



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:45 PM UTC

PDB ID : 1TD2 / pdb_00001td2
Title : Crystal Structure of the PdxY Protein from Escherichia coli
Authors : Safo, M.K.; Musayev, F.N.; Hunt, S.; di Salvo, M.; Scarsdale, N.; Schirch, V.
Deposited on : 2004-05-21
Resolution : 2.22 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

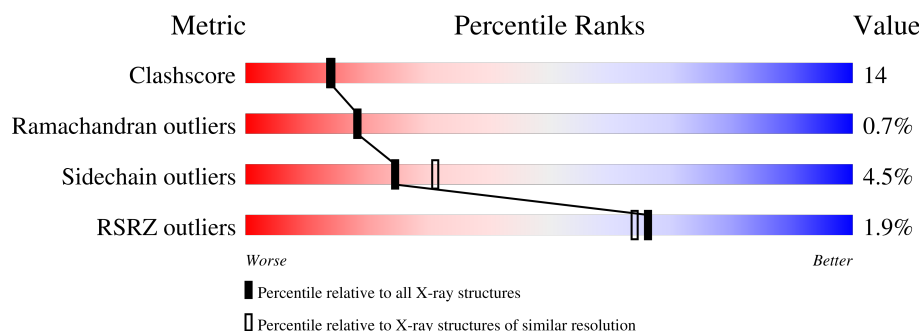
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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))
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	287	2% 70% 26% .
1	B	287	% 67% 29% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PXL	A	288	-	X	-	-

2 Entry composition [i](#)

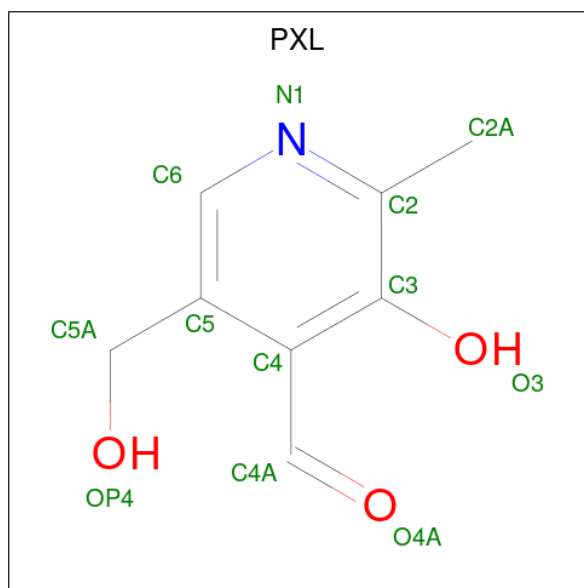
There are 4 unique types of molecules in this entry. The entry contains 4817 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyridoxamine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2201	1400	386	401	14			
1	B	287	Total	C	N	O	S	0	0	0
			2201	1400	386	401	14			

- Molecule 2 is 3-HYDROXY-5-(HYDROXYMETHYL)-2-METHYLISONICOTINALDEHYDE (CCD ID: PXL) (formula: C₈H₉NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	8	1	3		
2	B	1	Total	C	N	O	0	0
			12	8	1	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

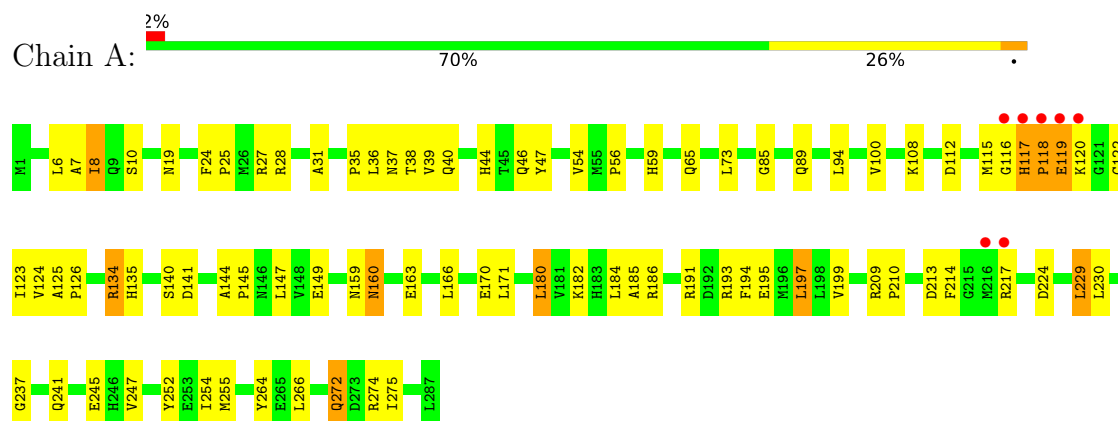
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		
4	B	171	Total	O	0	0
			171	171		

