



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:15 PM GMT

PDB ID : 1B4N
Title : FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE FROM PYRO-
COCCUS FURIOSUS, COMPLEXED WITH GLUTARATE
Authors : Hu, Y.L.; Faham, S.; Roy, R.; Adams, M.W.W.; Rees, D.C.
Deposited on : 1998-12-24
Resolution : 2.40 Å(reported)

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

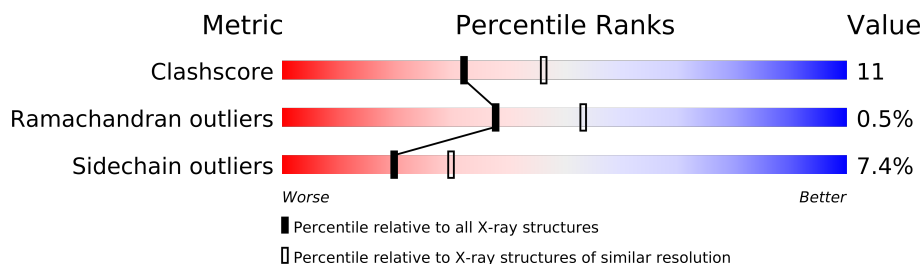
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	619	
1	B	619	
1	C	619	
1	D	619	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19600 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4786	3067	809	888	22			
1	B	611	Total	C	N	O	S	0	0	0
			4786	3067	809	888	22			
1	C	611	Total	C	N	O	S	0	0	0
			4786	3067	809	888	22			
1	D	611	Total	C	N	O	S	0	0	0
			4786	3067	809	888	22			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

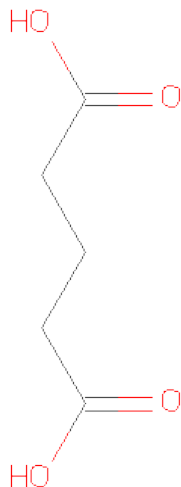
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



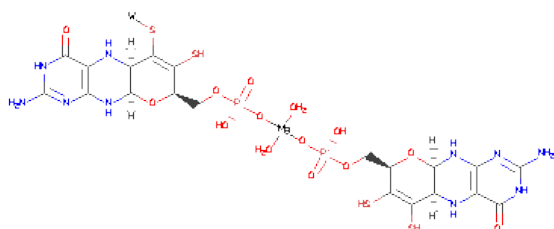
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is GLUTARIC ACID (three-letter code: GUA) (formula: C₅H₈O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 5 4	0	0
4	B	1	Total C O 9 5 4	0	0
4	C	1	Total C O 9 5 4	0	0
4	D	1	Total C O 9 5 4	0	0

- Molecule 5 is TUNGSTOPTERIN COFACTOR (three-letter code: PTE) (formula: $C_{20}H_{29}MgN_{10}O_{14}P_2S$)



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Mg N O P S W 50 20 1 10 12 2 4 1	0	0
5	B	1	Total C Mg N O P S W 50 20 1 10 12 2 4 1	0	0
5	C	1	Total C Mg N O P S W 50 20 1 10 12 2 4 1	0	0
5	D	1	Total C Mg N O P S W 50 20 1 10 12 2 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	38	Total O 38 38	0	0
6	B	46	Total O 46 46	0	0

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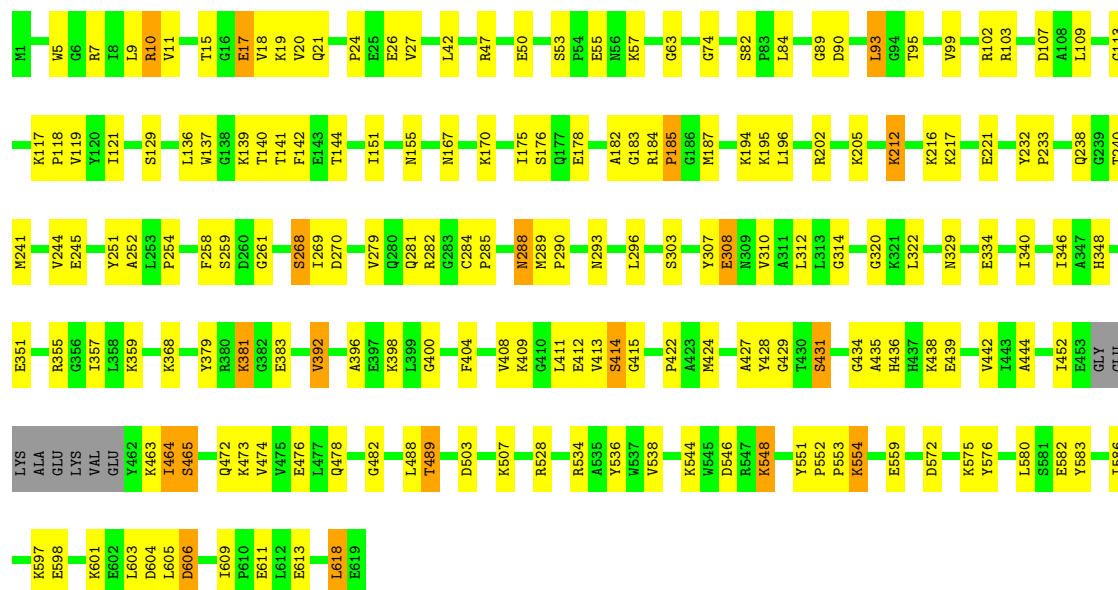
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	49	Total	O	0	0
			49	49		
6	D	51	Total	O	0	0
			51	51		



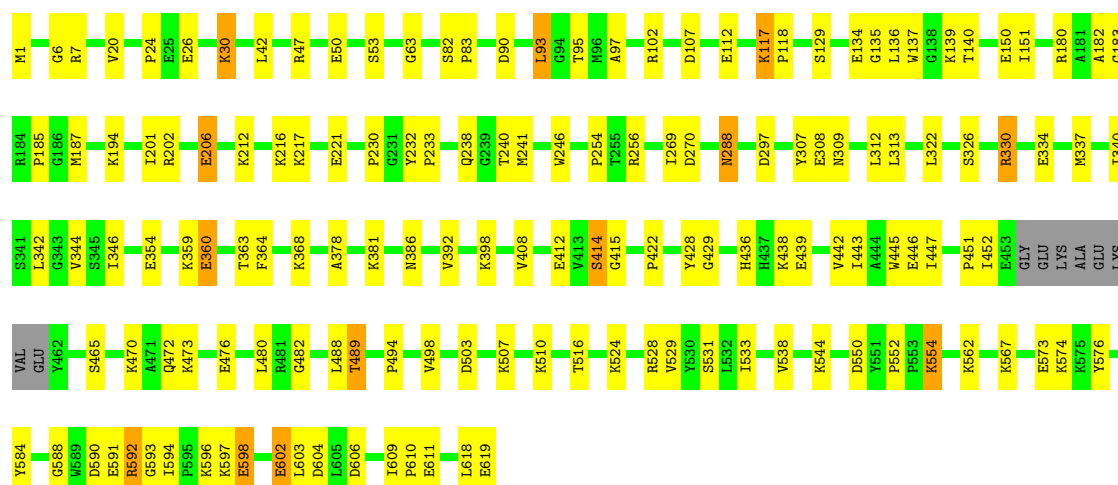
- Molecule 1: FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE

Chain C:



- Molecule 1: FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE

Chain D:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.40Å 170.50Å 180.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	77.0 (30.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.177 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19600	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTE, GUA, CA, SF4

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	0.40	0/4896	0.60	0/6619
1	B	0.41	0/4896	0.62	0/6619
1	C	0.42	0/4896	0.61	0/6619
1	D	0.40	0/4896	0.61	0/6619
All	All	0.41	0/19584	0.61	0/26476

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4786	0	4773	123	0
1	B	4786	0	4773	116	0
1	C	4786	0	4773	109	0
1	D	4786	0	4773	93	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	0	0	0
3	B	8	0	0	1	0
3	C	8	0	0	1	0
3	D	8	0	0	0	0
4	A	9	0	0	2	0
4	B	9	0	0	3	0
4	C	9	0	0	2	0
4	D	9	0	0	1	0
5	A	50	0	20	1	0
5	B	50	0	20	1	0
5	C	50	0	19	1	0
5	D	50	0	20	1	0
6	A	38	0	0	1	0
6	B	46	0	0	3	0
6	C	49	0	0	3	0
6	D	51	0	0	2	0
All	All	19600	0	19171	441	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (441) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:93:LEU:HB3	1:D:182:ALA:HB2	1.34	1.05
1:A:93:LEU:HB3	1:A:182:ALA:HB2	1.39	1.02
1:C:93:LEU:HB3	1:C:182:ALA:HB2	1.39	1.02
1:C:572:ASP:OD2	1:C:575:LYS:HG3	1.65	0.97
1:B:93:LEU:HB3	1:B:182:ALA:HB2	1.47	0.94
1:A:426:LEU:HD23	1:A:474:VAL:HG21	1.51	0.93
1:B:288:ASN:H	1:B:288:ASN:HD22	1.15	0.91
1:B:308:GLU:HG2	1:B:340:ILE:HD11	1.50	0.91
1:C:74:GLY:HA3	1:C:285:PRO:HG2	1.53	0.89
1:A:439:GLU:HG2	1:A:482:GLY:HA3	1.54	0.86
1:A:232:TYR:HB3	1:A:233:PRO:HD3	1.58	0.85
1:A:534:ARG:O	1:A:538:VAL:HG23	1.78	0.84
1:B:510:LYS:HB2	1:B:510:LYS:HZ2	1.43	0.83
1:B:26:GLU:O	1:B:30:LYS:HB2	1.80	0.82
1:C:103:ARG:O	1:C:205:LYS:HB2	1.80	0.81
1:C:268:SER:HB2	1:C:320:GLY:O	1.80	0.80
1:B:24:PRO:HB3	1:B:26:GLU:OE2	1.84	0.78
1:C:50:GLU:HB2	1:C:53:SER:HB3	1.67	0.77
1:C:9:LEU:HD23	1:C:109:LEU:HD13	1.68	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:572:ASP:OD2	1:B:575:LYS:HG3	1.86	0.76
1:D:308:GLU:HG2	1:D:340:ILE:HD11	1.69	0.75
1:C:444:ALA:HB3	6:C:639:HOH:O	1.86	0.74
1:A:572:ASP:OD2	1:A:575:LYS:HG3	1.88	0.73
1:A:214:GLU:OE1	1:A:217:LYS:HD3	1.88	0.72
1:D:340:ILE:O	1:D:344:VAL:HG23	1.90	0.72
1:A:345:SER:O	1:A:349:VAL:HG23	1.89	0.71
1:B:149:LYS:HD3	1:B:154:LYS:HA	1.71	0.71
1:D:297:ASP:HB3	1:D:326:SER:HB3	1.74	0.70
1:C:11:VAL:HG22	1:C:18:VAL:HG22	1.74	0.70
1:A:414:SER:HB2	1:A:428:TYR:OH	1.91	0.70
1:A:330:ARG:O	1:A:334:GLU:HG2	1.92	0.70
1:A:50:GLU:HB2	1:A:53:SER:HB3	1.72	0.69
1:B:7:ARG:NH1	1:B:20:VAL:HG11	2.07	0.69
1:C:284:CYS:HB3	1:C:285:PRO:HD2	1.75	0.68
1:C:308:GLU:HG2	1:C:340:ILE:HD11	1.76	0.66
1:D:136:LEU:O	1:D:139:LYS:HG3	1.95	0.66
1:B:256:ARG:HG2	1:B:364:PHE:CG	2.30	0.66
1:B:481:ARG:HH22	4:B:622:GUA:C1	2.09	0.66
1:B:93:LEU:HA	5:B:623:PTE:O5P	1.96	0.65
1:C:474:VAL:O	1:C:478:GLN:HG3	1.97	0.65
1:A:74:GLY:HA3	1:A:285:PRO:HG2	1.79	0.65
1:A:598:GLU:O	1:A:602:GLU:HB2	1.96	0.65
1:C:140:THR:HB	1:C:334:GLU:HB2	1.77	0.65
1:B:83:PRO:HD2	1:B:185:PRO:O	1.97	0.65
1:C:24:PRO:HD2	1:C:27:VAL:HG21	1.79	0.65
1:D:238:GLN:O	1:D:241:MET:HB2	1.96	0.64
1:C:381:LYS:NZ	1:C:381:LYS:HB3	2.13	0.64
1:B:50:GLU:HB2	1:B:53:SER:HB3	1.79	0.64
1:C:288:ASN:H	1:C:288:ASN:HD22	1.44	0.64
1:C:503:ASP:O	1:C:507:LYS:HG3	1.97	0.64
1:B:238:GLN:O	1:B:241:MET:HB2	1.98	0.64
1:C:238:GLN:O	1:C:241:MET:HB2	1.98	0.63
1:D:588:GLY:O	1:D:596:LYS:HG3	1.98	0.63
1:D:50:GLU:HB2	1:D:53:SER:HB3	1.80	0.63
1:B:288:ASN:N	1:B:288:ASN:HD22	1.90	0.62
1:C:183:GLY:HA3	1:C:187:MET:HB2	1.80	0.62
1:D:232:TYR:HB3	1:D:233:PRO:HD3	1.79	0.62
1:C:431:SER:HB3	1:C:434:GLY:O	1.99	0.62
1:A:288:ASN:HD22	1:A:288:ASN:H	1.47	0.62
1:C:424:MET:O	1:C:427:ALA:HB3	2.00	0.62
1:B:7:ARG:HH11	1:B:20:VAL:HG11	1.65	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:427:ALA:HB1	1:A:440:ALA:HB3	1.82	0.62
1:D:414:SER:HB3	1:D:428:TYR:OH	2.00	0.62
1:D:118:PRO:HB3	1:D:137:TRP:CE3	2.35	0.62
1:C:439:GLU:HG2	1:C:482:GLY:HA3	1.82	0.62
1:A:43:TRP:O	1:A:539:ARG:NH2	2.31	0.61
1:A:431:SER:HB3	1:A:434:GLY:O	2.00	0.61
1:D:7:ARG:NH1	1:D:20:VAL:HG11	2.16	0.61
1:B:148:LEU:HD23	1:C:151:ILE:HD12	1.82	0.60
1:A:63:GLY:HA3	1:A:488:LEU:O	2.02	0.60
1:B:13:LEU:HD12	1:B:194:LYS:HB3	1.83	0.60
1:B:308:GLU:OE2	1:B:415:GLY:N	2.28	0.60
1:C:99:VAL:O	1:C:103:ARG:HG3	2.01	0.59
1:C:281:GLN:NE2	1:C:293:ASN:OD1	2.35	0.59
1:D:381:LYS:NZ	1:D:381:LYS:HB3	2.17	0.59
1:B:566:HIS:O	1:B:569:GLU:HB2	2.02	0.59
1:B:503:ASP:O	1:B:506:PRO:HD2	2.03	0.59
1:D:342:LEU:O	1:D:346:ILE:HG13	2.01	0.59
1:C:355:ARG:HB2	1:C:357:ILE:HD12	1.85	0.59
1:D:254:PRO:HG2	1:D:415:GLY:HA2	1.84	0.58
1:C:308:GLU:OE2	1:C:415:GLY:N	2.33	0.58
1:C:47:ARG:NH1	1:C:611:GLU:OE2	2.36	0.58
1:A:151:ILE:HG13	1:D:151:ILE:HG13	1.84	0.58
1:B:381:LYS:NZ	1:B:381:LYS:HB3	2.19	0.58
1:B:429:GLY:O	1:B:550:ASP:HA	2.02	0.58
1:C:217:LYS:O	1:C:221:GLU:HG3	2.03	0.58
1:B:342:LEU:O	1:B:346:ILE:HG13	2.03	0.58
1:A:393:LYS:HD2	1:A:410:GLY:HA2	1.84	0.58
1:B:99:VAL:O	1:B:103:ARG:HG2	2.04	0.58
1:C:355:ARG:CB	1:C:357:ILE:HD12	2.34	0.58
1:B:431:SER:HB3	1:B:434:GLY:O	2.04	0.57
1:A:543:GLY:HA3	1:A:616:THR:HG23	1.84	0.57
1:A:441:TRP:HB2	1:A:481:ARG:NH2	2.20	0.57
