



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:21 am BST

PDB ID : 3NOE  
Title : Crystal Structure of Dihydrodipicolinate synthase from *Pseudomonas aeruginosa*  
Authors : Kaur, N.; Kumar, S.; Singh, N.; Gautam, A.; Sharma, R.; Sharma, S.; Tewari, R.; Singh, T.P.  
Deposited on : 2010-06-25  
Resolution : 2.95 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

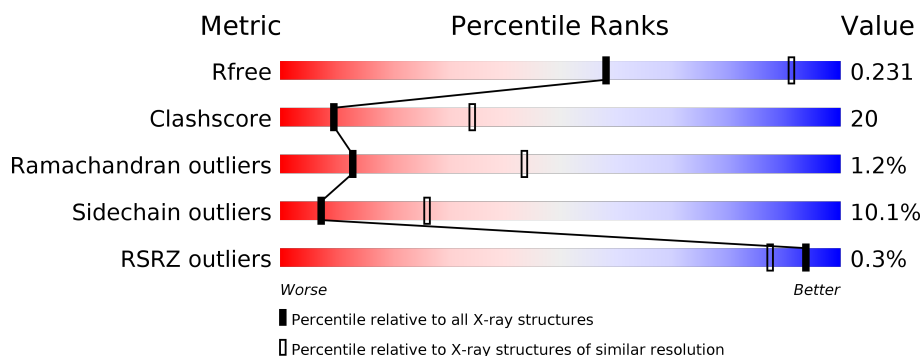
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 62% 33% 5%
1	B	292	 60% 34% 5%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4608 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.

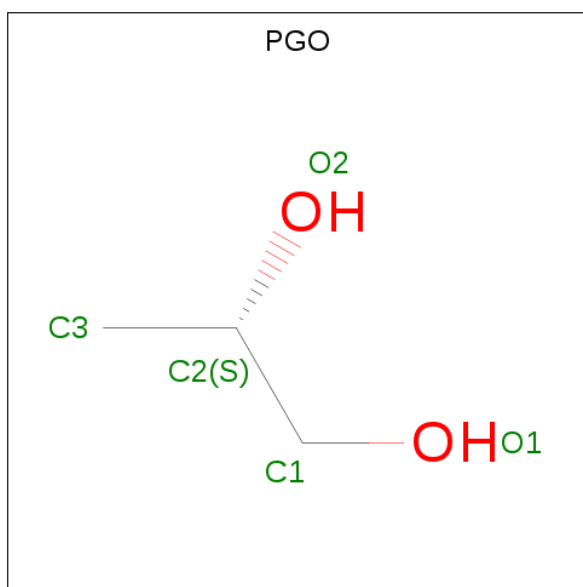
- Molecule 1 is a protein called Dihydrodipicolinate synthase.

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 (three-letter code: PGO) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).



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	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		

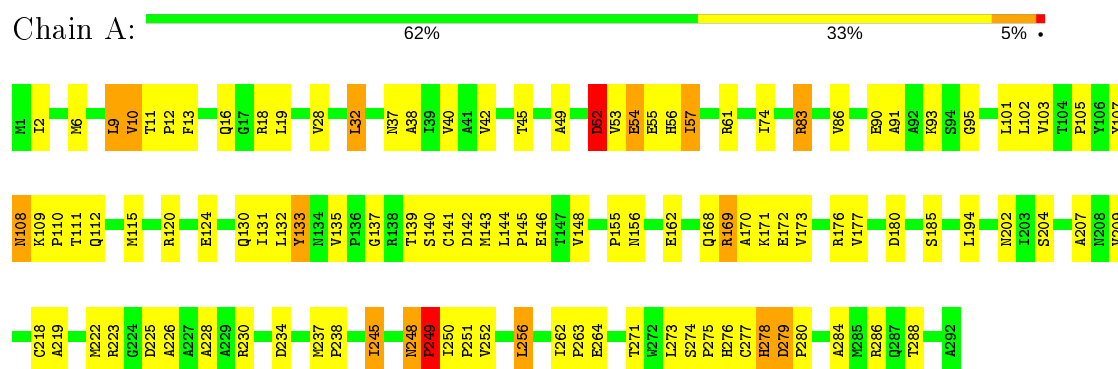
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	89	Total	O	0	0
			89	89		
3	B	79	Total	O	0	0
			79	79		

