33	0.46
1:B:169:ARG:O	1:B:173:VAL:HG23	2.15	0.46
1:A:108:ASN:ND2	1:B:269:PRO:HG3	2.30	0.46
1:B:250:ILE:HB	1:B:251:PRO:HD3	1.98	0.46
1:B:250:ILE:HG12	1:B:271:THR:O	2.14	0.46
1:A:107:TYR:CD1	1:B:138:ARG:HB3	2.51	0.45
1:A:173:VAL:O	1:A:177:VAL:HG22	2.16	0.45
1:B:192:VAL:HG23	1:B:229:ALA:HB1	1.97	0.45
1:A:109:LYS:HE2	1:B:137:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:CYS:O	1:A:280:PRO:HD2	2.16	0.45
1:A:10:VAL:HG23	1:A:11:THR:N	2.32	0.45
1:B:257:HIS:CD2	1:B:262:ILE:O	2.68	0.45
1:B:14:ASP:OD2	1:B:18:ARG:NH1	2.50	0.45
1:B:52:ASP:CB	1:B:55:GLU:HG3	2.47	0.45
1:B:67:VAL:HG11	1:B:71:ILE:O	2.17	0.45
1:B:275:PRO:HA	1:B:278:HIS:CD2	2.52	0.45
1:B:279:ASP:CG	1:B:280:PRO:HD3	2.42	0.44
1:B:107:TYR:O	1:B:107:TYR:CG	2.68	0.44
1:A:106:TYR:O	1:A:108:ASN:HB2	2.17	0.44
1:A:109:LYS:HZ2	1:A:109:LYS:HG2	1.46	0.44
1:A:32:LEU:HD21	1:A:70:ARG:CZ	2.47	0.44
1:A:80:ASN:OD1	1:A:80:ASN:C	2.60	0.44
1:A:233:ASN:HD21	1:A:237:MET:HE1	1.83	0.44
1:B:142:ASP:H	2:B:295:PGO:C1	2.31	0.44
1:A:273:LEU:HD23	1:A:278:HIS:HD2	1.83	0.44
1:B:42:VAL:HG12	1:B:42:VAL:O	2.18	0.44
1:B:6:MET:HE1	1:B:184:TYR:CE1	2.53	0.43
1:B:244:PHE:C	1:B:246:GLU:H	2.26	0.43
1:A:250:ILE:HG12	1:A:271:THR:O	2.18	0.43
1:A:279:ASP:N	1:A:280:PRO:CD	2.82	0.43
1:A:170:ALA:O	1:A:172:GLU:N	2.51	0.43
1:B:98:ASP:O	1:B:129:PRO:HG2	2.19	0.43
1:A:112:GLN:CB	2:A:294:PGO:H33	2.49	0.43
1:B:192:VAL:CG2	1:B:229:ALA:HB1	2.49	0.43
1:A:55:GLU:O	1:A:59:VAL:HG23	2.18	0.43
1:A:172:GLU:OE1	1:A:176:ARG:NH1	2.52	0.43
1:B:7:VAL:O	1:B:7:VAL:HG13	2.19	0.43
1:A:225:ASP:HB3	1:A:228:ALA:CB	2.45	0.42
1:B:33:GLN:HG2	1:B:34:ASP:N	2.31	0.42
1:A:52:ASP:CB	1:A:55:GLU:H	2.32	0.42
1:B:16:GLN:HB3	1:B:18:ARG:HH21	1.83	0.42
1:B:248:ASN:HA	1:B:249:PRO:HA	1.75	0.42
1:B:88:LEU:O	1:B:91:ALA:HB3	2.20	0.42
1:A:16:GLN:HB2	1:A:18:ARG:HH21	1.85	0.42
1:A:19:LEU:HD12	1:A:19:LEU:N	2.30	0.42
1:B:111:THR:O	1:B:115:MET:HE3	2.20	0.42
1:B:242:ALA:HB1	1:B:281:LEU:HD13	2.01	0.42
1:A:108:ASN:ND2	1:B:269:PRO:HG2	2.35	0.42
1:B:202:ASN:ND2	1:B:214:MET:HE2	2.34	0.42
1:B:282:ARG:O	1:B:286:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:SER:HA	1:B:181:PHE:CE1	2.54	0.41
1:A:101:LEU:HD12	1:A:131:ILE:O	2.20	0.41
1:A:120:ARG:O	1:A:124:GLU:HG3	2.20	0.41
1:B:42:VAL:HG11	1:B:56:HIS:CE1	2.56	0.41
1:A:225:ASP:CB	1:A:228:ALA:HB3	2.43	0.41
1:A:245:ILE:HA	1:A:245:ILE:HD12	1.75	0.41
1:A:49:ALA:HB1	1:B:80:ASN:HD21	1.85	0.41
1:A:52:ASP:C	1:A:54:GLU:N	2.77	0.41
1:B:42:VAL:HG13	1:B:51:LEU:HD12	2.02	0.41
1:B:57:ILE:H	1:B:57:ILE:HG13	1.61	0.41
1:B:246:GLU:O	1:B:251:PRO:HG2	2.21	0.41
1:A:105:PRO:HB2	1:A:110:PRO:CG	2.50	0.41
1:A:268:LEU:HB3	1:B:82:THR:OG1	2.19	0.41
1:B:219:ALA:HB1	1:B:223:ARG:NH1	2.36	0.41
1:B:256:LEU:HD13	1:B:256:LEU:HA	1.94	0.41
1:B:115:MET:O	1:B:118:HIS:HB3	2.20	0.41
1:B:279:ASP:N	1:B:280:PRO:HD2	2.36	0.41
1:A:248:ASN:CG	1:A:249:PRO:HA	2.45	0.40
1:B:2:ILE:HG22	1:B:184:TYR:OH	2.22	0.40
1:B:266:ILE:HG12	1:B:270:LEU:HB3	2.03	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	290/292 (99%)	267 (92%)	20 (7%)	3 (1%)	12	25
1	B	290/292 (99%)	263 (91%)	23 (8%)	4 (1%)	9	19
All	All	580/584 (99%)	530 (91%)	43 (7%)	7 (1%)	10	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	PRO
1	B	276	HIS
1	A	171	LYS
1	B	171	LYS
1	A	127	ALA
1	B	155	PRO
1	B	164	THR

