Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2025 – 11:39 AM EDT

PDB ID	:	2DDW / pdb_00002ddw
Title	:	Crystal Structure of Pyridoxal Kinase from the Escherichia coli PdxK gene complexed with pyridoxal at 3.2 A resolution
Authors	:	Safo, M.K.; Musayev, F.N.; di Salvo, M.L.; Hunt, S.; Claude, J.B.; Schirch, V.
Deposited on	:	2006-02-03
Resolution	:	3.20 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:

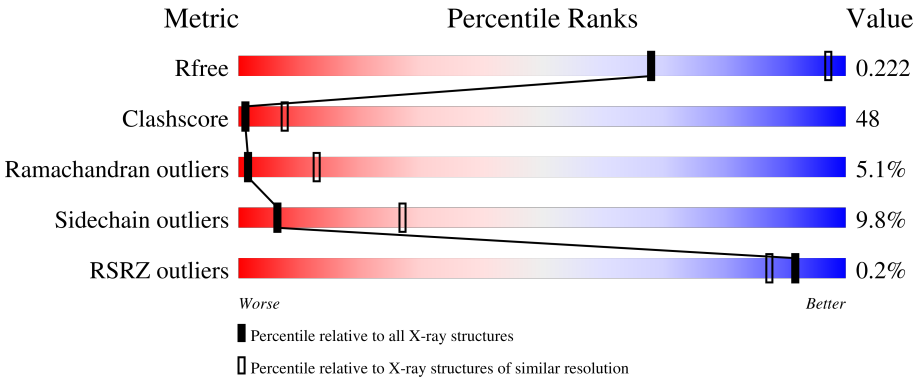
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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 <=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	283	30% 50% 11% • 7%
1	B	283	26% 56% 10% 8%

2 Entry composition

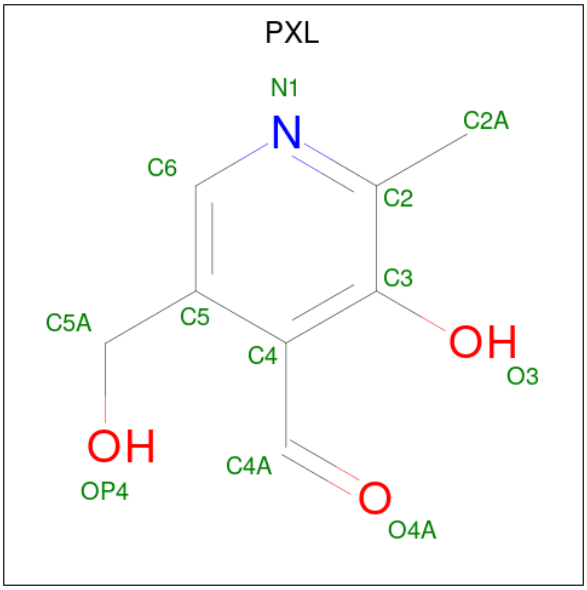
There are 3 unique types of molecules in this entry. The entry contains 4083 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyridoxine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2018	1289	343	380	6			
1	B	261	Total	C	N	O	S	0	0	0
			1992	1266	342	378	6			

- Molecule 2 is 3-HYDROXY-5-(HYDROXYMETHYL)-2-METHYLISONICOTINALDEHYDE (CCD ID: PXL) (formula: $C_8H_9NO_3$).



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 water.

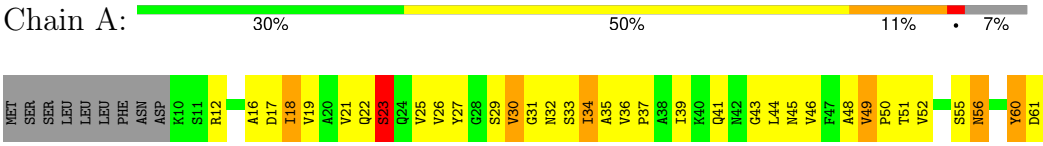
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	25	Total O 25 25	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

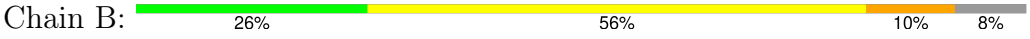
• Molecule 1: Pyridoxine kinase

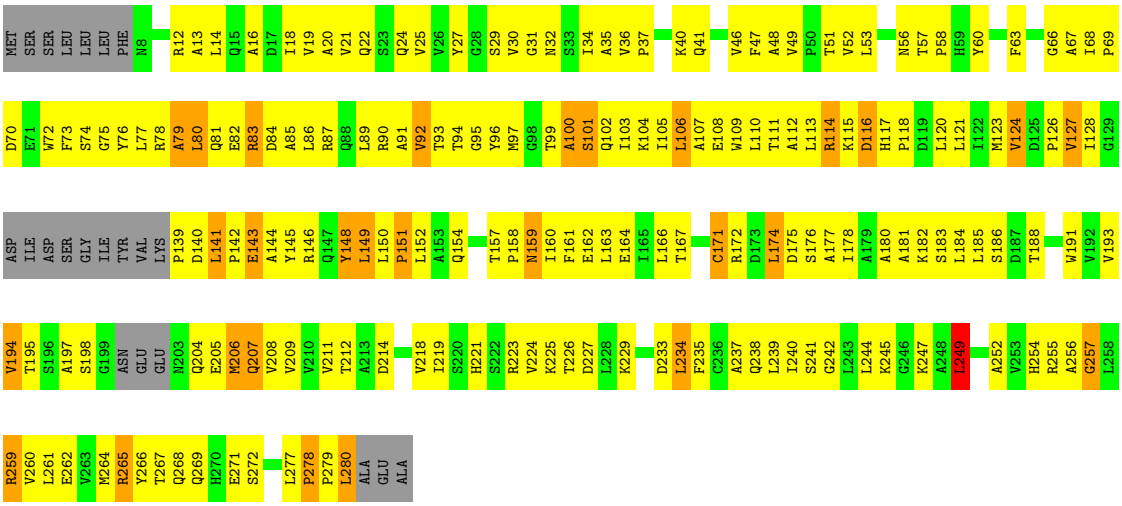
Chain A:



