



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:24 PM UTC

PDB ID : 3EB2 / pdb_00003eb2
Title : Crystal structure of Dihydrodipicolinate Synthase from *Rhodopseudomonas palustris* at 2.0Å resolution
Authors : Satyanarayana, L.; Eswaramoorthy, S.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-08-26
Resolution : 2.04 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)
Xtrriage (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

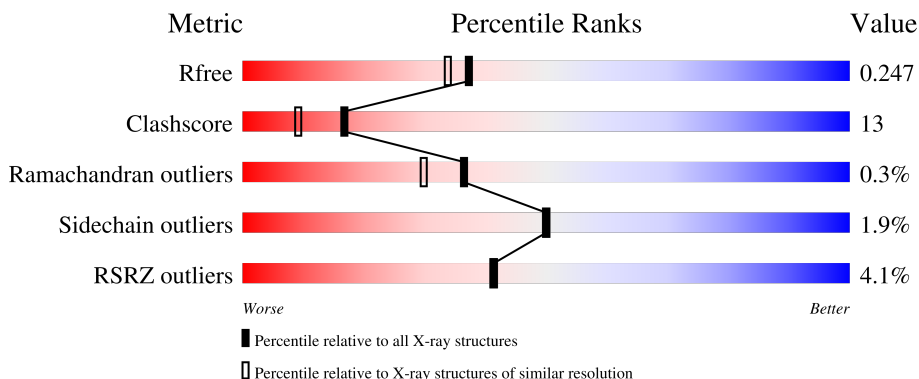
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	300	 73% 22% . .
1	B	300	 75% 21% . .
1	C	300	 12% 72% 23% . .
1	D	300	 2% 72% 22% . . .

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9399 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 Putative dihydrodipicolinate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2186	1393	384	400	9	0	0	0
1	B	291	2205	1404	387	405	9	0	0	0
1	C	288	2186	1393	384	400	9	0	0	0
1	D	290	2197	1398	386	404	9	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

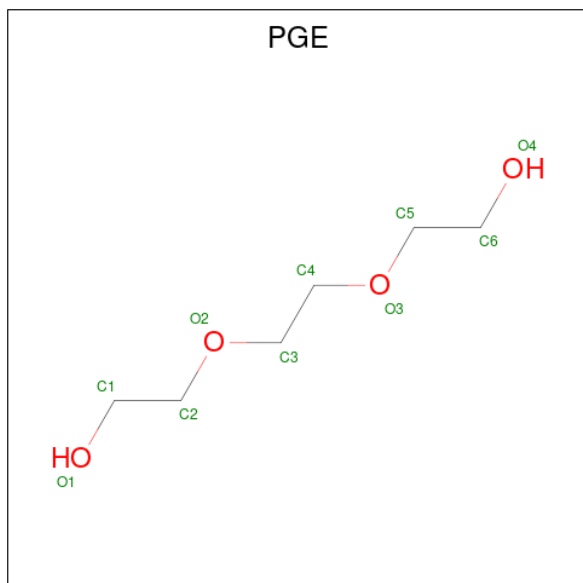
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q6N9H8
A	2	SER	-	expression tag	UNP Q6N9H8
A	3	LEU	-	expression tag	UNP Q6N9H8
A	293	GLU	-	expression tag	UNP Q6N9H8
A	294	GLY	-	expression tag	UNP Q6N9H8
A	295	HIS	-	expression tag	UNP Q6N9H8
A	296	HIS	-	expression tag	UNP Q6N9H8
A	297	HIS	-	expression tag	UNP Q6N9H8
A	298	HIS	-	expression tag	UNP Q6N9H8
A	299	HIS	-	expression tag	UNP Q6N9H8
A	300	HIS	-	expression tag	UNP Q6N9H8
B	1	MET	-	expression tag	UNP Q6N9H8
B	2	SER	-	expression tag	UNP Q6N9H8
B	3	LEU	-	expression tag	UNP Q6N9H8
B	293	GLU	-	expression tag	UNP Q6N9H8
B	294	GLY	-	expression tag	UNP Q6N9H8
B	295	HIS	-	expression tag	UNP Q6N9H8
B	296	HIS	-	expression tag	UNP Q6N9H8
B	297	HIS	-	expression tag	UNP Q6N9H8
B	298	HIS	-	expression tag	UNP Q6N9H8
B	299	HIS	-	expression tag	UNP Q6N9H8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	300	HIS	-	expression tag	UNP Q6N9H8
C	1	MET	-	expression tag	UNP Q6N9H8
C	2	SER	-	expression tag	UNP Q6N9H8
C	3	LEU	-	expression tag	UNP Q6N9H8
C	293	GLU	-	expression tag	UNP Q6N9H8
C	294	GLY	-	expression tag	UNP Q6N9H8
C	295	HIS	-	expression tag	UNP Q6N9H8
C	296	HIS	-	expression tag	UNP Q6N9H8
C	297	HIS	-	expression tag	UNP Q6N9H8
C	298	HIS	-	expression tag	UNP Q6N9H8
C	299	HIS	-	expression tag	UNP Q6N9H8
C	300	HIS	-	expression tag	UNP Q6N9H8
D	1	MET	-	expression tag	UNP Q6N9H8
D	2	SER	-	expression tag	UNP Q6N9H8
D	3	LEU	-	expression tag	UNP Q6N9H8
D	293	GLU	-	expression tag	UNP Q6N9H8
D	294	GLY	-	expression tag	UNP Q6N9H8
D	295	HIS	-	expression tag	UNP Q6N9H8
D	296	HIS	-	expression tag	UNP Q6N9H8
D	297	HIS	-	expression tag	UNP Q6N9H8
D	298	HIS	-	expression tag	UNP Q6N9H8
D	299	HIS	-	expression tag	UNP Q6N9H8
D	300	HIS	-	expression tag	UNP Q6N9H8

