Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:15 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

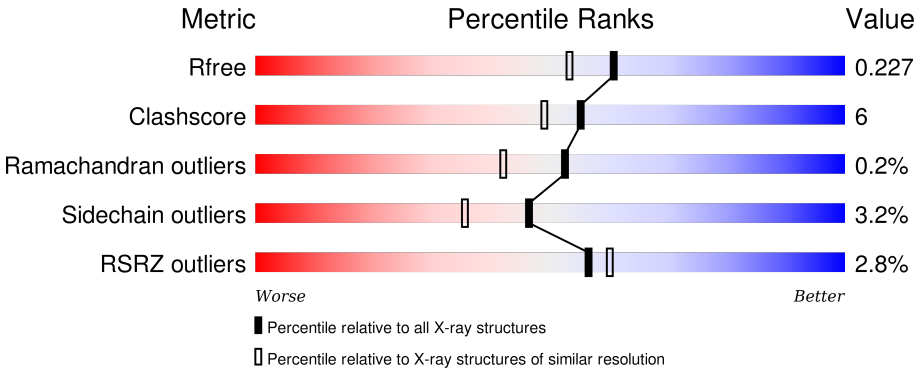
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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. 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	796	2% 81% 17%
1	B	796	3% 86% 12%
1	C	796	3% 85% 14%
1	D	796	4% 80% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	1795	-	-	-	X
3	PO4	B	1796	-	-	-	X
3	PO4	C	1796	-	-	-	X
3	PO4	D	1794	-	-	-	X
4	FMT	A	1796	-	-	-	X
4	FMT	A	1800	-	-	-	X
4	FMT	A	1801	-	-	-	X
4	FMT	A	1802	-	-	-	X
4	FMT	B	1800	-	-	-	X
4	FMT	D	1795	-	-	-	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 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.

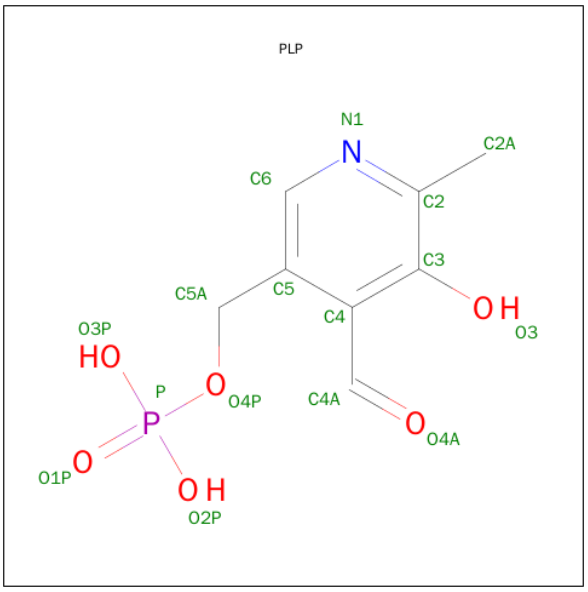
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE.

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:

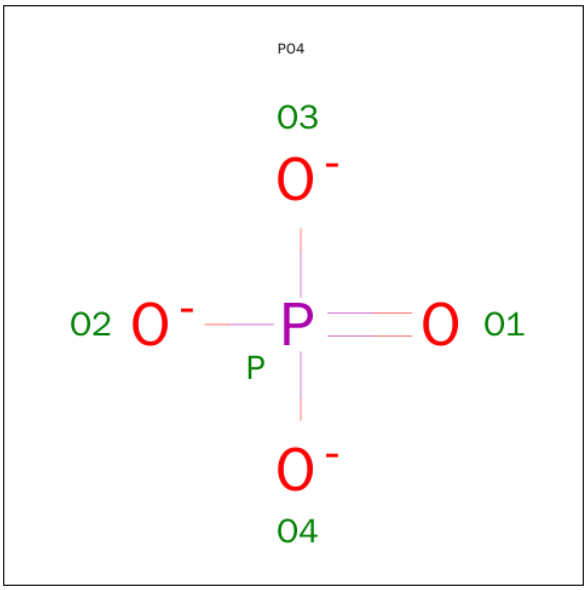
Chain	Residue	Modelled	Actual	Comment	Reference
A	224	ALA	SER	ENGINEERED MUTATION	UNP Q8KQ56
B	224	ALA	SER	ENGINEERED MUTATION	UNP Q8KQ56
C	224	ALA	SER	ENGINEERED MUTATION	UNP Q8KQ56
D	224	ALA	SER	ENGINEERED MUTATION	UNP Q8KQ56