• Molecule 1: Pyridoxine kinase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.67Å 75.03Å 109.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 3.20 19.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.4 (19.90-3.20) 94.1 (19.90-3.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.254 0.220 , 0.222	Depositor DCC
R_{free} test set	417 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	1.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 65.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4083	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.57	1/2053 (0.0%)	1.14	19/2796 (0.7%)
1	B	0.50	0/2025	1.06	12/2757 (0.4%)
All	All	0.54	1/4078 (0.0%)	1.10	31/5553 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	SER	CA-C	5.34	1.59	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	125	ASP	CA-C-N	8.95	131.03	119.84
1	A	125	ASP	C-N-CA	8.95	131.03	119.84
1	B	100	ALA	N-CA-C	-8.38	105.06	114.62
1	B	212	THR	N-CA-C	-8.16	100.00	110.53
1	A	172	ARG	N-CA-C	7.66	122.30	113.19
1	A	168	GLY	N-CA-C	-7.43	102.88	114.10
1	A	261	LEU	N-CA-C	-7.02	103.71	111.36
1	B	51	THR	N-CA-C	-6.93	106.72	114.62
1	A	68	ILE	CA-C-N	6.91	126.94	119.89
1	A	68	ILE	C-N-CA	6.91	126.94	119.89
1	B	148	TYR	N-CA-C	6.64	121.60	112.04
1	A	148	TYR	N-CA-C	6.54	121.63	112.93
1	A	218	VAL	N-CA-C	6.12	115.16	106.53
1	B	154	GLN	N-CA-C	-5.95	105.32	113.30
1	B	227	ASP	N-CA-C	-5.93	105.36	112.59
1	A	49	VAL	CA-C-N	5.92	125.68	119.76
1	A	49	VAL	C-N-CA	5.92	125.68	119.76
1	A	72	TRP	N-CA-C	-5.91	102.51	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	25	VAL	N-CA-C	5.74	116.56	108.36
1	A	18	ILE	N-CA-C	5.69	117.93	109.17
1	A	154	GLN	N-CA-C	-5.63	106.40	113.72
1	A	268	GLN	N-CA-C	-5.58	104.83	111.69
1	A	116	ASP	N-CA-C	-5.56	107.15	114.04
1	B	56	ASN	N-CA-C	-5.54	101.47	108.45
1	B	124	VAL	N-CA-C	5.35	115.75	107.78
1	A	149	LEU	N-CA-C	5.34	119.43	113.02
1	B	265	ARG	N-CA-C	-5.25	105.25	110.97
1	B	101	SER	N-CA-C	-5.18	105.71	111.36
1	A	162	GLU	N-CA-C	-5.13	106.86	113.01
1	B	257	GLY	N-CA-C	-5.12	106.30	112.49
1	A	191	TRP	N-CA-C	5.01	115.65	108.74

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	2018	0	2066	201	0
1	B	1992	0	2023	203	0
2	A	12	0	9	0	0
2	B	12	0	9	2	0
3	A	24	0	0	1	0
3	B	25	0	0	2	0
All	All	4083	0	4107	389	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 48.

