



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 04:18 AM GMT

PDB ID : 2C4M
Title : STARCH PHOSPHORYLASE: STRUCTURAL STUDIES EXPLAIN
OXYANION-DEPENDENT KINETIC STABILITY AND REGULATORY
CONTROL.
Authors : Purvis, A.; Nidetzky, B.; Watson, K.
Deposited on : 2005-10-20
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

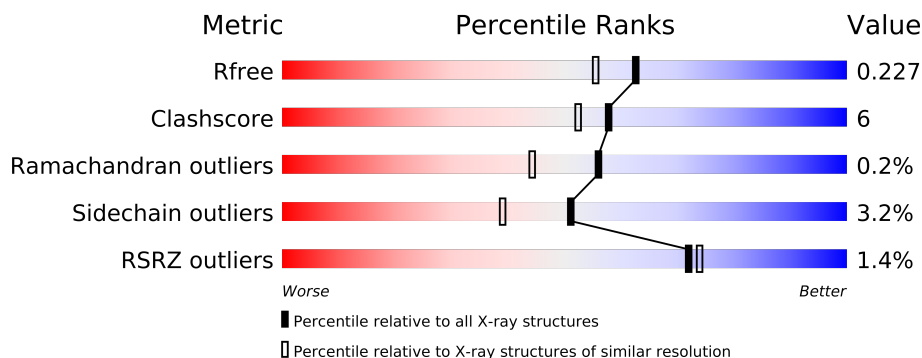
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	796	
1	B	796	
1	C	796	
1	D	796	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	PO4	B	1795	-	X
3	PO4	B	1796	-	X
3	PO4	C	1798	-	X
3	PO4	D	1794	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	FMT	A	1795	X	X
4	FMT	A	1796	X	X
4	FMT	A	1797	X	X
4	FMT	A	1798	X	-
4	FMT	A	1799	X	X
4	FMT	A	1800	X	X
4	FMT	A	1801	X	X
4	FMT	A	1802	X	X
4	FMT	A	1803	X	X
4	FMT	B	1799	X	-
4	FMT	B	1800	X	X
4	FMT	C	1799	X	X
4	FMT	C	1800	X	-
4	FMT	C	1801	X	-
4	FMT	C	1802	X	-
4	FMT	D	1795	X	X
4	FMT	D	1796	X	-
4	FMT	D	1797	X	-
4	FMT	D	1798	X	-
5	EDO	C	1803	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26654 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

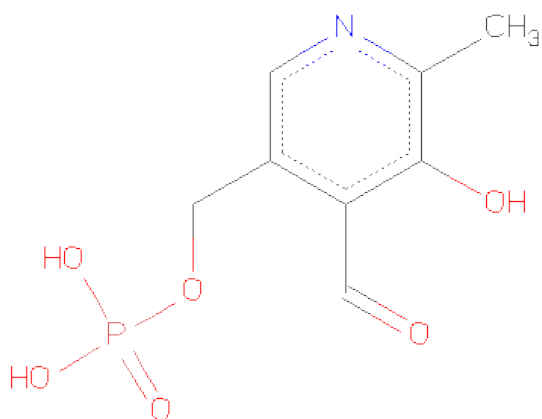
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	789	Total	C	N	O	S	63	0	1
			6328	4014	1088	1204	22			
1	B	789	Total	C	N	O	S	56	0	1
			6326	4014	1087	1203	22			
1	C	791	Total	C	N	O	S	57	0	1
			6344	4025	1091	1206	22			
1	D	789	Total	C	N	O	S	69	0	1
			6328	4014	1088	1204	22			

There are 4 discrepancies between the modelled and reference sequences:

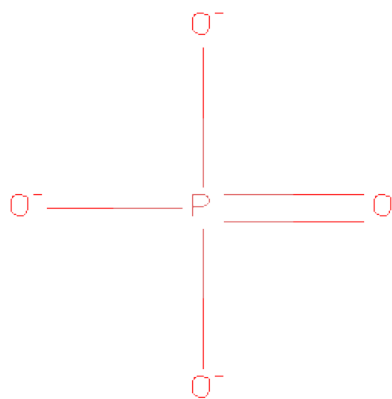
Chain	Residue	Modelled	Actual	Comment	Reference
A	224	ALA	SER	ENGINEERED MUTATION	UNP Q8KQ56
B	224	ALA	SER	ENGINEERED MUTATION	UNP Q8KQ56
C	224	ALA	SER	ENGINEERED MUTATION	UNP Q8KQ56
D	224	ALA	SER	ENGINEERED MUTATION	UNP Q8KQ56

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



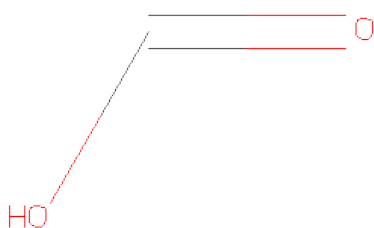
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



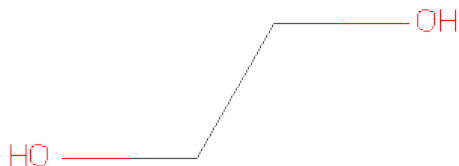
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

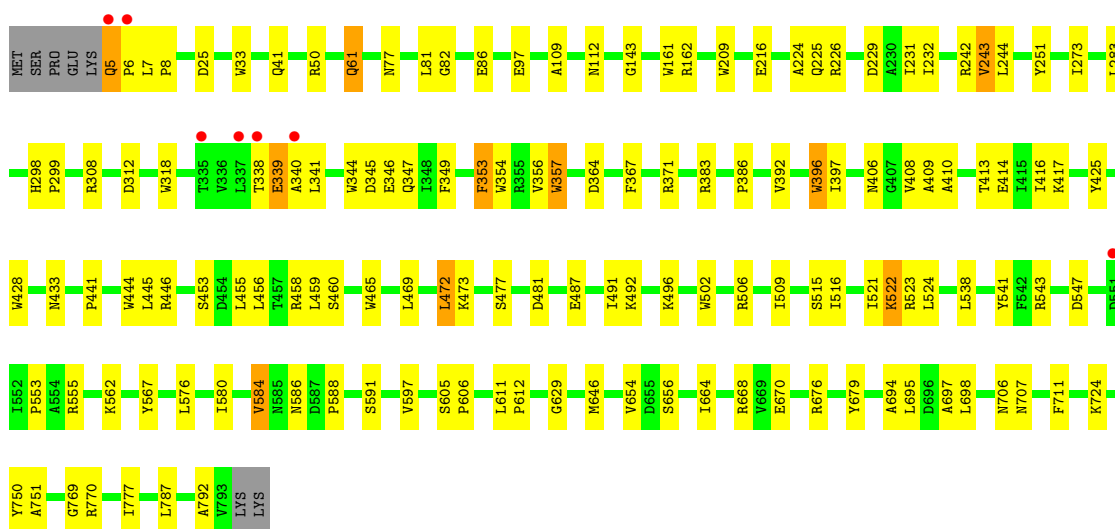
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	303	Total	O	0	0
			303	303		
6	B	306	Total	O	0	0
			306	306		
6	C	340	Total	O	0	0
			340	340		
6	D	205	Total	O	0	0
			205	205		

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 errors 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.