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



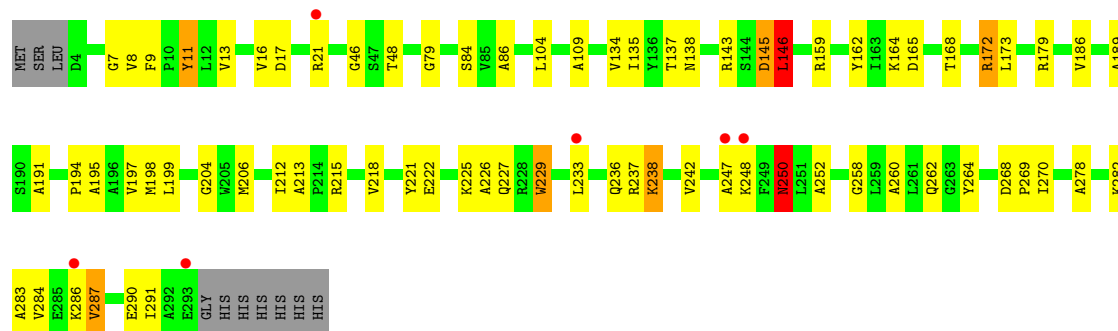
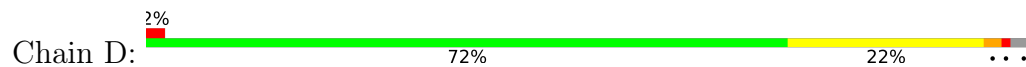
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	181	Total	O	0	0
			181	181		
3	B	154	Total	O	0	0
			154	154		
3	C	137	Total	O	0	0
			137	137		
3	D	133	Total	O	0	0
			133	133		



- Molecule 1: Putative dihydrodipicolinate synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.75Å 120.85Å 135.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.04 50.00 – 2.04	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.04) 95.5 (50.00-2.04)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 2.05Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.248 0.210 , 0.247	Depositor DCC
R_{free} test set	3207 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtrriage
Anisotropy	0.353	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9399	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: PGE