1:A:610:PRO:O	1:A:614:LYS:HG3	2.04	0.57
1:C:167:ASN:ND2	1:C:379:TYR:HA	2.20	0.57
1:A:308:GLU:CG	1:A:340:ILE:HD11	2.34	0.57
1:B:532:LEU:O	1:B:535:ALA:HB3	2.05	0.57
1:B:240:THR:O	1:B:307:TYR:HB2	2.04	0.57
1:C:392:VAL:CG2	1:C:412:GLU:HG3	2.35	0.57
1:B:185:PRO:HD3	6:B:629:HOH:O	2.05	0.56
1:D:354:GLU:OE2	1:D:363:THR:HB	2.05	0.56
1:A:63:GLY:N	1:A:66:ASN:OD1	2.39	0.56
1:A:429:GLY:O	1:A:550:ASP:HA	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:175:ILE:HG22	1:C:176:SER:N	2.19	0.56
1:C:212:LYS:O	1:C:216:LYS:HG3	2.05	0.56
1:A:45:GLU:HB3	1:A:57:LYS:HE2	1.87	0.56
1:A:93:LEU:HA	5:A:623:PTE:O5P	2.05	0.56
1:D:117:LYS:HB2	6:D:664:HOH:O	2.06	0.56
1:D:308:GLU:CG	1:D:340:ILE:HD11	2.36	0.55
1:C:142:PHE:CE1	1:C:178:GLU:HA	2.41	0.55
1:D:524:LYS:HE3	1:D:528:ARG:NH2	2.21	0.55
1:A:539:ARG:HD2	1:A:540:GLU:OE2	2.05	0.55
1:A:147:GLU:HB3	1:D:151:ILE:HD11	1.87	0.55
1:D:330:ARG:O	1:D:334:GLU:HG2	2.06	0.55
1:D:446:GLU:HG3	1:D:470:LYS:HE2	1.87	0.55
1:A:597:LYS:NZ	1:A:618:LEU:HB3	2.22	0.55
1:D:185:PRO:HD2	1:D:187:MET:CE	2.36	0.55
1:D:309:ASN:O	1:D:313:LEU:HB2	2.07	0.55
1:C:93:LEU:HA	5:C:623:PTE:O5P	2.07	0.55
1:A:308:GLU:HG2	1:A:340:ILE:HD11	1.88	0.54
1:D:598:GLU:O	1:D:602:GLU:HB2	2.07	0.54
1:D:312:LEU:HG	1:D:340:ILE:HG23	1.89	0.54
1:A:503:ASP:O	1:A:506:PRO:HD2	2.06	0.54
1:D:240:THR:O	1:D:307:TYR:HB2	2.07	0.54
1:A:52:LEU:HD22	1:A:193:SER:HB3	1.89	0.54
1:B:103:ARG:HB2	1:B:203:GLY:HA3	1.89	0.54
1:A:404:PHE:HB3	1:A:555:ARG:NH2	2.23	0.54
1:A:534:ARG:NH1	1:A:545:TRP:HE1	2.06	0.54
1:B:309:ASN:O	1:B:313:LEU:HB2	2.08	0.54
1:B:91:GLY:HA3	1:B:183:GLY:H	1.73	0.53
1:C:534:ARG:O	1:C:538:VAL:HG23	2.08	0.53
1:B:103:ARG:O	1:B:205:LYS:HB2	2.08	0.53
1:D:206:GLU:HG2	1:D:206:GLU:O	2.08	0.53
1:D:26:GLU:CD	1:D:26:GLU:H	2.12	0.53
1:A:76:LEU:HB2	1:A:98:SER:HB2	1.90	0.53
1:C:117:LYS:O	1:C:119:VAL:HG13	2.08	0.53
1:B:288:ASN:H	1:B:288:ASN:ND2	1.95	0.53
1:A:140:THR:HB	1:A:334:GLU:HB2	1.91	0.53
1:D:445:TRP:CD1	1:D:473:LYS:HE2	2.44	0.53
1:B:232:TYR:HB3	1:B:233:PRO:HD3	1.89	0.53
1:B:259:SER:HB2	6:B:656:HOH:O	2.09	0.52
1:D:93:LEU:HA	5:D:623:PTE:O5P	2.09	0.52
1:B:183:GLY:HA3	1:B:187:MET:HB2	1.90	0.52
1:D:185:PRO:HD2	1:D:187:MET:HE2	1.90	0.52
1:A:404:PHE:CD1	1:A:404:PHE:N	2.78	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:468:PRO:HB2	1:A:582:GLU:HG2	1.90	0.52
1:C:251:TYR:HA	1:C:261:GLY:O	2.09	0.52
1:A:226:ILE:HD11	1:A:494:PRO:HB3	1.91	0.52
1:C:55:GLU:O	1:C:57:LYS:NZ	2.41	0.52
1:B:31:PHE:O	1:B:33:GLY:N	2.39	0.52
1:B:63:GLY:HA3	1:B:488:LEU:O	2.10	0.52
1:D:288:ASN:H	1:D:288:ASN:HD22	1.58	0.52
1:A:232:TYR:HB3	1:A:233:PRO:CD	2.36	0.52
1:B:78:VAL:HG12	1:B:187:MET:HG3	1.92	0.52
1:C:436:HIS:CE1	1:C:438:LYS:HB2	2.44	0.52
1:A:603:LEU:O	1:A:604:ASP:HB2	2.08	0.52
1:B:78:VAL:HG12	1:B:187:MET:CG	2.39	0.51
1:B:414:SER:HB2	1:B:428:TYR:CE1	2.44	0.51
1:C:113:GLY:O	1:C:194:LYS:HG2	2.11	0.51
1:D:488:LEU:N	1:D:489:THR:HA	2.26	0.51
1:D:494:PRO:O	1:D:498:VAL:HG22	2.11	0.51
1:A:202:ARG:HG3	1:A:202:ARG:NH1	2.25	0.51
1:B:180:ARG:N	1:B:180:ARG:HD2	2.26	0.51
1:A:340:ILE:O	1:A:344:VAL:HG23	2.10	0.51
1:B:245:GLU:OE1	1:B:270:ASP:OD2	2.29	0.51
1:B:1:MET:SD	1:B:25:GLU:HG3	2.49	0.51
1:B:598:GLU:O	1:B:602:GLU:HB2	2.11	0.51
1:C:142:PHE:CD1	1:C:178:GLU:HG2	2.46	0.51
1:D:230:PRO:O	1:D:233:PRO:HD2	2.10	0.51
1:D:452:ILE:O	1:D:452:ILE:HG13	2.11	0.51
1:D:584:TYR:CE1	1:D:593:GLY:HA2	2.46	0.51
1:D:603:LEU:O	1:D:604:ASP:HB2	2.09	0.51
1:B:609:ILE:O	1:B:613:GLU:HB2	2.11	0.50
1:D:439:GLU:HG2	1:D:482:GLY:HA3	1.93	0.50
1:C:580:LEU:O	1:C:583:TYR:HB3	2.11	0.50
1:C:121:ILE:HG13	1:C:196:LEU:HD11	1.93	0.50
1:C:348:HIS:CG	1:C:392:VAL:HG12	2.46	0.50
1:D:562:LYS:O	1:D:567:LYS:HD2	2.12	0.50
1:A:47:ARG:NH1	1:A:611:GLU:OE2	2.44	0.50
1:D:140:THR:HB	1:D:334:GLU:HB2	1.92	0.50
1:A:28:ALA:O	1:A:32:ILE:N	2.41	0.50
1:C:442:VAL:HG22	1:C:442:VAL:O	2.11	0.50
1:D:180:ARG:N	1:D:180:ARG:HD2	2.25	0.50
1:B:308:GLU:OE1	4:B:622:GUA:O3	2.29	0.50
1:C:185:PRO:HD2	1:C:187:MET:CE	2.41	0.50
1:D:381:LYS:HB3	1:D:381:LYS:HZ2	1.76	0.50
1:D:392:VAL:HG22	1:D:412:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:256:ARG:HG2	1:D:364:PHE:CG	2.47	0.50
1:C:598:GLU:OE1	1:C:598:GLU:HA	2.12	0.50
1:C:414:SER:HB2	1:C:428:TYR:CE1	2.46	0.50
1:B:596:LYS:O	1:B:599:THR:HB	2.12	0.50
1:C:528:ARG:HG3	1:C:605:LEU:HD21	1.93	0.49
1:B:50:GLU:HB2	1:B:53:SER:CB	2.43	0.49
1:A:243:ALA:HB2	6:A:631:HOH:O	2.11	0.49
1:D:308:GLU:OE2	1:D:415:GLY:N	2.36	0.49
1:B:479:ARG:HD3	1:B:523:TYR:HB3	1.94	0.49
1:C:118:PRO:HB3	1:C:137:TRP:CE3	2.48	0.49
1:A:308:GLU:OE2	1:A:415:GLY:N	2.35	0.49
1:A:308:GLU:OE2	1:A:414:SER:HB3	2.13	0.49
1:A:47:ARG:HG3	1:A:539:ARG:CZ	2.43	0.49
1:A:26:GLU:O	1:A:30:LYS:HB2	2.12	0.49
1:D:97:ALA:HB1	1:D:201:ILE:HD12	1.95	0.49
1:C:554:LYS:HG2	1:C:554:LYS:O	2.12	0.49
1:A:597:LYS:HZ3	1:A:618:LEU:HB3	1.78	0.49
1:A:175:ILE:HG22	1:A:176:SER:N	2.28	0.49
1:B:88:TYR:HB3	1:B:533:ILE:HG23	1.95	0.49
1:D:288:ASN:HD22	1:D:288:ASN:N	2.10	0.49
1:B:74:GLY:HA3	1:B:285:PRO:HG2	1.95	0.49
1:A:145:GLU:O	1:A:149:LYS:HG3	2.12	0.49
1:C:408:VAL:O	1:C:409:LYS:HB2	2.13	0.48
1:C:597:LYS:O	1:C:601:LYS:HG3	2.13	0.48
1:A:31:PHE:O	1:A:33:GLY:N	2.42	0.48
4:D:622:GUA:C4	4:D:622:GUA:O1	2.66	0.48
1:C:184:ARG:HB2	1:C:185:PRO:HD3	1.95	0.48
1:B:344:VAL:HG12	1:B:392:VAL:HG11	1.95	0.48