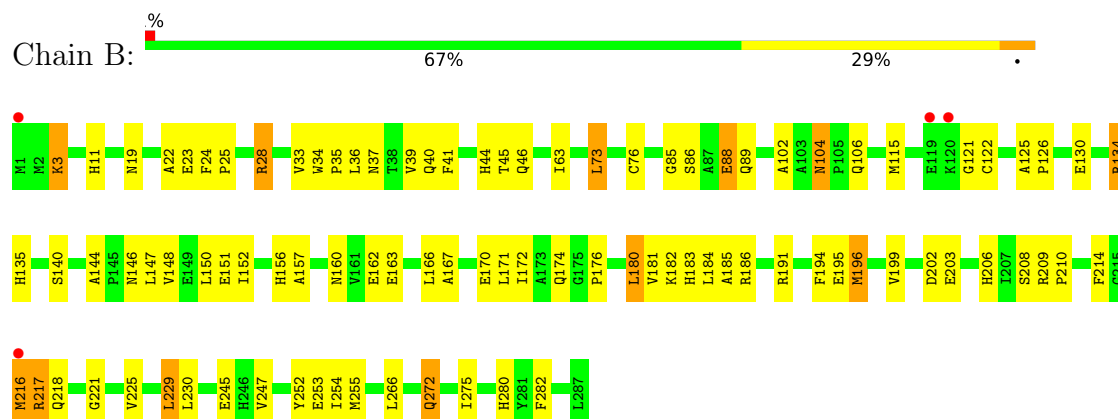
3 Residue-property plots

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: Pyridoxamine kinase



• Molecule 1: Pyridoxamine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.13Å 67.38Å 73.59Å 90.00° 93.67° 90.00°	Depositor
Resolution (Å)	38.20 – 2.22 38.20 – 2.22	Depositor EDS
% Data completeness (in resolution range)	90.4 (38.20-2.22) 90.3 (38.20-2.22)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.176 , 0.246 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4817	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.73% 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: SO4, PXL

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	0.66	0/2249	1.12	13/3058 (0.4%)
1	B	0.60	0/2249	1.07	14/3058 (0.5%)
All	All	0.63	0/4498	1.09	27/6116 (0.4%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	ILE	N-CA-C	-10.61	100.33	111.58
1	A	10	SER	N-CA-C	7.82	120.68	110.43
1	A	275	ILE	N-CA-C	-7.61	103.44	110.82
1	B	272	GLN	N-CA-C	6.83	119.60	111.33
1	A	182	LYS	N-CA-C	6.67	120.87	112.87
1	A	47	TYR	N-CA-C	-6.62	105.17	113.18
1	B	22	ALA	N-CA-C	6.26	119.38	111.69
1	B	146	ASN	N-CA-C	-5.97	100.48	109.79
1	B	199	VAL	N-CA-C	5.97	117.07	108.48
1	A	264	TYR	N-CA-C	-5.91	106.20	113.41
1	B	134	ARG	N-CA-C	5.87	120.50	113.23
1	B	23	GLU	N-CA-C	5.84	118.14	111.02
1	B	45	THR	N-CA-C	5.75	119.56	112.54
1	B	181	VAL	N-CA-C	-5.58	98.46	106.55
1	A	213	ASP	N-CA-C	5.50	117.20	108.67
1	B	221	GLY	N-CA-C	5.50	122.07	114.92
1	A	237	GLY	N-CA-C	5.37	122.73	115.32
1	A	140	SER	N-CA-C	5.35	118.04	110.50
1	A	112	ASP	N-CA-C	-5.34	98.13	108.59
1	A	272	GLN	N-CA-C	5.27	117.71	111.33
1	B	217	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	217	ARG	NE-CZ-NH2	5.27	123.94	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	SER	N-CA-C	5.17	118.13	110.48
1	A	199	VAL	N-CA-C	5.16	116.80	108.85
1	A	185	ALA	CB-CA-C	-5.13	110.64	116.54
1	B	104	ASN	CA-C-N	5.13	124.84	119.82
1	B	104	ASN	C-N-CA	5.13	124.84	119.82

