Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:20 PM GMT

PDB ID	:	1F3T
Title	:	CRYSTAL STRUCTURE OF TRYPANOSOMA BRUCEI ORNITHINE DECARBOXYLASE (ODC) COMPLEXED WITH PUTRESCINE, ODC'S REACTION PRODUCT.
Authors	:	Jackson, L.K.; Brooks, H.B.; Osterman, A.L.; Goldsmith, E.J.; Phillips, M.A.
Deposited on	:	2000-06-06
Resolution	:	2.00 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:

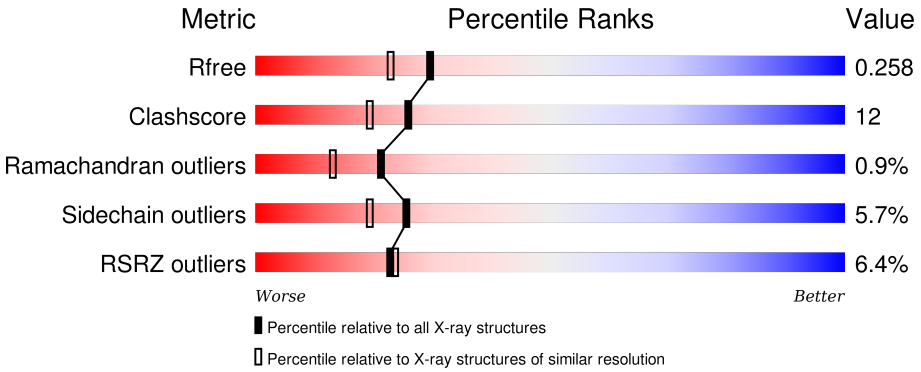
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	425	7% 68% 17% • 11%
1	B	425	5% 68% 19% • 10%
1	C	425	6% 67% 17% • 13%
1	D	425	4% 67% 17% • 14%

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	PUT	A	1002	-	-	-	X
3	PUT	B	1004	-	-	-	X
3	PUT	C	1006	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12201 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.

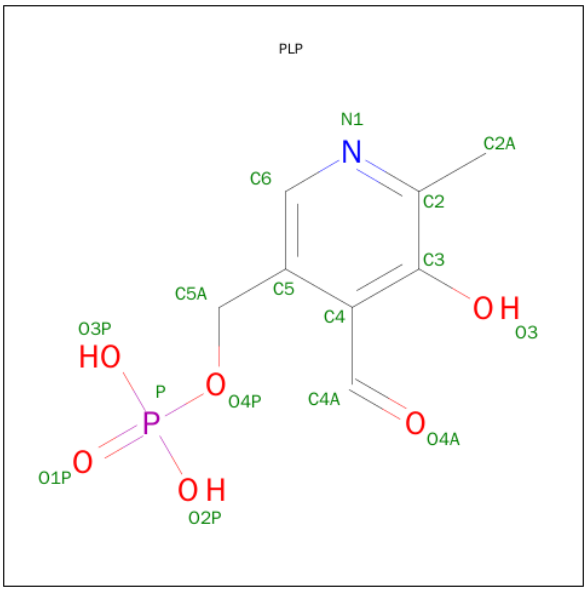
- Molecule 1 is a protein called ORNITHINE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2965	1905	497	547	16			
1	B	381	Total	C	N	O	S	0	0	0
			2987	1918	500	553	16			
1	C	370	Total	C	N	O	S	0	0	0
			2906	1866	486	538	16			
1	D	367	Total	C	N	O	S	0	0	0
			2879	1852	480	531	16			

There are 8 discrepancies between the modelled and reference sequences:

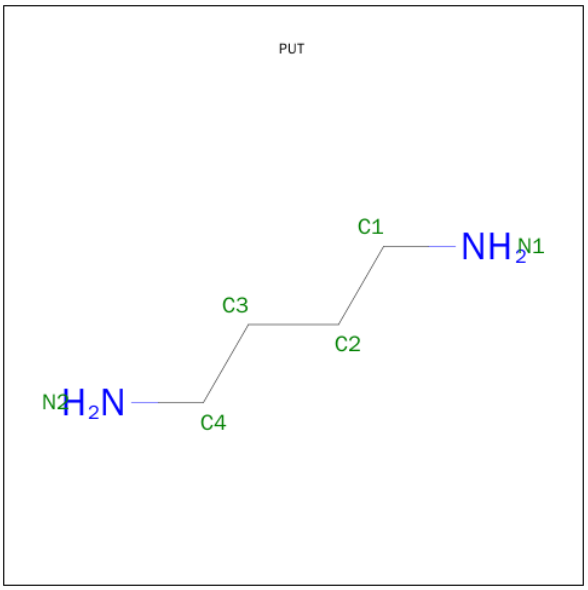
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P07805
A	2	ALA	-	CLONING ARTIFACT	UNP P07805
B	1	GLY	-	CLONING ARTIFACT	UNP P07805
B	2	ALA	-	CLONING ARTIFACT	UNP P07805
C	1	GLY	-	CLONING ARTIFACT	UNP P07805
C	2	ALA	-	CLONING ARTIFACT	UNP P07805
D	1	GLY	-	CLONING ARTIFACT	UNP P07805
D	2	ALA	-	CLONING ARTIFACT	UNP P07805

- 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 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 6 4 2	0	0
3	B	1	Total C N 6 4 2	0	0
3	C	1	Total C N 6 4 2	0	0
3	D	1	Total C N 6 4 2	0	0

- Molecule 4 is water.