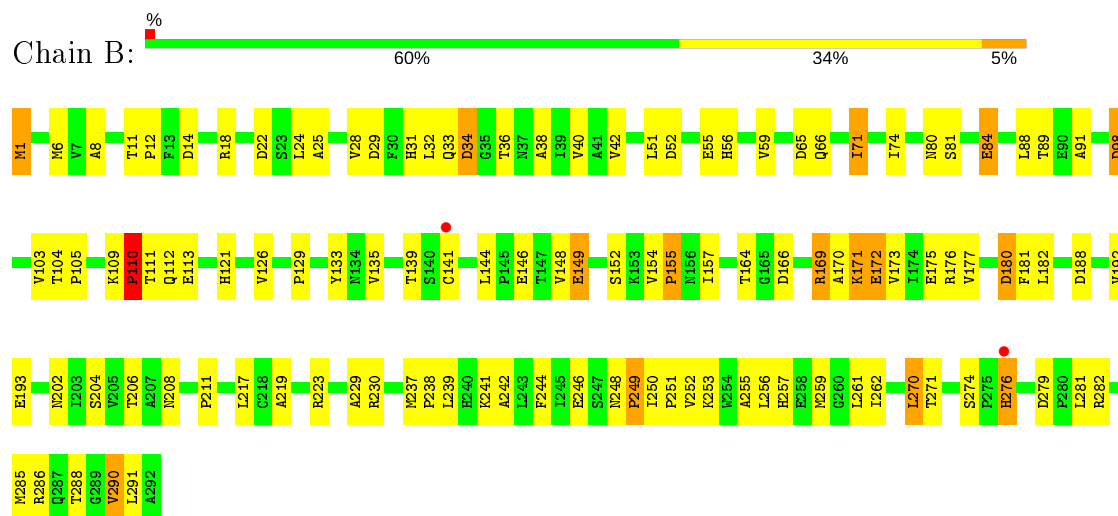
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	58.42Å 81.87Å 124.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.91 – 2.95 23.91 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.2 (23.91-2.95) 97.3 (23.91-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.94Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.202 , 0.234 0.201 , 0.231	Depositor DCC
$R_{free}$ test set	653 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.53	0/2239	1.08	9/3043 (0.3%)
1	B	0.44	0/2239	0.79	1/3043 (0.0%)
All	All	0.49	0/4478	0.94	10/6086 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	PRO	CA-N-CD	-24.84	76.72	111.50
1	A	249	PRO	N-CA-CB	16.50	123.10	103.30
1	A	249	PRO	N-CD-CG	14.55	125.03	103.20
1	A	248	ASN	C-N-CD	-9.45	99.81	120.60
1	A	107	TYR	CB-CG-CD2	6.10	124.66	121.00
1	B	110	PRO	CA-N-CD	-5.63	103.62	111.50
1	A	249	PRO	CA-CB-CG	-5.62	93.33	104.00
1	A	248	ASN	CA-CB-CG	-5.30	101.74	113.40
1	A	248	ASN	C-N-CA	5.11	143.47	122.00
1	A	52	ASP	CA-CB-CG	5.10	124.62	113.40

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	100	0
1	B	2200	0	2235	78	0
2	A	20	0	32	1	0
2	B	20	0	32	1	0
3	A	89	0	0	2	0
3	B	79	0	0	0	0
All	All	4608	0	4534	175	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 20.