1:B:254:PRO:HG2	1:B:415:GLY:HA2	1.95	0.48
1:A:488:LEU:N	1:A:489:THR:HA	2.28	0.48
1:C:232:TYR:HB3	1:C:233:PRO:HD3	1.95	0.48
1:C:488:LEU:N	1:C:489:THR:HA	2.29	0.48
4:C:622:GUA:C4	4:C:622:GUA:O1	2.66	0.48
1:C:452:ILE:HG13	1:C:452:ILE:O	2.13	0.48
1:A:183:GLY:HA3	1:A:187:MET:HB2	1.96	0.48
1:C:136:LEU:O	1:C:139:LYS:HG3	2.14	0.48
1:C:603:LEU:O	1:C:604:ASP:HB2	2.14	0.48
1:B:28:ALA:O	1:B:32:ILE:N	2.46	0.48
1:B:85:THR:HB	1:B:537:TRP:HH2	1.79	0.47
1:D:524:LYS:HE3	1:D:528:ARG:HH22	1.78	0.47
1:B:72:SER:HB3	3:B:621:SF4:S3	2.53	0.47
1:C:270:ASP:HB2	6:C:644:HOH:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:439:GLU:O	1:B:481:ARG:HB2	2.15	0.47
1:C:288:ASN:N	1:C:288:ASN:HD22	2.10	0.47
1:A:423:ALA:HB2	1:A:470:LYS:HD3	1.96	0.47
1:B:525:ALA:O	1:B:529:VAL:HG23	2.15	0.47
1:D:552:PRO:HD3	1:D:576:TYR:CZ	2.49	0.47
4:A:622:GUA:O1	4:A:622:GUA:C4	2.68	0.47
1:D:135:GLY:O	1:D:139:LYS:HE3	2.15	0.47
1:B:269:ILE:HA	1:B:322:LEU:HB2	1.96	0.47
1:C:408:VAL:HG11	1:C:429:GLY:HA2	1.96	0.47
1:D:1:MET:HE1	1:D:6:GLY:HA3	1.97	0.47
1:B:510:LYS:HA	1:B:515:VAL:O	2.15	0.47
1:C:312:LEU:HG	1:C:340:ILE:HG23	1.96	0.47
1:C:289:MET:N	1:C:290:PRO:CD	2.77	0.47
1:C:7:ARG:NH1	1:C:20:VAL:HG11	2.29	0.47
1:B:408:VAL:HB	1:B:435:ALA:HB2	1.96	0.47
1:C:63:GLY:HA3	1:C:488:LEU:O	2.15	0.47
1:B:140:THR:HB	1:B:334:GLU:HB2	1.95	0.47
1:D:429:GLY:O	1:D:550:ASP:HA	2.14	0.47
1:B:414:SER:HB2	1:B:428:TYR:OH	2.15	0.47
1:A:202:ARG:HH11	1:A:202:ARG:HG3	1.80	0.47
1:C:310:VAL:O	1:C:314:GLY:N	2.47	0.47
1:A:215:LEU:HD12	1:A:508:LEU:CD2	2.45	0.47
1:B:582:GLU:O	1:B:586:ILE:HG13	2.15	0.47
1:B:510:LYS:CB	1:B:510:LYS:HZ2	2.22	0.47
1:A:408:VAL:HB	1:A:435:ALA:HB2	1.96	0.47
1:B:538:VAL:HG21	1:B:594:ILE:HG12	1.97	0.47
1:B:209:VAL:HG11	1:B:212:LYS:HA	1.97	0.46
1:B:258:PHE:CD2	1:B:406:MET:HG3	2.49	0.46
4:B:622:GUA:C4	4:B:622:GUA:O1	2.67	0.46
1:B:441:TRP:HB2	1:B:481:ARG:NH2	2.30	0.46
1:D:359:LYS:C	1:D:360:GLU:HG2	2.36	0.46
1:D:597:LYS:HG2	1:D:618:LEU:HD23	1.97	0.46
1:C:582:GLU:O	1:C:586:ILE:HG13	2.15	0.46
1:A:439:GLU:HG2	1:A:482:GLY:CA	2.37	0.46
1:D:337:MET:HE1	1:D:378:ALA:HB2	1.96	0.46
1:C:175:ILE:CG2	1:C:176:SER:N	2.78	0.46
1:A:466:TYR:O	1:A:467:ASP:C	2.51	0.46
1:C:10:ARG:HD3	1:C:21:GLN:OE1	2.15	0.46
1:A:479:ARG:HD3	1:A:523:TYR:HB3	1.98	0.46
1:D:270:ASP:C	1:D:270:ASP:OD1	2.53	0.46
1:A:452:ILE:HG13	1:A:452:ILE:O	2.14	0.46
1:C:472:GLN:O	1:C:476:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:439:GLU:HG2	1:C:482:GLY:CA	2.45	0.46
1:A:240:THR:O	1:A:307:TYR:HB2	2.15	0.46
1:A:116:LYS:HG2	1:A:116:LYS:H	1.44	0.46
1:C:308:GLU:HG2	1:C:340:ILE:CD1	2.45	0.46
1:C:244:VAL:HB	6:C:644:HOH:O	2.15	0.46
1:D:117:LYS:HZ2	1:D:117:LYS:HB3	1.81	0.46
1:B:10:ARG:HD3	1:B:21:GLN:OE1	2.15	0.46
1:B:355:ARG:HB2	1:B:357:ILE:HD12	1.98	0.46
1:A:170:LYS:HD2	1:A:170:LYS:HA	1.68	0.46
1:B:101:LEU:HA	1:B:201:ILE:HG21	1.98	0.46
1:B:452:ILE:HG13	1:B:452:ILE:O	2.16	0.46
1:C:74:GLY:CA	1:C:285:PRO:HG2	2.36	0.45
1:B:235:TRP:CH2	1:B:493:LEU:HD13	2.51	0.45
1:A:534:ARG:HH11	1:A:545:TRP:HE1	1.64	0.45
1:C:411:LEU:O	1:C:435:ALA:HB3	2.16	0.45
1:A:359:LYS:HA	1:A:359:LYS:HD3	1.52	0.45
1:C:606:ASP:O	1:C:609:ILE:HG13	2.16	0.45
1:D:472:GLN:O	1:D:476:GLU:HG3	2.16	0.45
1:B:184:ARG:HB2	6:B:629:HOH:O	2.17	0.45
1:A:422:PRO:HD2	1:A:446:GLU:OE2	2.16	0.45
1:A:82:SER:HA	1:A:83:PRO:HD3	1.78	0.45
1:D:538:VAL:HG21	1:D:594:ILE:HG23	1.98	0.45
1:B:175:ILE:HG22	1:B:176:SER:N	2.30	0.45
1:D:269:ILE:HA	1:D:322:LEU:HB2	1.98	0.45
1:B:43:TRP:O	1:B:539:ARG:NH2	2.46	0.45
1:A:148:LEU:HD13	1:A:200:VAL:CG2	2.47	0.45
1:C:15:THR:OG1	1:C:17:GLU:HB2	2.17	0.45
1:D:609:ILE:HB	1:D:610:PRO:CD	2.47	0.45
1:A:270:ASP:OD1	1:A:270:ASP:C	2.55	0.45
1:A:546:ASP:OD1	1:A:546:ASP:C	2.54	0.45
1:C:240:THR:O	1:C:307:TYR:HB2	2.16	0.45
1:C:609:ILE:HG23	1:C:618:LEU:HD23	1.99	0.45
1:B:518:THR:O	1:B:521:ASP:HB2	2.17	0.45
1:B:373:LEU:O	1:B:377:ILE:HG13	2.16	0.45
1:A:418:CYS:SG	1:A:424:MET:HB3	2.57	0.45
1:A:546:ASP:OD1	1:A:548:LYS:HB2	2.17	0.44
1:A:117:LYS:O	1:A:119:VAL:HG13	2.16	0.44
1:C:102:ARG:NH1	1:C:107:ASP:OD1	2.50	0.44
1:A:423:ALA:HB1	1:A:442:VAL:HG21	2.00	0.44
1:C:396:ALA:O	1:C:400:GLY:N	2.49	0.44
1:A:350:MET:O	1:A:354:GLU:HG3	2.17	0.44
1:B:163:PRO:HA	1:B:166:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:548:LYS:HD2	1:B:548:LYS:HA	1.75	0.44
1:A:548:LYS:HD2	1:A:548:LYS:HA	1.53	0.44
1:C:548:LYS:O	1:C:551:TYR:HB2	2.18	0.44
1:B:488:LEU:N	1:B:489:THR:HA	2.32	0.44
1:C:351:GLU:HG2	1:C:404:PHE:CE2	2.53	0.44
1:B:597:LYS:HG3	1:B:618:LEU:HB3	2.00	0.44
1:D:503:ASP:O	1:D:507:LYS:HG3	2.18	0.44
1:D:183:GLY:HA3	1:D:187:MET:HB2	2.00	0.44
1:C:548:LYS:HE2	1:C:551:TYR:CE2	2.53	0.44
1:C:141:THR:OG1	1:C:334:GLU:HA	2.18	0.44
1:A:41:ILE:HG23	1:A:45:GLU:HG3	2.00	0.44
1:A:76:LEU:O	1:A:92:ASN:HA	2.18	0.44
1:D:246:TRP:CD2	1:D:451:PRO:HG3	2.52	0.44
1:B:551:TYR:HA	1:B:552:PRO:HD3	1.85	0.44
1:B:90:ASP:C	1:B:90:ASP:OD1	2.56	0.44
1:B:125:ASP:OD2	1:B:204:THR:OG1	2.36	0.44
1:A:423:ALA:HB3	1:A:446:GLU:OE1	2.18	0.44
1:B:534:ARG:HG3	1:B:595:PRO:HD3	1.99	0.44
1:A:170:LYS:HG2	1:A:390:GLU:HA	2.00	0.44
1:B:547:ARG:NH1	1:B:591:GLU:OE1	2.48	0.44
1:A:254:PRO:HB3	1:A:258:PHE:CD1	2.53	0.43
1:B:278:LYS:HE2	1:B:293:ASN:OD1	2.18	0.43
1:C:359:LYS:HA	1:C:359:LYS:HD3	1.78	0.43
1:A:534:ARG:HD3	1:A:534:ARG:HA	1.78	0.43