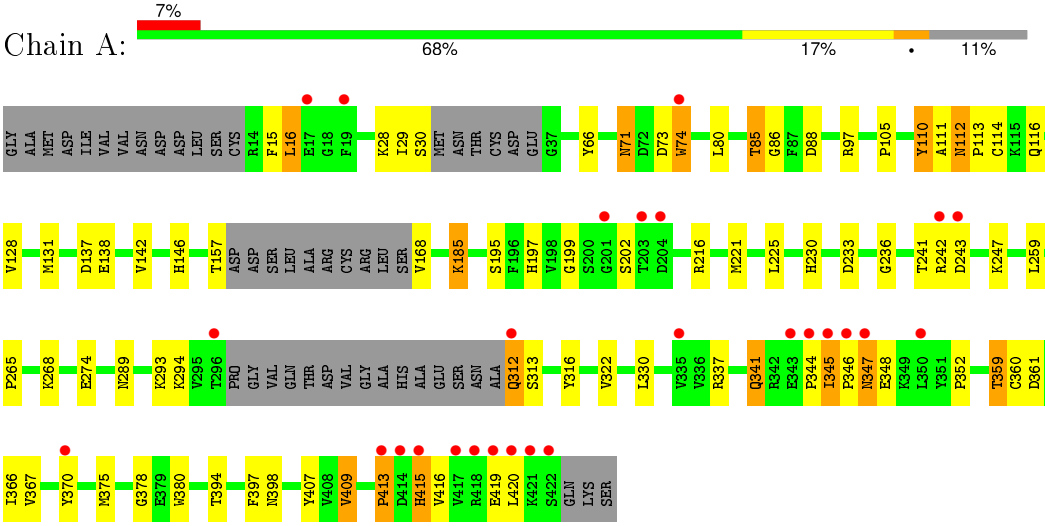
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	81	Total O 81 81	0	0
4	B	110	Total O 110 110	0	0
4	C	77	Total O 77 77	0	0
4	D	112	Total O 112 112	0	0

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.

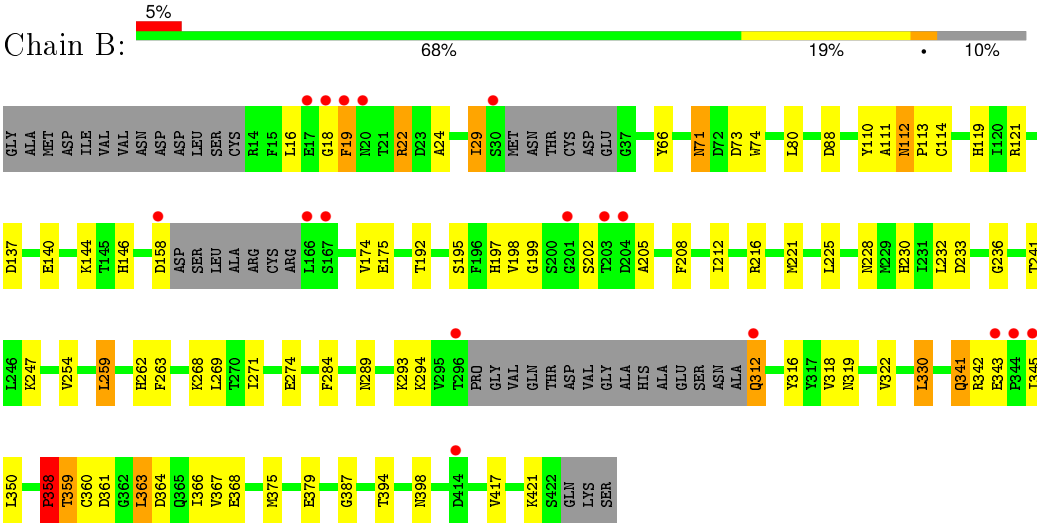
- Molecule 1: ORNITHINE DECARBOXYLASE

Chain A:



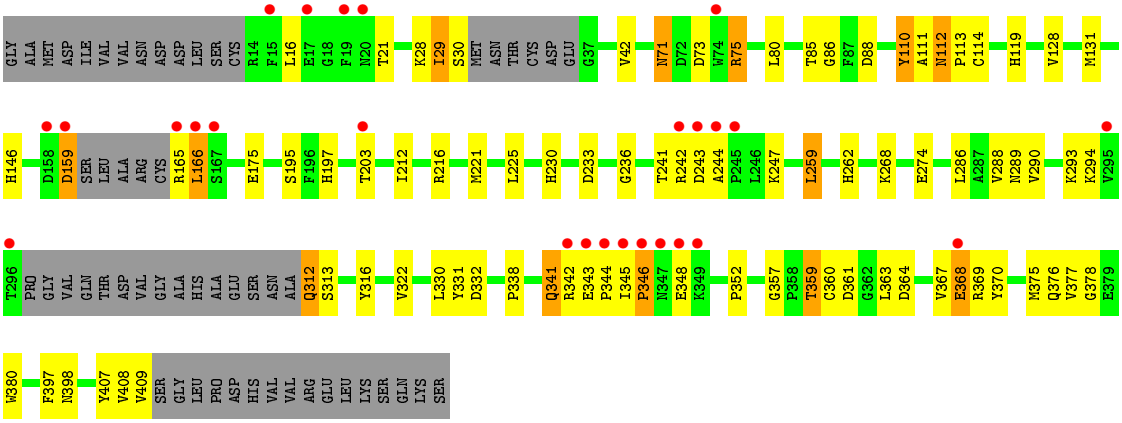
- Molecule 1: ORNITHINE DECARBOXYLASE

Chain B:



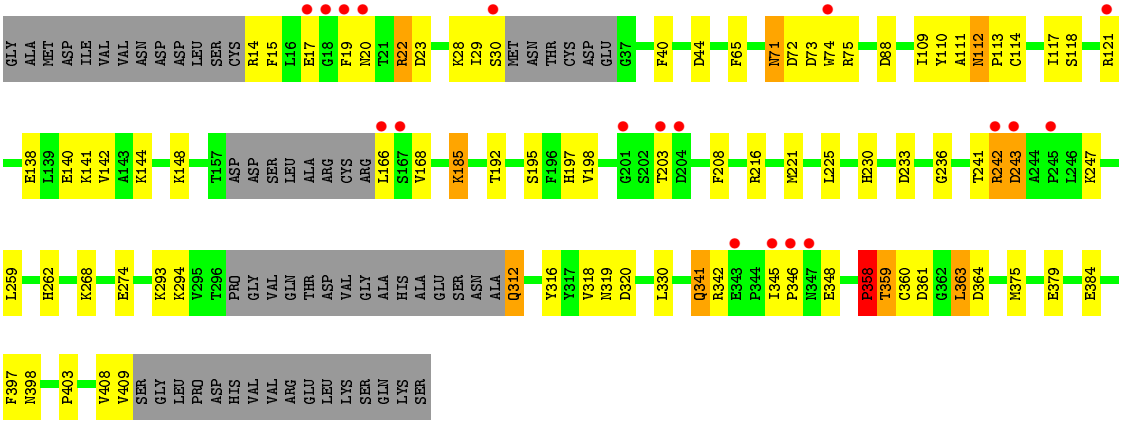
- Molecule 1: ORNITHINE DECARBOXYLASE

Chain C:



- Molecule 1: ORNITHINE DECARBOXYLASE

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	67.29Å 151.60Å 86.41Å 90.00° 103.18° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 19.91 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (8.00-2.00) 89.6 (19.91-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 1.90Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.237 , 0.280 0.222 , 0.258	Depositor DCC
R_{free} test set	2098 reflections (2.00%)	DCC
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	3 of 126566 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12201	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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 46.34 % 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 1.1616e-04.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: PUT, 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	0.46	0/3036	0.69	0/4115
1	B	0.50	1/3058 (0.0%)	0.75	2/4145 (0.0%)
1	C	0.45	0/2975	0.67	0/4032
1	D	0.47	0/2948	0.72	1/3996 (0.0%)
All	All	0.47	1/12017 (0.0%)	0.71	3/16288 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	PRO	N-CA	5.00	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	358	PRO	CA-N-CD	-11.61	95.25	111.50
1	D	358	PRO	CA-N-CD	-8.53	99.56	111.50
1	B	18	GLY	N-CA-C	-7.26	94.94	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	345	ILE	Mainchain

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	2965	0	2931	81	0
1	B	2987	0	2951	70	0
1	C	2906	0	2865	76	0
1	D	2879	0	2844	67	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
2	C	15	0	7	1	0
2	D	15	0	7	1	0
3	A	6	0	10	1	0
3	B	6	0	10	0	0
3	C	6	0	10	1	0
3	D	6	0	10	1	0
4	A	81	0	0	5	0
4	B	110	0	0	6	0
4	C	77	0	0	2	0
4	D	112	0	0	4	0
All	All	12201	0	11659	292	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 12.

