Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 02:56 pm 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 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

PERCENTILES INFOmissingINFO

1 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 26654 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.

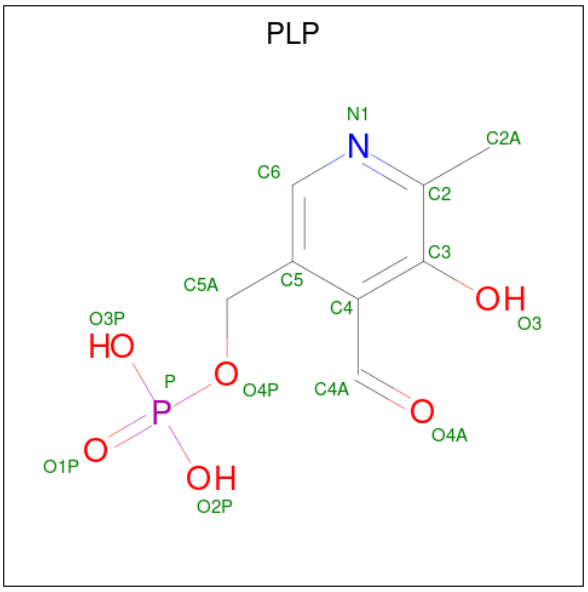
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE.

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:

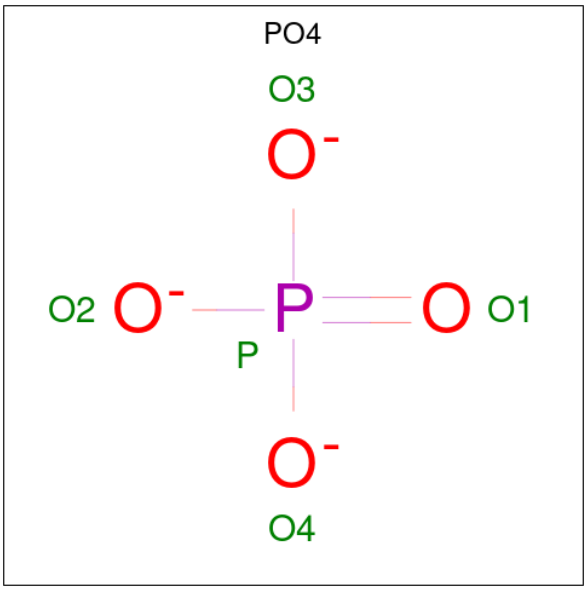
Chain	Residue	Modelled	Actual	Comment	Reference
A	224	ALA	SER	engineered mutation	UNP Q8KQ56
B	224	ALA	SER	engineered mutation	UNP Q8KQ56
C	224	ALA	SER	engineered mutation	UNP Q8KQ56
D	224	ALA	SER	engineered mutation	UNP Q8KQ56

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



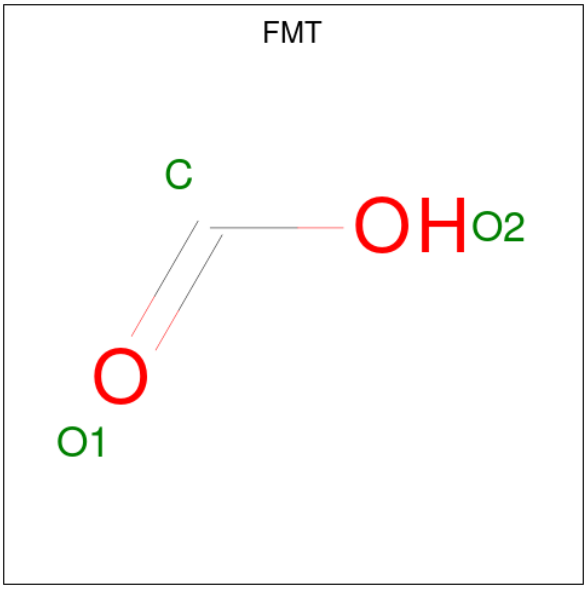
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 15 8 1 5 1	0	0
2	B	1	Total C N O P 15 8 1 5 1	0	0
2	C	1	Total C N O P 15 8 1 5 1	0	0
2	D	1	Total C N O P 15 8 1 5 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