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	232/232 (100%)	216 (93%)	16 (7%)	14	30
1	B	232/232 (100%)	217 (94%)	15 (6%)	15	32
All	All	464/464 (100%)	433 (93%)	31 (7%)	15	31

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	10	VAL
1	A	32	LEU
1	A	54	GLU
1	A	57	ILE
1	A	68	LYS
1	A	109	LYS
1	A	156	ASN
1	A	162	GLU
1	A	169	ARG
1	A	171	LYS
1	A	180	ASP
1	A	234	ASP
1	A	245	ILE
1	A	279	ASP
1	A	286	ARG
1	B	19	LEU

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Mol	Chain	Res	Type
1	B	29	ASP
1	B	32	LEU
1	B	34	ASP
1	B	65	ASP
1	B	71	ILE
1	B	84	GLU
1	B	105	PRO
1	B	130	GLN
1	B	172	GLU
1	B	175	GLU
1	B	182	LEU
1	B	270	LEU
1	B	279	ASP
1	B	290	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	56	HIS
1	A	58	GLN
1	A	108	ASN
1	A	117	GLN
1	A	202	ASN
1	A	233	ASN
1	B	31	HIS
1	B	58	GLN
1	B	121	HIS
1	B	168	GLN
1	B	202	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are 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	$\# Z > 2$
2	PGO	A	295	-	4,4,4	1.06	0	4,4,4	0.71	0
2	PGO	B	296	-	4,4,4	1.05	0	4,4,4	1.03	0
2	PGO	A	294	-	4,4,4	0.96	0	4,4,4	0.73	0
2	PGO	A	293	-	4,4,4	1.18	1 (25%)	4,4,4	0.89	0
2	PGO	B	293	-	4,4,4	1.24	1 (25%)	4,4,4	0.54	0
2	PGO	B	295	-	4,4,4	0.99	0	4,4,4	0.95	0
2	PGO	B	294	-	4,4,4	0.93	0	4,4,4	0.69	0

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
2	PGO	A	295	-	-	1/2/2/2	-
2	PGO	B	296	-	-	2/2/2/2	-
2	PGO	A	294	-	-	2/2/2/2	-
2	PGO	A	293	-	-	2/2/2/2	-
2	PGO	B	293	-	-	0/2/2/2	-
2	PGO	B	295	-	-	2/2/2/2	-
2	PGO	B	294	-	-	2/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	293	PGO	C1-C2	2.16	1.57	1.46
2	A	293	PGO	C1-C2	2.01	1.57	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	293	PGO	O1-C1-C2-C3
2	A	293	PGO	O1-C1-C2-O2
2	A	294	PGO	O1-C1-C2-C3
2	A	294	PGO	O1-C1-C2-O2
2	B	294	PGO	O1-C1-C2-C3
2	B	294	PGO	O1-C1-C2-O2
2	B	295	PGO	O1-C1-C2-C3
2	B	295	PGO	O1-C1-C2-O2
2	B	296	PGO	O1-C1-C2-C3
2	B	296	PGO	O1-C1-C2-O2
2	A	295	PGO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	294	PGO	2	0
2	B	295	PGO	3	0
2	B	294	PGO	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	292/292 (100%)	-0.22	1 (0%) 90 89	10, 23, 35, 46	0
1	B	292/292 (100%)	-0.17	0 100 100	10, 22, 37, 47	0
All	All	584/584 (100%)	-0.20	1 (0%) 91 91	10, 23, 36, 47	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	ASN	2.9

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](#)

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(Å ²)	Q<0.9
2	PGO	B	293	5/5	0.52	0.29	64,64,65,66	0
2	PGO	A	295	5/5	0.61	0.20	52,52,53,54	0
2	PGO	B	294	5/5	0.66	0.14	52,53,53,53	0
2	PGO	A	293	5/5	0.68	0.17	30,32,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PGO	B	296	5/5	0.80	0.17	57,57,58,58	0
2	PGO	A	294	5/5	0.81	0.14	41,42,43,44	0
2	PGO	B	295	5/5	0.89	0.14	49,50,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.