All (389) 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:91:ALA:O	1:B:92:VAL:HG23	1.64	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD22	1:B:178:ILE:HD11	1.44	0.97
1:A:22:GLN:HE21	1:A:95:GLY:HA3	1.33	0.92
1:B:280:LEU:HD13	1:B:280:LEU:H	1.33	0.91
1:B:157:THR:HG22	1:B:193:VAL:HB	1.53	0.88
1:A:92:VAL:HG11	1:A:110:LEU:HD21	1.55	0.87
1:A:128:ILE:HD11	1:A:135:ILE:HG12	1.58	0.86
1:A:278:PRO:HB2	1:A:279:PRO:HD2	1.57	0.86
1:B:167:THR:HG22	1:B:184:LEU:HD11	1.57	0.84
1:A:97:MET:HE2	1:A:103:ILE:HG12	1.58	0.83
1:B:143:GLU:CD	1:B:143:GLU:H	1.86	0.82
1:A:170:ASN:HB3	1:A:176:SER:HB3	1.62	0.81
1:A:23:SER:HB3	1:A:96:TYR:HB3	1.61	0.81
1:A:159:ASN:ND2	1:A:162:GLU:H	1.78	0.80
1:A:22:GLN:NE2	1:A:95:GLY:HA3	1.96	0.80
1:A:214:ASP:O	1:A:215:SER:HB3	1.81	0.80
1:A:126:PRO:O	1:A:128:ILE:HG22	1.81	0.79
1:B:19:VAL:HG23	1:B:89:LEU:HD11	1.65	0.79
1:B:195:THR:HG22	1:B:208:VAL:HG13	1.66	0.78
1:A:234:LEU:HD13	1:A:260:VAL:HG22	1.68	0.76
1:A:159:ASN:HD22	1:A:161:PHE:H	1.29	0.76
1:A:139:PRO:O	1:A:142:PRO:HD2	1.86	0.75
1:A:100:ALA:HB1	1:A:144:ALA:HB2	1.69	0.75
1:B:58:PRO:HD2	2:B:1005:PXL:O3	1.88	0.74
1:A:18:ILE:HB	1:A:46:VAL:HG23	1.71	0.72
1:A:205:GLU:HB2	1:A:223:ARG:HH21	1.54	0.72
1:B:19:VAL:HG23	1:B:89:LEU:CD1	2.19	0.72
1:B:103:ILE:HG23	1:B:149:LEU:HD22	1.69	0.72
1:B:240:ILE:HG13	1:B:244:LEU:CD1	2.20	0.72
1:A:96:TYR:HA	1:A:127:VAL:HG21	1.72	0.72
1:A:159:ASN:ND2	1:A:161:PHE:H	1.88	0.71
1:A:258:LEU:HA	1:A:261:LEU:HD12	1.71	0.71
1:B:83:ARG:HE	1:B:83:ARG:HA	1.53	0.71
1:A:116:ASP:C	1:A:118:PRO:HD3	2.16	0.71
1:A:267:THR:HG21	1:A:275:LEU:HA	1.72	0.71
1:B:126:PRO:O	1:B:128:ILE:HG13	1.91	0.70
1:A:29:SER:O	1:A:30:VAL:HG13	1.92	0.70
1:B:18:ILE:HG22	1:B:19:VAL:N	2.07	0.70
1:A:32:ASN:ND2	1:A:48:ALA:HB1	2.06	0.70
1:A:224:VAL:HG21	1:A:268:GLN:HE22	1.58	0.69
1:B:32:ASN:HA	1:B:35:ALA:HB3	1.75	0.69
1:A:264:MET:O	1:A:268:GLN:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:VAL:HG11	1:B:57:THR:HG21	1.76	0.68
1:B:159:ASN:ND2	1:B:162:GLU:H	1.91	0.68
1:B:280:LEU:H	1:B:280:LEU:CD1	2.04	0.68
1:A:172:ARG:N	1:A:172:ARG:HD2	2.08	0.68
1:B:267:THR:HG23	1:B:272:SER:HB3	1.75	0.67
1:B:126:PRO:HG2	1:B:158:PRO:HB3	1.75	0.67
1:B:104:LYS:O	1:B:107:ALA:HB3	1.95	0.67
1:A:159:ASN:OD1	1:A:162:GLU:HG3	1.95	0.67
1:A:267:THR:HG22	1:A:276:ILE:HG13	1.78	0.66
1:A:29:SER:CB	1:A:275:LEU:HB2	2.26	0.66
1:B:34:ILE:C	1:B:37:PRO:HD2	2.19	0.66
1:B:18:ILE:HG22	1:B:20:ALA:H	1.60	0.66
1:A:110:LEU:O	1:A:113:LEU:HB2	1.96	0.66
1:A:178:ILE:O	1:A:182:LYS:HG2	1.96	0.66
1:B:167:THR:CG2	1:B:184:LEU:HD11	2.26	0.66
1:A:86:LEU:HD22	1:A:89:LEU:HD22	1.77	0.66
1:A:234:LEU:HD11	1:A:263:VAL:HG21	1.77	0.65
1:B:183:SER:O	1:B:184:LEU:HG	1.96	0.65
1:B:278:PRO:HB2	1:B:279:PRO:HD2	1.77	0.65
1:B:242:GLY:O	1:B:247:LYS:HB2	1.96	0.65
1:A:19:VAL:HG23	1:A:89:LEU:CD1	2.27	0.64
1:A:185:LEU:HD13	1:A:213:ALA:HA	1.79	0.64
1:B:99:THR:OG1	1:B:102:GLN:HG3	1.98	0.64
1:B:209:VAL:HG22	1:B:218:VAL:HG22	1.78	0.64
1:A:19:VAL:HG12	1:A:19:VAL:O	1.97	0.63
1:A:130:ASP:CG	1:A:131:ILE:H	2.06	0.63
1:B:76:TYR:O	1:B:79:ALA:HB3	1.98	0.63
1:B:94:THR:OG1	1:B:124:VAL:HG13	1.99	0.63
1:B:86:LEU:HD22	1:B:89:LEU:HD22	1.79	0.63
1:B:22:GLN:HB3	1:B:95:GLY:HA3	1.81	0.63
1:A:135:ILE:C	1:A:137:VAL:H	2.05	0.62
1:A:97:MET:HG3	1:A:103:ILE:HD11	1.82	0.62
1:A:36:VAL:N	1:A:37:PRO:HD2	2.15	0.62
1:A:97:MET:CE	1:A:103:ILE:HG12	2.27	0.62
1:A:146:ARG:HD3	1:A:166:LEU:O	1.99	0.62
1:B:205:GLU:HG3	1:B:221:HIS:O	1.99	0.62
1:A:160:ILE:O	1:A:164:GLU:HG3	2.00	0.62
1:B:36:VAL:O	1:B:40:LYS:HB2	1.99	0.62
1:B:22:GLN:OE1	1:B:31:GLY:HA2	2.00	0.61
1:B:256:ALA:O	1:B:260:VAL:HG23	2.00	0.61
1:B:280:LEU:HD13	1:B:280:LEU:N	2.11	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:THR:HA	1:B:193:VAL:O	2.00	0.61
1:A:21:VAL:HG22	1:A:49:VAL:HB	1.81	0.60
1:B:191:TRP:CE3	1:B:193:VAL:HG23	2.35	0.60
1:A:150:LEU:C	1:A:152:LEU:H	2.09	0.60
1:B:94:THR:HG22	1:B:106:LEU:HD21	1.83	0.60
1:B:224:VAL:HG12	1:B:225:LYS:H	1.66	0.60
1:B:223:ARG:HD3	1:B:264:MET:HE1	1.84	0.60
1:A:156:ILE:HG13	1:A:158:PRO:HD3	1.83	0.60
1:B:21:VAL:HG22	1:B:49:VAL:HB	1.84	0.60
1:B:255:ARG:HG2	1:B:255:ARG:HH11	1.66	0.60
1:A:12:ARG:HH21	1:B:271:GLU:HB3	1.66	0.60
1:B:18:ILE:HG22	1:B:20:ALA:N	2.17	0.60