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



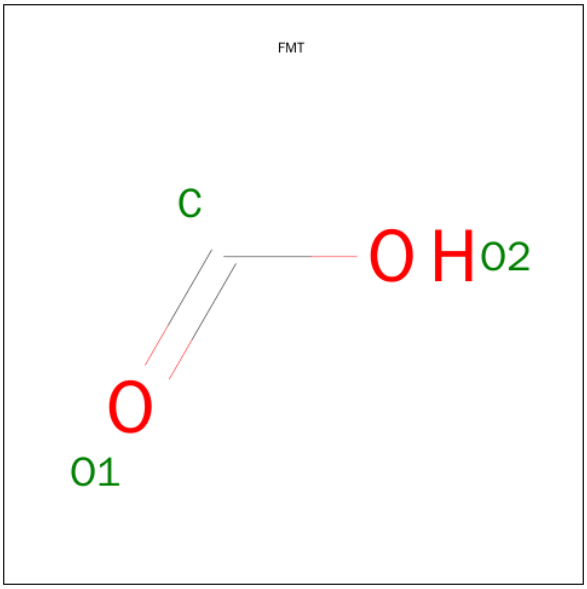
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

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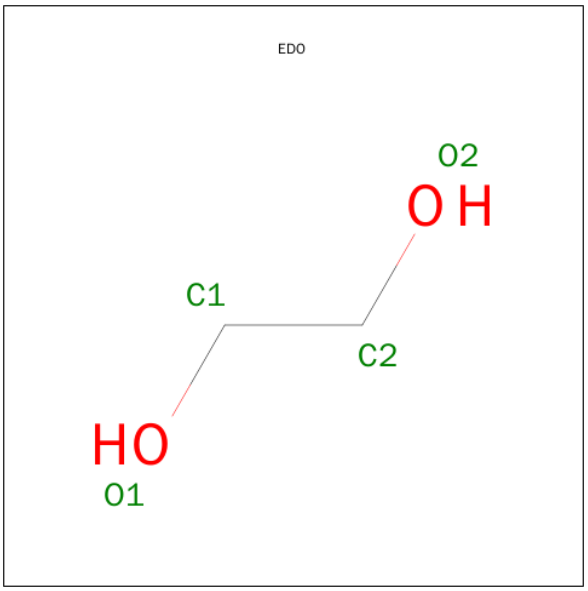
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0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

- 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.