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	0.41	0/2227	0.90	7/3029 (0.2%)
1	B	0.39	0/2246	0.88	7/3055 (0.2%)
1	C	0.37	0/2227	0.89	11/3029 (0.4%)
1	D	0.38	0/2238	0.91	9/3044 (0.3%)
All	All	0.39	0/8938	0.89	34/12157 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	VAL	N-CA-C	8.44	120.74	108.58
1	D	186	VAL	N-CA-C	8.43	120.42	108.36
1	B	186	VAL	N-CA-C	8.13	120.29	108.58
1	B	46	GLY	N-CA-C	-8.06	101.52	112.57
1	C	186	VAL	N-CA-C	7.92	119.68	108.36
1	B	250	ASN	N-CA-C	-7.60	98.42	109.59
1	D	46	GLY	N-CA-C	-7.35	101.35	112.60
1	A	46	GLY	N-CA-C	-7.13	101.69	112.60
1	D	8	VAL	N-CA-C	6.56	117.57	107.99
1	D	250	ASN	N-CA-C	-6.48	100.06	109.59
1	A	13	VAL	N-CA-C	-6.47	102.99	110.05
1	D	229	TRP	N-CA-C	6.43	119.11	111.33
1	B	234	MET	N-CA-C	-6.32	104.30	111.07
1	C	13	VAL	N-CA-C	-6.16	103.34	110.05
1	D	13	VAL	N-CA-C	-6.13	103.29	110.21
1	B	229	TRP	N-CA-C	6.06	117.88	111.28
1	C	138	ASN	CA-C-N	6.06	125.74	119.56
1	C	138	ASN	C-N-CA	6.06	125.74	119.56
1	D	146	LEU	N-CA-C	6.04	118.80	109.07
1	A	229	TRP	N-CA-C	5.84	117.65	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	VAL	N-CA-C	-5.75	103.79	110.05
1	C	250	ASN	N-CA-C	-5.67	101.26	109.59
1	C	229	TRP	N-CA-C	5.62	118.18	111.71
1	C	213	ALA	CA-C-N	5.57	124.77	118.97
1	C	213	ALA	C-N-CA	5.57	124.77	118.97
1	C	146	LEU	N-CA-C	5.54	117.99	109.07
1	C	46	GLY	N-CA-C	-5.51	104.17	112.60
1	C	110	TYR	N-CA-C	-5.41	103.28	111.34
1	D	138	ASN	CA-C-N	5.31	124.98	119.56
1	D	138	ASN	C-N-CA	5.31	124.98	119.56
1	A	138	ASN	CA-C-N	5.25	125.56	119.47
1	A	138	ASN	C-N-CA	5.25	125.56	119.47
1	B	110	TYR	N-CA-C	-5.23	103.55	111.34
1	A	207	ALA	N-CA-C	5.08	116.78	109.07

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	2186	0	2220	72	0
1	B	2205	0	2233	53	0
1	C	2186	0	2220	48	0
1	D	2197	0	2222	57	0
2	A	10	0	14	1	0
2	B	10	0	14	0	0
3	A	181	0	0	15	0
3	B	154	0	0	9	0
3	C	137	0	0	13	0
3	D	133	0	0	5	0
All	All	9399	0	8923	226	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 13.