1:B:159:ASN:C	1:B:159:ASN:HD22	2.10	0.59
1:B:150:LEU:HB3	1:B:151:PRO:HD3	1.84	0.59
1:A:29:SER:HB3	1:A:275:LEU:HB2	1.85	0.59
1:B:159:ASN:ND2	1:B:162:GLU:HG3	2.17	0.59
1:B:37:PRO:O	1:B:41:GLN:HG3	2.03	0.59
1:A:159:ASN:HD22	1:A:161:PHE:N	1.97	0.59
1:B:163:LEU:O	1:B:167:THR:HG23	2.03	0.59
1:A:49:VAL:HG21	1:A:77:LEU:HD23	1.85	0.58
1:B:121:LEU:C	1:B:121:LEU:HD23	2.27	0.58
1:A:259:ARG:O	1:A:262:GLU:HB3	2.03	0.58
1:A:267:THR:HG22	1:A:276:ILE:CG1	2.34	0.58
1:A:159:ASN:HD22	1:A:159:ASN:C	2.12	0.58
1:A:266:TYR:O	1:A:270:HIS:HB2	2.02	0.58
1:A:266:TYR:CD1	1:A:278:PRO:HB3	2.38	0.58
1:A:56:ASN:HD21	1:A:63:PHE:N	2.01	0.58
1:B:18:ILE:CG2	1:B:19:VAL:N	2.66	0.58
1:B:240:ILE:HG23	1:B:241:SER:N	2.17	0.58
1:B:31:GLY:O	1:B:34:ILE:HG22	2.04	0.58
1:A:134:GLY:HA3	1:A:161:PHE:CE1	2.39	0.57
1:A:205:GLU:HB2	1:A:223:ARG:NH2	2.19	0.57
1:A:34:ILE:O	1:A:37:PRO:HG2	2.03	0.57
1:A:83:ARG:HE	1:A:83:ARG:HA	1.69	0.57
1:B:19:VAL:HG12	1:B:19:VAL:O	2.03	0.57
1:B:259:ARG:HD3	1:B:262:GLU:OE1	2.05	0.57
1:B:240:ILE:CG2	1:B:241:SER:N	2.68	0.56
1:A:174:LEU:HD21	1:A:209:VAL:HG21	1.86	0.56
1:B:14:LEU:O	1:B:85:ALA:HB1	2.05	0.56
1:B:278:PRO:CB	1:B:279:PRO:HD2	2.35	0.56
1:A:114:ARG:HB3	1:A:114:ARG:NH1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ALA:O	1:B:108:GLU:C	2.49	0.56
1:A:19:VAL:HG23	1:A:89:LEU:HD13	1.86	0.56
1:A:159:ASN:HD21	1:A:162:GLU:H	1.53	0.56
1:A:278:PRO:HB2	1:A:279:PRO:CD	2.35	0.55
1:B:114:ARG:HG3	1:B:114:ARG:HH11	1.69	0.55
1:B:19:VAL:O	1:B:21:VAL:HG23	2.06	0.55
1:A:138:LYS:O	1:A:141:LEU:HG	2.05	0.55
1:A:241:SER:O	1:A:245:LYS:HG3	2.07	0.55
1:B:265:ARG:HG2	1:B:265:ARG:HH11	1.72	0.55
1:A:83:ARG:HA	1:A:83:ARG:NE	2.22	0.55
1:A:114:ARG:HB3	1:A:114:ARG:HH11	1.70	0.55
1:B:260:VAL:O	1:B:264:MET:HG3	2.08	0.54
1:A:271:GLU:HA	1:B:12:ARG:HH12	1.73	0.54
1:A:29:SER:HB3	1:A:34:ILE:HD13	1.89	0.54
1:B:92:VAL:HG11	1:B:110:LEU:HD21	1.88	0.54
1:A:12:ARG:NH2	1:B:271:GLU:HB3	2.22	0.54
1:A:61:ASP:HB3	1:B:83:ARG:HH22	1.72	0.54
1:A:172:ARG:HD2	1:A:172:ARG:H	1.71	0.54
1:A:271:GLU:HG3	1:B:12:ARG:NH1	2.23	0.54
1:B:116:ASP:OD2	1:B:116:ASP:N	2.39	0.54
1:B:142:PRO:HD2	1:B:143:GLU:OE2	2.07	0.54
1:B:241:SER:O	1:B:245:LYS:HG3	2.08	0.54
1:A:238:GLN:HB3	1:A:256:ALA:CB	2.38	0.53
1:B:233:ASP:OD2	2:B:1005:PXL:OP4	2.24	0.53
1:A:16:ALA:HA	1:A:45:ASN:HB2	1.91	0.53
1:A:94:THR:OG1	1:A:124:VAL:HG13	2.09	0.53
1:B:29:SER:HB3	1:B:34:ILE:HD13	1.90	0.53
1:B:249:LEU:O	1:B:252:ALA:N	2.42	0.53
1:A:101:SER:O	1:A:105:ILE:HG13	2.10	0.52
1:B:16:ALA:HB3	1:B:47:PHE:CD1	2.44	0.52
1:A:234:LEU:HD13	1:A:260:VAL:HA	1.89	0.52
1:B:106:LEU:HD12	1:B:106:LEU:O	2.08	0.52
1:A:43:GLY:C	1:A:44:LEU:HG	2.33	0.52
1:B:69:PRO:O	1:B:70:ASP:C	2.52	0.52
1:A:234:LEU:HB3	1:A:260:VAL:HG22	1.91	0.52
1:A:159:ASN:ND2	1:A:159:ASN:C	2.68	0.52
1:A:265:ARG:HH11	1:A:265:ARG:HG2	1.75	0.52
1:A:128:ILE:HD12	1:A:142:PRO:HG3	1.92	0.51
1:B:197:ALA:HA	1:B:205:GLU:O	2.10	0.51
1:A:18:ILE:HG22	1:A:19:VAL:N	2.25	0.51
1:A:19:VAL:HG11	1:A:109:TRP:CH2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:PHE:CE2	1:B:102:GLN:HB3	2.46	0.51
1:B:99:THR:OG1	1:B:100:ALA:N	2.42	0.51
1:A:27:TYR:OH	1:B:13:ALA:HB1	2.10	0.51
1:A:74:SER:HB2	1:A:105:ILE:HD13	1.93	0.51
1:A:110:LEU:HD13	1:A:122:ILE:HD13	1.90	0.51
1:B:77:LEU:O	1:B:78:ARG:C	2.53	0.51
1:A:149:LEU:O	1:A:149:LEU:HG	2.11	0.51
1:B:79:ALA:O	1:B:81:GLN:N	2.44	0.51
1:B:267:THR:CG2	1:B:272:SER:HB3	2.39	0.51
1:A:159:ASN:ND2	1:A:161:PHE:N	2.56	0.51
1:A:265:ARG:HA	1:A:268:GLN:OE1	2.10	0.51
1:A:17:ASP:O	1:A:89:LEU:HD12	2.11	0.51
1:B:24:GLN:O	1:B:53:LEU:HD12	2.11	0.51
1:B:159:ASN:HD22	1:B:161:PHE:N	2.08	0.51
1:A:117:HIS:N	1:A:118:PRO:HD3	2.26	0.51
1:A:267:THR:HG21	1:A:276:ILE:N	2.26	0.51
1:B:97:MET:HE2	1:B:103:ILE:HG12	1.92	0.51
1:B:198:SER:O	1:B:204:GLN:HA	2.11	0.51
1:B:204:GLN:HE21	1:B:223:ARG:HD2	1.76	0.51
1:A:146:ARG:HH11	1:A:146:ARG:HB2	1.77	0.50
1:A:174:LEU:O	1:A:178:ILE:HG13	2.11	0.50
1:A:113:LEU:HD13	1:A:120:LEU:HD11	1.92	0.50
1:B:159:ASN:ND2	1:B:159:ASN:C	2.69	0.50
1:A:167:THR:HG22	1:A:184:LEU:HD11	1.93	0.50
1:A:72:TRP:CZ2	1:B:66:GLY:HA3	2.45	0.50
1:A:83:ARG:NH1	1:B:60:TYR:HB3	2.27	0.50
1:B:27:TYR:C	1:B:27:TYR:CD2	2.88	0.50
1:A:126:PRO:O	1:A:127:VAL:C	2.54	0.50
1:A:247:LYS:CE	1:A:255:ARG:HE	2.25	0.50