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	2201	0	2210	66	0
1	B	2201	0	2211	64	0
2	A	12	0	8	2	0
2	B	12	0	9	2	0
3	B	5	0	0	1	0
4	A	215	0	0	3	0
4	B	171	0	0	5	0
All	All	4817	0	4438	127	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 (127) 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:159:ASN:HD22	1:A:186:ARG:NH2	1.56	1.03
1:A:159:ASN:ND2	1:A:186:ARG:HH22	1.56	1.01
1:A:186:ARG:HG2	4:A:386:HOH:O	1.61	0.98
1:A:8:ILE:N	1:A:8:ILE:HD13	1.85	0.90
1:A:6:LEU:HG	1:A:8:ILE:HD11	1.55	0.88
1:A:229:LEU:HB3	1:A:247:VAL:HG22	1.63	0.80
1:B:3:LYS:HD2	1:B:3:LYS:N	1.98	0.78
1:A:19:ASN:HD22	1:A:37:ASN:HD22	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ALA:C	1:A:8:ILE:HD13	2.15	0.71
1:A:160:ASN:ND2	1:A:163:GLU:HG3	2.06	0.70
1:A:85:GLY:H	1:A:89:GLN:HE22	1.42	0.68
1:A:122:CYS:SG	2:A:288:PXL:C4	2.82	0.68
1:A:40:GLN:HE22	1:B:37:ASN:HB2	1.59	0.66
1:B:88:GLU:H	1:B:88:GLU:CD	2.01	0.66
1:A:117:HIS:O	1:A:119:GLU:N	2.29	0.66
1:A:85:GLY:H	1:A:89:GLN:NE2	1.95	0.65
1:A:184:LEU:HD12	1:A:195:GLU:HB3	1.79	0.64
1:A:19:ASN:HD22	1:A:37:ASN:ND2	1.95	0.64
1:A:44:HIS:HD2	1:A:46:GLN:H	1.43	0.64
1:B:229:LEU:HB3	1:B:247:VAL:HG22	1.79	0.63
1:B:44:HIS:HD2	1:B:46:GLN:H	1.46	0.63
1:B:85:GLY:H	1:B:89:GLN:NE2	1.97	0.63
1:A:44:HIS:HE1	4:A:330:HOH:O	1.83	0.61
1:A:160:ASN:HD21	1:A:163:GLU:HG3	1.64	0.61
1:B:216:MET:O	1:B:217:ARG:CG	2.49	0.61
1:B:174:GLN:HG3	4:B:620:HOH:O	2.00	0.61
1:B:130:GLU:O	1:B:134:ARG:HG2	2.01	0.60
1:A:241:GLN:O	1:A:245:GLU:HG3	2.02	0.60
1:B:216:MET:C	1:B:217:ARG:HG3	2.27	0.60
1:A:214:PHE:HE1	1:A:255:MET:HE3	1.67	0.59
1:B:160:ASN:ND2	1:B:162:GLU:HB3	2.17	0.59
1:B:85:GLY:H	1:B:89:GLN:HE22	1.51	0.58
1:A:116:GLY:C	1:A:118:PRO:HD3	2.28	0.58
1:A:180:LEU:HG	1:A:230:LEU:HD22	1.85	0.58
1:B:216:MET:O	1:B:217:ARG:HG3	2.03	0.58
1:A:118:PRO:HA	1:A:123:ILE:HD13	1.86	0.58
1:B:245:GLU:HG2	1:B:282:PHE:O	2.04	0.58
1:A:73:LEU:HD22	1:A:100:VAL:HG22	1.86	0.57
1:B:147:LEU:HD22	1:B:184:LEU:O	2.04	0.57
1:B:210:PRO:HG2	1:B:252:TYR:CE1	2.39	0.57