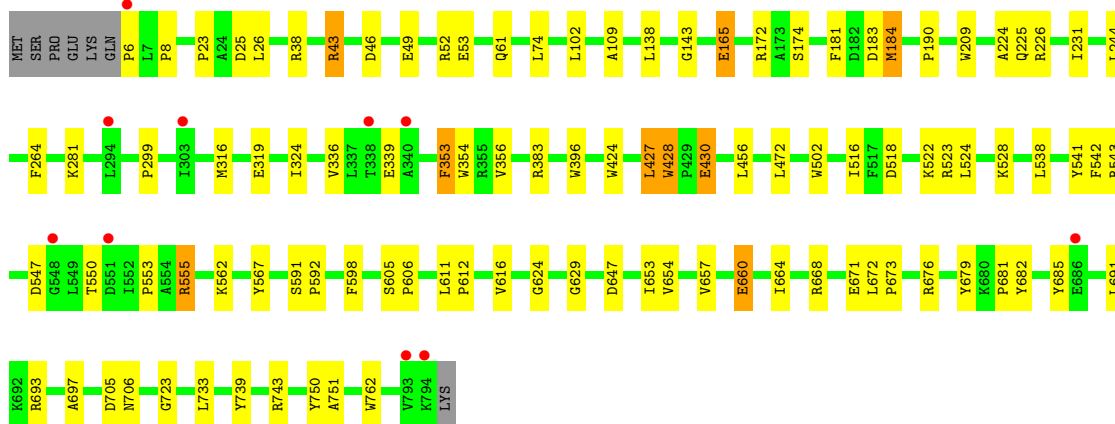
• Molecule 1: GLYCOGEN PHOSPHORYLASE

Chain A: 



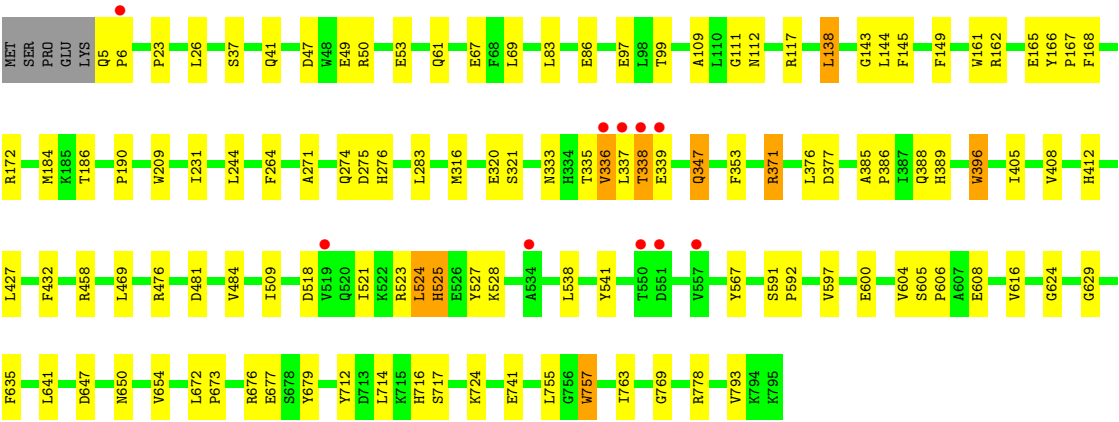
• Molecule 1: GLYCOGEN PHOSPHORYLASE

Chain B: 



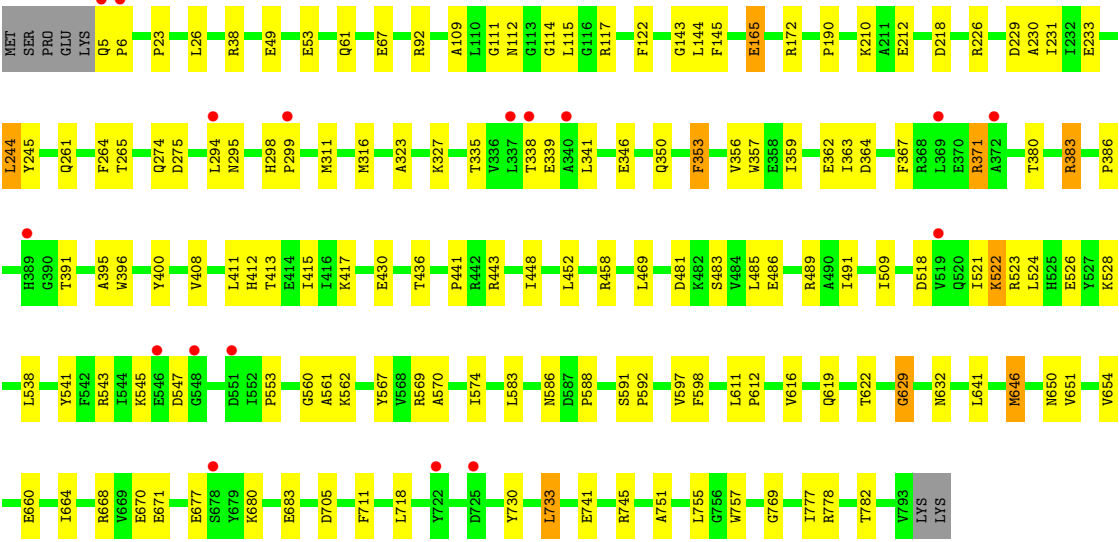
• Molecule 1: GLYCOGEN PHOSPHORYLASE

Chain C: 



• Molecule 1: GLYCOGEN PHOSPHORYLASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.27Å 187.62Å 129.31Å 90.00° 112.48° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.3 (30.00-1.90) 89.5 (29.93-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.232 0.210 , 0.227	Depositor DCC
R_{free} test set	15209 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.2	EDS
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 306185 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26654	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.29 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7096e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, FMT, EDO, PLP

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	0.71	12/6478 (0.2%)	0.89	0/8801
1	B	0.56	5/6476 (0.1%)	0.73	0/8798
1	C	0.48	1/6494 (0.0%)	0.72	0/8822
1	D	0.47	0/6478	0.70	0/8801
All	All	0.56	18/25926 (0.1%)	0.76	0/35222