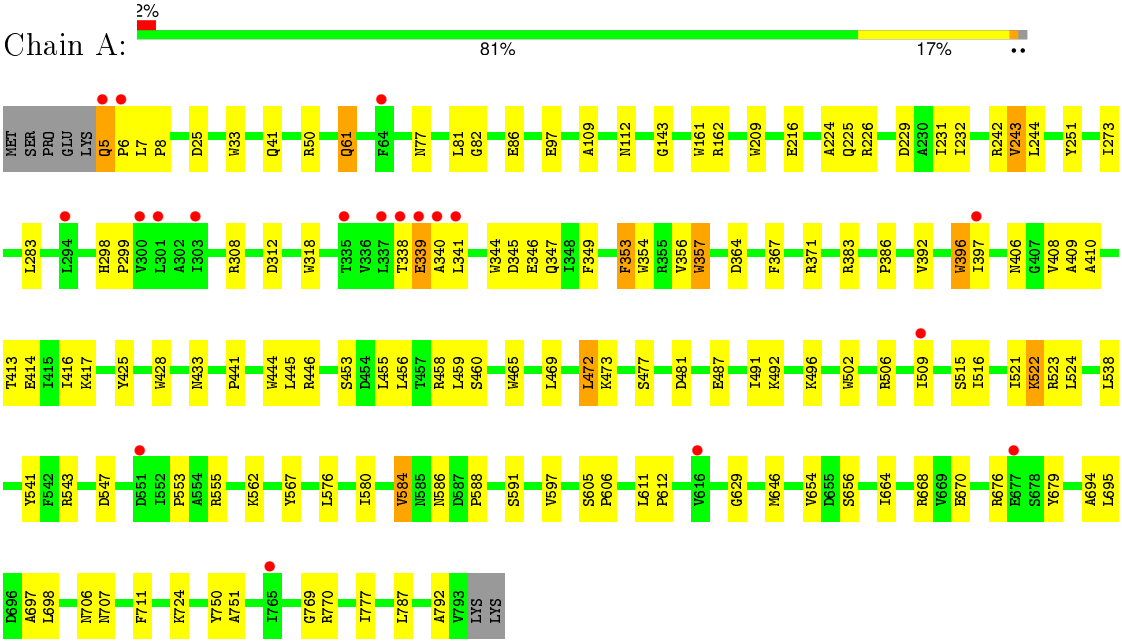
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	303	Total O 303 303	0	0
6	B	306	Total O 306 306	0	0
6	C	340	Total O 340 340	0	0
6	D	205	Total O 205 205	0	0

3 Residue-property plots (i)

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.

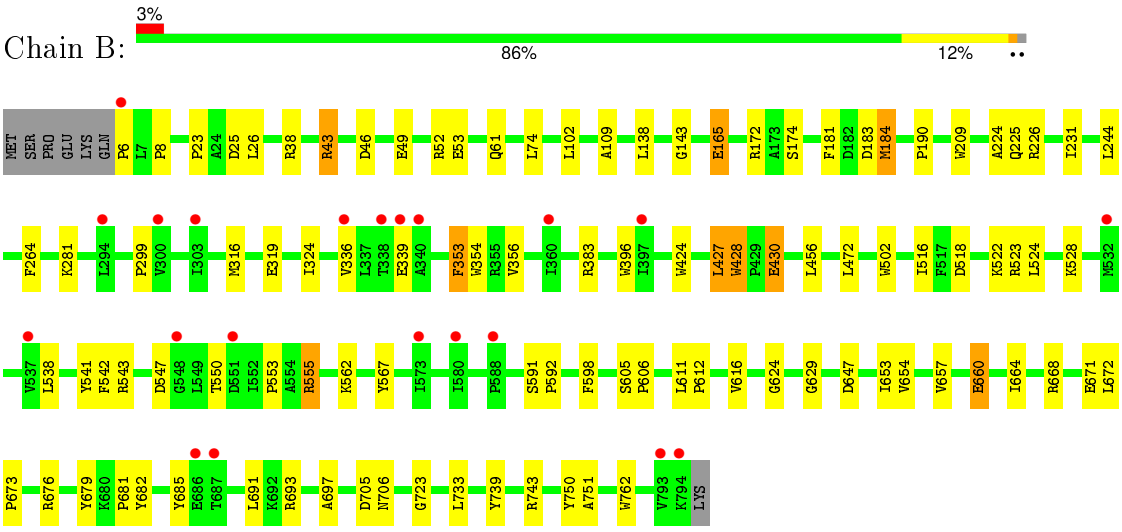
- Molecule 1: GLYCOGEN PHOSPHORYLASE

Chain A:



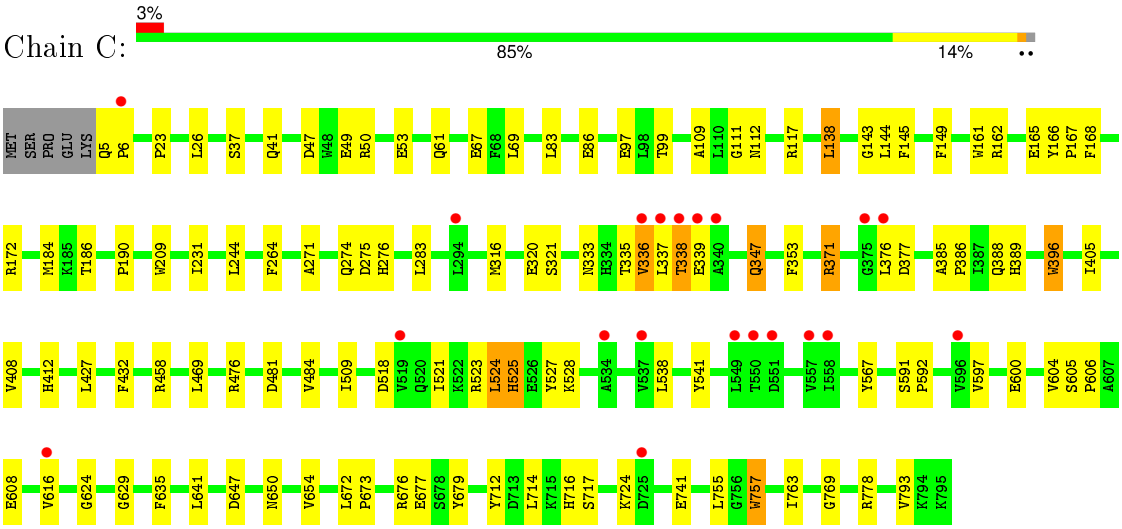
- Molecule 1: GLYCOGEN PHOSPHORYLASE

Chain B:



- Molecule 1: GLYCOGEN PHOSPHORYLASE

Chain C:



- Molecule 1: GLYCOGEN PHOSPHORYLASE

Chain D:

4 Data and refinement statistics (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 0.210 , 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)	0.35 , 42.0	EDS
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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

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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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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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: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: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

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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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	787/796 (99%)	752 (96%)	32 (4%)	3 (0%)	39	27
1	B	787/796 (99%)	760 (97%)	25 (3%)	2 (0%)	46	35
1	C	789/796 (99%)	762 (97%)	26 (3%)	1 (0%)	56	46
1	D	787/796 (99%)	761 (97%)	25 (3%)	1 (0%)	56	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3150/3184 (99%)	3035 (96%)	108 (3%)	7 (0%)	52 42

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

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	660/668 (99%)	642 (97%)	18 (3%)	52 43
1	B	660/668 (99%)	636 (96%)	24 (4%)	42 30
1	C	662/668 (99%)	641 (97%)	21 (3%)	46 35
1	D	660/668 (99%)	638 (97%)	22 (3%)	45 34
All	All	2642/2672 (99%)	2557 (97%)	85 (3%)	46 35

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

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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

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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

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

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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

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 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	15,15,16	2.14	6 (40%)	21,22,23	1.94	6 (28%)
3	PO4	A	1794	-	4,4,4	0.72	0	6,6,6	0.30	0
4	FMT	A	1795	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	1796	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	1797	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	1798	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	1799	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	1800	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	1801	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	1802	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	1803	-	0,2,2	0.00	-	0,1,1	0.00	-
2	PLP	B	1634	1	15,15,16	1.86	6 (40%)	21,22,23	2.12	8 (38%)
3	PO4	B	1795	-	4,4,4	0.87	0	6,6,6	0.30	0
3	PO4	B	1796	-	4,4,4	0.86	0	6,6,6	0.30	0
3	PO4	B	1797	-	4,4,4	0.52	0	6,6,6	0.29	0
3	PO4	B	1798	-	4,4,4	0.72	0	6,6,6	0.30	0
4	FMT	B	1799	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	1800	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	B	1801	-	3,3,3	0.47	0	2,2,2	0.42	0
5	EDO	B	1802	-	3,3,3	0.47	0	2,2,2	0.42	0
2	PLP	C	1634	1	15,15,16	2.06	7 (46%)	21,22,23	2.16	8 (38%)
3	PO4	C	1796	-	4,4,4	0.96	0	6,6,6	0.30	0
3	PO4	C	1797	-	4,4,4	0.66	0	6,6,6	0.29	0
3	PO4	C	1798	-	4,4,4	0.72	0	6,6,6	0.30	0
4	FMT	C	1799	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	1800	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	1801	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	1802	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	C	1803	-	3,3,3	0.47	0	2,2,2	0.42	0
2	PLP	D	1634	1	15,15,16	2.11	5 (33%)	21,22,23	2.27	8 (38%)
3	PO4	D	1794	-	4,4,4	0.93	0	6,6,6	0.30	0
4	FMT	D	1795	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	1796	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	1797	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	1798	-	0,2,2	0.00	-	0,1,1	0.00	-