1:A:267:THR:CG2	1:A:276:ILE:N	2.75	0.50
1:B:144:ALA:O	1:B:148:TYR:HB2	2.11	0.50
1:A:26:VAL:HG12	1:A:26:VAL:O	2.12	0.50
1:A:62:THR:O	1:A:63:PHE:CD2	2.65	0.50
1:B:143:GLU:CD	1:B:143:GLU:N	2.64	0.50
1:A:234:LEU:HD11	1:A:263:VAL:CB	2.42	0.49
1:B:69:PRO:O	1:B:72:TRP:N	2.45	0.49
1:A:30:VAL:O	1:A:33:SER:HB2	2.13	0.49
1:A:52:VAL:HA	1:A:67:ALA:HA	1.94	0.49
1:A:173:ASP:HB2	1:A:176:SER:OG	2.12	0.49
1:A:247:LYS:NZ	1:A:255:ARG:HE	2.10	0.49
1:B:160:ILE:O	1:B:164:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:MET:O	1:B:207:GLN:C	2.55	0.49
1:A:35:ALA:O	1:A:39:ILE:HG13	2.12	0.49
1:B:36:VAL:N	1:B:37:PRO:CD	2.75	0.49
1:B:255:ARG:HG2	1:B:255:ARG:NH1	2.26	0.49
1:B:24:GLN:NE2	1:B:53:LEU:HD11	2.27	0.49
1:B:99:THR:HG1	1:B:102:GLN:HG3	1.77	0.49
1:A:94:THR:CG2	1:A:106:LEU:HD21	2.42	0.49
1:A:238:GLN:HB3	1:A:256:ALA:HB1	1.94	0.49
1:B:150:LEU:CB	1:B:151:PRO:HD3	2.43	0.49
1:A:238:GLN:CG	1:A:256:ALA:HA	2.43	0.48
1:A:219:ILE:H	1:A:219:ILE:HD12	1.78	0.48
1:B:36:VAL:HB	1:B:37:PRO:HD3	1.94	0.48
1:B:113:LEU:C	1:B:115:LYS:H	2.21	0.48
1:A:130:ASP:CG	1:A:131:ILE:N	2.71	0.48
1:A:160:ILE:HG23	1:A:196:SER:HB2	1.93	0.48
1:A:175:ASP:O	1:A:176:SER:C	2.56	0.48
1:A:237:ALA:O	1:A:240:ILE:HG22	2.14	0.48
1:B:123:MET:HE1	1:B:240:ILE:HB	1.94	0.48
1:A:129:GLY:HA3	1:A:161:PHE:CD1	2.49	0.48
1:A:219:ILE:HD11	1:A:250:THR:HG23	1.94	0.48
1:B:16:ALA:HB3	1:B:47:PHE:CE1	2.49	0.48
1:B:104:LYS:O	1:B:108:GLU:HG3	2.13	0.48
1:B:141:LEU:N	1:B:142:PRO:CD	2.77	0.48
1:B:197:ALA:HB1	1:B:204:GLN:HB2	1.95	0.48
1:B:224:VAL:HG12	1:B:225:LYS:N	2.28	0.48
1:A:55:SER:OG	1:A:63:PHE:HA	2.13	0.48
1:A:167:THR:HG22	1:A:184:LEU:CD1	2.44	0.48
1:B:69:PRO:HD2	1:B:72:TRP:CE3	2.49	0.48
1:A:62:THR:OG1	1:B:83:ARG:NH1	2.46	0.48
1:A:110:LEU:HD23	1:A:113:LEU:HD12	1.95	0.48
1:A:234:LEU:HD11	1:A:263:VAL:CG2	2.41	0.48
1:A:240:ILE:HG13	1:A:244:LEU:HD12	1.94	0.48
1:B:113:LEU:O	1:B:115:LYS:N	2.47	0.47
1:A:150:LEU:N	1:A:151:PRO:CD	2.77	0.47
1:B:240:ILE:HG13	1:B:244:LEU:HD13	1.96	0.47
1:B:278:PRO:CB	1:B:279:PRO:CD	2.92	0.47
1:A:32:ASN:CG	1:A:48:ALA:HB1	2.39	0.47
1:B:174:LEU:HD22	1:B:178:ILE:CD1	2.32	0.47
1:A:93:THR:HG22	1:A:123:MET:HB3	1.96	0.47
1:A:121:LEU:HD23	1:A:240:ILE:CD1	2.44	0.47
1:A:135:ILE:C	1:A:137:VAL:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LYS:HE3	1:A:251:ASP:OD2	2.14	0.47
1:B:269:GLN:C	1:B:271:GLU:H	2.20	0.47
1:B:32:ASN:ND2	1:B:48:ALA:HB1	2.30	0.47
1:B:109:TRP:O	1:B:110:LEU:C	2.57	0.47
1:B:149:LEU:O	1:B:150:LEU:C	2.58	0.47
1:B:191:TRP:NE1	3:B:1009:HOH:O	2.42	0.47
1:A:117:HIS:N	1:A:117:HIS:ND1	2.62	0.47
1:A:137:VAL:HB	1:A:141:LEU:HD12	1.97	0.47
1:A:138:LYS:HB3	1:A:140:ASP:OD1	2.14	0.47
1:A:150:LEU:H	1:A:151:PRO:CD	2.27	0.47
1:B:79:ALA:O	1:B:80:LEU:C	2.58	0.46
1:B:95:GLY:O	1:B:96:TYR:C	2.58	0.46
1:B:159:ASN:HD21	1:B:162:GLU:HG3	1.80	0.46
1:A:179:ALA:O	1:A:182:LYS:N	2.48	0.46
1:B:160:ILE:HG21	1:B:172:ARG:NH1	2.31	0.46
1:A:167:THR:OG1	1:A:169:LYS:HB2	2.16	0.46
1:A:159:ASN:H	1:A:162:GLU:HB2	1.80	0.46
1:A:262:GLU:O	1:A:263:VAL:C	2.59	0.46
1:A:271:GLU:HG3	1:B:12:ARG:HH11	1.81	0.46
1:B:30:VAL:HG11	1:B:57:THR:CG2	2.45	0.46
1:A:109:TRP:CZ3	1:A:113:LEU:HD11	2.51	0.46
1:A:267:THR:CG2	1:A:276:ILE:H	2.29	0.46
1:A:27:TYR:CE1	1:B:14:LEU:HB2	2.51	0.46
1:B:16:ALA:HB1	1:B:46:VAL:HA	1.98	0.46
1:B:238:GLN:O	1:B:239:LEU:C	2.60	0.45
1:B:91:ALA:O	1:B:92:VAL:CG2	2.51	0.45
1:B:107:ALA:O	1:B:110:LEU:N	2.49	0.45
1:B:280:LEU:HD22	1:B:280:LEU:O	2.16	0.45
1:A:76:TYR:O	1:A:77:LEU:C	2.59	0.45
1:A:94:THR:HG22	1:A:106:LEU:HD21	1.98	0.45
1:B:206:MET:O	1:B:207:GLN:O	2.34	0.45
1:A:99:THR:OG1	1:A:102:GLN:HG3	2.16	0.45
1:B:114:ARG:HG3	1:B:114:ARG:NH1	2.31	0.45
1:B:278:PRO:HB2	1:B:279:PRO:CD	2.46	0.45
1:B:235:PHE:HB2	1:B:260:VAL:HG21	1.99	0.45
1:A:63:PHE:O	1:A:63:PHE:CG	2.69	0.45
1:A:249:LEU:O	1:A:250:THR:C	2.60	0.45
1:B:206:MET:HB2	1:B:221:HIS:HB2	1.98	0.45
1:A:272:SER:C	1:A:274:GLU:H	2.25	0.45
1:A:41:GLN:C	1:A:43:GLY:H	2.24	0.44
1:A:97:MET:HG3	1:A:103:ILE:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLU:OE2	1:A:143:GLU:HA	2.17	0.44
1:A:62:THR:HG21	1:B:82:GLU:OE2	2.17	0.44
1:A:60:TYR:HB3	1:A:61:ASP:H	1.46	0.44
1:A:99:THR:HG1	1:A:102:GLN:HG3	1.82	0.44
1:A:150:LEU:O	1:A:152:LEU:N	2.50	0.44