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	428	TRP	NE1-CE2	8.84	1.49	1.37
1	B	502	TRP	NE1-CE2	8.79	1.49	1.37
1	A	354	TRP	NE1-CE2	8.77	1.49	1.37
1	C	757	TRP	NE1-CE2	8.75	1.49	1.37
1	A	502	TRP	NE1-CE2	8.70	1.48	1.37
1	A	344	TRP	NE1-CE2	8.68	1.48	1.37
1	B	424	TRP	NE1-CE2	8.62	1.48	1.37
1	A	465	TRP	NE1-CE2	8.59	1.48	1.37
1	A	357	TRP	NE1-CE2	8.57	1.48	1.37
1	A	444	TRP	NE1-CE2	8.55	1.48	1.37
1	A	318	TRP	NE1-CE2	8.55	1.48	1.37
1	A	209	TRP	NE1-CE2	8.41	1.48	1.37
1	B	428	TRP	NE1-CE2	8.36	1.48	1.37
1	B	762	TRP	NE1-CE2	7.93	1.47	1.37
1	B	354	TRP	NE1-CE2	7.72	1.47	1.37
1	A	33	TRP	NE1-CE2	7.54	1.47	1.37
1	A	396	TRP	NE1-CE2	7.28	1.47	1.37
1	A	792	ALA	C-N	-5.19	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6328	0	6116	80	0
1	B	6326	0	6118	54	0
1	C	6344	0	6138	77	0
1	D	6328	0	6116	103	0
2	A	15	0	7	0	0
2	B	15	0	7	0	0
2	C	15	0	7	0	0
2	D	15	0	7	2	0
3	A	5	0	0	0	0
3	B	20	0	0	1	0
3	C	15	0	0	0	0
3	D	5	0	0	0	0
4	A	27	0	18	0	0
4	B	6	0	4	0	0
4	C	12	0	8	0	0
4	D	12	0	8	0	0
5	B	8	0	12	2	0
5	C	4	0	6	0	0
6	A	303	0	0	7	0
6	B	306	0	0	3	0
6	C	340	0	0	3	0
6	D	205	0	0	1	0
All	All	26654	0	24572	310	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (310) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:6:PRO:HG2	1:C:86:GLU:HG2	1.56	0.85
1:B:6:PRO:HB2	1:B:8:PRO:HD3	1.60	0.83
1:D:244:LEU:HD12	1:D:245:TYR:HD1	1.45	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:112:ASN:HB2	1:C:244:LEU:HD21	1.64	0.79
1:D:380:THR:HA	1:D:383:ARG:HD3	1.64	0.78
1:A:5:GLN:O	1:A:8:PRO:HD3	1.85	0.76
1:A:523:ARG:HD3	1:A:562:LYS:O	1.86	0.75
1:B:172:ARG:HB2	1:B:190:PRO:HG2	1.69	0.74
1:C:408:VAL:H	1:C:412:HIS:HD2	1.32	0.74
1:A:86:GLU:N	1:A:86:GLU:OE1	2.20	0.74
1:D:244:LEU:HD12	1:D:245:TYR:CD1	2.24	0.72
1:D:650:ASN:O	1:D:654:VAL:HG22	1.90	0.71
1:D:38:ARG:NH2	1:D:165:GLU:HG2	2.06	0.71
1:D:23:PRO:HG2	1:D:26:LEU:HD12	1.73	0.71
1:D:646:MET:HE1	1:D:654:VAL:HG21	1.73	0.70
1:D:543:ARG:HA	1:D:547:ASP:HB2	1.73	0.70
1:D:646:MET:CE	1:D:654:VAL:HG21	2.22	0.69
1:D:509:ILE:HD13	1:D:597:VAL:HG22	1.74	0.69
1:D:458:ARG:HH11	1:D:458:ARG:HG2	1.57	0.69
1:A:509:ILE:HD13	1:A:597:VAL:HG22	1.75	0.69
1:B:523:ARG:HD3	1:B:562:LYS:O	1.93	0.68
1:C:149:PHE:CD2	1:C:600:GLU:HG3	2.30	0.67
1:A:109:ALA:HB1	1:A:143:GLY:HA3	1.76	0.67
1:C:605:SER:HB2	1:C:606:PRO:HD3	1.75	0.67
1:C:676:ARG:HD3	6:C:2309:HOH:O	1.94	0.67
1:C:6:PRO:HB2	1:C:83:LEU:CD2	2.25	0.67
1:C:376:LEU:HD12	1:C:377:ASP:H	1.57	0.67
1:C:109:ALA:HB1	1:C:143:GLY:HA3	1.77	0.66
1:D:718:LEU:HB3	1:D:733:LEU:HD21	1.77	0.66
1:D:112:ASN:HB2	1:D:244:LEU:HD11	1.77	0.66
1:A:605:SER:HB3	1:A:606:PRO:HD3	1.78	0.66
1:D:641:LEU:HD12	1:D:757:TRP:CZ2	2.30	0.65
1:A:251:TYR:OH	1:A:347:GLN:HG3	1.97	0.65
1:A:347:GLN:HB3	1:C:347:GLN:NE2	2.13	0.64
1:A:345:ASP:HB3	1:C:347:GLN:OE1	1.98	0.64
1:D:541:TYR:O	1:D:545:LYS:HB2	1.97	0.64
1:A:580:ILE:O	1:A:584:VAL:HG13	1.99	0.63
1:D:38:ARG:HH22	1:D:165:GLU:HG2	1.62	0.63
1:A:521:ILE:O	1:A:522:LYS:HG2	1.98	0.62
1:D:408:VAL:H	1:D:412:HIS:HD2	1.48	0.62
1:C:650:ASN:O	1:C:654:VAL:HG23	1.99	0.62
1:C:676:ARG:HA	1:C:679:TYR:HB2	1.82	0.62
1:D:523:ARG:HD3	1:D:562:LYS:O	2.00	0.61
1:C:149:PHE:CE2	1:C:600:GLU:HG3	2.35	0.61
1:A:668:ARG:HB3	1:A:670:GLU:OE2	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:538:LEU:O	1:B:541:TYR:HB3	2.00	0.61
1:D:718:LEU:HB3	1:D:733:LEU:CD2	2.31	0.60
1:D:413:THR:HG22	1:D:417:LYS:HE3	1.82	0.60
1:C:161:TRP:CZ2	1:C:162:ARG:HD2	2.37	0.60
1:D:109:ALA:HB1	1:D:143:GLY:HA3	1.85	0.59
1:C:23:PRO:HG2	1:C:26:LEU:HD12	1.84	0.59
1:D:430:GLU:N	1:D:430:GLU:OE1	2.31	0.59
1:B:109:ALA:HB1	1:B:143:GLY:HA3	1.83	0.59
1:A:367:PHE:O	1:A:371:ARG:HG2	2.01	0.59
1:D:522:LYS:HE2	2:D:1634:PLP:O2P	2.03	0.59
1:D:49:GLU:O	1:D:53:GLU:HG3	2.02	0.58
1:D:524:LEU:HD13	1:D:574:ILE:HG13	1.84	0.58
1:D:641:LEU:HD12	1:D:757:TRP:CH2	2.38	0.58
1:C:521:ILE:HD11	1:C:635:PHE:CZ	2.38	0.58
1:D:143:GLY:C	1:D:244:LEU:HD23	2.23	0.58
1:C:509:ILE:HD13	1:C:597:VAL:HG22	1.83	0.58
1:B:183:ASP:O	1:B:184:MET:HB2	2.03	0.58
1:C:190:PRO:HB3	1:C:209:TRP:CZ3	2.39	0.58
1:A:654:VAL:HG21	1:A:664:ILE:HG13	1.86	0.58
1:D:5:GLN:HB3	1:D:6:PRO:HD3	1.85	0.58
1:D:670:GLU:CD	1:D:670:GLU:H	2.07	0.58
1:B:660:GLU:CD	1:B:660:GLU:H	2.08	0.57
1:B:676:ARG:O	1:B:723:GLY:HA2	2.05	0.57
1:B:654:VAL:HG21	1:B:664:ILE:HG13	1.87	0.57
1:B:353:PHE:HB3	5:B:1801:EDO:H21	1.87	0.56
1:D:172:ARG:HB2	1:D:190:PRO:HG2	1.86	0.56
1:B:676:ARG:HA	1:B:679:TYR:HB2	1.88	0.56
1:B:316:MET:HE1	1:B:324:ILE:HD12	1.87	0.56
1:C:166:TYR:CE2	1:C:168:PHE:HB2	2.41	0.55
1:B:430:GLU:H	1:B:430:GLU:CD	2.09	0.55
1:C:481:ASP:OD2	1:C:484:VAL:HG23	2.06	0.55
1:B:427:LEU:HD22	1:B:428:TRP:CE2	2.42	0.55
1:C:525:HIS:HB2	1:C:528:LYS:HD3	1.89	0.55
1:A:273:ILE:HG23	1:A:283:LEU:HD21	1.89	0.55
1:B:654:VAL:HG21	1:B:664:ILE:CG1	2.37	0.54
1:A:242:ARG:HG2	1:A:243:VAL:CG1	2.37	0.54
1:A:646:MET:CE	1:A:664:ILE:HG21	2.38	0.54
1:B:555:ARG:HD2	6:B:2245:HOH:O	2.08	0.54
1:C:67:GLU:HB2	1:C:111:GLY:HA2	1.88	0.54
1:D:408:VAL:H	1:D:412:HIS:CD2	2.25	0.54
1:C:97:GLU:HG3	1:C:99:THR:HG22	1.89	0.54