All (175) 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:HD2	1.07	1.18
1:A:42:VAL:HG11	1:A:56:HIS:CD2	1.91	1.04
1:A:45:THR:HA	1:A:249:PRO:CG	1.95	0.96
1:A:45:THR:HA	1:A:249:PRO:HG2	1.50	0.93
1:A:256:LEU:HB3	1:A:262:ILE:HG12	1.52	0.91
1:B:149:GLU:HG3	1:B:176:ARG:HB3	1.58	0.85
1:A:105:PRO:HB2	1:A:110:PRO:HG2	1.63	0.81
1:A:103:VAL:HA	1:A:133:TYR:HB3	1.62	0.80
1:A:83:ARG:HH21	1:A:83:ARG:HG2	1.44	0.80
1:A:9:LEU:HD23	1:A:10:VAL:O	1.83	0.78
1:B:256:LEU:HB3	1:B:262:ILE:HG12	1.66	0.78
1:B:6:MET:HG2	1:B:38:ALA:HB3	1.67	0.77
1:B:252:VAL:O	1:B:256:LEU:HD23	1.86	0.76
1:B:36:THR:O	1:B:71:ILE:HD11	1.89	0.72
1:A:40:VAL:HG22	1:A:74:ILE:HB	1.71	0.72
1:A:139:THR:O	1:A:140:SER:HB2	1.88	0.72
1:B:172:GLU:O	1:B:176:ARG:HG3	1.90	0.71
1:B:111:THR:HG22	1:B:113:GLU:H	1.56	0.70
1:B:249:PRO:HD2	1:B:270:LEU:HD21	1.74	0.69
1:A:225:ASP:HB3	1:A:228:ALA:HB3	1.73	0.69
1:A:45:THR:CA	1:A:249:PRO:HG2	2.23	0.68
1:A:19:LEU:H	1:A:19:LEU:HD12	1.59	0.68
1:A:53:VAL:HG23	1:A:54:GLU:N	2.10	0.66
1:B:286:ARG:HA	1:B:291:LEU:O	1.95	0.66
1:A:170:ALA:C	1:A:172:GLU:H	1.97	0.66
1:A:250:ILE:HB	1:A:251:PRO:CD	2.26	0.66
1:A:45:THR:HA	1:A:249:PRO:HG3	1.78	0.66
1:B:285:MET:HB3	1:B:290:VAL:HG22	1.78	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:HD22	1:A:108:ASN:H	1.44	0.65
1:A:226:ALA:O	1:A:230:ARG:HG3	1.97	0.65
1:B:237:MET:HG3	1:B:241:LYS:HE3	1.79	0.65
1:B:31:HIS:HD2	1:B:211:PRO:HB3	1.63	0.64
1:A:132:LEU:HD13	1:A:143:MET:HE3	1.79	0.64
1:B:81:SER:HB3	1:B:84:GLU:HG3	1.78	0.64
1:B:202:ASN:ND2	1:B:204:SER:HB2	2.13	0.63
1:B:144:LEU:O	1:B:148:VAL:HG23	1.98	0.63
1:B:180:ASP:OD2	1:B:180:ASP:N	2.31	0.63
1:A:2:ILE:HG21	1:A:74:ILE:HD11	1.82	0.62
1:B:154:VAL:HB	1:B:157:ILE:HD12	1.81	0.62
1:B:173:VAL:O	1:B:177:VAL:HG22	1.99	0.62
1:A:137:GLY:O	1:B:109:LYS:HE2	2.00	0.61
1:A:169:ARG:O	1:A:173:VAL:HG23	2.01	0.61
1:A:202:ASN:ND2	1:A:204:SER:HB2	2.16	0.60
1:B:8:ALA:HA	1:B:40:VAL:HB	1.83	0.60
1:B:1:MET:SD	2:B:294:PGO:H31	2.41	0.60
1:B:274:SER:OG	1:B:276:HIS:HB2	2.01	0.60
1:A:28:VAL:O	1:A:32:LEU:HB2	2.02	0.59
1:B:111:THR:HG22	1:B:112:GLN:N	2.17	0.59
1:B:55:GLU:O	1:B:59:VAL:HG23	2.02	0.59
1:A:83:ARG:HG2	1:A:83:ARG:NH2	2.16	0.58
1:B:248:ASN:OD1	1:B:249:PRO:HA	2.02	0.58
1:B:31:HIS:CD2	1:B:211:PRO:HB3	2.39	0.58
1:B:253:LYS:O	1:B:262:ILE:HD11	2.02	0.58
1:A:273:LEU:O	1:A:278:HIS:HE1	1.86	0.57
1:A:6:MET:HG2	1:A:38:ALA:HB3	1.87	0.57
1:A:135:VAL:O	1:A:135:VAL:HG13	2.05	0.56
1:A:132:LEU:HD13	1:A:143:MET:CE	2.35	0.56
1:B:52:ASP:HB3	1:B:55:GLU:HG3	1.87	0.56
1:A:249:PRO:O	1:A:252:VAL:HG12	2.05	0.56
1:A:145:PRO:HG2	1:A:146:GLU:OE1	2.06	0.56
1:A:42:VAL:HG12	1:A:42:VAL:O	2.06	0.55
1:A:250:ILE:HB	1:A:251:PRO:HD3	1.89	0.55