All (292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:VAL:O	1:B:358:PRO:HD3	1.37	1.18
1:D:318:VAL:O	1:D:358:PRO:HD3	1.55	1.05
1:A:312:GLN:HE21	1:A:312:GLN:HA	1.25	1.01
1:A:409:VAL:HG21	1:A:419:GLU:OE1	1.62	0.98
1:C:359:THR:HG23	1:C:361:ASP:H	1.31	0.96
1:A:359:THR:HG23	1:A:361:ASP:H	1.34	0.93
1:B:16:LEU:CD1	1:B:24:ALA:HB1	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:HIS:HD2	1:B:236:GLY:H	1.20	0.87
1:A:15:PHE:CE2	1:A:420:LEU:HD22	2.10	0.86
1:D:197:HIS:HD2	1:D:236:GLY:H	1.20	0.86
1:B:22:ARG:HB2	1:B:22:ARG:NH1	1.92	0.84
1:B:312:GLN:HE21	1:B:312:GLN:HA	1.42	0.83
1:A:221:MET:O	1:A:225:LEU:HD23	1.80	0.81
1:D:312:GLN:HE21	1:D:312:GLN:HA	1.45	0.81
1:B:345:ILE:O	1:B:348:GLU:HG3	1.78	0.81
1:A:185:LYS:O	1:A:185:LYS:HE3	1.81	0.80
1:C:221:MET:O	1:C:225:LEU:HD23	1.80	0.80
1:C:197:HIS:HD2	1:C:236:GLY:H	1.29	0.79
1:C:341:GLN:HG2	1:C:380:TRP:HB2	1.64	0.79
1:D:359:THR:HG23	1:D:361:ASP:H	1.47	0.79
1:B:318:VAL:O	1:B:358:PRO:CD	2.28	0.76
1:A:197:HIS:HD2	1:A:236:GLY:H	1.33	0.76
1:B:322:VAL:HB	1:B:330:LEU:HD21	1.67	0.76
1:B:16:LEU:HD11	1:B:24:ALA:HB1	1.68	0.75
1:A:419:GLU:HG3	1:A:420:LEU:HD23	1.69	0.75
1:D:140:GLU:O	1:D:144:LYS:HD3	1.86	0.75
1:D:345:ILE:O	1:D:348:GLU:HG3	1.87	0.75
1:B:216:ARG:HD3	1:B:262:HIS:O	1.86	0.74
1:D:319:ASN:HA	1:D:358:PRO:HG3	1.71	0.73
1:A:345:ILE:O	1:A:348:GLU:HG3	1.89	0.73
1:C:21:THR:HG23	1:C:42:VAL:HG11	1.70	0.72
1:C:316:TYR:CE2	1:C:375:MET:HB2	2.23	0.72
1:B:22:ARG:HH11	1:B:22:ARG:HB2	1.54	0.72
1:C:312:GLN:HA	1:C:312:GLN:HE21	1.55	0.72
1:D:185:LYS:O	1:D:185:LYS:HE3	1.89	0.72
1:A:416:VAL:HA	1:A:419:GLU:OE1	1.90	0.71
1:A:341:GLN:HG2	1:A:380:TRP:HB2	1.72	0.71
1:C:322:VAL:HB	1:C:330:LEU:HD21	1.73	0.70
1:A:359:THR:CG2	1:A:361:ASP:H	2.04	0.70
1:D:216:ARG:HD3	1:D:262:HIS:O	1.91	0.69
1:C:112:ASN:C	1:C:112:ASN:HD22	1.95	0.69
1:B:197:HIS:CD2	1:B:236:GLY:H	2.08	0.68
1:A:195:SER:CB	1:A:233:ASP:HB3	2.24	0.68
1:B:140:GLU:O	1:B:144:LYS:HD3	1.94	0.68
1:D:197:HIS:CD2	1:D:236:GLY:H	2.09	0.68
1:A:416:VAL:O	1:A:420:LEU:HG	1.92	0.68
1:B:359:THR:HG23	1:B:361:ASP:H	1.58	0.67
1:C:80:LEU:HB3	1:C:85:THR:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:THR:CG2	1:D:361:ASP:H	2.08	0.66
1:B:319:ASN:HA	1:B:358:PRO:HG3	1.78	0.66
1:B:359:THR:HB	1:B:364:ASP:OD2	1.95	0.66
1:B:71:ASN:HD22	1:B:71:ASN:C	1.99	0.66
1:C:290:VAL:HG23	1:C:377:VAL:HA	1.77	0.66
1:B:359:THR:CG2	1:B:361:ASP:H	2.09	0.66
1:A:71:ASN:ND2	1:A:73:ASP:H	1.94	0.65
1:C:359:THR:CG2	1:C:361:ASP:H	2.08	0.65
1:D:195:SER:CB	1:D:233:ASP:HB3	2.25	0.65
1:B:16:LEU:HD13	1:B:24:ALA:HB1	1.79	0.65
1:A:312:GLN:NE2	1:A:312:GLN:HA	2.06	0.65
1:B:366:ILE:HG22	1:B:367:VAL:HG23	1.77	0.65
1:A:71:ASN:C	1:A:71:ASN:HD22	2.00	0.65
1:B:322:VAL:HB	1:B:330:LEU:CD2	2.27	0.65
1:D:44:ASP:HA	1:D:408:VAL:HG13	1.79	0.65
1:A:367:VAL:HG11	1:A:370:TYR:HB2	1.77	0.65
1:A:88:ASP:OD1	1:A:111:ALA:HB3	1.96	0.65
1:D:71:ASN:HD22	1:D:71:ASN:C	1.99	0.65
1:A:85:THR:HG23	1:A:86:GLY:O	1.96	0.64
1:A:71:ASN:HD22	1:A:73:ASP:H	1.45	0.64
1:A:316:TYR:CE2	1:A:375:MET:HB2	2.33	0.64
1:C:21:THR:HG23	1:C:42:VAL:CG1	2.27	0.64
1:A:74:TRP:HD1	1:A:97:ARG:NH2	1.96	0.64
1:C:197:HIS:CD2	1:C:236:GLY:H	2.15	0.63
1:D:185:LYS:HG2	4:D:723:HOH:O	1.98	0.63
1:A:312:GLN:HE21	1:A:312:GLN:CA	2.00	0.62
1:B:341:GLN:O	1:B:341:GLN:NE2	2.32	0.62
1:C:341:GLN:NE2	1:C:341:GLN:O	2.30	0.62
1:A:112:ASN:HD22	1:A:112:ASN:C	2.02	0.62
1:D:88:ASP:OD1	1:D:111:ALA:HB3	1.99	0.62
1:B:230:HIS:HB2	1:B:268:LYS:O	2.00	0.62
1:A:337:ARG:HB3	1:A:337:ARG:HH21	1.63	0.61
1:C:71:ASN:HD22	1:C:73:ASP:H	1.47	0.61
1:A:409:VAL:HG11	1:A:416:VAL:HG13	1.81	0.61
1:C:290:VAL:O	1:C:290:VAL:HG23	1.99	0.61
1:C:359:THR:HB	1:C:364:ASP:OD2	2.01	0.61
1:D:221:MET:O	1:D:225:LEU:HD23	2.01	0.61
1:C:293:LYS:HG2	1:C:294:LYS:N	2.15	0.60
1:B:146:HIS:HD2	4:B:756:HOH:O	1.84	0.60
1:D:44:ASP:HA	1:D:408:VAL:CG1	2.32	0.60
1:C:71:ASN:HD22	1:C:71:ASN:C	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ILE:O	1:C:30:SER:HB3	2.01	0.60
1:A:322:VAL:HB	1:A:330:LEU:HD21	1.83	0.60
1:D:241:THR:O	1:D:243:ASP:N	2.34	0.59
1:B:312:GLN:HA	1:B:312:GLN:NE2	2.16	0.59
1:C:312:GLN:CA	1:C:312:GLN:HE21	2.15	0.59
1:D:241:THR:C	1:D:243:ASP:H	2.05	0.59
1:A:216:ARG:HD3	1:A:262:HIS:O	2.02	0.59
1:D:112:ASN:C	1:D:112:ASN:HD22	2.05	0.59
1:B:112:ASN:C	1:B:112:ASN:HD22	2.06	0.59