1:C:49:GLU:O	1:C:53:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:538:LEU:O	1:A:541:TYR:HB3	2.08	0.54
1:D:359:ILE:O	1:D:363:ILE:HG13	2.08	0.54
1:B:224:ALA:O	1:B:225:GLN:HB2	2.07	0.54
1:B:591:SER:OG	1:B:592:PRO:HD3	2.07	0.53
1:B:336:VAL:HG22	6:B:2173:HOH:O	2.07	0.53
1:B:38:ARG:NH2	1:B:165:GLU:HG2	2.23	0.53
1:B:23:PRO:HG2	1:B:26:LEU:HD12	1.89	0.53
1:C:172:ARG:HB2	1:C:190:PRO:HG2	1.89	0.53
1:C:316:MET:CE	1:C:320:GLU:HG2	2.39	0.53
1:A:242:ARG:HG2	1:A:243:VAL:HG13	1.90	0.53
1:D:458:ARG:HG2	1:D:458:ARG:NH1	2.22	0.53
1:D:668:ARG:HB2	1:D:671:GLU:HG3	1.89	0.52
1:B:553:PRO:HB3	1:B:751:ALA:HB2	1.92	0.52
1:D:443:ARG:O	1:D:448:ILE:HG23	2.10	0.52
1:A:229:ASP:HA	1:A:232:ILE:HD12	1.90	0.52
1:B:672:LEU:N	1:B:673:PRO:HD2	2.24	0.52
1:C:476:ARG:HG3	1:C:763:ILE:HD13	1.91	0.52
1:D:591:SER:N	1:D:592:PRO:HD2	2.25	0.51
1:A:161:TRP:CZ2	1:A:162:ARG:HD2	2.46	0.51
1:D:114:GLY:HA2	2:D:1634:PLP:H5A2	1.93	0.50
1:B:522:LYS:HD2	1:B:528:LYS:HE3	1.92	0.50
1:D:521:ILE:O	1:D:521:ILE:HG13	2.11	0.50
1:D:654:VAL:HG11	1:D:664:ILE:HG13	1.94	0.50
1:A:492:LYS:O	1:A:496:LYS:HG3	2.12	0.50
1:A:646:MET:HE2	1:A:664:ILE:HG21	1.94	0.50
1:B:691:LEU:HD21	1:B:733:LEU:HD22	1.93	0.50
1:B:591:SER:N	1:B:592:PRO:HD2	2.27	0.50
1:D:380:THR:HA	1:D:383:ARG:HH11	1.77	0.50
1:C:37:SER:HB2	1:C:167:PRO:HG2	1.94	0.50
1:A:487:GLU:O	1:A:491:ILE:HG13	2.10	0.50
1:B:682:TYR:O	1:B:685:TYR:HB3	2.11	0.50
1:D:430:GLU:H	1:D:430:GLU:CD	2.15	0.50
1:D:122:PHE:CG	1:D:777:ILE:HD11	2.47	0.50
1:B:611:LEU:HB2	1:B:612:PRO:HD3	1.94	0.50
1:D:452:LEU:HA	1:D:491:ILE:HD13	1.95	0.49
1:A:417:LYS:HD3	1:A:425:TYR:CE1	2.48	0.49
1:D:641:LEU:HD12	1:D:757:TRP:CE2	2.48	0.49
1:C:316:MET:HE1	1:C:320:GLU:HG2	1.93	0.49
1:A:112:ASN:HB2	1:A:244:LEU:HD21	1.93	0.49
1:A:455:LEU:O	1:A:459:LEU:HG	2.13	0.49
1:A:706:ASN:O	1:A:707:ASN:HB2	2.12	0.49
1:C:408:VAL:H	1:C:412:HIS:CD2	2.23	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:604:VAL:O	1:C:608:GLU:HG3	2.13	0.49
1:A:553:PRO:HB3	1:A:751:ALA:HB2	1.94	0.49
1:D:611:LEU:HB2	1:D:612:PRO:HD3	1.93	0.49
1:A:413:THR:O	1:A:417:LYS:HG3	2.13	0.49
1:B:231:ILE:HD12	1:B:231:ILE:C	2.33	0.48
1:D:778:ARG:O	1:D:782:THR:HG23	2.13	0.48
1:A:41:GLN:HA	1:A:41:GLN:OE1	2.13	0.48
1:A:506:ARG:HD2	6:A:2220:HOH:O	2.13	0.48
1:D:298:HIS:HB2	1:D:299:PRO:HD3	1.96	0.48
1:D:339:GLU:C	1:D:341:LEU:H	2.16	0.48
1:B:624:GLY:H	1:B:647:ASP:CG	2.17	0.48
1:A:364:ASP:OD1	1:A:386:PRO:HD2	2.13	0.48
1:A:446:ARG:HA	1:A:453:SER:OG	2.13	0.48
1:C:714:LEU:O	1:C:717:SER:OG	2.31	0.48
1:A:695:LEU:O	1:A:698:LEU:HB2	2.14	0.47
1:D:651:VAL:O	1:D:654:VAL:HG23	2.15	0.47
1:A:515:SER:HB2	1:A:555:ARG:HA	1.96	0.47
1:D:411:LEU:O	1:D:415:ILE:HG13	2.14	0.47
1:A:82:GLY:HA2	6:A:2041:HOH:O	2.15	0.47
1:D:538:LEU:O	1:D:541:TYR:HB3	2.14	0.47
1:C:138:LEU:HD13	1:C:264:PHE:HB3	1.95	0.47
1:D:371:ARG:HD3	1:D:371:ARG:HA	1.61	0.47
1:C:469:LEU:HB3	1:C:769:GLY:HA2	1.97	0.47
1:A:670:GLU:CD	1:A:670:GLU:H	2.18	0.47
1:D:411:LEU:HG	6:D:2180:HOH:O	2.15	0.47
1:A:231:ILE:HD12	1:A:231:ILE:C	2.35	0.47
6:A:2173:HOH:O	1:C:347:GLN:NE2	2.48	0.47
1:D:518:ASP:HA	1:D:616:VAL:HB	1.97	0.47
1:D:629:GLY:O	1:D:632:ASN:HB2	2.15	0.47
1:C:672:LEU:N	1:C:673:PRO:HD2	2.29	0.47
1:B:174:SER:HB3	3:B:1795:PO4:O1	2.15	0.47
1:A:543:ARG:HA	1:A:547:ASP:HB2	1.97	0.47
1:C:376:LEU:HD12	1:C:377:ASP:N	2.29	0.46
1:A:386:PRO:HB3	1:A:397:ILE:HG13	1.97	0.46
1:C:371:ARG:HA	1:C:371:ARG:NE	2.30	0.46
1:B:516:ILE:HG12	1:B:750:TYR:CD1	2.50	0.46
1:C:6:PRO:HG3	1:C:86:GLU:OE2	2.15	0.46
1:D:646:MET:HE3	1:D:654:VAL:HG21	1.96	0.46
1:D:670:GLU:CD	1:D:670:GLU:N	2.68	0.46
1:A:413:THR:O	1:A:416:ILE:HG12	2.15	0.46
1:C:144:LEU:O	1:C:145:PHE:HB3	2.15	0.46
1:D:486:GLU:OE2	1:D:489:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:115:LEU:HD11	1:D:295:ASN:OD1	2.15	0.46
1:D:586:ASN:O	1:D:588:PRO:HD3	2.16	0.46
1:A:216:GLU:HG2	6:A:2116:HOH:O	2.16	0.46
1:B:671:GLU:C	1:B:673:PRO:HD2	2.36	0.46
1:B:190:PRO:HB3	1:B:209:TRP:CZ3	2.51	0.46
1:B:316:MET:HE3	1:B:316:MET:HB3	1.78	0.46
1:D:668:ARG:HB3	1:D:670:GLU:OE2	2.15	0.45
1:C:316:MET:HE2	1:C:321:SER:HA	1.98	0.45
1:B:138:LEU:CD2	1:B:264:PHE:HB3	2.46	0.45
1:C:338:THR:HG23	1:C:338:THR:O	2.15	0.45
1:A:481:ASP:OD1	1:A:481:ASP:C	2.55	0.45
1:A:112:ASN:HB2	1:A:244:LEU:CD2	2.46	0.45
1:C:524:LEU:C	1:C:524:LEU:CD1	2.84	0.45
1:A:694:ALA:O	1:A:697:ALA:HB3	2.16	0.45
1:A:347:GLN:NE2	1:C:347:GLN:HG2	2.31	0.45
1:D:553:PRO:HB3	1:D:751:ALA:HB2	1.99	0.45
1:D:469:LEU:HG	1:D:769:GLY:HA2	1.99	0.45
1:D:469:LEU:CG	1:D:769:GLY:HA2	2.47	0.45
1:C:337:LEU:HD23	1:C:337:LEU:HA	1.81	0.45
1:C:388:GLN:O	1:C:389:HIS:HB3	2.17	0.45
1:C:591:SER:N	1:C:592:PRO:HD2	2.32	0.45
1:C:538:LEU:O	1:C:541:TYR:HB3	2.17	0.45
1:B:74:LEU:HD23	1:B:102:LEU:HD23	1.98	0.45
1:C:641:LEU:HD12	1:C:757:TRP:CZ2	2.52	0.45
1:A:339:GLU:HB3	1:A:340:ALA:H	1.67	0.45
1:D:341:LEU:HD22	1:D:395:ALA:HB2	1.99	0.45
1:C:271:ALA:HA	1:C:274:GLN:HE21	1.82	0.45
1:D:619:GLN:HB2	1:D:650:ASN:HD21	1.83	0.44
1:A:473:LYS:HD2	6:A:2294:HOH:O	2.16	0.44
1:A:226:ARG:HH11	1:A:226:ARG:HD2	1.63	0.44
1:D:231:ILE:HD12	1:D:231:ILE:C	2.37	0.44