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
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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1634	PLP	P-O4P	-3.29	1.49	1.60
2	A	1634	PLP	P-O4P	-3.27	1.49	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1634	PLP	P-O4P	-3.06	1.50	1.60
2	C	1634	PLP	P-O4P	-2.79	1.50	1.60
2	A	1634	PLP	C2A-C2	-2.28	1.45	1.50
2	C	1634	PLP	C2-N1	2.03	1.38	1.34
2	C	1634	PLP	C6-N1	2.17	1.39	1.34
2	B	1634	PLP	C3-C2	2.19	1.42	1.40
2	B	1634	PLP	C6-N1	2.26	1.39	1.34
2	C	1634	PLP	P-O1P	2.26	1.58	1.51
2	A	1634	PLP	C6-N1	2.32	1.39	1.34
2	C	1634	PLP	P-O2P	2.35	1.63	1.54
2	A	1634	PLP	P-O1P	2.45	1.59	1.51
2	B	1634	PLP	C2-N1	2.58	1.39	1.34
2	D	1634	PLP	C6-N1	2.59	1.40	1.34
2	B	1634	PLP	C6-C5	2.61	1.43	1.37
2	B	1634	PLP	P-O1P	2.90	1.60	1.51
2	C	1634	PLP	C6-C5	2.90	1.44	1.37
2	D	1634	PLP	P-O1P	2.93	1.60	1.51
2	A	1634	PLP	C6-C5	3.11	1.44	1.37
2	D	1634	PLP	C6-C5	3.14	1.44	1.37
2	D	1634	PLP	C3-C2	4.00	1.43	1.40
2	A	1634	PLP	C3-C2	4.47	1.43	1.40
2	C	1634	PLP	C3-C2	4.55	1.43	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1634	PLP	C5-C6-N1	-3.80	117.26	123.86
2	C	1634	PLP	C5A-C5-C6	-3.67	112.34	119.28
2	D	1634	PLP	O4P-C5A-C5	-3.44	103.31	108.99
2	C	1634	PLP	C5-C6-N1	-3.31	118.11	123.86
2	D	1634	PLP	C5-C6-N1	-3.18	118.35	123.86
2	B	1634	PLP	C5A-C5-C6	-3.17	113.29	119.28
2	A	1634	PLP	C5-C6-N1	-3.15	118.40	123.86
2	D	1634	PLP	O2P-P-O4P	-2.92	98.14	106.56
2	B	1634	PLP	C4A-C4-C3	-2.91	115.09	120.36
2	A	1634	PLP	C5A-C5-C6	-2.90	113.80	119.28
2	D	1634	PLP	C5A-C5-C6	-2.60	114.37	119.28
2	B	1634	PLP	C3-C2-N1	-2.44	117.23	120.61
2	A	1634	PLP	C4A-C4-C3	-2.36	116.08	120.36
2	C	1634	PLP	C3-C2-N1	-2.18	117.60	120.61
2	D	1634	PLP	C6-N1-C2	2.09	123.54	119.28
2	C	1634	PLP	O3-C3-C4	2.11	124.06	118.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1634	PLP	C6-N1-C2	2.25	123.87	119.28
2	B	1634	PLP	C6-N1-C2	2.49	124.36	119.28
2	B	1634	PLP	O2P-P-O4P	2.50	113.75	106.56
2	C	1634	PLP	C3-C4-C5	2.75	121.78	118.78
2	C	1634	PLP	O3P-P-O4P	3.04	115.31	106.56
2	D	1634	PLP	C3-C4-C5	3.23	122.31	118.78
2	A	1634	PLP	O2P-P-O4P	3.29	116.03	106.56
2	A	1634	PLP	C3-C4-C5	3.35	122.44	118.78
2	B	1634	PLP	C3-C4-C5	3.48	122.58	118.78
2	D	1634	PLP	C5A-C5-C4	4.39	127.47	121.65
2	A	1634	PLP	C5A-C5-C4	4.48	127.59	121.65
2	B	1634	PLP	C5A-C5-C4	4.71	127.89	121.65
2	D	1634	PLP	O3P-P-O4P	4.95	120.81	106.56
2	C	1634	PLP	C5A-C5-C4	5.43	128.84	121.65