1:A:409:VAL:CG1	1:A:416:VAL:HG13	2.33	0.58
1:C:367:VAL:HG11	1:C:370:TYR:HB2	1.86	0.58
1:B:394:THR:HG21	4:B:799:HOH:O	2.03	0.58
1:B:293:LYS:HG2	1:B:294:LYS:N	2.16	0.58
1:D:312:GLN:NE2	1:D:312:GLN:HA	2.18	0.58
1:D:71:ASN:ND2	1:D:73:ASP:H	2.02	0.57
1:C:71:ASN:ND2	1:C:73:ASP:H	2.02	0.57
1:B:195:SER:CB	1:B:233:ASP:HB3	2.34	0.57
1:C:341:GLN:C	1:C:341:GLN:HE21	2.07	0.57
1:A:195:SER:HB3	1:A:233:ASP:HB3	1.86	0.57
1:D:22:ARG:HA	1:D:22:ARG:HH11	1.69	0.57
1:A:16:LEU:HD21	1:A:28:LYS:HD2	1.87	0.57
1:C:75:ARG:HH11	1:C:75:ARG:HG2	1.71	0.56
1:C:195:SER:CB	1:C:233:ASP:HB3	2.36	0.56
1:D:195:SER:HB3	1:D:233:ASP:HB3	1.86	0.56
1:C:29:ILE:O	1:C:29:ILE:HG22	2.05	0.56
1:B:88:ASP:OD1	1:B:111:ALA:HB3	2.06	0.56
1:C:343:GLU:HA	1:C:343:GLU:OE2	2.05	0.56
3:A:1002:PUT:H11	1:B:360:CYS:SG	2.46	0.56
1:D:341:GLN:O	1:D:341:GLN:NE2	2.39	0.55
1:C:146:HIS:HD2	4:C:546:HOH:O	1.88	0.55
1:A:29:ILE:O	1:A:30:SER:CB	2.54	0.55
1:D:17:GLU:OE2	1:D:17:GLU:HA	2.06	0.55
1:C:397:PHE:O	1:C:398:ASN:HB2	2.05	0.55
1:B:241:THR:O	1:B:243:ASP:N	2.38	0.55
1:B:360:CYS:HB3	4:B:689:HOH:O	2.07	0.55
1:C:322:VAL:HB	1:C:330:LEU:CD2	2.35	0.54
1:D:242:ARG:HG3	4:D:755:HOH:O	2.07	0.54
1:B:241:THR:C	1:B:243:ASP:H	2.12	0.54
1:D:230:HIS:HB2	1:D:268:LYS:O	2.07	0.54
1:C:241:THR:HB	1:C:243:ASP:OD1	2.08	0.53
1:D:29:ILE:O	1:D:30:SER:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ARG:HB3	1:C:165:ARG:CZ	2.38	0.53
1:D:138:GLU:O	1:D:142:VAL:HG23	2.09	0.53
1:A:289:ASN:HD21	1:A:378:GLY:HA2	1.74	0.53
1:C:216:ARG:HD3	1:C:262:HIS:O	2.08	0.52
1:B:71:ASN:ND2	1:B:73:ASP:H	2.07	0.52
1:B:316:TYR:CE2	1:B:375:MET:HB2	2.44	0.52
1:D:20:ASN:HB2	1:D:23:ASP:HB2	1.92	0.52
1:D:192:THR:HB	1:D:230:HIS:CE1	2.45	0.52
1:A:367:VAL:CG1	1:A:370:TYR:HB2	2.39	0.52
1:C:112:ASN:ND2	1:C:112:ASN:C	2.63	0.51
1:C:338:PRO:HD3	1:C:367:VAL:HG21	1.93	0.51
1:A:157:THR:HG22	1:A:157:THR:O	2.09	0.51
1:B:319:ASN:HA	1:B:358:PRO:CG	2.41	0.51
1:A:360:CYS:HB3	4:A:568:HOH:O	2.10	0.51
1:C:112:ASN:ND2	1:C:114:CYS:H	2.09	0.51
1:C:29:ILE:O	1:C:30:SER:CB	2.59	0.51
1:A:366:ILE:HG22	1:A:367:VAL:HG23	1.94	0.50
1:A:409:VAL:O	1:A:409:VAL:HG22	2.11	0.50
1:A:322:VAL:HB	1:A:330:LEU:CD2	2.41	0.50
1:D:359:THR:HB	1:D:364:ASP:OD2	2.11	0.50
1:A:29:ILE:O	1:A:30:SER:HB3	2.12	0.50
1:C:289:ASN:HD21	1:C:378:GLY:HA2	1.76	0.50
1:B:221:MET:O	1:B:225:LEU:HD23	2.10	0.50
1:D:71:ASN:HD22	1:D:73:ASP:H	1.59	0.50
1:D:293:LYS:HG2	1:D:294:LYS:N	2.27	0.50
1:C:241:THR:C	1:C:243:ASP:H	2.15	0.50
1:A:146:HIS:HD2	4:A:505:HOH:O	1.95	0.50
1:B:66:TYR:CG	1:B:80:LEU:HD13	2.47	0.49
1:A:337:ARG:HB3	1:A:337:ARG:NH2	2.25	0.49
1:B:360:CYS:H	1:B:398:ASN:HD21	1.59	0.49
1:B:128:VAL:O	1:B:146:HIS:HE1	1.95	0.49
1:C:128:VAL:O	1:C:146:HIS:HE1	1.95	0.49
1:A:359:THR:HB	1:A:364:ASP:OD2	2.12	0.49
1:D:168:VAL:HG12	4:D:859:HOH:O	2.12	0.49
1:A:241:THR:C	1:A:243:ASP:H	2.15	0.49
1:C:322:VAL:CG2	1:C:364:ASP:HA	2.42	0.49
1:A:341:GLN:HG3	4:A:576:HOH:O	2.12	0.49
1:D:112:ASN:ND2	1:D:114:CYS:H	2.10	0.49
1:C:332:ASP:OD2	3:C:1006:PUT:N2	2.45	0.49
1:C:159:ASP:N	1:C:159:ASP:OD2	2.46	0.49
1:A:112:ASN:HD22	1:A:113:PRO:N	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:O	1:A:146:HIS:HE1	1.96	0.49
1:D:117:ILE:HG22	1:D:121:ARG:NH2	2.28	0.49
1:C:16:LEU:HD21	1:C:28:LYS:HD2	1.95	0.49
1:C:313:SER:HB3	1:C:352:PRO:HG2	1.95	0.48
1:C:322:VAL:HG22	1:C:364:ASP:HA	1.93	0.48
1:C:312:GLN:HA	1:C:312:GLN:NE2	2.26	0.48
1:B:112:ASN:HD22	1:B:113:PRO:N	2.12	0.48
1:C:119:HIS:HE1	4:D:913:HOH:O	1.96	0.48
1:B:175:GLU:CD	1:B:175:GLU:H	2.15	0.48
1:B:202:SER:HB2	4:B:878:HOH:O	2.12	0.48
1:A:330:LEU:N	1:A:330:LEU:HD22	2.28	0.48
1:A:394:THR:HG21	4:A:650:HOH:O	2.13	0.47
1:B:228:ASN:HB2	4:B:678:HOH:O	2.13	0.47
1:A:112:ASN:ND2	1:A:112:ASN:C	2.67	0.47
1:B:29:ILE:HD12	1:B:341:GLN:OE1	2.15	0.47
1:C:75:ARG:HB2	1:C:407:TYR:CE2	2.49	0.47
1:C:88:ASP:OD1	1:C:111:ALA:HB3	2.15	0.47
1:B:71:ASN:HD22	1:B:73:ASP:H	1.62	0.47
1:A:29:ILE:O	1:A:29:ILE:HG22	2.15	0.47
1:D:360:CYS:H	1:D:398:ASN:HD21	1.62	0.47
1:C:112:ASN:HD22	1:C:113:PRO:N	2.13	0.47
1:A:112:ASN:ND2	1:A:114:CYS:H	2.13	0.47
1:C:344:PRO:C	1:C:345:ILE:HD12	2.36	0.47
1:D:316:TYR:CE2	1:D:375:MET:HB2	2.50	0.46
1:C:341:GLN:HG3	4:C:575:HOH:O	2.14	0.46
1:A:195:SER:HB2	1:A:233:ASP:HB3	1.95	0.46
1:C:85:THR:HG23	1:C:86:GLY:O	2.16	0.46
1:A:241:THR:O	1:A:243:ASP:N	2.41	0.46