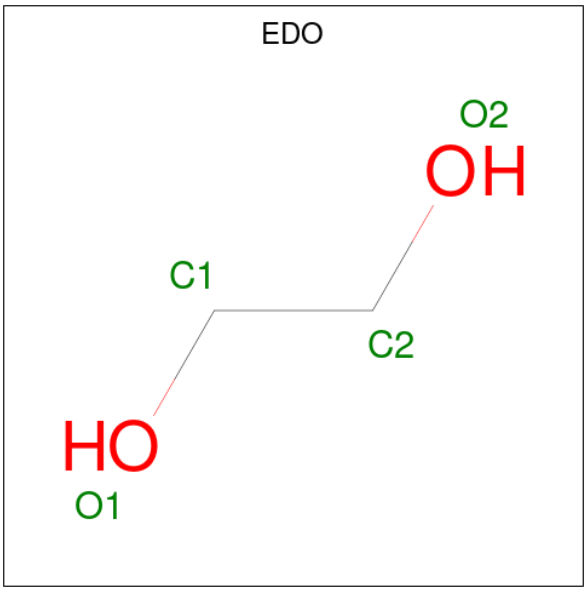
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0

Continued on next page...

Continued from previous page...

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	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		
4	D	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

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

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.35 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.232 0.203 , 0.220	Depositor DCC
R_{free} test set	15209 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	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.*

[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.

3 Model quality (i)

3.1 Standard geometry (i)

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

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.

3.2 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	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

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 6.