1:A:53:VAL:CG2	1:A:54:GLU:N	2.70	0.55
1:A:250:ILE:HD13	1:A:271:THR:O	2.07	0.55
1:A:49:ALA:HB1	1:B:80:ASN:ND2	2.21	0.55
1:A:170:ALA:C	1:A:172:GLU:N	2.61	0.54
1:B:255:ALA:HB1	1:B:285:MET:CE	2.37	0.54
1:A:108:ASN:N	1:A:108:ASN:HD22	2.05	0.54
1:A:13:PHE:O	1:A:263:PRO:HB2	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:MET:HB2	1:B:261:LEU:HD12	1.88	0.54
1:A:133:TYR:HE1	1:A:135:VAL:HB	1.73	0.54
1:B:103:VAL:HA	1:B:133:TYR:HB3	1.90	0.54
1:A:53:VAL:O	1:A:57:ILE:HG12	2.09	0.53
1:B:42:VAL:HG13	1:B:51:LEU:CD1	2.39	0.53
1:B:28:VAL:HB	1:B:66:GLN:NE2	2.24	0.53
1:B:89:THR:HG22	1:B:126:VAL:HG11	1.89	0.53
1:A:185:SER:HB2	1:A:194:LEU:HD22	1.92	0.52
1:A:250:ILE:CB	1:A:251:PRO:CD	2.88	0.52
1:B:257:HIS:HD2	1:B:262:ILE:O	1.93	0.52
1:B:219:ALA:O	1:B:223:ARG:HG3	2.10	0.52
1:A:277:CYS:C	1:A:280:PRO:HD2	2.30	0.51
1:A:10:VAL:HG23	1:A:11:THR:N	2.26	0.51
1:A:102:LEU:HD11	1:A:130:GLN:HG2	1.92	0.51
1:A:284:ALA:O	1:A:288:THR:HG22	2.09	0.51
1:B:206:THR:HG23	1:B:239:LEU:HD23	1.93	0.51
1:A:112:GLN:HB2	2:A:294:PGO:H33	1.92	0.51
1:B:217:LEU:C	1:B:217:LEU:HD23	2.31	0.50
1:B:36:THR:HG22	1:B:38:ALA:H	1.77	0.49
1:A:93:LYS:C	1:A:95:GLY:H	2.15	0.49
1:A:52:ASP:O	1:A:55:GLU:HB2	2.13	0.49
1:B:42:VAL:HG13	1:B:51:LEU:HD12	1.93	0.49
1:B:166:ASP:OD1	1:B:169:ARG:N	2.43	0.48
1:B:239:LEU:HD22	1:B:288:THR:HG21	1.96	0.48
1:A:52:ASP:O	1:A:55:GLU:N	2.47	0.48
1:A:45:THR:HG23	1:A:249:PRO:HG3	1.96	0.48
1:A:57:ILE:CG2	1:A:91:ALA:HB1	2.44	0.48
1:A:49:ALA:HB1	1:B:80:ASN:HD21	1.79	0.47
1:B:192:VAL:CG2	1:B:229:ALA:HB1	2.44	0.47
1:B:88:LEU:O	1:B:91:ALA:HB3	2.15	0.47
1:B:257:HIS:CD2	1:B:262:ILE:O	2.68	0.47
1:A:141:CYS:HB3	3:A:343:HOH:O	2.15	0.47
1:A:146:GLU:HG3	1:A:176:ARG:NH2	2.30	0.47
1:A:120:ARG:O	1:A:124:GLU:HG3	2.14	0.47
1:B:250:ILE:HB	1:B:251:PRO:HD3	1.97	0.47
1:A:279:ASP:N	1:A:280:PRO:CD	2.78	0.47
1:B:25:ALA:HA	1:B:66:GLN:OE1	2.15	0.47
1:B:192:VAL:HG13	1:B:193:GLU:N	2.30	0.46
1:B:192:VAL:HG23	1:B:229:ALA:HB1	1.97	0.46
1:A:105:PRO:HB2	1:A:110:PRO:CG	2.40	0.46
1:A:173:VAL:O	1:A:177:VAL:HG22	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLN:HG2	1:B:34:ASP:N	2.31	0.46
1:A:277:CYS:O	1:A:280:PRO:HD2	2.16	0.46
1:A:112:GLN:HG3	1:A:144:LEU:HD12	1.98	0.45
1:A:86:VAL:O	1:A:90:GLU:HB2	2.17	0.45
1:A:218:CYS:O	1:A:222:MET:HG3	2.15	0.45
1:B:208:ASN:HB3	1:B:256:LEU:HD21	1.99	0.45
1:A:45:THR:CA	1:A:249:PRO:CG	2.81	0.45
1:A:250:ILE:CB	1:A:251:PRO:HD3	2.45	0.45
1:A:42:VAL:CG1	1:A:56:HIS:HD2	1.99	0.45
1:B:121:HIS:C	1:B:121:HIS:CD2	2.90	0.45
1:B:166:ASP:O	1:B:169:ARG:HB2	2.17	0.45
1:B:282:ARG:O	1:B:286:ARG:HG3	2.18	0.44
1:A:37:ASN:ND2	3:A:306:HOH:O	2.50	0.44
1:A:108:ASN:H	1:A:108:ASN:ND2	2.13	0.44
1:A:133:TYR:CE1	1:A:135:VAL:HB	2.52	0.44