1:C:290:VAL:O	1:C:290:VAL:CG2	2.62	0.46
1:D:28:LYS:HD3	1:D:40:PHE:CE1	2.50	0.46
1:C:290:VAL:HG21	1:C:376:GLN:O	2.16	0.46
1:A:110:TYR:HB3	1:A:131:MET:HG2	1.98	0.46
1:C:110:TYR:HB3	1:C:131:MET:HG2	1.98	0.46
1:A:359:THR:HG23	1:A:360:CYS:N	2.30	0.46
1:C:75:ARG:HH11	1:C:75:ARG:CG	2.26	0.45
1:D:185:LYS:HA	1:D:185:LYS:HE3	1.97	0.45
1:D:320:ASP:OD2	1:D:403:PRO:HG2	2.15	0.45
1:D:274:GLU:O	2:D:1007:PLP:H6	2.17	0.45
1:B:174:VAL:HG23	1:B:175:GLU:N	2.30	0.45
1:A:293:LYS:HG2	1:A:294:LYS:N	2.30	0.45
1:A:313:SER:HB3	1:A:352:PRO:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:CD2	1:A:420:LEU:HD22	2.49	0.45
1:A:230:HIS:HB2	1:A:268:LYS:O	2.17	0.45
1:C:212:ILE:HD13	1:C:259:LEU:HD13	1.99	0.45
1:D:195:SER:HB2	1:D:233:ASP:HB3	1.98	0.45
1:C:230:HIS:HB2	1:C:268:LYS:O	2.16	0.45
1:B:232:LEU:HD23	1:B:271:ILE:HD12	1.98	0.45
1:A:409:VAL:CG2	1:A:419:GLU:OE1	2.50	0.45
1:D:112:ASN:HD22	1:D:113:PRO:N	2.15	0.45
1:D:14:ARG:HH11	1:D:14:ARG:HG3	1.82	0.45
1:B:198:VAL:HG23	1:B:199:GLY:O	2.17	0.44
1:C:359:THR:HG23	1:C:360:CYS:N	2.32	0.44
1:D:312:GLN:CA	1:D:312:GLN:HE21	2.15	0.44
1:C:166:LEU:HD13	1:C:166:LEU:N	2.32	0.44
1:D:363:LEU:HA	1:D:363:LEU:HD12	1.78	0.44
1:B:345:ILE:H	1:B:348:GLU:CD	2.21	0.44
1:C:331:TYR:CE2	1:D:330:LEU:HD12	2.52	0.44
1:D:198:VAL:HG21	1:D:208:PHE:CE2	2.53	0.44
1:B:192:THR:HB	1:B:230:HIS:CE1	2.53	0.44
1:C:195:SER:HB3	1:C:233:ASP:HB3	1.99	0.44
1:B:198:VAL:HG21	1:B:208:PHE:CE2	2.53	0.44
1:D:71:ASN:HD22	1:D:72:ASP:N	2.16	0.44
1:D:15:PHE:HZ	1:D:75:ARG:HE	1.64	0.44
1:B:417:VAL:CG1	1:B:421:LYS:HE3	2.47	0.43
1:B:349:LYS:HD3	1:B:350:LEU:H	1.83	0.43
1:A:397:PHE:O	1:A:398:ASN:HB2	2.18	0.43
1:C:357:GLY:HA3	1:C:364:ASP:OD1	2.18	0.43
1:C:360:CYS:SG	3:D:1008:PUT:H11	2.58	0.43
1:C:225:LEU:HD22	1:C:225:LEU:N	2.34	0.43
1:A:105:PRO:HB2	1:A:127:GLY:O	2.19	0.43
1:A:197:HIS:CE1	1:A:199:GLY:HA2	2.53	0.43
1:B:19:PHE:CD2	1:B:19:PHE:C	2.90	0.43
1:B:212:ILE:HD13	1:B:259:LEU:HD13	2.00	0.43
1:A:116:GLN:NE2	1:B:319:ASN:HD22	2.17	0.43
1:A:66:TYR:CG	1:A:80:LEU:HD13	2.53	0.43
1:A:202:SER:HB2	4:A:733:HOH:O	2.17	0.43
1:A:312:GLN:NE2	1:A:312:GLN:CA	2.70	0.43
1:A:409:VAL:HG11	1:A:419:GLU:OE1	2.19	0.43
1:A:347:ASN:C	1:A:347:ASN:HD22	2.22	0.43
1:A:168:VAL:O	1:A:168:VAL:HG22	2.18	0.43
1:A:344:PRO:C	1:A:345:ILE:HD12	2.39	0.43
1:B:263:PHE:HB3	1:B:269:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ILE:HD11	1:D:141:LYS:HD3	2.01	0.42
1:A:185:LYS:HA	1:A:185:LYS:HD2	1.84	0.42
1:B:195:SER:HB3	1:B:233:ASP:HB3	2.01	0.42
1:B:289:ASN:ND2	4:B:673:HOH:O	2.52	0.42
1:A:413:PRO:O	1:A:415:HIS:N	2.42	0.42
1:A:138:GLU:O	1:A:142:VAL:HG23	2.20	0.42
1:D:342:ARG:HD2	1:D:379:GLU:OE2	2.20	0.42
1:B:205:ALA:HB3	1:B:254:VAL:HG21	2.02	0.42
1:B:121:ARG:HG3	1:B:124:ARG:NH2	2.34	0.42
1:B:342:ARG:HD2	1:B:379:GLU:OE2	2.20	0.42
1:A:15:PHE:HA	1:A:407:TYR:O	2.19	0.42
1:A:195:SER:HA	1:A:233:ASP:O	2.19	0.42
1:D:19:PHE:HD1	1:D:19:PHE:O	2.02	0.42
1:D:19:PHE:CE2	1:D:409:VAL:O	2.73	0.42
1:D:22:ARG:NH2	1:D:384:GLU:OE2	2.52	0.41
1:C:75:ARG:NH1	1:C:75:ARG:CG	2.81	0.41
1:A:264:PRO:HA	1:A:265:PRO:HD3	1.95	0.41
1:B:363:LEU:HA	1:B:363:LEU:HD12	1.81	0.41
1:D:241:THR:C	1:D:243:ASP:N	2.73	0.41
1:D:397:PHE:O	1:D:398:ASN:HB2	2.20	0.41
1:A:274:GLU:O	2:A:1001:PLP:H6	2.21	0.41
1:D:166:LEU:HD23	1:D:197:HIS:ND1	2.35	0.41
1:B:112:ASN:C	1:B:112:ASN:ND2	2.72	0.41
1:B:112:ASN:ND2	1:B:114:CYS:H	2.18	0.41
1:C:75:ARG:HD2	1:C:75:ARG:N	2.36	0.41
1:C:368:GLU:OE1	1:C:369:ARG:HG3	2.19	0.41
1:D:65:PHE:CD2	1:D:109:ILE:HG13	2.56	0.41
1:D:148:LYS:HE2	1:D:148:LYS:HB3	1.86	0.41
1:A:71:ASN:C	1:A:71:ASN:ND2	2.71	0.41
1:C:367:VAL:CG1	1:C:370:TYR:HB2	2.50	0.41
1:D:29:ILE:O	1:D:30:SER:CB	2.69	0.41
1:C:286:LEU:HG	1:C:288:VAL:HG13	2.03	0.41
1:C:274:GLU:O	2:C:1005:PLP:H6	2.20	0.41
1:C:342:ARG:NH2	1:C:348:GLU:OE1	2.54	0.41
1:B:274:GLU:O	2:B:1003:PLP:H6	2.21	0.41
1:B:22:ARG:CZ	1:B:22:ARG:HB2	2.49	0.40
1:D:112:ASN:C	1:D:112:ASN:ND2	2.73	0.40
1:D:118:SER:HA	1:D:121:ARG:NH1	2.36	0.40
1:B:284:PHE:HB2	1:B:387:GLY:CA	2.51	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	370/425 (87%)	351 (95%)	16 (4%)	3 (1%)	24	15
1	B	373/425 (88%)	356 (95%)	13 (4%)	4 (1%)	17	9
1	C	362/425 (85%)	341 (94%)	17 (5%)	4 (1%)	17	9
1	D	359/425 (84%)	345 (96%)	12 (3%)	2 (1%)	30	22
All	All	1464/1700 (86%)	1393 (95%)	58 (4%)	13 (1%)	21	13