1:A:175:ASP:CG	1:A:176:SER:N	2.76	0.44
1:B:159:ASN:ND2	1:B:161:PHE:N	2.66	0.44
1:A:56:ASN:HD21	1:A:63:PHE:CA	2.31	0.44
1:A:64:TYR:HH	1:B:82:GLU:CD	2.26	0.44
1:A:173:ASP:HB3	1:A:175:ASP:OD1	2.17	0.44
1:B:158:PRO:HB2	1:B:162:GLU:HB2	2.00	0.44
1:A:56:ASN:HD21	1:A:63:PHE:H	1.65	0.44
1:A:256:ALA:O	1:A:260:VAL:HG23	2.16	0.44
1:A:262:GLU:O	1:A:265:ARG:N	2.49	0.44
1:A:110:LEU:O	1:A:113:LEU:N	2.51	0.44
1:B:180:ALA:HA	1:B:183:SER:OG	2.18	0.44
1:B:116:ASP:C	1:B:118:PRO:HD3	2.43	0.44
1:B:182:LYS:HA	1:B:185:LEU:HD11	2.00	0.44
1:A:129:GLY:HA2	1:A:134:GLY:HA2	1.99	0.43
1:A:271:GLU:CG	1:B:12:ARG:HH11	2.31	0.43
1:B:112:ALA:O	1:B:113:LEU:C	2.60	0.43
1:B:229:LYS:N	1:B:229:LYS:HD2	2.33	0.43
1:B:105:ILE:O	1:B:106:LEU:C	2.61	0.43
1:B:181:ALA:HB3	1:B:211:VAL:HG11	2.00	0.43
1:B:87:ARG:NH1	1:B:87:ARG:HG2	2.33	0.43
1:A:31:GLY:C	1:A:33:SER:N	2.74	0.43
1:A:97:MET:HG3	1:A:103:ILE:CD1	2.46	0.43
1:B:117:HIS:O	1:B:120:LEU:HB2	2.18	0.43
1:A:22:GLN:O	1:A:50:PRO:HA	2.17	0.43
1:B:58:PRO:HA	1:B:63:PHE:CD1	2.53	0.43
1:A:224:VAL:HG21	1:A:268:GLN:NE2	2.30	0.43
1:B:19:VAL:O	1:B:20:ALA:C	2.62	0.43
1:B:52:VAL:HA	1:B:67:ALA:HA	2.01	0.43
1:B:101:SER:O	1:B:105:ILE:HG13	2.19	0.43
1:B:171:CYS:CB	1:B:176:SER:HB3	2.49	0.43
1:B:182:LYS:C	1:B:184:LEU:H	2.27	0.43
1:B:234:LEU:O	1:B:237:ALA:HB3	2.18	0.43
1:B:254:HIS:O	1:B:257:GLY:N	2.52	0.43
1:A:265:ARG:HH11	1:A:265:ARG:CG	2.31	0.43
1:B:32:ASN:C	1:B:34:ILE:N	2.75	0.43
1:B:150:LEU:HD11	1:B:166:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLY:O	1:A:34:ILE:HG22	2.19	0.42
1:A:117:HIS:O	1:A:120:LEU:HB2	2.19	0.42
1:A:230:GLY:O	1:A:231:THR:C	2.62	0.42
1:B:146:ARG:O	1:B:151:PRO:HD3	2.20	0.42
1:B:74:SER:O	1:B:75:GLY:C	2.61	0.42
1:B:96:TYR:N	1:B:127:VAL:HG21	2.34	0.42
1:B:177:ALA:O	1:B:180:ALA:HB3	2.19	0.42
1:B:234:LEU:O	1:B:235:PHE:C	2.61	0.42
1:A:128:ILE:CD1	1:A:142:PRO:HG3	2.50	0.42
1:B:110:LEU:O	1:B:111:THR:C	2.62	0.42
1:B:223:ARG:HG2	1:B:224:VAL:N	2.35	0.42
1:B:277:LEU:HA	1:B:278:PRO:HD3	1.73	0.42
1:A:212:THR:HG22	1:A:213:ALA:H	1.84	0.42
1:B:269:GLN:C	1:B:271:GLU:N	2.76	0.42
1:B:83:ARG:HE	1:B:83:ARG:CA	2.28	0.42
1:A:36:VAL:N	1:A:37:PRO:CD	2.82	0.42
1:A:238:GLN:HB3	1:A:256:ALA:HA	2.01	0.42
1:B:191:TRP:CZ3	1:B:193:VAL:HG23	2.54	0.42
1:A:219:ILE:HG22	1:A:220:SER:N	2.34	0.42
1:B:149:LEU:HD12	1:B:149:LEU:HA	1.82	0.42
1:B:159:ASN:CG	1:B:162:GLU:HG3	2.45	0.42
1:A:90:ARG:NH2	1:A:244:LEU:O	2.52	0.41
1:B:150:LEU:C	1:B:152:LEU:H	2.28	0.41
1:B:171:CYS:HB3	1:B:176:SER:HB3	2.01	0.41
1:B:237:ALA:O	1:B:240:ILE:HG22	2.20	0.41
1:B:261:LEU:O	1:B:265:ARG:HG3	2.20	0.41
1:A:128:ILE:HD12	1:A:142:PRO:CG	2.51	0.41
1:A:175:ASP:CG	1:A:176:SER:H	2.28	0.41
1:B:139:PRO:C	1:B:141:LEU:H	2.28	0.41
1:A:146:ARG:HB2	1:A:146:ARG:NH1	2.34	0.41
1:A:171:CYS:HB2	1:A:172:ARG:H	1.56	0.41
1:A:223:ARG:HH11	1:A:264:MET:HE1	1.85	0.41
1:B:145:TYR:O	1:B:150:LEU:HB2	2.20	0.41
1:A:75:GLY:O	1:A:79:ALA:N	2.48	0.41
1:A:234:LEU:HD11	1:A:263:VAL:HG11	2.02	0.41
1:B:78:ARG:O	1:B:79:ALA:C	2.63	0.41
1:B:211:VAL:O	1:B:211:VAL:HG12	2.20	0.41
1:B:240:ILE:O	1:B:241:SER:C	2.63	0.41
1:B:265:ARG:O	1:B:266:TYR:C	2.61	0.41
1:B:83:ARG:O	1:B:84:ASP:HB3	2.21	0.41
1:A:125:ASP:CG	3:A:1008:HOH:O	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:THR:HG23	3:B:1028:HOH:O	2.20	0.41
1:B:265:ARG:O	1:B:268:GLN:N	2.54	0.41
1:A:37:PRO:O	1:A:41:GLN:HG3	2.20	0.41
1:A:51:THR:HG21	1:A:97:MET:SD	2.61	0.41
1:A:179:ALA:O	1:A:182:LYS:HB2	2.21	0.41
1:A:250:THR:O	1:A:251:ASP:C	2.63	0.41
1:B:68:ILE:HA	1:B:69:PRO:HD3	1.79	0.41
1:B:140:ASP:O	1:B:143:GLU:HG2	2.21	0.41
1:A:276:ILE:O	1:A:278:PRO:HD3	2.21	0.41
1:B:87:ARG:HG2	1:B:87:ARG:HH11	1.85	0.41
1:A:178:ILE:HD13	1:A:216:VAL:HG11	2.02	0.40
1:B:93:THR:HG22	1:B:123:MET:HB3	2.03	0.40
1:B:194:VAL:HG13	1:B:209:VAL:HB	2.04	0.40
1:B:254:HIS:O	1:B:255:ARG:C	2.64	0.40
1:A:65:GLY:HA2	1:B:72:TRP:CG	2.57	0.40
1:B:114:ARG:O	1:B:114:ARG:HG2	2.21	0.40
1:A:68:ILE:HA	1:A:69:PRO:HD3	1.95	0.40
1:B:89:LEU:HG	1:B:90:ARG:N	2.36	0.40
1:B:207:GLN:HE21	1:B:207:GLN:HB3	1.53	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	259/283 (92%)	189 (73%)	55 (21%)	15 (6%)	1 10
1	B	255/283 (90%)	179 (70%)	65 (26%)	11 (4%)	2 16
All	All	514/566 (91%)	368 (72%)	120 (23%)	26 (5%)	1 13