All (226) 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:B:231:GLU:HA	1:B:234:MET:HE3	1.47	0.95
1:B:250:ASN:HD21	1:B:273:GLN:HE21	1.13	0.92
1:A:71:GLN:HB2	1:A:73:ARG:NH1	1.85	0.92
1:A:200:ILE:HG13	3:A:971:HOH:O	1.71	0.89
1:A:172:ARG:HG3	3:A:1029:HOH:O	1.76	0.85
1:A:164:LYS:HG2	3:A:1025:HOH:O	1.79	0.82
1:A:256:LYS:HE3	3:A:972:HOH:O	1.79	0.82
1:D:283:ALA:O	1:D:286:LYS:HG2	1.79	0.82
1:A:261:LEU:HD21	1:A:281:ARG:HD3	1.61	0.81
1:A:242:VAL:CG2	1:A:291:ILE:HD11	2.13	0.78
1:A:216:GLN:HE21	1:A:291:ILE:HG22	1.50	0.77
1:A:257:ALA:O	1:A:261:LEU:HD23	1.87	0.75
1:D:250:ASN:C	1:D:250:ASN:HD22	1.95	0.75
1:D:238:LYS:HE2	1:D:238:LYS:HA	1.69	0.74
1:D:195:ALA:H	1:D:236:GLN:HE21	1.37	0.73
1:B:134:VAL:HG12	3:B:1152:HOH:O	1.90	0.70
1:C:9:PHE:HB2	1:C:206:MET:HG2	1.72	0.70
1:C:17:ASP:OD2	1:C:21:ARG:HB2	1.91	0.69
1:A:71:GLN:HB2	1:A:73:ARG:HH12	1.57	0.69
1:D:286:LYS:O	1:D:290:GLU:HG3	1.91	0.69
1:B:149:ASP:O	1:B:153:ARG:HG3	1.92	0.68
1:A:242:VAL:HA	1:A:287:VAL:HG21	1.74	0.68
1:B:248:LYS:HE3	1:B:249:PHE:CZ	2.29	0.68
1:B:36:GLN:HG3	3:B:1143:HOH:O	1.94	0.67
1:C:248:LYS:HB3	3:C:365:HOH:O	1.95	0.67
1:D:134:VAL:HG22	1:D:162:TYR:HB2	1.76	0.67
1:B:164:LYS:NZ	1:B:189:ALA:HB2	2.09	0.66
1:D:86:ALA:HB3	3:D:414:HOH:O	1.95	0.65
1:A:243:ASN:HB3	3:A:979:HOH:O	1.95	0.65
1:A:242:VAL:HG22	1:A:291:ILE:HD11	1.79	0.65
1:C:123:ARG:HD2	3:C:367:HOH:O	1.95	0.65
1:A:231:GLU:HA	1:A:234:MET:HE3	1.79	0.64
1:B:11:TYR:OH	1:B:164:LYS:HE2	1.95	0.64
1:A:227:GLN:HE21	1:A:229:TRP:HE1	1.45	0.63
1:C:30:LEU:O	1:C:34:LEU:HG	1.98	0.63
1:B:231:GLU:HA	1:B:234:MET:CE	2.26	0.63
1:C:212:ILE:HD12	1:C:288:LEU:HD21	1.81	0.63
1:A:272:PRO:HD3	1:C:84:SER:HA	1.82	0.62
1:B:195:ALA:H	1:B:236:GLN:HE21	1.47	0.61
1:A:73:ARG:HG3	1:A:73:ARG:HH11	1.66	0.61
1:D:195:ALA:H	1:D:236:GLN:NE2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LYS:HD2	1:B:206:MET:HE3	1.83	0.60
1:D:11:TYR:CZ	1:D:164:LYS:HE3	2.36	0.60
1:A:119:GLU:O	1:A:123:ARG:HG3	2.01	0.60
1:A:195:ALA:H	1:A:236:GLN:HE21	1.50	0.60
1:C:249:PHE:HB2	1:C:254:CYS:SG	2.42	0.59
1:A:141:PHE:O	2:A:888:PGE:H5	2.02	0.59
1:A:164:LYS:HD2	1:A:206:MET:HE2	1.84	0.59
1:D:221:TYR:OH	1:D:225:LYS:HD2	2.03	0.59
1:A:104:LEU:HD22	1:A:206:MET:HE1	1.84	0.58
1:A:164:LYS:HE3	1:A:206:MET:HB2	1.85	0.58
1:B:104:LEU:HD13	1:B:206:MET:HE1	1.84	0.58
1:C:251:LEU:HD23	3:C:336:HOH:O	2.03	0.58
1:B:220:LEU:HD22	1:B:239:LEU:HD12	1.85	0.58
1:A:216:GLN:NE2	1:A:291:ILE:HG22	2.17	0.58
1:D:16:VAL:HG21	1:D:270:ILE:HD11	1.83	0.58
1:A:84:SER:HA	1:C:272:PRO:HD3	1.85	0.58
1:A:72:ARG:NH1	1:A:72:ARG:HB2	2.19	0.58
1:C:9:PHE:CB	1:C:206:MET:HG2	2.33	0.58
1:D:194:PRO:HD2	1:D:236:GLN:HE22	1.69	0.58
1:A:73:ARG:NE	3:A:998:HOH:O	2.35	0.58
1:C:245:ALA:CB	1:C:287:VAL:HG11	2.33	0.57
1:D:146:LEU:HD12	1:D:146:LEU:N	2.18	0.57
1:B:165:ASP:HB3	1:B:173:LEU:HD21	1.86	0.57
1:D:165:ASP:HB3	1:D:173:LEU:HD21	1.86	0.57
1:C:165:ASP:HB3	1:C:173:LEU:HD21	1.87	0.57
1:A:146:LEU:HD12	1:A:146:LEU:N	2.20	0.57
1:B:172:ARG:HB3	3:B:1047:HOH:O	2.04	0.57
1:A:176:ILE:HG13	3:A:1029:HOH:O	2.03	0.56
1:B:146:LEU:N	1:B:146:LEU:HD12	2.20	0.56
1:A:71:GLN:HB2	1:A:73:ARG:HH11	1.66	0.56
1:A:9:PHE:HB2	1:A:206:MET:HG2	1.87	0.56
1:C:97:LYS:HE2	3:C:390:HOH:O	2.06	0.56
1:C:229:TRP:O	1:C:233:LEU:HG	2.06	0.56
1:D:283:ALA:O	1:D:287:VAL:HG13	2.06	0.56
1:A:73:ARG:CZ	3:A:998:HOH:O	2.55	0.55
1:B:135:ILE:C	3:B:1152:HOH:O	2.48	0.55
1:C:55:GLY:O	1:C:59:ARG:HG3	2.07	0.54