All (310) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:LEU:HD12	1:D:245:TYR:HD1	1.45	0.79
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:A:86:GLU:OE1	1:A:86:GLU:N	2.20	0.74
1:C:408:VAL:H	1:C:412:HIS:HD2	1.32	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:458:ARG:HG2	1:D:458:ARG:HH11	1.57	0.69
1:D:509:ILE:HD13	1:D:597:VAL:HG22	1.74	0.69
1:D:646:MET:CE	1:D:654:VAL:HG21	2.22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ARG:HB3	1:A:670:GLU:OE2	2.00	0.61
1:C:149:PHE:CE2	1:C:600:GLU:HG3	2.35	0.61
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:C:161:TRP:CZ2	1:C:162:ARG:HD2	2.37	0.60
1:D:413:THR:HG22	1:D:417:LYS:HE3	1.82	0.60
1:C:23:PRO:HG2	1:C:26:LEU:HD12	1.84	0.59
1:D:109:ALA:HB1	1:D:143:GLY:HA3	1.85	0.59
1:D:430:GLU:OE1	1:D:430:GLU:N	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:CD	1:B:430:GLU:H	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:GLU:HG3	1:C:99:THR:HG22	1.89	0.54
1:D:408:VAL:H	1:D:412:HIS:CD2	2.25	0.54
1:A:538:LEU:O	1:A:541:TYR:HB3	2.08	0.54
1:C:49:GLU:O	1:C:53:GLU:HG3	2.07	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:336:VAL:HG22	6:B:2173:HOH:O	2.07	0.53
1:B:591:SER:OG	1:B:592:PRO:HD3	2.07	0.53
1:B:23:PRO:HG2	1:B:26:LEU:HD12	1.89	0.53
1:B:38:ARG:NH2	1:B:165:GLU:HG2	2.23	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:A:161:TRP:CZ2	1:A:162:ARG:HD2	2.46	0.51
1:D:591:SER:N	1:D:592:PRO:HD2	2.25	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:HG13	1:D:521:ILE:O	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: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:C:37:SER:HB2	1:C:167:PRO:HG2	1.94	0.50
1:D:380:THR:HA	1:D:383:ARG:HH11	1.77	0.50
1:B:611:LEU:HB2	1:B:612:PRO:HD3	1.94	0.50
1:D:122:PHE:CG	1:D:777:ILE:HD11	2.47	0.50
1:D:430:GLU:H	1:D:430:GLU:CD	2.15	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:553:PRO:HB3	1:A:751:ALA:HB2	1.94	0.49
1:C:408:VAL:H	1:C:412:HIS:CD2	2.23	0.49
1:C:604:VAL:O	1:C:608:GLU:HG3	2.13	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:OE1	1:A:41:GLN:HA	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: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:D:651:VAL:O	1:D:654:VAL:HG23	2.15	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:C:469:LEU:HB3	1:C:769:GLY:HA2	1.97	0.47
1:D:371:ARG:HA	1:D:371:ARG:HD3	1.61	0.47
1:A:231:ILE:C	1:A:231:ILE:HD12	2.35	0.47
1:A:670:GLU:H	1:A:670:GLU:CD	2.18	0.47
1:D:411:LEU:HG	6:D:2180:HOH:O	2.15	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:B:174:SER:HB3	3:B:1795:PO4:O1	2.15	0.47
1:C:672:LEU:N	1:C:673:PRO:HD2	2.29	0.47
1:D:629:GLY:O	1:D:632:ASN:HB2	2.15	0.47
1:A:543:ARG:HA	1:A:547:ASP:HB2	1.97	0.47
1:A:386:PRO:HB3	1:A:397:ILE:HG13	1.97	0.46
1:B:516:ILE:HG12	1:B:750:TYR:CD1	2.50	0.46
1:C:371:ARG:HA	1:C:371:ARG:NE	2.30	0.46
1:C:376:LEU:HD12	1:C:377:ASP:N	2.29	0.46
1:C:6:PRO:HG3	1:C:86:GLU:OE2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HB3	1:B:316:MET:HE3	1.78	0.46
1:D:668:ARG:HB3	1:D:670:GLU:OE2	2.15	0.45
1:A:481:ASP:C	1:A:481:ASP:OD1	2.55	0.45
1:B:138:LEU:CD2	1:B:264:PHE:HB3	2.46	0.45
1:C:316:MET:HE2	1:C:321:SER:HA	1.98	0.45
1:C:338:THR:HG23	1:C:338:THR:O	2.15	0.45
1:A:112:ASN:HB2	1:A:244:LEU:CD2	2.46	0.45
1:C:524:LEU:CD1	1:C:524:LEU:C	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:469:LEU:HG	1:D:769:GLY:HA2	1.99	0.45
1:D:553:PRO:HB3	1:D:751:ALA:HB2	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:A:339:GLU:HB3	1:A:340:ALA:H	1.67	0.45
1:B:74:LEU:HD23	1:B:102:LEU:HD23	1.98	0.45
1:C:538:LEU:O	1:C:541:TYR:HB3	2.17	0.45
1:C:641:LEU:HD12	1:C:757:TRP:CZ2	2.52	0.45
1:C:271:ALA:HA	1:C:274:GLN:HE21	1.82	0.45
1:D:341:LEU:HD22	1:D:395:ALA:HB2	1.99	0.45
1:A:473:LYS:HD2	6:A:2294:HOH:O	2.16	0.44
1:D:619:GLN:HB2	1:D:650:ASN:HD21	1.83	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: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:C:5:GLN:HA	1:C:6:PRO:HD2	1.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ALA:O	1:A:414:GLU:HG2	2.17	0.44