1:A:117:HIS:N	1:A:118:PRO:HD3	2.20	0.56
1:A:186:ARG:HB3	1:A:191:ARG:NH1	2.21	0.56
1:B:167:ALA:O	1:B:171:LEU:HD13	2.06	0.56
1:A:254:ILE:HG22	1:A:266:LEU:HD22	1.86	0.56
1:B:180:LEU:HD13	1:B:182:LYS:HB3	1.87	0.56
1:B:253:GLU:OE1	1:B:280:HIS:HD2	1.88	0.56
1:A:8:ILE:HD12	1:A:36:LEU:HB3	1.88	0.56
1:A:214:PHE:CE1	1:A:255:MET:HE3	2.42	0.55
1:A:159:ASN:HD22	1:A:186:ARG:HH22	0.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PHE:HB3	1:A:25:PRO:HD3	1.90	0.54
1:B:180:LEU:HG	1:B:230:LEU:HD22	1.89	0.54
1:A:65:GLN:HA	1:A:65:GLN:OE1	2.08	0.53
1:B:194:PHE:O	1:B:208:SER:HA	2.08	0.53
3:B:288:SO4:O4	2:B:289:PXL:H5A1	2.09	0.53
1:B:144:ALA:HA	1:B:180:LEU:O	2.08	0.53
1:B:24:PHE:HB3	1:B:25:PRO:HD3	1.92	0.52
1:A:94:LEU:HD11	1:A:135:HIS:HB3	1.92	0.52
1:A:39:VAL:HG12	1:A:54:VAL:HA	1.92	0.52
1:A:274:ARG:NH1	4:A:326:HOH:O	2.24	0.52
1:B:160:ASN:ND2	1:B:163:GLU:H	2.06	0.52
1:A:8:ILE:N	1:A:8:ILE:CD1	2.59	0.51
1:A:254:ILE:CG2	1:A:266:LEU:HD22	2.39	0.51
1:A:186:ARG:HB3	1:A:191:ARG:HH11	1.75	0.51
1:A:94:LEU:CD1	1:A:135:HIS:HB3	2.41	0.51
1:B:225:VAL:HG12	1:B:229:LEU:HD22	1.92	0.51
1:B:195:GLU:OE1	1:B:206:HIS:HE1	1.93	0.50
1:B:28:ARG:HD3	1:B:272:GLN:HB2	1.94	0.50
1:A:193:ARG:NH1	1:A:210:PRO:HG3	2.27	0.49
1:B:202:ASP:OD1	1:B:203:GLU:HG2	2.11	0.49
1:B:195:GLU:OE1	1:B:206:HIS:CE1	2.65	0.49
1:A:6:LEU:HG	1:A:8:ILE:CD1	2.36	0.49
1:B:36:LEU:HD13	1:B:63:ILE:HG21	1.95	0.49
1:A:44:HIS:HD2	1:A:46:GLN:N	2.10	0.48
1:A:159:ASN:ND2	1:A:186:ARG:NH2	2.34	0.48
1:A:184:LEU:HD21	1:A:197:LEU:HD22	1.96	0.48
1:B:254:ILE:HG21	1:B:266:LEU:HG	1.96	0.47
1:B:19:ASN:HD22	1:B:37:ASN:HD22	1.62	0.47
1:B:88:GLU:CD	1:B:88:GLU:N	2.72	0.47
1:B:182:LYS:HA	1:B:196:MET:HG2	1.96	0.47
1:B:214:PHE:HB2	1:B:218:GLN:OE1	2.15	0.47
1:A:166:LEU:O	1:A:170:GLU:HG3	2.14	0.47
1:A:147:LEU:HD13	1:A:147:LEU:C	2.40	0.47
1:B:44:HIS:HD2	1:B:46:GLN:N	2.13	0.47
1:A:56:PRO:HG2	1:A:59:HIS:HB2	1.97	0.46
1:B:104:ASN:ND2	1:B:106:GLN:H	2.13	0.46
1:B:115:MET:SD	1:B:152:ILE:HD12	2.56	0.46
1:B:172:ILE:HA	1:B:176:PRO:O	2.15	0.46