1:C:146:LEU:H	1:C:146:LEU:HD12	1.73	0.54
1:A:165:ASP:HB3	1:A:173:LEU:HD21	1.87	0.54
1:D:218:VAL:O	1:D:222:GLU:HG3	2.08	0.54
1:A:71:GLN:OE1	1:A:73:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ALA:H	1:B:236:GLN:NE2	2.06	0.54
1:A:199:LEU:HD22	1:B:199:LEU:HD22	1.90	0.54
1:B:194:PRO:HD2	1:B:236:GLN:HE22	1.73	0.54
1:D:17:ASP:OD2	1:D:21:ARG:HB3	2.08	0.54
1:D:278:ALA:O	1:D:282:LYS:HG3	2.09	0.53
1:D:194:PRO:HD2	1:D:236:GLN:NE2	2.23	0.53
1:A:145:ASP:C	1:A:146:LEU:HD12	2.33	0.53
1:A:194:PRO:HD2	1:A:236:GLN:HE22	1.74	0.53
1:C:291:ILE:HG22	3:C:429:HOH:O	2.09	0.53
1:C:251:LEU:O	1:C:255:ILE:HG12	2.09	0.52
1:C:214:PRO:HD3	3:C:369:HOH:O	2.08	0.52
1:D:198:MET:HE1	1:D:204:GLY:N	2.24	0.52
1:D:9:PHE:O	1:D:206:MET:HA	2.10	0.52
1:A:195:ALA:H	1:A:236:GLN:NE2	2.06	0.52
1:C:239:LEU:HD23	1:C:291:ILE:HD12	1.92	0.52
1:B:268:ASP:HB3	1:B:269:PRO:HD2	1.91	0.52
1:B:60:GLU:OE1	1:B:64:ARG:NH1	2.39	0.52
1:B:179:ARG:HG3	1:B:179:ARG:HH11	1.73	0.51
1:D:109:ALA:O	1:D:143:ARG:HD2	2.09	0.51
1:B:104:LEU:CD1	3:B:1152:HOH:O	2.57	0.51
1:B:277:THR:OG1	1:B:280:GLU:HG3	2.10	0.51
1:D:242:VAL:HG21	1:D:291:ILE:HD13	1.91	0.51
1:A:164:LYS:CE	1:A:206:MET:HB2	2.39	0.51
1:B:286:LYS:O	1:B:290:GLU:HG3	2.10	0.51
1:B:246:PHE:CD1	1:B:254:CYS:SG	3.04	0.51
1:A:231:GLU:HG3	3:A:963:HOH:O	2.10	0.51
1:A:71:GLN:CB	1:A:73:ARG:HH12	2.24	0.50
1:C:286:LYS:HB2	3:C:413:HOH:O	2.10	0.50
1:D:164:LYS:NZ	1:D:189:ALA:HB2	2.26	0.50
1:A:165:ASP:C	3:A:1025:HOH:O	2.54	0.50
1:B:54:LEU:HD21	1:B:270:ILE:HD11	1.93	0.50
1:C:146:LEU:HD12	1:C:146:LEU:N	2.27	0.50
1:A:177:ILE:CD1	3:A:971:HOH:O	2.58	0.50
1:A:233:LEU:O	1:A:237:ARG:HG3	2.12	0.49
1:C:283:ALA:HA	3:C:413:HOH:O	2.11	0.49
1:B:54:LEU:CD2	1:B:270:ILE:HD11	2.42	0.49
1:C:134:VAL:HG22	1:C:162:TYR:HB2	1.95	0.49
1:D:221:TYR:CZ	1:D:225:LYS:HD2	2.48	0.49
1:A:43:THR:HG21	1:A:206:MET:HE3	1.94	0.49
1:A:36:GLN:HG3	3:A:995:HOH:O	2.13	0.49
1:A:164:LYS:CD	1:A:206:MET:HE2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:PHE:HB2	1:D:206:MET:HG2	1.94	0.48
1:B:172:ARG:HD3	3:B:1047:HOH:O	2.13	0.48
1:B:9:PHE:O	1:B:206:MET:HA	2.13	0.48
1:B:53:TYR:HB2	1:B:270:ILE:HD12	1.94	0.48
1:B:104:LEU:HD12	3:B:1152:HOH:O	2.12	0.48
1:D:284:VAL:O	1:D:287:VAL:HG22	2.14	0.48
1:D:172:ARG:HG2	3:D:413:HOH:O	2.14	0.48
1:B:164:LYS:HZ1	1:B:189:ALA:HB2	1.76	0.48
1:C:164:LYS:NZ	1:C:189:ALA:HB2	2.27	0.48
1:A:165:ASP:OD2	1:A:172:ARG:NH1	2.47	0.47
1:C:277:THR:OG1	1:C:280:GLU:HG3	2.14	0.47
1:D:79:GLY:HA2	1:D:104:LEU:HB3	1.96	0.47
1:A:190:SER:O	1:A:243:ASN:ND2	2.48	0.47
1:A:291:ILE:HG22	1:A:291:ILE:O	2.13	0.47
1:B:242:VAL:HG21	1:B:291:ILE:HD13	1.94	0.47
1:C:10:PRO:HD2	1:C:41:GLY:O	2.15	0.47
1:A:17:ASP:OD2	1:A:21:ARG:HB3	2.13	0.47
1:A:207:ALA:HB3	3:A:1018:HOH:O	2.15	0.47
1:B:218:VAL:O	1:B:222:GLU:HG3	2.13	0.47
1:C:268:ASP:HB3	1:C:269:PRO:HD2	1.96	0.47
1:D:137:THR:OG1	1:D:145:ASP:OD2	2.27	0.47
1:A:277:THR:OG1	1:A:280:GLU:HG3	2.15	0.46
1:D:11:TYR:OH	1:D:164:LYS:HE3	2.16	0.46
1:A:73:ARG:NH1	1:A:73:ARG:HG3	2.29	0.46
1:D:268:ASP:HB3	1:D:269:PRO:HD2	1.98	0.46
1:C:199:LEU:HD22	1:D:199:LEU:HD22	1.96	0.46
1:D:212:ILE:HD12	1:D:213:ALA:N	2.31	0.46
1:B:22:VAL:HG21	1:B:61:ALA:HB3	1.98	0.46
1:D:159:ARG:HH11	1:D:159:ARG:HG3	1.81	0.46
1:A:9:PHE:O	1:A:206:MET:HA	2.15	0.45
1:A:287:VAL:O	1:A:291:ILE:HG13	2.15	0.45
1:D:197:VAL:HG12	1:D:198:MET:HE2	1.99	0.45
1:B:11:TYR:HB3	1:B:48:THR:HB	1.98	0.45