1:D:346:GLU:HB2	1:D:357:TRP:CZ3	2.53	0.44
1:B:49:GLU:O	1:B:53:GLU:HG3	2.17	0.44
1:B:353:PHE:CD1	1:B:356:VAL:HB	2.53	0.44
1:A:308:ARG:O	1:A:312:ASP:HB2	2.18	0.44
1:C:41:GLN:HA	1:C:41:GLN:OE1	2.18	0.44
1:D:226:ARG:NH1	1:D:229:ASP:OD2	2.50	0.44
1:D:346:GLU:O	1:D:350:GLN:HG3	2.17	0.44
1:D:632:ASN:OD1	1:D:632:ASN:N	2.50	0.44
1:C:165:GLU:HG2	6:C:2103:HOH:O	2.17	0.43
1:C:396:TRP:HA	1:C:396:TRP:CE3	2.53	0.43
1:C:458:ARG:HH11	1:C:458:ARG:HG2	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:61:GLN:HB3	1:A:787:LEU:HD11	2.01	0.43
1:A:496:LYS:HD3	6:A:2217:HOH:O	2.18	0.43
1:A:298:HIS:HB2	1:A:299:PRO:HD3	2.00	0.43
1:C:336:VAL:HG13	1:C:337:LEU:H	1.84	0.43
1:D:524:LEU:HD22	1:D:570:ALA:HA	2.01	0.43
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:C	1:C:231:ILE:HD12	2.40	0.42
1:C:527:TYR:CE1	1:C:528:LYS:HD2	2.54	0.42
1:C:712:TYR:CE1	1:C:716:HIS:HE1	2.37	0.42
1:A:224:ALA:O	1:A:225:GLN:HB2	2.20	0.42
1:C:53:GLU:OE1	1:C:793:VAL:HG21	2.19	0.42
1:A:371:ARG:HA	1:A:371:ARG:NE	2.34	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:B:49:GLU:HA	1:B:52:ARG:HH11	1.84	0.42
1:A:50:ARG:HH11	1:A:50:ARG:HD2	1.62	0.42
1:C:673:PRO:HG2	6:C:2291:HOH:O	2.19	0.42
1:D:362:GLU:HA	1:D:362:GLU:OE1	2.20	0.42
1:A:777:ILE:HD13	1:A:777:ILE:HA	1.86	0.42
1:D:408:VAL:O	1:D:436:THR:HA	2.19	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:B:605:SER:HB3	1:B:606:PRO:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:PHE:HB2	1:D:400:TYR:CE2	2.55	0.42
1:C:276:HIS:CD2	1:C:283:LEU:HD23	2.55	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:A:383:ARG:HH11	1:A:383:ARG:HD3	1.60	0.42
1:A:408:VAL:O	1:A:409:ALA:HB2	2.19	0.42
1:D:117:ARG:HA	1:D:117:ARG:HD2	1.83	0.42
1:D:526:GLU:OE2	1:D:569:ARG:HD3	2.20	0.42
1:D:646:MET:HE2	1:D:664:ILE:HG21	2.02	0.42
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:C:396:TRP:HA	1:C:396:TRP:HE3	1.85	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:323:ALA:O	1:D:327:LYS:HG3	2.20	0.41
1:D:441:PRO:HB3	1:D:469:LEU:HD22	2.01	0.41
1:A:538:LEU:HD21	1:A:697:ALA:HB3	2.02	0.41
1:A:611:LEU:HB2	1:A:612:PRO:HD3	2.02	0.41
1:C:117:ARG:HA	1:C:117:ARG:HD2	1.92	0.41
1:D:67:GLU:HB2	1:D:111:GLY:HA2	2.03	0.41
1:D:338:THR:HG22	1:D:341:LEU:HD12	2.02	0.41
1:D:660:GLU:H	1:D:660:GLU:CD	2.24	0.41
1:C:518:ASP:HA	1:C:616:VAL:HB	2.02	0.41
1:A:441:PRO:O	1:A:445:LEU:HB3	2.20	0.41
1:A:458:ARG:NH1	1:A:458:ARG:HG2	2.35	0.41
1:A:576:LEU:HA	1:A:711:PHE:CZ	2.56	0.41
1:C:336:VAL:H	1:C:336:VAL:HG12	1.52	0.41
1:D:364:ASP:HA	1:D:386:PRO:HG2	2.02	0.41
1:C:385:ALA:HA	1:C:386:PRO:HD3	2.00	0.41
1:C:624:GLY:H	1:C:647:ASP:CG	2.24	0.41
1:D:622:THR:OG1	1:D:730:TYR:HB3	2.21	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:226:ARG:HH11	1:B:226:ARG:HD2	1.61	0.41
1:B:518:ASP:HA	1:B:616:VAL:HB	2.02	0.41
1:B:538:LEU:HD21	1:B:697:ALA:HB3	2.03	0.41
1:B:739:TYR:OH	1:B:743:ARG:NH1	2.54	0.41
1:C:335:THR:O	1:C:412:HIS:HE1	2.04	0.41
1:D:481:ASP:OD2	1:D:483:SER:HB3	2.21	0.41
1:A:77:ASN:O	1:A:81:LEU:HG	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASN:HA	1:A:433:ASN:O	2.22	0.40
1:B:6:PRO:HG2	1:B:43:ARG:HH21	1.86	0.40
1:C:405:ILE:O	1:C:432:PHE:HA	2.21	0.40
1:D:522:LYS:HD3	1:D:528:LYS:HE3	2.03	0.40
1:A:353:PHE:CD1	1:A:356:VAL:HB	2.56	0.40
1:B:456:LEU:HD22	1:B:472:LEU:HD22	2.03	0.40
1:B:676:ARG:HH11	1:B:676:ARG:HD2	1.67	0.40
1:C:69:LEU:HD12	1:C:69:LEU:HA	1.93	0.40
1:D:144:LEU:O	1:D:145:PHE:HB3	2.21	0.40
1:D:346:GLU:HB2	1:D:357:TRP:CH2	2.56	0.40
1:A:668:ARG:HH11	1:A:668:ARG:HD3	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:A:346:GLU:HB2	1:A:357:TRP:CZ3	2.56	0.40
1:A:347:GLN:HB3	1:C:347:GLN:CD	2.42	0.40
1:A:349:PHE:HE2	1:A:392:VAL:HG11	1.87	0.40
1:C:408:VAL:HG22	1:C:412:HIS:CD2	2.57	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:D:543:ARG:CA	1:D:547:ASP:HB2	2.46	0.40
1:D:646:MET:HE1	1:D:654:VAL:CG2	2.49	0.40