1:B:653:ILE:O	1:B:657:VAL:HG22	2.18	0.44
1:D:353:PHE:CD1	1:D:356:VAL:HB	2.52	0.44
1:C:5:GLN:HA	1:C:6:PRO:HD2	1.86	0.44
1:B:353:PHE:CB	5:B:1801:EDO:H21	2.47	0.44
1:B:542:PHE:HB3	1:B:693:ARG:CZ	2.47	0.44
1:D:346:GLU:HB2	1:D:357:TRP:CZ3	2.53	0.44
1:A:410:ALA:O	1:A:414:GLU:HG2	2.17	0.44
1:B:353:PHE:CD1	1:B:356:VAL:HB	2.53	0.44
1:B:49:GLU:O	1:B:53:GLU:HG3	2.17	0.44
1:D:632:ASN:OD1	1:D:632:ASN:N	2.50	0.44
1:D:346:GLU:O	1:D:350:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:226:ARG:NH1	1:D:229:ASP:OD2	2.50	0.44
1:C:41:GLN:HA	1:C:41:GLN:OE1	2.18	0.44
1:A:308:ARG:O	1:A:312:ASP:HB2	2.18	0.44
1:C:165:GLU:HG2	6:C:2103:HOH:O	2.17	0.43
1:C:396:TRP:CE3	1:C:396:TRP:HA	2.53	0.43
1:C:458:ARG:HG2	1:C:458:ARG:HH11	1.84	0.43
1:D:485:LEU:HD12	1:D:755:LEU:HD12	2.00	0.43
1:D:705:ASP:HB3	1:D:711:PHE:CD2	2.53	0.43
1:D:560:GLY:O	1:D:561:ALA:HB2	2.18	0.43
1:D:741:GLU:OE2	1:D:745:ARG:HD3	2.19	0.43
1:A:496:LYS:HD3	6:A:2217:HOH:O	2.18	0.43
1:A:61:GLN:HB3	1:A:787:LEU:HD11	2.01	0.43
1:D:524:LEU:HD22	1:D:570:ALA:HA	2.01	0.43
1:C:336:VAL:HG13	1:C:337:LEU:H	1.84	0.43
1:A:298:HIS:HB2	1:A:299:PRO:HD3	2.00	0.43
1:C:527:TYR:CE1	1:C:528:LYS:HD2	2.54	0.42
1:B:543:ARG:HA	1:B:547:ASP:HB2	2.00	0.42
1:C:184:MET:HG2	1:C:186:THR:HG23	2.01	0.42
1:C:231:ILE:HD12	1:C:231:ILE:C	2.40	0.42
1:C:712:TYR:CE1	1:C:716:HIS:HE1	2.37	0.42
1:C:53:GLU:OE1	1:C:793:VAL:HG21	2.19	0.42
1:A:224:ALA:O	1:A:225:GLN:HB2	2.20	0.42
1:A:371:ARG:HA	1:A:371:ARG:NE	2.34	0.42
1:B:49:GLU:HA	1:B:52:ARG:HH11	1.84	0.42
1:A:456:LEU:HD13	1:A:472:LEU:HD21	2.01	0.42
1:A:516:ILE:HG12	1:A:750:TYR:CE2	2.54	0.42
1:C:673:PRO:HG2	6:C:2291:HOH:O	2.19	0.42
1:D:362:GLU:OE1	1:D:362:GLU:HA	2.20	0.42
1:A:50:ARG:HH11	1:A:50:ARG:HD2	1.62	0.42
1:D:408:VAL:O	1:D:436:THR:HA	2.19	0.42
1:A:777:ILE:HD13	1:A:777:ILE:HA	1.86	0.42
1:C:641:LEU:HD12	1:C:757:TRP:CH2	2.54	0.42
1:D:210:LYS:HE2	1:D:212:GLU:OE2	2.20	0.42
1:A:586:ASN:O	1:A:588:PRO:HD3	2.19	0.42
1:D:367:PHE:HB2	1:D:400:TYR:CE2	2.55	0.42
1:B:605:SER:HB3	1:B:606:PRO:HD3	2.01	0.42
1:D:144:LEU:N	1:D:244:LEU:HD23	2.35	0.42
1:D:524:LEU:C	1:D:524:LEU:HD23	2.39	0.42
1:D:680:LYS:O	1:D:683:GLU:HB3	2.20	0.42
1:C:276:HIS:CD2	1:C:283:LEU:HD23	2.55	0.42
1:D:646:MET:HE2	1:D:664:ILE:HG21	2.02	0.42
1:D:526:GLU:OE2	1:D:569:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:117:ARG:HA	1:D:117:ARG:HD2	1.83	0.42
1:A:383:ARG:HD3	1:A:383:ARG:HH11	1.60	0.42
1:A:408:VAL:O	1:A:409:ALA:HB2	2.19	0.42
1:C:396:TRP:HE3	1:C:396:TRP:HA	1.85	0.41
1:A:469:LEU:HB3	1:A:769:GLY:HA2	2.02	0.41
1:A:676:ARG:HA	1:A:679:TYR:HB2	2.01	0.41
1:D:261:GLN:O	1:D:265:THR:HG23	2.20	0.41
1:B:181:PHE:HB2	1:B:184:MET:HB3	2.02	0.41
1:D:441:PRO:HB3	1:D:469:LEU:HD22	2.01	0.41
1:D:323:ALA:O	1:D:327:LYS:HG3	2.20	0.41
1:A:538:LEU:HD21	1:A:697:ALA:HB3	2.02	0.41
1:C:117:ARG:HD2	1:C:117:ARG:HA	1.92	0.41
1:A:611:LEU:HB2	1:A:612:PRO:HD3	2.02	0.41
1:D:338:THR:HG22	1:D:341:LEU:HD12	2.02	0.41
1:D:660:GLU:CD	1:D:660:GLU:H	2.24	0.41
1:D:67:GLU:HB2	1:D:111:GLY:HA2	2.03	0.41
1:C:518:ASP:HA	1:C:616:VAL:HB	2.02	0.41
1:C:336:VAL:H	1:C:336:VAL:HG12	1.52	0.41
1:A:576:LEU:HA	1:A:711:PHE:CZ	2.56	0.41
1:A:458:ARG:NH1	1:A:458:ARG:HG2	2.35	0.41
1:D:364:ASP:HA	1:D:386:PRO:HG2	2.02	0.41
1:A:441:PRO:O	1:A:445:LEU:HB3	2.20	0.41
1:C:624:GLY:H	1:C:647:ASP:CG	2.24	0.41
1:C:385:ALA:HA	1:C:386:PRO:HD3	2.00	0.41
1:D:622:THR:OG1	1:D:730:TYR:HB3	2.21	0.41
1:C:335:THR:O	1:C:412:HIS:HE1	2.04	0.41
1:B:538:LEU:HD21	1:B:697:ALA:HB3	2.03	0.41
1:B:518:ASP:HA	1:B:616:VAL:HB	2.02	0.41
1:A:460:SER:HB2	6:A:2212:HOH:O	2.21	0.41
1:A:656:SER:HG	1:A:770:ARG:HH11	1.68	0.41
1:B:739:TYR:OH	1:B:743:ARG:NH1	2.54	0.41
1:B:226:ARG:HH11	1:B:226:ARG:HD2	1.61	0.41
1:D:481:ASP:OD2	1:D:483:SER:HB3	2.21	0.41
1:B:6:PRO:HG2	1:B:43:ARG:HH21	1.86	0.40
1:D:522:LYS:HD3	1:D:528:LYS:HE3	2.03	0.40
1:A:77:ASN:O	1:A:81:LEU:HG	2.21	0.40
1:A:406:ASN:HA	1:A:433:ASN:O	2.22	0.40
1:C:405:ILE:O	1:C:432:PHE:HA	2.21	0.40
1:D:144:LEU:O	1:D:145:PHE:HB3	2.21	0.40
1:B:676:ARG:HD2	1:B:676:ARG:HH11	1.67	0.40
1:D:346:GLU:HB2	1:D:357:TRP:CH2	2.56	0.40
1:B:456:LEU:HD22	1:B:472:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:69:LEU:HA	1:C:69:LEU:HD12	1.93	0.40
1:A:353:PHE:CD1	1:A:356:VAL:HB	2.56	0.40
1:A:668:ARG:HD3	1:A:668:ARG:HH11	1.60	0.40
1:C:47:ASP:HA	1:C:50:ARG:NH1	2.36	0.40
1:B:681:PRO:HG3	6:B:2280:HOH:O	2.21	0.40
1:C:408:VAL:HG22	1:C:412:HIS:CD2	2.57	0.40
1:D:646:MET:HE1	1:D:654:VAL:CG2	2.49	0.40
1:D:543:ARG:CA	1:D:547:ASP:HB2	2.46	0.40
1:A:347:GLN:HB3	1:C:347:GLN:CD	2.42	0.40
1:D:218:ASP:HB3	1:D:230:ALA:HA	2.03	0.40
1:D:311:MET:HG2	1:D:316:MET:O	2.21	0.40
1:A:346:GLU:HB2	1:A:357:TRP:CZ3	2.56	0.40
1:A:349:PHE:HE2	1:A:392:VAL:HG11	1.87	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	787/796 (99%)	752 (96%)	32 (4%)	3 (0%)	43	29
1	B	787/796 (99%)	760 (97%)	25 (3%)	2 (0%)	50	37
1	C	789/796 (99%)	762 (97%)	26 (3%)	1 (0%)	59	48
1	D	787/796 (99%)	761 (97%)	25 (3%)	1 (0%)	59	48
All	All	3150/3184 (99%)	3035 (96%)	108 (3%)	7 (0%)	56	44