1:B:484:LEU:O	1:B:488:LEU:HG	2.17	0.43
1:A:148:LEU:HD13	1:A:200:VAL:HG22	2.00	0.43
1:D:24:PRO:HB3	1:D:26:GLU:OE2	2.18	0.43
1:D:246:TRP:CE3	1:D:451:PRO:HG3	2.54	0.43
1:C:89:GLY:O	1:C:90:ASP:HB3	2.18	0.43
1:D:529:VAL:O	1:D:533:ILE:HD12	2.18	0.43
1:A:142:PHE:CD1	1:A:142:PHE:N	2.86	0.43
1:D:422:PRO:HD2	1:D:446:GLU:OE2	2.19	0.43
1:D:47:ARG:NH1	1:D:611:GLU:OE2	2.50	0.43
1:A:312:LEU:HD22	1:A:312:LEU:N	2.33	0.43
1:D:554:LYS:HG2	1:D:554:LYS:O	2.18	0.43
1:B:185:PRO:HD2	1:B:187:MET:CE	2.48	0.43
1:A:493:LEU:N	1:A:494:PRO:CD	2.82	0.43
1:A:78:VAL:HG12	1:A:187:MET:HG3	2.00	0.43
1:A:141:THR:OG1	1:A:334:GLU:HA	2.17	0.43
1:D:26:GLU:O	1:D:30:LYS:HB2	2.19	0.43
1:B:284:CYS:HB3	1:B:285:PRO:HD2	2.00	0.43
1:A:50:GLU:CB	1:A:53:SER:HB3	2.46	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:414:SER:HB2	1:B:428:TYR:HE1	1.84	0.43
1:C:546:ASP:C	1:C:546:ASP:OD1	2.57	0.43
1:B:26:GLU:H	1:B:26:GLU:CD	2.22	0.43
1:A:102:ARG:HA	1:A:106:TYR:O	2.18	0.43
1:A:25:GLU:HG2	1:A:29:LYS:HE3	2.00	0.43
1:A:75:LYS:HD2	1:A:92:ASN:OD1	2.19	0.43
1:B:76:LEU:HB2	1:B:98:SER:HB2	2.00	0.43
1:A:66:ASN:HB2	1:A:102:ARG:HG3	2.00	0.42
1:B:408:VAL:HG11	1:B:429:GLY:HA2	2.01	0.42
1:A:312:LEU:HA	1:A:312:LEU:HD13	1.77	0.42
1:D:42:LEU:HD23	1:D:42:LEU:HA	1.88	0.42
1:C:24:PRO:HD2	1:C:27:VAL:CG2	2.47	0.42
1:D:117:LYS:NZ	1:D:117:LYS:HB3	2.33	0.42
1:A:202:ARG:NH2	1:D:134:GLU:OE2	2.52	0.42
1:D:82:SER:HA	1:D:83:PRO:HD3	1.78	0.42
1:B:178:GLU:O	1:B:282:ARG:NH1	2.52	0.42
1:D:93:LEU:HB3	1:D:182:ALA:CB	2.25	0.42
1:A:29:LYS:HA	1:A:517:TYR:OH	2.19	0.42
1:D:436:HIS:CE1	1:D:438:LYS:HB2	2.54	0.42
1:A:59:ILE:HG23	1:A:110:VAL:HG22	2.02	0.42
1:D:408:VAL:HG11	1:D:429:GLY:HA2	2.01	0.42
1:A:284:CYS:HB3	1:A:285:PRO:HD2	2.02	0.42
1:C:5:TRP:HB3	1:C:7:ARG:HG3	2.00	0.42
1:D:90:ASP:C	1:D:90:ASP:OD1	2.58	0.42
1:C:183:GLY:HA2	1:C:187:MET:HE3	2.01	0.42
1:A:548:LYS:O	1:A:551:TYR:HB2	2.20	0.42
1:C:42:LEU:O	1:C:536:TYR:HE2	2.02	0.42
1:C:552:PRO:HD3	1:C:576:TYR:CZ	2.55	0.42
1:D:597:LYS:N	1:D:619:GLU:O	2.38	0.42
1:A:466:TYR:N	1:A:466:TYR:CD1	2.87	0.42
1:C:269:ILE:HA	1:C:322:LEU:HB2	2.02	0.42
1:D:590:ASP:C	1:D:592:ARG:H	2.23	0.42
1:B:467:ASP:CG	1:B:469:ILE:HG22	2.40	0.42
1:A:609:ILE:O	1:A:613:GLU:HB2	2.19	0.42
1:B:75:LYS:HD2	1:B:92:ASN:OD1	2.19	0.42
1:C:355:ARG:HB3	1:C:357:ILE:HD12	2.01	0.42
1:C:183:GLY:O	1:C:184:ARG:C	2.57	0.41
1:C:422:PRO:HG2	1:C:465:SER:O	2.20	0.41
1:D:112:GLU:HA	1:D:194:LYS:HE3	2.01	0.41
1:A:308:GLU:OE1	4:A:622:GUA:O3	2.38	0.41
1:D:139:LYS:HA	6:D:660:HOH:O	2.19	0.41
1:B:392:VAL:HG22	1:B:412:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:495:TRP:O	1:B:499:GLY:HA2	2.21	0.41
1:B:590:ASP:C	1:B:592:ARG:H	2.24	0.41
1:C:251:TYR:O	1:C:261:GLY:HA3	2.21	0.41
1:D:442:VAL:O	1:D:442:VAL:HG22	2.20	0.41
1:C:413:VAL:HG21	1:C:553:PRO:HG2	2.02	0.41
1:B:479:ARG:HD3	1:B:523:TYR:CB	2.50	0.41
1:A:505:TYR:HB2	1:A:506:PRO:HD3	2.02	0.41
1:A:257:ASN:ND2	1:A:404:PHE:HB2	2.35	0.41
1:D:529:VAL:HG12	1:D:533:ILE:HD12	2.02	0.41
1:A:525:ALA:O	1:A:528:ARG:HB3	2.20	0.41
1:D:63:GLY:HA3	1:D:488:LEU:O	2.20	0.41
1:A:552:PRO:HD3	1:A:576:TYR:CZ	2.55	0.41
1:B:82:SER:HB3	1:B:85:THR:OG1	2.20	0.41
1:A:597:LYS:O	1:A:601:LYS:HG3	2.20	0.41
1:A:282:ARG:CZ	1:A:294:VAL:HG21	2.51	0.41
1:C:252:ALA:O	1:C:254:PRO:HD3	2.21	0.41
1:A:94:GLY:HA3	1:A:284:CYS:SG	2.61	0.41
1:B:72:SER:N	1:B:286:TYR:O	2.49	0.41
1:A:10:ARG:HD3	1:A:21:GLN:OE1	2.19	0.41
1:A:126:ASP:OD2	1:A:205:LYS:NZ	2.54	0.41
1:A:9:LEU:HD23	1:A:109:LEU:HD13	2.02	0.41
1:B:409:LYS:HG2	1:B:549:MET:HE3	2.03	0.41
1:A:585:ARG:NH1	1:A:585:ARG:HG2	2.36	0.41
1:C:279:VAL:HG11	1:C:296:LEU:HG	2.03	0.41
1:C:254:PRO:HG2	1:C:415:GLY:HA2	2.03	0.41
1:B:285:PRO:O	1:B:286:TYR:HB2	2.21	0.41
1:C:84:LEU:HD13	1:C:170:LYS:HB3	2.03	0.41
1:B:213:GLU:HA	1:B:213:GLU:OE1	2.16	0.41
1:C:136:LEU:HD22	1:C:144:THR:HG23	2.02	0.40
1:D:510:LYS:NZ	1:D:516:THR:OG1	2.49	0.40
1:C:308:GLU:OE1	4:C:622:GUA:O3	2.39	0.40
1:A:123:ILE:O	1:A:201:ILE:HA	2.20	0.40
1:B:82:SER:HA	1:B:83:PRO:HD3	1.68	0.40
1:A:288:ASN:N	1:A:288:ASN:HD22	2.14	0.40
1:A:582:GLU:HA	1:A:582:GLU:OE1	2.21	0.40
1:B:516:THR:HG22	1:B:516:THR:O	2.20	0.40
1:D:443:ILE:O	1:D:447:ILE:HG13	2.21	0.40
1:B:326:SER:O	1:B:329:ASN:HB3	2.22	0.40
1:C:290:PRO:HA	3:C:621:SF4:S2	2.62	0.40
1:A:537:TRP:O	1:A:541:PHE:HB2	2.21	0.40
1:D:217:LYS:O	1:D:221:GLU:HG3	2.21	0.40
1:B:184:ARG:HB2	1:B:185:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:451:PRO:C	1:B:453:GLU:H	2.25	0.40
1:D:102:ARG:NH1	1:D:107:ASP:OD1	2.55	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	607/619 (98%)	570 (94%)	34 (6%)	3 (0%)	38	53
1	B	607/619 (98%)	572 (94%)	31 (5%)	4 (1%)	30	43
1	C	607/619 (98%)	569 (94%)	35 (6%)	3 (0%)	38	53
1	D	607/619 (98%)	572 (94%)	34 (6%)	1 (0%)	56	74
All	All	2428/2476 (98%)	2283 (94%)	134 (6%)	11 (0%)	38	53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	B	24	PRO
1	B	178	GLU
1	D	591	GLU
1	C	258	PHE
1	A	32	ILE
1	A	414	SER
1	B	32	ILE
1	B	185	PRO
1	C	464	ILE
1	C	185	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	493/499 (99%)	454 (92%)	39 (8%)	18	26
1	B	493/499 (99%)	456 (92%)	37 (8%)	19	29
1	C	493/499 (99%)	453 (92%)	40 (8%)	17	25
1	D	493/499 (99%)	464 (94%)	29 (6%)	28	42
All	All	1972/1996 (99%)	1827 (93%)	145 (7%)	20	30