There are no symmetry-related clashes.

3.3 Torsion angles (i)

3.3.1 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	787/796 (99%)	752 (96%)	32 (4%)	3 (0%)	34	24
1	B	787/796 (99%)	760 (97%)	25 (3%)	2 (0%)	41	31
1	C	789/796 (99%)	762 (97%)	26 (3%)	1 (0%)	51	42
1	D	787/796 (99%)	761 (97%)	25 (3%)	1 (0%)	51	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3150/3184 (99%)	3035 (96%)	108 (3%)	7 (0%)	47 38

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
1	A	629	GLY
1	C	629	GLY

3.3.2 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	660/668 (99%)	642 (97%)	18 (3%)	44 38
1	B	660/668 (99%)	636 (96%)	24 (4%)	35 26
1	C	662/668 (99%)	641 (97%)	21 (3%)	39 30
1	D	660/668 (99%)	638 (97%)	22 (3%)	38 29
All	All	2642/2672 (99%)	2557 (97%)	85 (3%)	39 30

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

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	61	GLN
1	A	279	HIS
1	A	280	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

3.3.3 RNA (i)

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains (i)

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

3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

3.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	FMT	D	1796	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
4	FMT	A	1803	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
4	FMT	B	1800	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
4	FMT	C	1802	-	2,2,2	5.51	2 (100%)	1,1,1	1.32	0
3	PO4	B	1796	-	4,4,4	1.30	1 (25%)	6,6,6	0.94	0
3	PO4	B	1795	-	4,4,4	1.59	1 (25%)	6,6,6	0.89	0
4	FMT	A	1800	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
3	PO4	C	1798	-	4,4,4	1.38	1 (25%)	6,6,6	0.86	0
3	PO4	A	1794	-	4,4,4	1.37	1 (25%)	6,6,6	0.86	0
2	PLP	B	1634	1	15,15,16	1.89	5 (33%)	20,22,23	2.06	7 (35%)
4	FMT	A	1801	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
3	PO4	C	1796	-	4,4,4	1.81	1 (25%)	6,6,6	0.92	0
4	FMT	A	1799	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
4	FMT	C	1800	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
4	FMT	C	1801	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
2	PLP	D	1634	1	15,15,16	2.05	6 (40%)	20,22,23	2.23	8 (40%)
4	FMT	A	1797	-	2,2,2	5.50	2 (100%)	1,1,1	1.31	0
4	FMT	D	1795	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
5	EDO	C	1803	-	3,3,3	0.46	0	2,2,2	0.33	0
3	PO4	D	1794	-	4,4,4	1.68	1 (25%)	6,6,6	0.91	0
2	PLP	A	1634	1	15,15,16	2.06	7 (46%)	20,22,23	1.83	6 (30%)
4	FMT	A	1795	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
4	FMT	B	1799	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
5	EDO	B	1801	-	3,3,3	0.45	0	2,2,2	0.33	0
2	PLP	C	1634	1	15,15,16	1.93	7 (46%)	20,22,23	1.98	7 (35%)
5	EDO	B	1802	-	3,3,3	0.45	0	2,2,2	0.33	0
3	PO4	B	1798	-	4,4,4	1.36	1 (25%)	6,6,6	0.86	0
4	FMT	D	1797	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
3	PO4	C	1797	-	4,4,4	1.30	1 (25%)	6,6,6	0.84	0
4	FMT	D	1798	-	2,2,2	5.51	2 (100%)	1,1,1	1.32	0
3	PO4	B	1797	-	4,4,4	1.28	1 (25%)	6,6,6	0.82	0
4	FMT	A	1798	-	2,2,2	5.49	2 (100%)	1,1,1	1.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FMT	A	1802	-	2,2,2	5.49	2 (100%)	1,1,1	1.32	0
4	FMT	A	1796	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	0
4	FMT	C	1799	-	2,2,2	5.50	2 (100%)	1,1,1	1.32	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
5	EDO	C	1803	-	-	0/1/1/1	-
2	PLP	B	1634	1	-	3/6/6/8	0/1/1/1
5	EDO	B	1802	-	-	1/1/1/1	-
5	EDO	B	1801	-	-	1/1/1/1	-
2	PLP	A	1634	1	-	4/6/6/8	0/1/1/1
2	PLP	C	1634	1	-	3/6/6/8	0/1/1/1
2	PLP	D	1634	1	-	5/6/6/8	0/1/1/1