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	GLU
1	A	338	THR
1	B	184	MET
1	B	629	GLY
1	D	629	GLY

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Mol	Chain	Res	Type
1	A	629	GLY
1	C	629	GLY

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	660/668 (99%)	642 (97%)	18 (3%)	57	47
1	B	660/668 (99%)	636 (96%)	24 (4%)	47	33
1	C	662/668 (99%)	641 (97%)	21 (3%)	51	39
1	D	660/668 (99%)	638 (97%)	22 (3%)	50	37
All	All	2642/2672 (99%)	2557 (97%)	85 (3%)	51	39

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	6	PRO
1	A	7	LEU
1	A	25	ASP
1	A	61	GLN
1	A	97	GLU
1	A	243	VAL
1	A	341	LEU
1	A	353	PHE
1	A	396	TRP
1	A	472	LEU
1	A	477	SER
1	A	522	LYS
1	A	524	LEU
1	A	567	TYR
1	A	584	VAL
1	A	591	SER
1	A	724	LYS
1	B	25	ASP
1	B	43	ARG

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Mol	Chain	Res	Type
1	B	46	ASP
1	B	61	GLN
1	B	165	GLU
1	B	244	LEU
1	B	281	LYS
1	B	299	PRO
1	B	319	GLU
1	B	339	GLU
1	B	353	PHE
1	B	383	ARG
1	B	396	TRP
1	B	427	LEU
1	B	430	GLU
1	B	524	LEU
1	B	550	THR
1	B	555	ARG
1	B	567	TYR
1	B	598	PHE
1	B	660	GLU
1	B	668	ARG
1	B	705	ASP
1	B	706	ASN
1	C	61	GLN
1	C	138	LEU
1	C	275	ASP
1	C	333	ASN
1	C	336	VAL
1	C	338	THR
1	C	339	GLU
1	C	347	GLN
1	C	353	PHE
1	C	371	ARG
1	C	396	TRP
1	C	427	LEU
1	C	523	ARG
1	C	524	LEU
1	C	525	HIS
1	C	567	TYR
1	C	677	GLU
1	C	724	LYS
1	C	741	GLU
1	C	755	LEU

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Mol	Chain	Res	Type
1	C	778	ARG
1	D	61	GLN
1	D	92	ARG
1	D	165	GLU
1	D	233	GLU
1	D	244	LEU
1	D	264	PHE
1	D	274	GLN
1	D	275	ASP
1	D	294	LEU
1	D	335	THR
1	D	353	PHE
1	D	371	ARG
1	D	383	ARG
1	D	391	THR
1	D	396	TRP
1	D	522	LYS
1	D	567	TYR
1	D	583	LEU
1	D	598	PHE
1	D	646	MET
1	D	677	GLU
1	D	733	LEU

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

Mol	Chain	Res	Type
1	A	61	GLN
1	A	279	HIS
1	A	280	HIS
1	A	347	GLN
1	A	716	HIS
1	B	201	HIS
1	B	280	HIS
1	B	298	HIS
1	B	333	ASN
1	B	347	GLN
1	B	437	ASN
1	C	61	GLN
1	C	223	ASN
1	C	274	GLN
1	C	333	ASN

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Mol	Chain	Res	Type
1	C	412	HIS
1	C	707	ASN
1	C	716	HIS
1	D	106	ASN
1	D	274	GLN
1	D	412	HIS
1	D	706	ASN
1	D	720	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