1:B:46:GLN:HG3	1:B:121:GLY:HA3	1.97	0.45
1:B:86:SER:OG	1:B:88:GLU:HG2	2.16	0.45
1:B:216:MET:C	1:B:217:ARG:CG	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PRO:HG3	1:A:124:VAL:H	1.80	0.45
1:A:209:ARG:HD3	1:A:252:TYR:CD1	2.52	0.45
1:B:34:TRP:CZ3	1:B:76:CYS:HB2	2.52	0.45
1:A:144:ALA:HA	1:A:180:LEU:O	2.17	0.45
1:B:134:ARG:HG3	1:B:135:HIS:CD2	2.51	0.45
1:A:27:ARG:HA	1:A:31:ALA:O	2.17	0.45
1:B:156:HIS:HE2	1:B:170:GLU:CD	2.24	0.45
1:B:148:VAL:HG23	4:B:487:HOH:O	2.16	0.44
1:A:194:PHE:HB3	1:A:209:ARG:CG	2.47	0.44
1:A:38:THR:HB	1:A:89:GLN:HE22	1.83	0.44
1:A:37:ASN:H	1:B:40:GLN:HE22	1.64	0.44
1:B:102:ALA:HB3	4:B:479:HOH:O	2.18	0.43
1:B:195:GLU:HG2	1:B:208:SER:HB3	2.00	0.43
1:B:254:ILE:CG2	1:B:266:LEU:HG	2.48	0.43
1:A:40:GLN:HE22	1:B:37:ASN:CB	2.28	0.43
1:B:39:VAL:HB	1:B:41:PHE:CE2	2.54	0.43
1:B:216:MET:HG2	4:B:667:HOH:O	2.19	0.43
1:B:122:CYS:SG	2:B:289:PXL:C4A	3.07	0.43
1:A:209:ARG:O	1:A:209:ARG:HG3	2.15	0.42
1:B:151:GLU:OE2	1:B:157:ALA:HA	2.19	0.42
1:B:194:PHE:HB3	1:B:209:ARG:HG3	2.01	0.42
1:A:8:ILE:HG22	1:A:38:THR:CG2	2.49	0.42
1:A:108:LYS:HE2	1:A:141:ASP:CG	2.44	0.42
1:B:184:LEU:O	1:B:185:ALA:HB3	2.20	0.42
1:A:56:PRO:O	1:A:59:HIS:HB3	2.19	0.42
1:B:33:VAL:O	1:B:35:PRO:HD3	2.19	0.42
1:B:73:LEU:HB2	4:B:631:HOH:O	2.19	0.42
1:B:104:ASN:ND2	1:B:104:ASN:C	2.77	0.41
1:A:115:MET:HG3	1:A:149:GLU:HG2	2.03	0.41
1:A:24:PHE:HE1	1:A:272:GLN:HB3	1.85	0.41
1:A:134:ARG:HH11	1:A:134:ARG:HA	1.86	0.41
1:A:224:ASP:OD2	2:A:288:PXL:OP4	2.35	0.41
1:A:125:ALA:HA	1:A:126:PRO:HD3	1.93	0.40
1:B:28:ARG:CD	1:B:272:GLN:HB2	2.51	0.40
1:A:35:PRO:O	1:B:11:HIS:HE1	2.03	0.40
1:B:125:ALA:HA	1:B:126:PRO:HD3	1.95	0.40
1:B:186:ARG:HA	1:B:191:ARG:HG2	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	285/287 (99%)	276 (97%)	7 (2%)	2 (1%)	18	18
1	B	285/287 (99%)	270 (95%)	13 (5%)	2 (1%)	18	18
All	All	570/574 (99%)	546 (96%)	20 (4%)	4 (1%)	18	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	PRO
1	A	119	GLU
1	B	183	HIS
1	B	216	MET