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	45	GLU
1	A	65	PHE
1	A	93	LEU
1	A	95	THR
1	A	116	LYS
1	A	117	LYS
1	A	154	LYS
1	A	170	LYS
1	A	187	MET
1	A	195	LYS
1	A	202	ARG
1	A	213	GLU
1	A	216	LYS
1	A	245	GLU
1	A	267	ARG
1	A	268	SER
1	A	288	ASN
1	A	359	LYS
1	A	381	LYS
1	A	397	GLU
1	A	398	LYS
1	A	404	PHE
1	A	431	SER
1	A	433	ILE
1	A	465	SER

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Mol	Chain	Res	Type
1	A	469	ILE
1	A	473	LYS
1	A	489	THR
1	A	510	LYS
1	A	544	LYS
1	A	548	LYS
1	A	554	LYS
1	A	573	GLU
1	A	574	LYS
1	A	590	ASP
1	A	592	ARG
1	A	601	LYS
1	A	618	LEU
1	B	10	ARG
1	B	19	LYS
1	B	21	GLN
1	B	29	LYS
1	B	30	LYS
1	B	90	ASP
1	B	93	LEU
1	B	117	LYS
1	B	154	LYS
1	B	187	MET
1	B	195	LYS
1	B	209	VAL
1	B	213	GLU
1	B	216	LYS
1	B	220	GLN
1	B	245	GLU
1	B	267	ARG
1	B	268	SER
1	B	280	GLN
1	B	288	ASN
1	B	304	GLU
1	B	360	GLU
1	B	368	LYS
1	B	386	ASN
1	B	431	SER
1	B	473	LYS
1	B	489	THR
1	B	507	LYS
1	B	510	LYS