There are no chirality outliers.

There are no torsion outliers.

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
5	B	1801	EDO	2	0
2	D	1634	PLP	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	789/796 (99%)	0.02	19 (2%)	62	66	15, 29, 46, 75	16 (2%)
1	B	789/796 (99%)	0.01	21 (2%)	58	61	15, 28, 48, 69	14 (1%)
1	C	791/796 (99%)	-0.01	20 (2%)	61	64	15, 27, 45, 74	15 (1%)
1	D	789/796 (99%)	0.18	30 (3%)	44	48	20, 34, 52, 71	16 (2%)
All	All	3158/3184 (99%)	0.05	90 (2%)	56	60	15, 29, 48, 75	61 (1%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	THR	6.1
1	D	340	ALA	5.5
1	C	336	VAL	5.4
1	A	340	ALA	4.4
1	B	793	VAL	4.4
1	A	337	LEU	4.4
1	D	294	LEU	4.4
1	C	339	GLU	4.3
1	A	5	GLN	4.2
1	B	6	PRO	4.0
1	C	337	LEU	3.8
1	A	551	ASP	3.7
1	D	722	TYR	3.7
1	D	372	ALA	3.5
1	C	534	ALA	3.4
1	D	725	ASP	3.4
1	B	294	LEU	3.3
1	C	557	VAL	3.3
1	C	550	THR	3.3
1	A	338	THR	3.3
1	C	519	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	335	THR	3.1
1	C	537	VAL	2.9
1	D	519	VAL	2.9
1	B	551	ASP	2.9
1	C	6	PRO	2.9
1	B	336	VAL	2.9
1	B	548	GLY	2.9
1	C	294	LEU	2.9
1	C	551	ASP	2.9
1	D	548	GLY	2.9
1	D	299	PRO	2.8
1	B	303	ILE	2.8
1	B	340	ALA	2.8
1	D	300	VAL	2.8
1	A	294	LEU	2.8
1	D	551	ASP	2.8
1	A	300	VAL	2.7
1	B	794	LYS	2.7
1	B	397	ILE	2.7
1	B	687	THR	2.7
1	A	509	ILE	2.6
1	B	338	THR	2.6
1	B	686	GLU	2.6
1	D	6	PRO	2.6
1	C	725	ASP	2.6
1	A	6	PRO	2.5
1	D	389	HIS	2.5
1	A	339	GLU	2.5
1	D	550	THR	2.5
1	C	340	ALA	2.5
1	D	546	GLU	2.5
1	D	534	ALA	2.5
1	D	64	PHE	2.5
1	D	674	ALA	2.4
1	D	337	LEU	2.4
1	B	300	VAL	2.4
1	B	339	GLU	2.4
1	D	369	LEU	2.4
1	D	5	GLN	2.3
1	D	792	ALA	2.3
1	B	580	ILE	2.3
1	C	376	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	678	SER	2.3
1	C	616	VAL	2.3
1	C	375	GLY	2.3
1	D	588	PRO	2.3
1	C	558	ILE	2.3
1	A	64	PHE	2.2
1	A	303	ILE	2.2
1	B	360	ILE	2.2
1	D	338	THR	2.2
1	B	573	ILE	2.2
1	B	532	MET	2.2
1	D	57	ALA	2.2
1	A	616	VAL	2.2
1	D	303	ILE	2.1
1	A	301	LEU	2.1
1	D	375	GLY	2.1
1	A	341	LEU	2.1