35 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	PLP	A	1634	1	14,15,16	2.15	7 (50%)	20,22,23	1.54	4 (20%)
3	PO4	A	1794	-	4,4,4	0.65	0	6,6,6	0.33	0
4	FMT	A	1795	-	2,2,2	5.54	2 (100%)	1,1,1	1.17	0
4	FMT	A	1796	-	2,2,2	5.54	2 (100%)	1,1,1	1.17	0
4	FMT	A	1797	-	2,2,2	5.54	2 (100%)	1,1,1	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMT	A	1798	-	2,2,2	5.53	2 (100%)	1,1,1	1.17	0
4	FMT	A	1799	-	2,2,2	5.54	2 (100%)	1,1,1	1.17	0
4	FMT	A	1800	-	2,2,2	5.53	2 (100%)	1,1,1	1.17	0
4	FMT	A	1801	-	2,2,2	5.54	2 (100%)	1,1,1	1.17	0
4	FMT	A	1802	-	2,2,2	5.53	2 (100%)	1,1,1	1.17	0
4	FMT	A	1803	-	2,2,2	5.53	2 (100%)	1,1,1	1.17	0
2	PLP	B	1634	1	14,15,16	1.85	6 (42%)	20,22,23	1.70	6 (30%)
3	PO4	B	1795	-	4,4,4	0.78	0	6,6,6	0.33	0
3	PO4	B	1796	-	4,4,4	0.82	0	6,6,6	0.33	0
3	PO4	B	1797	-	4,4,4	0.44	0	6,6,6	0.33	0
3	PO4	B	1798	-	4,4,4	0.65	0	6,6,6	0.33	0
4	FMT	B	1799	-	2,2,2	5.53	2 (100%)	1,1,1	1.17	0
4	FMT	B	1800	-	2,2,2	5.53	2 (100%)	1,1,1	1.17	0
5	EDO	B	1801	-	3,3,3	0.54	0	2,2,2	0.37	0
5	EDO	B	1802	-	3,3,3	0.54	0	2,2,2	0.37	0
2	PLP	C	1634	1	14,15,16	2.06	7 (50%)	20,22,23	1.82	6 (30%)
3	PO4	C	1796	-	4,4,4	0.85	0	6,6,6	0.33	0
3	PO4	C	1797	-	4,4,4	0.59	0	6,6,6	0.33	0
3	PO4	C	1798	-	4,4,4	0.65	0	6,6,6	0.33	0
4	FMT	C	1799	-	2,2,2	5.54	2 (100%)	1,1,1	1.17	0
4	FMT	C	1800	-	2,2,2	5.54	2 (100%)	1,1,1	1.17	0
4	FMT	C	1801	-	2,2,2	5.53	2 (100%)	1,1,1	1.17	0
4	FMT	C	1802	-	2,2,2	5.55	2 (100%)	1,1,1	1.17	0
5	EDO	C	1803	-	3,3,3	0.55	0	2,2,2	0.37	0
2	PLP	D	1634	1	14,15,16	2.11	6 (42%)	20,22,23	2.13	7 (35%)
3	PO4	D	1794	-	4,4,4	0.83	0	6,6,6	0.33	0
4	FMT	D	1795	-	2,2,2	5.54	2 (100%)	1,1,1	1.17	0
4	FMT	D	1796	-	2,2,2	5.53	2 (100%)	1,1,1	1.17	0
4	FMT	D	1797	-	2,2,2	5.53	2 (100%)	1,1,1	1.17	0
4	FMT	D	1798	-	2,2,2	5.54	2 (100%)	1,1,1	1.17	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	PLP	A	1634	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	1794	-	-	0/0/0/0	0/0/0/0
4	FMT	A	1795	-	-	0/0/0/0	0/0/0/0
4	FMT	A	1796	-	-	0/0/0/0	0/0/0/0
4	FMT	A	1797	-	-	0/0/0/0	0/0/0/0
4	FMT	A	1798	-	-	0/0/0/0	0/0/0/0
4	FMT	A	1799	-	-	0/0/0/0	0/0/0/0
4	FMT	A	1800	-	-	0/0/0/0	0/0/0/0
4	FMT	A	1801	-	-	0/0/0/0	0/0/0/0
4	FMT	A	1802	-	-	0/0/0/0	0/0/0/0
4	FMT	A	1803	-	-	0/0/0/0	0/0/0/0
2	PLP	B	1634	1	-	0/6/6/8	0/1/1/1
3	PO4	B	1795	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1796	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1797	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1798	-	-	0/0/0/0	0/0/0/0
4	FMT	B	1799	-	-	0/0/0/0	0/0/0/0
4	FMT	B	1800	-	-	0/0/0/0	0/0/0/0
5	EDO	B	1801	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1802	-	-	0/1/1/1	0/0/0/0
2	PLP	C	1634	1	-	0/6/6/8	0/1/1/1
3	PO4	C	1796	-	-	0/0/0/0	0/0/0/0
3	PO4	C	1797	-	-	0/0/0/0	0/0/0/0
3	PO4	C	1798	-	-	0/0/0/0	0/0/0/0
4	FMT	C	1799	-	-	0/0/0/0	0/0/0/0
4	FMT	C	1800	-	-	0/0/0/0	0/0/0/0
4	FMT	C	1801	-	-	0/0/0/0	0/0/0/0
4	FMT	C	1802	-	-	0/0/0/0	0/0/0/0
5	EDO	C	1803	-	-	0/1/1/1	0/0/0/0
2	PLP	D	1634	1	-	0/6/6/8	0/1/1/1
3	PO4	D	1794	-	-	0/0/0/0	0/0/0/0
4	FMT	D	1795	-	-	0/0/0/0	0/0/0/0
4	FMT	D	1796	-	-	0/0/0/0	0/0/0/0
4	FMT	D	1797	-	-	0/0/0/0	0/0/0/0
4	FMT	D	1798	-	-	0/0/0/0	0/0/0/0