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	ARG
1	A	346	PRO
1	B	346	PRO
1	C	346	PRO
1	D	242	ARG
1	B	242	ARG
1	C	242	ARG
1	B	29	ILE
1	B	244	ALA
1	C	244	ALA
1	A	413	PRO
1	C	29	ILE
1	D	346	PRO

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	323/362 (89%)	305 (94%)	18 (6%)	26	20
1	B	326/362 (90%)	304 (93%)	22 (7%)	20	14
1	C	316/362 (87%)	298 (94%)	18 (6%)	25	19
1	D	313/362 (86%)	298 (95%)	15 (5%)	31	26
All	All	1278/1448 (88%)	1205 (94%)	73 (6%)	25	19

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	71	ASN
1	A	74	TRP
1	A	85	THR
1	A	110	TYR
1	A	112	ASN
1	A	119	HIS
1	A	137	ASP
1	A	185	LYS
1	A	247	LYS
1	A	259	LEU
1	A	312	GLN
1	A	341	GLN
1	A	347	ASN
1	A	359	THR
1	A	363	LEU
1	A	409	VAL
1	A	415	HIS
1	B	19	PHE
1	B	22	ARG
1	B	71	ASN
1	B	74	TRP
1	B	110	TYR
1	B	112	ASN
1	B	119	HIS
1	B	137	ASP
1	B	158	ASP
1	B	243	ASP
1	B	247	LYS
1	B	259	LEU
1	B	312	GLN
1	B	330	LEU
1	B	341	GLN

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Mol	Chain	Res	Type
1	B	343	GLU
1	B	346	PRO
1	B	347	ASN
1	B	358	PRO
1	B	359	THR
1	B	363	LEU
1	B	368	GLU
1	C	71	ASN
1	C	75	ARG
1	C	110	TYR
1	C	112	ASN
1	C	159	ASP
1	C	166	LEU
1	C	175	GLU
1	C	203	THR
1	C	247	LYS
1	C	259	LEU
1	C	312	GLN
1	C	341	GLN
1	C	346	PRO
1	C	359	THR
1	C	363	LEU
1	C	368	GLU
1	C	408	VAL
1	C	409	VAL
1	D	22	ARG
1	D	71	ASN
1	D	74	TRP
1	D	110	TYR
1	D	112	ASN
1	D	185	LYS
1	D	203	THR
1	D	243	ASP
1	D	247	LYS
1	D	259	LEU
1	D	312	GLN
1	D	341	GLN
1	D	358	PRO
1	D	359	THR
1	D	363	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	96	GLN
1	A	112	ASN
1	A	116	GLN
1	A	119	HIS
1	A	146	HIS
1	A	197	HIS
1	A	210	GLN
1	A	230	HIS
1	A	256	ASN
1	A	289	ASN
1	A	312	GLN
1	A	341	GLN
1	B	71	ASN
1	B	112	ASN
1	B	116	GLN
1	B	119	HIS
1	B	146	HIS
1	B	197	HIS
1	B	256	ASN
1	B	289	ASN
1	B	312	GLN
1	B	401	GLN
1	C	71	ASN
1	C	112	ASN
1	C	116	GLN
1	C	119	HIS
1	C	146	HIS
1	C	197	HIS
1	C	210	GLN
1	C	230	HIS
1	C	256	ASN
1	C	262	HIS
1	C	289	ASN
1	C	312	GLN
1	D	71	ASN
1	D	112	ASN
1	D	116	GLN
1	D	146	HIS
1	D	197	HIS
1	D	256	ASN
1	D	289	ASN
1	D	312	GLN

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Mol	Chain	Res	Type
1	D	401	GLN