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1802	FMT	O1-C	5.71	1.52	1.22
4	A	1797	FMT	O1-C	5.70	1.52	1.22
4	A	1795	FMT	O1-C	5.70	1.52	1.22
4	A	1801	FMT	O1-C	5.70	1.52	1.22
4	D	1795	FMT	O1-C	5.69	1.52	1.22
4	A	1799	FMT	O1-C	5.69	1.52	1.22
4	D	1798	FMT	O1-C	5.69	1.52	1.22
4	C	1799	FMT	O1-C	5.69	1.52	1.22
4	A	1803	FMT	O1-C	5.69	1.52	1.22
4	C	1800	FMT	O1-C	5.69	1.52	1.22
4	A	1796	FMT	O1-C	5.69	1.52	1.22
4	B	1799	FMT	O1-C	5.69	1.52	1.22
4	D	1797	FMT	O1-C	5.69	1.52	1.22
4	A	1800	FMT	O1-C	5.69	1.52	1.22
4	B	1800	FMT	O1-C	5.69	1.52	1.22
4	D	1796	FMT	O1-C	5.69	1.52	1.22
4	A	1798	FMT	O1-C	5.69	1.52	1.22
4	A	1802	FMT	O1-C	5.68	1.52	1.22
4	C	1801	FMT	O1-C	5.68	1.52	1.22
4	D	1798	FMT	O2-C	5.31	1.55	1.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1801	FMT	O2-C	5.31	1.55	1.28
4	C	1800	FMT	O2-C	5.31	1.55	1.28
4	A	1796	FMT	O2-C	5.31	1.55	1.28
4	A	1800	FMT	O2-C	5.31	1.55	1.28
4	B	1800	FMT	O2-C	5.30	1.55	1.28
4	B	1799	FMT	O2-C	5.30	1.55	1.28
4	A	1797	FMT	O2-C	5.30	1.55	1.28
4	D	1797	FMT	O2-C	5.30	1.55	1.28
4	A	1801	FMT	O2-C	5.30	1.55	1.28
4	A	1795	FMT	O2-C	5.30	1.55	1.28
4	C	1799	FMT	O2-C	5.30	1.55	1.28
4	C	1802	FMT	O2-C	5.30	1.55	1.28
4	A	1799	FMT	O2-C	5.30	1.55	1.28
4	D	1796	FMT	O2-C	5.30	1.55	1.28
4	D	1795	FMT	O2-C	5.30	1.55	1.28
4	A	1803	FMT	O2-C	5.30	1.55	1.28
4	A	1798	FMT	O2-C	5.29	1.55	1.28
4	A	1802	FMT	O2-C	5.29	1.55	1.28
2	D	1634	PLP	P-O4P	-3.41	1.49	1.60
2	A	1634	PLP	P-O4P	-3.39	1.49	1.60
2	D	1634	PLP	C6-C5	3.30	1.44	1.37
3	C	1796	PO4	P-O1	3.29	1.58	1.50
2	A	1634	PLP	C6-C5	3.27	1.44	1.37
2	D	1634	PLP	P-O1P	3.18	1.60	1.50
2	B	1634	PLP	P-O4P	-3.17	1.50	1.60
2	B	1634	PLP	P-O1P	3.15	1.60	1.50
2	C	1634	PLP	C6-C5	3.04	1.44	1.37
2	C	1634	PLP	C3-C2	3.01	1.43	1.40
2	B	1634	PLP	C2-N1	3.01	1.39	1.33
3	D	1794	PO4	P-O1	2.97	1.57	1.50
2	A	1634	PLP	C3-C2	2.96	1.43	1.40
2	C	1634	PLP	P-O4P	-2.89	1.50	1.60
3	B	1795	PO4	P-O1	2.75	1.57	1.50
2	B	1634	PLP	C6-C5	2.72	1.43	1.37
2	A	1634	PLP	C2A-C2	-2.71	1.45	1.50
2	A	1634	PLP	P-O1P	2.69	1.59	1.50
2	D	1634	PLP	C6-N1	2.64	1.40	1.34
2	D	1634	PLP	C3-C2	2.64	1.43	1.40
2	C	1634	PLP	P-O1P	2.50	1.58	1.50
3	C	1798	PO4	P-O1	2.40	1.56	1.50
2	C	1634	PLP	C2-N1	2.39	1.38	1.33
3	B	1797	PO4	P-O1	2.37	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1634	PLP	C6-N1	2.37	1.39	1.34
3	A	1794	PO4	P-O1	2.36	1.56	1.50
3	B	1798	PO4	P-O1	2.35	1.56	1.50
2	B	1634	PLP	C6-N1	2.31	1.39	1.34
2	A	1634	PLP	C2-N1	2.27	1.38	1.33
3	C	1797	PO4	P-O1	2.25	1.56	1.50
2	D	1634	PLP	C2-N1	2.23	1.38	1.33
2	C	1634	PLP	C6-N1	2.22	1.39	1.34
2	C	1634	PLP	P-O2P	2.16	1.63	1.54
3	B	1796	PO4	P-O1	2.03	1.55	1.50