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1802	FMT	O1-C	6.12	1.52	1.21
4	A	1797	FMT	O1-C	6.10	1.52	1.21
4	A	1795	FMT	O1-C	6.10	1.52	1.21
4	A	1801	FMT	O1-C	6.10	1.52	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1795	FMT	O1-C	6.09	1.52	1.21
4	A	1799	FMT	O1-C	6.09	1.52	1.21
4	C	1799	FMT	O1-C	6.09	1.52	1.21
4	D	1798	FMT	O1-C	6.09	1.52	1.21
4	A	1803	FMT	O1-C	6.09	1.52	1.21
4	C	1800	FMT	O1-C	6.09	1.52	1.21
4	A	1796	FMT	O1-C	6.09	1.52	1.21
4	D	1796	FMT	O1-C	6.09	1.52	1.21
4	A	1798	FMT	O1-C	6.09	1.52	1.21
4	D	1797	FMT	O1-C	6.09	1.52	1.21
4	A	1800	FMT	O1-C	6.09	1.52	1.21
4	B	1799	FMT	O1-C	6.09	1.52	1.21
4	B	1800	FMT	O1-C	6.09	1.52	1.21
4	A	1802	FMT	O1-C	6.08	1.52	1.21
4	C	1801	FMT	O1-C	6.08	1.52	1.21
4	D	1798	FMT	O2-C	4.93	1.55	1.28
4	C	1800	FMT	O2-C	4.92	1.55	1.28
4	C	1801	FMT	O2-C	4.92	1.55	1.28
4	A	1796	FMT	O2-C	4.92	1.55	1.28
4	A	1800	FMT	O2-C	4.92	1.55	1.28
4	B	1800	FMT	O2-C	4.92	1.55	1.28
4	A	1797	FMT	O2-C	4.92	1.55	1.28
4	B	1799	FMT	O2-C	4.92	1.55	1.28
4	D	1797	FMT	O2-C	4.92	1.55	1.28
4	A	1801	FMT	O2-C	4.92	1.55	1.28
4	C	1799	FMT	O2-C	4.92	1.55	1.28
4	A	1795	FMT	O2-C	4.92	1.55	1.28
4	D	1796	FMT	O2-C	4.91	1.55	1.28
4	A	1799	FMT	O2-C	4.91	1.55	1.28
4	C	1802	FMT	O2-C	4.92	1.55	1.28
4	D	1795	FMT	O2-C	4.91	1.55	1.28
4	A	1803	FMT	O2-C	4.91	1.55	1.28
4	A	1798	FMT	O2-C	4.91	1.55	1.28
4	A	1802	FMT	O2-C	4.90	1.55	1.28
2	C	1634	PLP	C3-C2	4.40	1.43	1.40
2	A	1634	PLP	C3-C2	4.32	1.43	1.40
2	D	1634	PLP	C3-C2	3.87	1.43	1.40
2	D	1634	PLP	P-O4P	-3.14	1.49	1.60
2	A	1634	PLP	P-O4P	-3.12	1.49	1.60
2	B	1634	PLP	C2-N1	3.05	1.39	1.33
2	D	1634	PLP	C6-C5	2.99	1.44	1.37
2	A	1634	PLP	C6-C5	2.96	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1634	PLP	P-O4P	-2.92	1.50	1.60
2	D	1634	PLP	P-O1P	2.86	1.60	1.51
2	B	1634	PLP	P-O1P	2.83	1.60	1.51
2	C	1634	PLP	C6-C5	2.76	1.44	1.37
2	C	1634	PLP	P-O4P	-2.66	1.50	1.60
2	B	1634	PLP	C6-C5	2.48	1.43	1.37
2	D	1634	PLP	C6-N1	2.47	1.40	1.34
2	C	1634	PLP	C2-N1	2.42	1.38	1.33
2	A	1634	PLP	P-O1P	2.39	1.59	1.51
2	C	1634	PLP	P-O2P	2.31	1.63	1.54
2	A	1634	PLP	C2-N1	2.30	1.38	1.33
2	A	1634	PLP	C2A-C2	-2.28	1.45	1.50
2	D	1634	PLP	C2-N1	2.26	1.38	1.33
2	A	1634	PLP	C6-N1	2.21	1.39	1.34
2	C	1634	PLP	P-O1P	2.21	1.58	1.51
2	B	1634	PLP	C6-N1	2.15	1.39	1.34
2	B	1634	PLP	C3-C2	2.12	1.42	1.40
2	C	1634	PLP	C6-N1	2.07	1.39	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1634	PLP	O3P-P-O4P	5.13	120.81	106.65
2	C	1634	PLP	C5A-C5-C6	-3.67	112.34	119.28
2	B	1634	PLP	C5-C6-N1	-3.66	117.26	123.86
2	D	1634	PLP	P-O4P-C5A	3.56	134.06	121.22
2	A	1634	PLP	O2P-P-O4P	3.40	116.03	106.65
2	C	1634	PLP	C5A-C5-C4	3.19	128.84	121.41
2	C	1634	PLP	C5-C6-N1	-3.19	118.11	123.86
2	B	1634	PLP	C5A-C5-C6	-3.16	113.29	119.28
2	C	1634	PLP	O3P-P-O4P	3.14	115.31	106.65
2	D	1634	PLP	O2P-P-O4P	-3.08	98.14	106.65
2	D	1634	PLP	C5-C6-N1	-3.06	118.35	123.86
2	A	1634	PLP	C5-C6-N1	-3.03	118.40	123.86
2	D	1634	PLP	O4P-C5A-C5	-2.93	103.31	109.26
2	A	1634	PLP	C5A-C5-C6	-2.89	113.80	119.28
2	B	1634	PLP	C5A-C5-C4	2.79	127.89	121.41
2	A	1634	PLP	C5A-C5-C4	2.66	127.59	121.41
2	D	1634	PLP	C5A-C5-C4	2.60	127.47	121.41
2	D	1634	PLP	C5A-C5-C6	-2.60	114.37	119.28
2	B	1634	PLP	O2P-P-O4P	2.57	113.75	106.65
2	B	1634	PLP	C3-C2-N1	-2.50	117.23	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1634	PLP	C6-N1-C2	2.37	124.36	119.28
2	C	1634	PLP	C3-C2-N1	-2.23	117.60	120.66
2	C	1634	PLP	C6-N1-C2	2.14	123.87	119.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	789/796 (99%)	-0.11	7 (0%) 81 83	15, 29, 46, 75	16 (2%)
1	B	789/796 (99%)	-0.11	10 (1%) 74 75	15, 28, 48, 69	14 (1%)
1	C	791/796 (99%)	-0.15	10 (1%) 74 75	15, 27, 45, 74	15 (1%)
1	D	789/796 (99%)	0.03	17 (2%) 59 60	20, 34, 52, 71	16 (2%)
All	All	3158/3184 (99%)	-0.09	44 (1%) 72 74	15, 29, 48, 75	61 (1%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	THR	5.1
1	D	340	ALA	4.3
1	B	793	VAL	4.2
1	C	336	VAL	4.0
1	A	5	GLN	3.7
1	A	337	LEU	3.5
1	C	339	GLU	3.5
1	B	6	PRO	3.4
1	A	551	ASP	3.2
1	D	294	LEU	3.1
1	A	340	ALA	3.1
1	C	337	LEU	3.1
1	D	722	TYR	3.1
1	C	557	VAL	2.7
1	D	372	ALA	2.7
1	C	534	ALA	2.7
1	C	550	THR	2.6
1	D	725	ASP	2.6
1	C	6	PRO	2.5
1	A	335	THR	2.5
1	B	338	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	340	ALA	2.5
1	A	338	THR	2.5
1	B	794	LYS	2.4
1	D	299	PRO	2.4
1	B	548	GLY	2.4
1	C	519	VAL	2.4
1	B	551	ASP	2.3
1	D	6	PRO	2.3
1	B	686	GLU	2.2
1	A	6	PRO	2.2
1	D	369	LEU	2.2
1	D	5	GLN	2.2
1	D	519	VAL	2.2
1	D	551	ASP	2.2
1	D	337	LEU	2.2
1	D	546	GLU	2.1
1	C	551	ASP	2.1
1	D	389	HIS	2.1
1	B	303	ILE	2.1
1	D	338	THR	2.1
1	D	678	SER	2.0
1	B	294	LEU	2.0
1	D	548	GLY	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	FMT	A	1802	3/3	0.15	8.51	42,42,42,42	0
4	FMT	D	1795	3/3	0.17	6.44	32,32,33,36	0
4	FMT	A	1796	3/3	0.16	4.99	39,39,39,41	0
5	EDO	C	1803	4/4	0.14	3.65	26,27,30,33	0
3	PO4	B	1796	5/5	0.13	3.56	38,38,40,41	3
4	FMT	B	1800	3/3	0.14	3.43	32,32,36,37	0
4	FMT	C	1799	3/3	0.12	2.86	36,36,38,38	0
4	FMT	A	1801	3/3	0.14	2.78	35,35,36,38	0
4	FMT	A	1803	3/3	0.14	2.62	39,39,39,40	0
3	PO4	D	1794	5/5	0.12	2.56	37,39,41,41	3
3	PO4	B	1795	5/5	0.13	2.49	37,38,39,39	4
4	FMT	A	1797	3/3	0.13	2.39	38,38,38,39	0
3	PO4	C	1798	5/5	0.17	2.38	56,57,58,58	2
4	FMT	A	1795	3/3	0.17	2.30	41,41,43,43	0
4	FMT	A	1799	3/3	0.13	2.04	39,39,40,41	0
4	FMT	A	1800	3/3	0.17	2.01	38,38,40,40	0
3	PO4	C	1797	5/5	0.09	1.70	36,38,40,41	0
4	FMT	C	1802	3/3	0.14	1.63	36,36,38,39	0
3	PO4	C	1796	5/5	0.11	1.56	36,39,41,42	4
4	FMT	D	1797	3/3	0.12	1.41	36,36,37,38	0
4	FMT	C	1801	3/3	0.12	1.33	35,35,37,38	0
3	PO4	B	1798	5/5	0.14	1.30	55,56,57,57	3
4	FMT	D	1796	3/3	0.11	0.98	35,35,37,37	0
3	PO4	A	1794	5/5	0.14	0.85	56,57,57,57	3
5	EDO	B	1802	4/4	0.11	0.71	27,27,31,34	0
4	FMT	B	1799	3/3	0.10	0.49	37,37,40,40	0
4	FMT	A	1798	3/3	0.09	0.41	23,23,26,28	0
2	PLP	B	1634	15/16	0.08	0.08	19,21,42,44	0
2	PLP	D	1634	15/16	0.09	0.08	28,30,48,48	0
5	EDO	B	1801	4/4	0.09	-0.07	41,42,43,43	0
2	PLP	C	1634	15/16	0.09	-0.10	23,24,42,43	0
4	FMT	D	1798	3/3	0.09	-0.19	40,40,40,40	0
3	PO4	B	1797	5/5	0.09	-0.34	37,39,41,41	0
2	PLP	A	1634	15/16	0.08	-0.54	21,24,42,43	0
4	FMT	C	1800	3/3	0.07	-0.66	33,33,35,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.