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Mol	Chain	Res	Type
1	B	516	THR
1	B	544	LYS
1	B	554	LYS
1	B	574	LYS
1	B	602	GLU
1	B	606	ASP
1	B	613	GLU
1	B	618	LEU
1	C	10	ARG
1	C	17	GLU
1	C	19	LYS
1	C	26	GLU
1	C	82	SER
1	C	93	LEU
1	C	95	THR
1	C	129	SER
1	C	155	ASN
1	C	195	LYS
1	C	202	ARG
1	C	212	LYS
1	C	245	GLU
1	C	259	SER
1	C	268	SER
1	C	282	ARG
1	C	288	ASN
1	C	303	SER
1	C	308	GLU
1	C	329	ASN
1	C	346	ILE
1	C	368	LYS
1	C	381	LYS
1	C	383	GLU
1	C	392	VAL
1	C	398	LYS
1	C	414	SER
1	C	431	SER
1	C	463	LYS
1	C	464	ILE
1	C	465	SER
1	C	473	LYS
1	C	489	THR
1	C	544	LYS

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Mol	Chain	Res	Type
1	C	548	LYS
1	C	554	LYS
1	C	559	GLU
1	C	606	ASP
1	C	613	GLU
1	C	618	LEU
1	D	30	LYS
1	D	93	LEU
1	D	95	THR
1	D	117	LYS
1	D	129	SER
1	D	150	GLU
1	D	202	ARG
1	D	206	GLU
1	D	212	LYS
1	D	216	LYS
1	D	288	ASN
1	D	330	ARG
1	D	360	GLU
1	D	368	LYS
1	D	386	ASN
1	D	398	LYS
1	D	414	SER
1	D	465	SER
1	D	480	LEU
1	D	489	THR
1	D	531	SER
1	D	544	LYS
1	D	554	LYS
1	D	573	GLU
1	D	574	LYS
1	D	592	ARG
1	D	598	GLU
1	D	602	GLU
1	D	606	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	A	288	ASN
1	A	293	ASN