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

8 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	1001	3	15,15,16	2.40	5 (33%)	21,22,23	1.42	3 (14%)
3	PUT	A	1002	2	5,5,5	0.50	0	4,4,4	0.67	0
2	PLP	B	1003	3	15,15,16	2.11	3 (20%)	21,22,23	1.17	2 (9%)
3	PUT	B	1004	2	5,5,5	0.41	0	4,4,4	0.71	0
2	PLP	C	1005	3	15,15,16	2.94	4 (26%)	21,22,23	1.46	4 (19%)
3	PUT	C	1006	2	5,5,5	0.35	0	4,4,4	0.94	0
2	PLP	D	1007	3	15,15,16	2.30	4 (26%)	21,22,23	1.63	3 (14%)
3	PUT	D	1008	2	5,5,5	0.32	0	4,4,4	0.86	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	1001	3	-	0/6/6/8	0/1/1/1
3	PUT	A	1002	2	-	0/3/3/3	0/0/0/0
2	PLP	B	1003	3	-	0/6/6/8	0/1/1/1
3	PUT	B	1004	2	-	0/3/3/3	0/0/0/0
2	PLP	C	1005	3	-	0/6/6/8	0/1/1/1
3	PUT	C	1006	2	-	0/3/3/3	0/0/0/0
2	PLP	D	1007	3	-	0/6/6/8	0/1/1/1
3	PUT	D	1008	2	-	0/3/3/3	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	PLP	C2A-C2	2.24	1.54	1.50
2	A	1001	PLP	C4A-C4	2.36	1.56	1.51
2	C	1005	PLP	C6-C5	2.79	1.43	1.37
2	B	1003	PLP	C6-C5	2.97	1.44	1.37
2	A	1001	PLP	C6-C5	2.97	1.44	1.37
2	D	1007	PLP	C4A-C4	3.05	1.57	1.51
2	C	1005	PLP	C2A-C2	3.05	1.56	1.50
2	D	1007	PLP	C6-C5	3.35	1.45	1.37
2	A	1001	PLP	C3-C2	4.18	1.43	1.40
2	B	1003	PLP	C3-C2	4.34	1.43	1.40
2	D	1007	PLP	C3-C2	4.67	1.44	1.40
2	B	1003	PLP	C5-C4	5.07	1.46	1.40
2	D	1007	PLP	C5-C4	5.42	1.46	1.40
2	A	1001	PLP	C5-C4	6.74	1.48	1.40
2	C	1005	PLP	C3-C2	6.85	1.45	1.40
2	C	1005	PLP	C5-C4	7.34	1.49	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1007	PLP	C4A-C4-C3	-2.64	115.58	120.36
2	C	1005	PLP	C5-C6-N1	-2.20	120.05	123.86
2	A	1001	PLP	C5-C6-N1	-2.02	120.36	123.86
2	C	1005	PLP	O4P-P-O1P	2.03	112.32	107.14
2	B	1003	PLP	C6-N1-C2	2.05	123.47	119.28
2	A	1001	PLP	O4P-P-O1P	2.22	112.80	107.14
2	B	1003	PLP	C5A-C5-C4	2.54	125.01	121.65
2	C	1005	PLP	O3-C3-C2	2.91	122.72	117.66
2	D	1007	PLP	C5A-C5-C4	2.95	125.56	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1005	PLP	C5A-C5-C4	3.15	125.82	121.65
2	A	1001	PLP	C5A-C5-C4	3.72	126.57	121.65
2	D	1007	PLP	C4A-C4-C5	4.55	125.62	120.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	PLP	1	0
3	A	1002	PUT	1	0
2	B	1003	PLP	1	0
2	C	1005	PLP	1	0
3	C	1006	PUT	1	0
2	D	1007	PLP	1	0
3	D	1008	PUT	1	0

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, 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	378/425 (88%)	0.09	28 (7%)	17	18	13, 25, 64, 83	0
1	B	381/425 (89%)	0.08	22 (5%)	26	28	10, 23, 55, 85	0
1	C	370/425 (87%)	0.15	26 (7%)	19	21	13, 26, 63, 88	0
1	D	367/425 (86%)	0.07	19 (5%)	31	33	11, 25, 54, 81	0
All	All	1496/1700 (88%)	0.10	95 (6%)	23	24	10, 25, 60, 88	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	PHE	14.2
1	D	19	PHE	9.6
1	B	18	GLY	8.7
1	A	347	ASN	6.9
1	D	166	LEU	6.3
1	D	167	SER	5.8
1	B	203	THR	5.6
1	C	74	TRP	5.6
1	A	345	ILE	5.4
1	B	346	PRO	5.3
1	B	158	ASP	5.2
1	A	242	ARG	5.2
1	B	30	SER	5.2
1	B	347	ASN	5.2
1	A	346	PRO	5.0
1	C	159	ASP	4.7
1	D	74	TRP	4.7
1	A	243	ASP	4.7
1	C	158	ASP	4.7
1	C	343	GLU	4.6
1	C	17	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	243	ASP	4.5
1	D	242	ARG	4.5
1	A	415	HIS	4.4
1	C	344	PRO	4.4
1	C	165	ARG	4.4
1	A	421	LYS	4.3
1	C	347	ASN	4.2
1	D	243	ASP	4.1
1	A	420	LEU	3.9
1	B	345	ILE	3.9
1	C	19	PHE	3.8
1	D	18	GLY	3.8
1	B	201	GLY	3.7
1	A	418	ARG	3.6
1	C	296	THR	3.6
1	C	244	ALA	3.5
1	C	345	ILE	3.5
1	C	203	THR	3.5
1	D	203	THR	3.4
1	B	17	GLU	3.4
1	A	344	PRO	3.4
1	D	201	GLY	3.4
1	D	204	ASP	3.3
1	A	203	THR	3.3
1	C	346	PRO	3.2
1	A	74	TRP	3.1
1	D	345	ILE	3.1
1	A	417	VAL	3.1
1	B	343	GLU	3.0
1	B	242	ARG	3.0
1	B	245	PRO	3.0
1	B	20	ASN	2.9
1	A	413	PRO	2.9
1	B	166	LEU	2.9
1	A	419	GLU	2.9
1	B	204	ASP	2.9
1	C	242	ARG	2.9
1	B	167	SER	2.9
1	D	20	ASN	2.9
1	A	422	SER	2.8
1	B	296	THR	2.8
1	A	335	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	414	ASP	2.7
1	C	368	GLU	2.7
1	D	346	PRO	2.6
1	A	296	THR	2.6
1	A	204	ASP	2.6
1	A	17	GLU	2.6
1	B	312	GLN	2.6
1	C	295	VAL	2.6
1	C	349	LYS	2.5
1	B	243	ASP	2.5
1	B	344	PRO	2.4
1	D	245	PRO	2.4
1	D	17	GLU	2.4
1	C	166	LEU	2.4
1	D	121	ARG	2.4
1	C	245	PRO	2.4
1	D	343	GLU	2.3
1	C	15	PHE	2.3
1	C	342	ARG	2.3
1	A	350	LEU	2.2
1	A	19	PHE	2.2
1	C	167	SER	2.2
1	A	312	GLN	2.2
1	A	363	LEU	2.2
1	D	347	ASN	2.2
1	A	343	GLU	2.2
1	A	201	GLY	2.2
1	D	30	SER	2.2
1	C	348	GLU	2.1
1	A	370	TYR	2.1
1	B	414	ASP	2.1
1	C	20	ASN	2.1

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

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
3	PUT	B	1004	6/6	0.68	0.34	19.21	44,51,55,59	0
3	PUT	A	1002	6/6	0.65	0.32	15.44	40,46,48,51	0
3	PUT	C	1006	6/6	0.76	0.27	12.38	43,49,53,53	0
3	PUT	D	1008	6/6	0.60	0.25	1.29	43,50,54,55	0
2	PLP	B	1003	15/16	0.97	0.10	-0.07	14,22,30,34	0
2	PLP	A	1001	15/16	0.98	0.09	-0.37	15,23,29,31	0
2	PLP	C	1005	15/16	0.97	0.09	-0.39	16,22,31,34	0
2	PLP	D	1007	15/16	0.97	0.08	-0.48	13,23,28,34	0

6.5 Other polymers

There are no such residues in this entry.