1:B:212:ILE:HD12	1:B:212:ILE:C	2.42	0.45
3:C:403:HOH:O	1:D:179:ARG:HB2	2.16	0.45
1:B:228:ARG:NH2	3:B:1125:HOH:O	2.50	0.45
1:A:126:ALA:HB1	1:A:157:HIS:CE1	2.52	0.45
1:B:242:VAL:CG2	1:B:291:ILE:HG21	2.47	0.45
1:C:214:PRO:HB3	3:C:369:HOH:O	2.16	0.45
1:C:237:ARG:HG2	1:C:237:ARG:HH11	1.82	0.45
1:D:229:TRP:O	1:D:233:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ARG:NH2	3:C:358:HOH:O	2.50	0.45
1:C:79:GLY:HA2	1:C:104:LEU:HB3	1.98	0.44
1:C:94:LEU:O	1:C:98:LEU:HG	2.17	0.44
1:A:256:LYS:CE	3:A:972:HOH:O	2.49	0.44
1:D:212:ILE:HD12	1:D:212:ILE:C	2.43	0.44
1:D:233:LEU:O	1:D:237:ARG:HG3	2.17	0.44
1:B:238:LYS:HE3	3:B:1021:HOH:O	2.17	0.44
1:A:194:PRO:HD2	1:A:236:GLN:NE2	2.31	0.44
1:C:63:VAL:HG21	1:C:95:TYR:CE1	2.51	0.44
1:C:64:ARG:O	1:C:68:GLU:HG2	2.18	0.44
1:A:94:LEU:O	1:A:98:LEU:HG	2.18	0.44
1:A:37:ALA:HA	1:A:215:ARG:NH1	2.32	0.44
1:D:258:GLY:O	1:D:262:GLN:HG3	2.18	0.44
1:B:137:THR:OG1	1:B:145:ASP:OD2	2.27	0.44
1:C:137:THR:OG1	1:C:145:ASP:OD2	2.30	0.43
1:D:84:SER:HB2	3:D:414:HOH:O	2.18	0.43
1:D:194:PRO:CD	1:D:236:GLN:HE22	2.31	0.43
1:A:137:THR:OG1	1:A:145:ASP:OD2	2.33	0.43
1:D:283:ALA:HB1	1:D:286:LYS:HE2	2.00	0.43
1:B:79:GLY:HA2	1:B:104:LEU:HB3	1.99	0.43
1:D:7:GLY:HA2	1:D:221:TYR:CE1	2.54	0.43
1:A:43:THR:HG21	1:A:206:MET:CE	2.48	0.43
1:B:212:ILE:HD12	1:B:213:ALA:N	2.33	0.43
1:C:126:ALA:HB1	1:C:157:HIS:CE1	2.54	0.43
1:D:215:ARG:HD2	3:D:356:HOH:O	2.19	0.43
1:C:72:ARG:HA	3:C:414:HOH:O	2.17	0.43
1:D:194:PRO:HB2	1:D:236:GLN:HE22	1.84	0.43
1:A:35:ILE:HG21	1:A:73:ARG:HE	1.84	0.42
1:B:194:PRO:HD2	1:B:236:GLN:NE2	2.34	0.42
1:D:164:LYS:CE	1:D:206:MET:HB2	2.49	0.42
1:A:75:PRO:HA	1:A:101:ASP:OD2	2.20	0.42
1:C:233:LEU:O	1:C:237:ARG:HG3	2.19	0.42
1:C:168:THR:HG22	1:C:191:ALA:HB1	2.01	0.42
1:C:9:PHE:O	1:C:206:MET:HA	2.20	0.42
1:D:250:ASN:ND2	1:D:252:ALA:H	2.18	0.42
1:B:230:ASP:O	1:B:234:MET:HG3	2.20	0.42
1:D:16:VAL:HG21	1:D:270:ILE:CD1	2.50	0.42
1:C:51:PHE:CD1	1:C:51:PHE:C	2.98	0.42
1:D:250:ASN:C	1:D:250:ASN:ND2	2.68	0.41
1:A:207:ALA:HB1	1:A:209:PRO:HD2	2.02	0.41
1:D:11:TYR:HB3	1:D:48:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LYS:HA	1:B:187:PHE:O	2.21	0.41
1:A:71:GLN:CG	1:A:73:ARG:HH12	2.33	0.41
1:A:29:ARG:O	1:A:29:ARG:HD3	2.21	0.41
1:D:226:ALA:O	1:D:227:GLN:HB2	2.20	0.41
1:A:73:ARG:NH2	3:A:998:HOH:O	2.54	0.41
1:B:9:PHE:HB2	1:B:206:MET:HG2	2.02	0.41
1:B:71:GLN:OE1	1:B:71:GLN:HA	2.21	0.41
1:B:164:LYS:HZ2	1:B:189:ALA:HB2	1.84	0.41
1:A:148:LEU:HD21	1:A:175:SER:HB3	2.03	0.41
1:A:208:GLY:N	1:A:209:PRO:CD	2.84	0.41
1:C:109:ALA:O	1:C:143:ARG:HD2	2.20	0.41
1:D:135:ILE:HG21	1:D:146:LEU:HD21	2.02	0.41
1:A:146:LEU:N	1:A:146:LEU:CD1	2.84	0.41
1:D:168:THR:HG22	1:D:191:ALA:HB1	2.03	0.41
1:B:122:PHE:CD1	1:B:135:ILE:HD12	2.56	0.40
1:C:146:LEU:HA	3:C:322:HOH:O	2.21	0.40
1:C:237:ARG:NH1	3:D:370:HOH:O	2.53	0.40
1:D:260:ALA:HA	1:D:264:TYR:O	2.20	0.40
1:C:218:VAL:O	1:C:222:GLU:HG3	2.22	0.40
1:D:135:ILE:HG21	1:D:146:LEU:CD2	2.51	0.40
1:B:168:THR:HG22	1:B:191:ALA:HB1	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	286/300 (95%)	282 (99%)	4 (1%)	0	100	100
1	B	289/300 (96%)	282 (98%)	7 (2%)	0	100	100
1	C	286/300 (95%)	282 (99%)	3 (1%)	1 (0%)	36	30
1	D	288/300 (96%)	284 (99%)	2 (1%)	2 (1%)	18	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1149/1200 (96%)	1130 (98%)	16 (1%)	3 (0%)	36 30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	248	LYS
1	D	247	ALA
1	C	247	ALA