1:B:170:ALA:O	1:B:171:LYS:HB2	2.18	0.44
1:B:288:THR:O	1:B:288:THR:HG22	2.17	0.44
1:B:193:GLU:CD	1:B:230:ARG:HH21	2.21	0.44
1:A:237:MET:N	1:A:238:PRO:HD2	2.33	0.44
1:B:98:ASP:O	1:B:129:PRO:HG2	2.18	0.44
1:A:170:ALA:O	1:A:172:GLU:N	2.51	0.43
1:A:249:PRO:O	1:A:250:ILE:C	2.55	0.43
1:A:53:VAL:CG2	1:A:54:GLU:H	2.31	0.43
1:B:135:VAL:HG13	1:B:135:VAL:O	2.18	0.43
1:A:219:ALA:O	1:A:223:ARG:HG3	2.19	0.43
1:B:250:ILE:HG12	1:B:271:THR:O	2.17	0.43
1:A:274:SER:HA	1:A:275:PRO:HD3	1.91	0.43
1:B:146:GLU:CD	1:B:146:GLU:H	2.22	0.43
1:B:244:PHE:C	1:B:246:GLU:N	2.73	0.42
1:B:256:LEU:HD13	1:B:256:LEU:HA	1.90	0.42
1:A:279:ASP:N	1:A:280:PRO:HD3	2.34	0.42
1:B:255:ALA:HB1	1:B:285:MET:HE3	2.01	0.42
1:A:156:ASN:N	1:A:156:ASN:OD1	2.49	0.42
1:B:104:THR:HG23	1:B:133:TYR:O	2.20	0.42
1:A:250:ILE:HG22	1:A:251:PRO:HD3	2.01	0.42
1:A:256:LEU:HB3	1:A:262:ILE:CG1	2.37	0.42
1:B:11:THR:HA	1:B:12:PRO:HD2	1.87	0.42
1:B:242:ALA:HB1	1:B:281:LEU:HD13	2.01	0.42
1:B:111:THR:CG2	1:B:112:GLN:N	2.81	0.42
1:A:276:HIS:CD2	1:A:276:HIS:C	2.92	0.42
1:A:209:VAL:HG12	1:A:256:LEU:HD13	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HD12	1:A:131:ILE:O	2.19	0.42
1:A:250:ILE:HB	1:A:251:PRO:HD2	1.98	0.42
1:B:152:SER:HA	1:B:181:PHE:CE1	2.54	0.42
1:B:14:ASP:OD2	1:B:18:ARG:NH1	2.53	0.42
1:B:237:MET:N	1:B:238:PRO:CD	2.83	0.41
1:A:142:ASP:OD2	1:A:169:ARG:NH2	2.54	0.41
1:A:252:VAL:O	1:A:252:VAL:HG22	2.20	0.41
1:A:143:MET:HG2	1:A:148:VAL:HG23	2.02	0.41
1:A:248:ASN:CG	1:A:249:PRO:N	2.73	0.41
1:A:168:GLN:O	1:A:172:GLU:HB2	2.20	0.41
1:A:57:ILE:O	1:A:61:ARG:HG3	2.21	0.41
1:A:11:THR:HA	1:A:12:PRO:HD3	1.87	0.41
1:B:24:LEU:O	1:B:28:VAL:HG23	2.20	0.41
1:B:22:ASP:O	1:B:25:ALA:HB3	2.20	0.41
1:A:16:GLN:HB2	1:A:18:ARG:HH21	1.87	0.40
1:A:273:LEU:O	1:A:278:HIS:CE1	2.71	0.40
1:A:19:LEU:HD12	1:A:19:LEU:N	2.32	0.40
1:B:135:VAL:O	1:B:139:THR:HG23	2.20	0.40
1:A:250:ILE:CG2	1:A:251:PRO:HD3	2.52	0.40
1:A:133:TYR:C	1:A:133:TYR:CD1	2.95	0.40
1:A:245:ILE:HD12	1:A:245:ILE:HA	1.83	0.40
1:B:42:VAL:HG11	1:B:56:HIS:CE1	2.57	0.40
1:B:40:VAL:HA	1:B:74:ILE:O	2.22	0.40
1:A:110:PRO:HB2	1:A:115:MET:HG3	2.03	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	290/292 (99%)	262 (90%)	25 (9%)	3 (1%)	15 48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	290/292 (99%)	264 (91%)	22 (8%)	4 (1%)	11	39
All	All	580/584 (99%)	526 (91%)	47 (8%)	7 (1%)	13	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	PRO
1	A	249	PRO
1	B	171	LYS
1	B	155	PRO
1	B	110	PRO
1	B	164	THR
1	A	207	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	232/232 (100%)	209 (90%)	23 (10%)	8	27
1	B	232/232 (100%)	208 (90%)	24 (10%)	7	25
All	All	464/464 (100%)	417 (90%)	47 (10%)	7	26