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%)	221 (95%)	11 (5%)	23	29
1	B	232/232 (100%)	222 (96%)	10 (4%)	26	33
All	All	464/464 (100%)	443 (96%)	21 (4%)	24	31

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	28	ARG

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Mol	Chain	Res	Type
1	A	117	HIS
1	A	120	LYS
1	A	134	ARG
1	A	145	PRO
1	A	160	ASN
1	A	171	LEU
1	A	180	LEU
1	A	197	LEU
1	A	229	LEU
1	B	3	LYS
1	B	28	ARG
1	B	73	LEU
1	B	88	GLU
1	B	150	LEU
1	B	166	LEU
1	B	180	LEU
1	B	196	MET
1	B	229	LEU
1	B	255	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	37	ASN
1	A	40	GLN
1	A	44	HIS
1	A	89	GLN
1	A	104	ASN
1	A	159	ASN
1	A	160	ASN
1	A	236	GLN
1	A	280	HIS
1	B	11	HIS
1	B	37	ASN
1	B	40	GLN
1	B	44	HIS
1	B	89	GLN
1	B	104	ASN
1	B	135	HIS
1	B	160	ASN
1	B	174	GLN

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Mol	Chain	Res	Type
1	B	177	GLN
1	B	206	HIS
1	B	267	GLN
1	B	280	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	PXL	A	288	1	12,12,12	3.10	9 (75%)	15,16,16	2.13	2 (13%)
3	SO4	B	288	-	4,4,4	0.58	0	6,6,6	0.24	0
2	PXL	B	289	-	12,12,12	3.12	7 (58%)	15,16,16	1.55	3 (20%)

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	PXL	A	288	1	-	4/4/4/4	0/1/1/1
2	PXL	B	289	-	-	0/4/4/4	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	288	PXL	O4A-C4A	5.95	1.42	1.21
2	B	289	PXL	C2-N1	5.45	1.43	1.33
2	B	289	PXL	C6-N1	4.79	1.44	1.34
2	A	288	PXL	C3-C2	3.91	1.45	1.41
2	B	289	PXL	C3-C2	3.87	1.45	1.41
2	A	288	PXL	C6-N1	3.67	1.41	1.34
2	B	289	PXL	C6-C5	3.43	1.44	1.37
2	A	288	PXL	C4-C5	3.20	1.46	1.42
2	B	289	PXL	C4-C3	3.18	1.46	1.41
2	B	289	PXL	C4-C4A	3.17	1.53	1.46
2	A	288	PXL	C2-N1	3.16	1.39	1.33
2	A	288	PXL	C4-C4A	3.10	1.53	1.46
2	B	289	PXL	C4-C5	3.08	1.46	1.42
2	A	288	PXL	C4-C3	2.53	1.45	1.41
2	A	288	PXL	C6-C5	2.31	1.42	1.37
2	A	288	PXL	C2A-C2	2.29	1.54	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	288	PXL	O4A-C4A-C4	-6.56	109.26	124.80
2	B	289	PXL	O4A-C4A-C4	-3.06	117.53	124.80
2	A	288	PXL	C5-C6-N1	-2.77	119.32	123.83
2	B	289	PXL	C5-C6-N1	-2.61	119.59	123.83
2	B	289	PXL	C3-C4-C5	2.29	120.12	118.28

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	288	PXL	C3-C4-C4A-O4A
2	A	288	PXL	C6-C5-C5A-OP4
2	A	288	PXL	C4-C5-C5A-OP4
2	A	288	PXL	C5-C4-C4A-O4A

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	288	PXL	2	0
3	B	288	SO4	1	0
2	B	289	PXL	2	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	287/287 (100%)	-0.35	7 (2%) 59 57	10, 20, 40, 94	0
1	B	287/287 (100%)	-0.17	4 (1%) 73 72	12, 24, 48, 74	0
All	All	574/574 (100%)	-0.26	11 (1%) 66 64	10, 21, 45, 94	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	PRO	3.5
1	B	216	MET	3.4
1	B	1	MET	3.3
1	A	216	MET	3.0
1	B	120	LYS	2.9
1	A	117	HIS	2.9
1	A	119	GLU	2.9
1	A	120	LYS	2.6
1	A	116	GLY	2.2
1	A	217	ARG	2.1
1	B	119	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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
3	SO4	B	288	5/5	0.87	0.22	49,54,65,69	0
2	PXL	A	288	12/12	0.93	0.10	14,18,35,36	0
2	PXL	B	289	12/12	0.95	0.08	13,23,31,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.