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	221/231 (96%)	218 (99%)	3 (1%)	59 60
1	B	222/231 (96%)	218 (98%)	4 (2%)	51 51
1	C	221/231 (96%)	218 (99%)	3 (1%)	59 60
1	D	221/231 (96%)	214 (97%)	7 (3%)	34 29
All	All	885/924 (96%)	868 (98%)	17 (2%)	50 50

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TYR
1	A	146	LEU
1	A	238	LYS
1	B	11	TYR
1	B	56	THR
1	B	179	ARG
1	B	250	ASN
1	C	11	TYR
1	C	145	ASP
1	C	146	LEU
1	D	11	TYR
1	D	145	ASP

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Mol	Chain	Res	Type
1	D	146	LEU
1	D	172	ARG
1	D	238	LYS
1	D	250	ASN
1	D	287	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	138	ASN
1	A	140	GLN
1	A	227	GLN
1	A	236	GLN
1	A	262	GLN
1	B	236	GLN
1	B	262	GLN
1	B	273	GLN
1	C	140	GLN
1	D	236	GLN
1	D	250	ASN
1	D	262	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	PGE	B	999	-	9,9,9	0.59	0	8,8,8	0.91	0
2	PGE	A	888	-	9,9,9	0.60	0	8,8,8	0.92	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	PGE	B	999	-	-	4/7/7/7	-
2	PGE	A	888	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	888	PGE	O2-C3-C4-O3
2	B	999	PGE	C6-C5-O3-C4
2	B	999	PGE	C1-C2-O2-C3
2	A	888	PGE	C1-C2-O2-C3
2	A	888	PGE	O3-C5-C6-O4
2	B	999	PGE	O3-C5-C6-O4
2	B	999	PGE	C3-C4-O3-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	888	PGE	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