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1634	PLP	O3P-P-O4P	5.29	120.81	106.73
2	C	1634	PLP	C5A-C5-C6	-4.28	112.34	119.37
2	B	1634	PLP	C5-C6-N1	-3.94	117.26	123.82
2	B	1634	PLP	C5A-C5-C6	-3.70	113.29	119.37
2	B	1634	PLP	C3-C4-C5	3.56	122.58	118.74
2	A	1634	PLP	O2P-P-O4P	3.49	116.03	106.73
2	C	1634	PLP	C5-C6-N1	-3.43	118.11	123.82
2	A	1634	PLP	C3-C4-C5	3.43	122.44	118.74
2	A	1634	PLP	C5A-C5-C6	-3.39	113.80	119.37
2	D	1634	PLP	C3-C4-C5	3.30	122.31	118.74
2	D	1634	PLP	C5-C6-N1	-3.29	118.35	123.82
2	A	1634	PLP	C5-C6-N1	-3.25	118.40	123.82
2	D	1634	PLP	O2P-P-O4P	-3.23	98.14	106.73
2	C	1634	PLP	O3P-P-O4P	3.22	115.31	106.73
2	B	1634	PLP	C4A-C4-C3	-3.19	115.09	120.50
2	D	1634	PLP	O4P-C5A-C5	-3.17	103.31	109.35
2	D	1634	PLP	C5A-C5-C6	-3.04	114.37	119.37
2	C	1634	PLP	C3-C4-C5	2.81	121.78	118.74
2	B	1634	PLP	C6-N1-C2	2.80	124.36	119.17
2	B	1634	PLP	C3-C2-N1	-2.73	117.23	120.77
2	B	1634	PLP	O2P-P-O4P	2.64	113.75	106.73
2	A	1634	PLP	C4A-C4-C3	-2.61	116.08	120.50
2	C	1634	PLP	C6-N1-C2	2.54	123.87	119.17
2	C	1634	PLP	C3-C2-N1	-2.45	117.60	120.77
2	D	1634	PLP	C6-N1-C2	2.36	123.54	119.17
2	C	1634	PLP	O3-C3-C4	2.26	124.06	118.10
2	D	1634	PLP	C3-C2-N1	-2.17	117.96	120.77
2	A	1634	PLP	C6-N1-C2	2.12	123.10	119.17

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1634	PLP	C5A-O4P-P-O2P
2	A	1634	PLP	C5A-O4P-P-O3P
2	B	1634	PLP	C5A-O4P-P-O3P
2	C	1634	PLP	C5A-O4P-P-O2P
2	C	1634	PLP	C5A-O4P-P-O3P
2	D	1634	PLP	C5A-O4P-P-O2P
5	B	1801	EDO	O1-C1-C2-O2
2	A	1634	PLP	C5A-O4P-P-O1P
2	B	1634	PLP	C5A-O4P-P-O1P
2	C	1634	PLP	C5A-O4P-P-O1P
2	D	1634	PLP	C5A-O4P-P-O1P
2	D	1634	PLP	C6-C5-C5A-O4P
2	B	1634	PLP	C5A-O4P-P-O2P
2	D	1634	PLP	C4-C5-C5A-O4P
5	B	1802	EDO	O1-C1-C2-O2
2	D	1634	PLP	C5A-O4P-P-O3P
2	A	1634	PLP	C4-C5-C5A-O4P

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1795	PO4	1	0
2	D	1634	PLP	2	0
5	B	1801	EDO	2	0

3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 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	789/796 (99%)	-0.01	17 (2%)	62	64	15, 29, 46, 75	16 (2%)
1	B	789/796 (99%)	-0.02	20 (2%)	57	60	15, 28, 48, 69	14 (1%)
1	C	791/796 (99%)	-0.04	18 (2%)	60	63	15, 27, 45, 74	15 (1%)
1	D	789/796 (99%)	0.15	29 (3%)	41	44	20, 34, 52, 71	16 (2%)
All	All	3158/3184 (99%)	0.02	84 (2%)	54	57	15, 29, 48, 75	61 (1%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	THR	6.0
1	D	340	ALA	5.4
1	C	336	VAL	5.3
1	A	337	LEU	4.3
1	B	793	VAL	4.3
1	A	340	ALA	4.3
1	D	294	LEU	4.3
1	C	339	GLU	4.2
1	A	5	GLN	4.2
1	B	6	PRO	3.9
1	C	337	LEU	3.7
1	A	551	ASP	3.7
1	D	722	TYR	3.6
1	D	372	ALA	3.4
1	C	534	ALA	3.3
1	D	725	ASP	3.3
1	C	550	THR	3.2
1	B	294	LEU	3.2
1	C	557	VAL	3.2
1	A	338	THR	3.2
1	C	519	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	335	THR	3.0
1	C	6	PRO	2.9
1	B	551	ASP	2.9
1	C	537	VAL	2.8
1	D	519	VAL	2.8
1	B	336	VAL	2.8
1	C	551	ASP	2.8
1	D	299	PRO	2.8
1	B	548	GLY	2.8
1	C	294	LEU	2.8
1	D	548	GLY	2.7
1	B	303	ILE	2.7
1	D	300	VAL	2.7
1	A	294	LEU	2.7
1	D	551	ASP	2.7
1	B	340	ALA	2.7
1	B	794	LYS	2.6
1	B	686	GLU	2.6
1	A	300	VAL	2.6
1	B	687	THR	2.6
1	B	397	ILE	2.6
1	B	338	THR	2.6
1	A	509	ILE	2.5
1	A	6	PRO	2.5
1	C	725	ASP	2.5
1	D	6	PRO	2.5
1	A	339	GLU	2.5
1	D	389	HIS	2.5
1	D	546	GLU	2.5
1	C	340	ALA	2.5
1	D	550	THR	2.5
1	D	534	ALA	2.4
1	D	64	PHE	2.4
1	D	674	ALA	2.3
1	D	5	GLN	2.3
1	D	337	LEU	2.3
1	B	339	GLU	2.3
1	B	300	VAL	2.3
1	D	678	SER	2.3
1	C	376	LEU	2.3
1	D	369	LEU	2.3
1	C	616	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	792	ALA	2.2
1	C	375	GLY	2.2
1	B	580	ILE	2.2
1	D	588	PRO	2.2
1	C	558	ILE	2.2
1	A	64	PHE	2.2
1	A	303	ILE	2.1
1	B	532	MET	2.1
1	B	360	ILE	2.1
1	B	573	ILE	2.1
1	D	338	THR	2.1
1	D	57	ALA	2.1
1	D	339	GLU	2.1
1	D	303	ILE	2.1
1	A	301	LEU	2.1
1	D	375	GLY	2.1
1	A	616	VAL	2.0
1	A	341	LEU	2.0
1	D	707	ASN	2.0
1	B	588	PRO	2.0
1	A	677	GLU	2.0