All (47) 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	52	ASP
1	A	54	GLU
1	A	57	ILE
1	A	83	ARG
1	A	108	ASN
1	A	109	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	111	THR
1	A	133	TYR
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	249	PRO
1	A	256	LEU
1	A	264	GLU
1	A	278	HIS
1	A	279	ASP
1	A	286	ARG
1	B	1	MET
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	98	ASP
1	B	105	PRO
1	B	110	PRO
1	B	141	CYS
1	B	149	GLU
1	B	155	PRO
1	B	169	ARG
1	B	172	GLU
1	B	175	GLU
1	B	180	ASP
1	B	182	LEU
1	B	188	ASP
1	B	249	PRO
1	B	270	LEU
1	B	276	HIS
1	B	279	ASP
1	B	290	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	121	HIS
1	A	202	ASN
1	A	233	ASN
1	A	276	HIS
1	A	278	HIS
1	B	31	HIS
1	B	121	HIS
1	B	202	ASN
1	B	257	HIS

### 5.3.3 RNA [i](#)

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	-	3,4,4	0.73	0	1,4,4	0.82	0
2	PGO	B	293	-	3,4,4	0.76	0	1,4,4	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PGO	A	293	-	3,4,4	0.88	0	1,4,4	0.89	0
2	PGO	A	296	-	3,4,4	0.63	0	1,4,4	0.80	0
2	PGO	B	296	-	3,4,4	0.68	0	1,4,4	0.66	0
2	PGO	B	295	-	3,4,4	0.75	0	1,4,4	0.76	0
2	PGO	A	294	-	3,4,4	0.72	0	1,4,4	0.85	0
2	PGO	B	294	-	3,4,4	0.65	0	1,4,4	0.73	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	293	-	-	0/2/2/2	-
2	PGO	A	293	-	-	2/2/2/2	-
2	PGO	A	296	-	-	1/2/2/2	-
2	PGO	B	296	-	-	2/2/2/2	-
2	PGO	B	295	-	-	2/2/2/2	-
2	PGO	A	294	-	-	2/2/2/2	-
2	PGO	B	294	-	-	2/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) 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	B	296	PGO	O1-C1-C2-C3
2	B	296	PGO	O1-C1-C2-O2
2	B	295	PGO	O1-C1-C2-C3
2	B	295	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-O2
2	A	296	PGO	O1-C1-C2-O2
2	B	294	PGO	O1-C1-C2-C3
2	A	295	PGO	O1-C1-C2-O2



There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	294	PGO	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	292/292 (100%)	-0.43	0 100 100	13, 26, 39, 49	0
1	B	292/292 (100%)	-0.39	2 (0%) 87 76	14, 26, 40, 50	0
All	All	584/584 (100%)	-0.41	2 (0%) 94 87	13, 26, 40, 50	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	CYS	2.4
1	B	276	HIS	2.1

### 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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PGO	A	293	5/5	0.77	0.23	36,37,37,38	0
2	PGO	A	295	5/5	0.79	0.38	54,55,55,55	0
2	PGO	B	293	5/5	0.82	0.40	68,69,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PGO	B	296	5/5	0.85	0.42	61,61,62,62	0
2	PGO	A	296	5/5	0.86	0.64	70,70,70,70	0
2	PGO	A	294	5/5	0.86	0.27	42,42,43,43	0
2	PGO	B	295	5/5	0.87	0.22	52,53,53,53	0
2	PGO	B	294	5/5	0.90	0.45	55,56,56,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.