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	TYR
1	A	127	VAL
1	A	170	ASN
1	A	215	SER
1	B	92	VAL
1	B	207	GLN
1	B	249	LEU
1	A	63	PHE
1	A	126	PRO
1	A	249	LEU
1	B	79	ALA
1	B	80	LEU
1	B	114	ARG
1	A	130	ASP
1	A	186	SER
1	B	127	VAL
1	A	71	GLU
1	A	279	PRO
1	B	174	LEU
1	B	186	SER
1	A	151	PRO
1	B	278	PRO
1	A	34	ILE
1	A	263	VAL
1	B	151	PRO
1	A	128	ILE

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	221/238 (93%)	196 (89%)	25 (11%)	4 22
1	B	217/238 (91%)	199 (92%)	18 (8%)	9 35
All	All	438/476 (92%)	395 (90%)	43 (10%)	6 27

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	25	VAL
1	A	30	VAL
1	A	56	ASN
1	A	63	PHE
1	A	83	ARG
1	A	103	ILE
1	A	117	HIS
1	A	120	LEU
1	A	127	VAL
1	A	128	ILE
1	A	131	ILE
1	A	159	ASN
1	A	171	CYS
1	A	174	LEU
1	A	189	LEU
1	A	206	MET
1	A	215	SER
1	A	221	HIS
1	A	234	LEU
1	A	249	LEU
1	A	270	HIS
1	A	271	GLU
1	A	273	ASP
1	A	277	LEU
1	B	83	ARG
1	B	106	LEU
1	B	116	ASP
1	B	141	LEU
1	B	143	GLU
1	B	149	LEU
1	B	159	ASN
1	B	171	CYS
1	B	175	ASP
1	B	188	THR
1	B	194	VAL
1	B	206	MET
1	B	214	ASP
1	B	219	ILE
1	B	234	LEU
1	B	249	LEU
1	B	259	ARG
1	B	280	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	24	GLN
1	A	32	ASN
1	A	59	HIS
1	A	81	GLN
1	A	159	ASN
1	A	207	GLN
1	B	8	ASN
1	B	15	GLN
1	B	24	GLN
1	B	32	ASN
1	B	42	ASN
1	B	159	ASN
1	B	204	GLN
1	B	207	GLN
1	B	221	HIS
1	B	238	GLN
1	B	254	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	PXL	B	1005	-	12,12,12	3.39	8 (66%)	15,16,16	1.40	3 (20%)
2	PXL	A	1003	-	12,12,12	3.20	6 (50%)	15,16,16	1.65	4 (26%)