1	D	339	GLU	2.1
1	D	707	ASN	2.1
1	B	588	PRO	2.1
1	C	596	VAL	2.1
1	B	537	VAL	2.1
1	A	677	GLU	2.0
1	A	397	ILE	2.0
1	C	549	LEU	2.0
1	D	377	ASP	2.0
1	A	765	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	FMT	D	1795	3/3	0.90	0.18	8.22	32,32,33,36	0
4	FMT	A	1802	3/3	0.73	0.16	7.62	42,42,42,42	0
4	FMT	A	1796	3/3	0.86	0.17	5.17	39,39,39,41	0
3	PO4	B	1796	5/5	0.97	0.14	3.46	38,38,40,41	3
4	FMT	B	1800	3/3	0.85	0.14	3.36	32,32,36,37	0
5	EDO	C	1803	4/4	0.91	0.14	2.96	26,27,30,33	0
4	FMT	A	1800	3/3	0.89	0.19	2.83	38,38,40,40	0
4	FMT	A	1801	3/3	0.83	0.14	2.39	35,35,36,38	0
3	PO4	D	1794	5/5	0.97	0.11	2.22	37,39,41,41	3
3	PO4	B	1795	5/5	0.98	0.12	2.02	37,38,39,39	4
3	PO4	C	1796	5/5	0.97	0.12	2.00	36,39,41,42	4
4	FMT	A	1797	3/3	0.85	0.14	1.95	38,38,38,39	0
3	PO4	C	1797	5/5	0.99	0.10	1.90	36,38,40,41	0
4	FMT	A	1803	3/3	0.85	0.12	1.84	39,39,39,40	0
4	FMT	A	1795	3/3	0.87	0.15	1.71	41,41,43,43	0
4	FMT	A	1798	3/3	0.96	0.12	1.71	23,23,26,28	0
4	FMT	A	1799	3/3	0.83	0.13	1.46	39,39,40,41	0
4	FMT	C	1799	3/3	0.87	0.10	1.34	36,36,38,38	0
4	FMT	C	1801	3/3	0.87	0.12	1.16	35,35,37,38	0
4	FMT	D	1797	3/3	0.79	0.13	1.12	36,36,37,38	0
4	FMT	C	1802	3/3	0.64	0.12	1.04	36,36,38,39	0
3	PO4	B	1798	5/5	0.93	0.14	0.85	55,56,57,57	3
5	EDO	B	1802	4/4	0.89	0.11	0.44	27,27,31,34	0
4	FMT	D	1796	3/3	0.89	0.10	0.22	35,35,37,37	0
2	PLP	B	1634	15/16	0.95	0.09	0.07	19,21,42,44	0
2	PLP	C	1634	15/16	0.94	0.10	-0.02	23,24,42,43	0
4	FMT	B	1799	3/3	0.93	0.09	-0.06	37,37,40,40	0
5	EDO	B	1801	4/4	0.94	0.09	-0.23	41,42,43,43	0
2	PLP	D	1634	15/16	0.96	0.09	-0.46	28,30,48,48	0
2	PLP	A	1634	15/16	0.95	0.09	-0.50	21,24,42,43	0
4	FMT	C	1800	3/3	0.96	0.07	-0.74	33,33,35,36	0
3	PO4	B	1797	5/5	0.99	0.09	-0.84	37,39,41,41	0
4	FMT	D	1798	3/3	0.93	0.08	-0.89	40,40,40,40	0
3	PO4	A	1794	5/5	0.88	0.15	-	56,57,57,57	3
3	PO4	C	1798	5/5	0.85	0.17	-	56,57,58,58	2

6.5 Other polymers (i)

There are no such residues in this entry.