4.2 Non-standard residues in protein, DNA, RNA chains (i)

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

4.3 Carbohydrates (i)

There are no monosaccharides in this entry.

4.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
4	FMT	C	1802	3/3	0.64	0.12	36,36,38,39	0
4	FMT	A	1802	3/3	0.72	0.16	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FMT	D	1797	3/3	0.78	0.13	36,36,37,38	0
4	FMT	A	1801	3/3	0.83	0.14	35,35,36,38	0
4	FMT	A	1799	3/3	0.84	0.13	39,39,40,41	0
4	FMT	A	1803	3/3	0.85	0.12	39,39,39,40	0
4	FMT	B	1800	3/3	0.85	0.14	32,32,36,37	0
4	FMT	A	1797	3/3	0.85	0.13	38,38,38,39	0
3	PO4	C	1798	5/5	0.85	0.17	56,57,58,58	2
4	FMT	A	1796	3/3	0.86	0.17	39,39,39,41	0
4	FMT	C	1801	3/3	0.87	0.12	35,35,37,38	0
4	FMT	A	1795	3/3	0.87	0.15	41,41,43,43	0
4	FMT	C	1799	3/3	0.87	0.10	36,36,38,38	0
3	PO4	A	1794	5/5	0.88	0.14	56,57,57,57	3
4	FMT	D	1796	3/3	0.89	0.11	35,35,37,37	0
5	EDO	B	1802	4/4	0.89	0.11	27,27,31,34	0
4	FMT	D	1795	3/3	0.90	0.18	32,32,33,36	0
4	FMT	A	1800	3/3	0.90	0.19	38,38,40,40	0
5	EDO	C	1803	4/4	0.91	0.14	26,27,30,33	0
4	FMT	D	1798	3/3	0.93	0.08	40,40,40,40	0
4	FMT	B	1799	3/3	0.93	0.09	37,37,40,40	0
3	PO4	B	1798	5/5	0.93	0.14	55,56,57,57	3
2	PLP	C	1634	15/16	0.94	0.10	23,24,42,43	0
5	EDO	B	1801	4/4	0.94	0.09	41,42,43,43	0
2	PLP	A	1634	15/16	0.95	0.09	21,24,42,43	0
2	PLP	B	1634	15/16	0.95	0.09	19,21,42,44	0
2	PLP	D	1634	15/16	0.96	0.09	28,30,48,48	0
4	FMT	A	1798	3/3	0.96	0.12	23,23,26,28	0
4	FMT	C	1800	3/3	0.96	0.07	33,33,35,36	0
3	PO4	B	1796	5/5	0.97	0.14	38,38,40,41	3
3	PO4	D	1794	5/5	0.97	0.11	37,39,41,41	3
3	PO4	C	1796	5/5	0.97	0.12	36,39,41,42	4
3	PO4	B	1795	5/5	0.98	0.12	37,38,39,39	4
3	PO4	B	1797	5/5	0.99	0.09	37,39,41,41	0
3	PO4	C	1797	5/5	0.99	0.10	36,38,40,41	0

4.5 Other polymers (i)

There are no such residues in this entry.