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	B	1005	-	-	2/4/4/4	0/1/1/1
2	PXL	A	1003	-	-	2/4/4/4	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1005	PXL	C3-C2	5.63	1.46	1.41
2	B	1005	PXL	C2-N1	5.24	1.43	1.33
2	A	1003	PXL	C2-N1	4.92	1.42	1.33
2	A	1003	PXL	C3-C2	4.63	1.45	1.41
2	A	1003	PXL	C4-C4A	4.38	1.56	1.46
2	B	1005	PXL	C4-C4A	4.32	1.56	1.46
2	A	1003	PXL	C4-C3	4.25	1.48	1.41
2	B	1005	PXL	C6-N1	3.92	1.42	1.34
2	A	1003	PXL	C6-N1	3.91	1.42	1.34
2	B	1005	PXL	C4-C3	3.64	1.47	1.41
2	A	1003	PXL	C6-C5	3.55	1.44	1.37
2	B	1005	PXL	C4-C5	3.47	1.46	1.42
2	B	1005	PXL	C6-C5	3.07	1.43	1.37
2	B	1005	PXL	C2A-C2	2.15	1.53	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1003	PXL	C4-C3-C2	-3.21	118.34	120.14
2	A	1003	PXL	O4A-C4A-C4	-2.87	117.99	124.80
2	A	1003	PXL	C5-C6-N1	-2.69	119.46	123.83
2	B	1005	PXL	C5-C6-N1	-2.48	119.81	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1005	PXL	O4A-C4A-C4	-2.35	119.22	124.80
2	A	1003	PXL	C3-C4-C4A	2.20	122.87	119.84
2	B	1005	PXL	C4-C3-C2	-2.20	118.91	120.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1005	PXL	C6-C5-C5A-OP4
2	A	1003	PXL	C6-C5-C5A-OP4
2	A	1003	PXL	C4-C5-C5A-OP4
2	B	1005	PXL	C4-C5-C5A-OP4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1005	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

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, 95^{th} 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	263/283 (92%)	-0.09	1 (0%) 89 81	8, 28, 67, 95	0
1	B	261/283 (92%)	-0.16	0 100 100	8, 30, 65, 95	0
All	All	524/566 (92%)	-0.13	1 (0%) 92 87	8, 29, 66, 95	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	ASN	3.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	PXL	A	1003	12/12	0.84	0.24	40,56,60,62	0
2	PXL	B	1005	12/12	0.89	0.13	27,57,63,75	0

6.5 Other polymers (i)

There are no such residues in this entry.