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	288/300 (96%)	-0.22	2 (0%) 84 85	10, 18, 29, 38	0
1	B	291/300 (97%)	-0.03	4 (1%) 73 75	13, 21, 35, 44	0
1	C	288/300 (96%)	0.62	36 (12%) 8 7	13, 27, 49, 64	0
1	D	290/300 (96%)	0.13	6 (2%) 63 65	14, 23, 35, 43	0
All	All	1157/1200 (96%)	0.12	48 (4%) 41 41	10, 22, 40, 64	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	71	GLN	3.8
1	C	72	ARG	3.5
1	D	247	ALA	3.4
1	C	18	ALA	3.3
1	C	74	VAL	3.3
1	C	291	ILE	3.3
1	C	73	ARG	3.2
1	C	4	ASP	3.2
1	C	34	LEU	3.1
1	C	35	ILE	3.1
1	C	29	ARG	3.0
1	C	37	ALA	2.9
1	C	95	TYR	2.8
1	C	5	PHE	2.8
1	C	30	LEU	2.8
1	D	286	LYS	2.8
1	D	21	ARG	2.7
1	C	247	ALA	2.7
1	C	24	ALA	2.6
1	C	248	LYS	2.6
1	C	233	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	36	GLN	2.4
1	C	22	VAL	2.4
1	C	182	ASP	2.3
1	C	67	ILE	2.3
1	C	69	ALA	2.3
1	C	25	ASP	2.3
1	C	32	ASP	2.3
1	A	291	ILE	2.3
1	C	23	ARG	2.3
1	C	94	LEU	2.2
1	B	130	GLU	2.2
1	C	281	ARG	2.2
1	C	39	VAL	2.2
1	C	243	ASN	2.2
1	C	282	LYS	2.1
1	B	182	ASP	2.1
1	B	153	ARG	2.1
1	C	26	VAL	2.1
1	C	70	ALA	2.1
1	A	21	ARG	2.1
1	C	65	ALA	2.1
1	B	3	LEU	2.0
1	D	233	LEU	2.0
1	C	11	TYR	2.0
1	D	293	GLU	2.0
1	D	248	LYS	2.0
1	C	7	GLY	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](#)

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	PGE	B	999	10/10	0.56	0.21	18,20,23,25	0
2	PGE	A	888	10/10	0.64	0.22	18,20,23,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.