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Mol	Chain	Res	Type
1	B	288	ASN
1	C	280	GLN
1	C	288	ASN
1	D	288	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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	$\# Z > 2$
3	SF4	A	621	1	12,12,12	6.18	12 (100%)	0,24,24	0.00	-
4	GUA	A	622	5	8,8,8	0.87	0	9,9,9	0.93	0
5	PTE	A	623	1,2,4,6	52,55,57	2.34	16 (30%)	68,84,89	4.93	32 (47%)
3	SF4	B	621	1	12,12,12	4.94	10 (83%)	0,24,24	0.00	-
4	GUA	B	622	5	8,8,8	0.94	0	9,9,9	0.85	0
5	PTE	B	623	1,2,4,6	52,55,57	2.54	14 (26%)	68,84,89	3.47	29 (42%)
3	SF4	C	621	1	12,12,12	4.97	11 (91%)	0,24,24	0.00	-
4	GUA	C	622	5	8,8,8	0.86	0	9,9,9	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PTE	C	623	1,2,4,6	52,55,57	2.50	14 (26%)	68,84,89	4.34	30 (44%)
3	SF4	D	621	1	12,12,12	3.83	11 (91%)	0,24,24	0.00	-
4	GUA	D	622	5	8,8,8	0.91	0	9,9,9	0.88	0
5	PTE	D	623	1,2,4,6	52,55,57	2.35	17 (32%)	68,84,89	3.17	30 (44%)

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
3	SF4	A	621	1	-	0/0/48/48	0/0/5/5
4	GUA	A	622	5	-	0/6/6/6	0/0/0/0
5	PTE	A	623	1,2,4,6	-	0/12/78/82	0/0/6/6
3	SF4	B	621	1	-	0/0/48/48	0/0/5/5
4	GUA	B	622	5	-	0/6/6/6	0/0/0/0
5	PTE	B	623	1,2,4,6	-	0/12/78/82	0/0/6/6
3	SF4	C	621	1	-	0/0/48/48	0/0/5/5
4	GUA	C	622	5	-	0/6/6/6	0/0/0/0
5	PTE	C	623	1,2,4,6	-	0/12/78/82	0/0/6/6
3	SF4	D	621	1	-	0/0/48/48	0/0/5/5
4	GUA	D	622	5	-	0/6/6/6	0/0/0/0
5	PTE	D	623	1,2,4,6	-	0/12/78/82	0/0/6/6

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	621	SF4	S4-FE1	-10.18	2.26	2.33
5	B	623	PTE	O28-C28	9.14	1.42	1.24
3	A	621	SF4	S3-FE4	-8.88	2.27	2.33
3	B	621	SF4	S3-FE4	-8.53	2.27	2.33
5	C	623	PTE	O8-C8	8.46	1.41	1.24
5	B	623	PTE	O8-C8	8.35	1.40	1.24
5	C	623	PTE	O28-C28	8.04	1.40	1.24
3	B	621	SF4	S4-FE1	-8.02	2.27	2.33
5	D	623	PTE	O28-C28	7.82	1.39	1.24
3	C	621	SF4	S3-FE1	-7.79	2.28	2.33
5	D	623	PTE	O8-C8	7.77	1.39	1.24
3	D	621	SF4	S4-FE1	-7.66	2.28	2.33
3	C	621	SF4	S3-FE2	-7.51	2.28	2.33
5	A	623	PTE	O28-C28	7.36	1.38	1.24
3	A	621	SF4	S4-FE3	-7.30	2.28	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	621	SF4	S3-FE2	-7.28	2.28	2.33
3	B	621	SF4	S3-FE2	-6.81	2.28	2.33
5	A	623	PTE	O8-C8	6.59	1.37	1.24
3	C	621	SF4	S4-FE1	-6.53	2.28	2.33
3	A	621	SF4	S4-FE2	-6.47	2.28	2.33
3	C	621	SF4	S4-FE2	-5.64	2.29	2.33
5	A	623	PTE	P1-O1P	5.29	1.62	1.51
3	C	621	SF4	S1-FE3	-5.14	2.29	2.33
3	B	621	SF4	S4-FE3	-5.11	2.29	2.33
3	B	621	SF4	S1-FE2	-5.08	2.29	2.33
3	D	621	SF4	S4-FE2	-5.06	2.29	2.33
5	B	623	PTE	P2-O5P	4.91	1.61	1.51
3	D	621	SF4	S3-FE2	-4.87	2.30	2.33
5	C	623	PTE	P2-O5P	4.84	1.61	1.51
3	C	621	SF4	S1-FE4	-4.72	2.30	2.33
3	A	621	SF4	S3-FE1	-4.67	2.30	2.33
5	B	623	PTE	P1-O1P	4.53	1.60	1.51
3	A	621	SF4	S2-FE1	-4.50	2.30	2.33
3	A	621	SF4	S1-FE2	-4.46	2.30	2.33
3	A	621	SF4	S2-FE4	-4.38	2.30	2.33
5	C	623	PTE	C27-C32	4.38	1.47	1.41
5	D	623	PTE	P2-O5P	4.34	1.60	1.51
3	A	621	SF4	S1-FE4	-4.24	2.30	2.33
5	D	623	PTE	P1-O1P	4.09	1.60	1.51
3	A	621	SF4	S1-FE3	-4.00	2.30	2.33
5	A	623	PTE	P2-O5P	3.97	1.59	1.51
5	A	623	PTE	C27-C32	3.87	1.46	1.41
3	C	621	SF4	S2-FE3	-3.86	2.30	2.33
5	D	623	PTE	C7-C12	3.85	1.46	1.41
5	B	623	PTE	C27-C32	3.85	1.46	1.41
5	C	623	PTE	P1-O1P	3.83	1.59	1.51
5	B	623	PTE	C7-C12	3.70	1.46	1.41
3	B	621	SF4	S2-FE1	-3.61	2.30	2.33
5	A	623	PTE	C2-C3	3.59	1.57	1.51
3	A	621	SF4	S2-FE3	-3.56	2.30	2.33
5	C	623	PTE	C10-N11	3.53	1.38	1.33
3	C	621	SF4	S2-FE1	-3.53	2.30	2.33
5	D	623	PTE	C27-C32	3.50	1.46	1.41
5	B	623	PTE	C25-C24	3.47	1.55	1.50
5	A	623	PTE	C30-N31	3.45	1.37	1.33
5	C	623	PTE	O2-C14	-3.37	1.39	1.44
3	B	621	SF4	S2-FE3	-3.36	2.31	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	621	SF4	S2-FE4	-3.35	2.31	2.33
3	D	621	SF4	S3-FE1	-3.33	2.31	2.33
5	C	623	PTE	C7-C12	3.28	1.46	1.41
3	D	621	SF4	S3-FE4	-3.27	2.31	2.33
5	D	623	PTE	C25-N26	3.25	1.50	1.45
5	C	623	PTE	C2-C3	3.25	1.57	1.51
3	B	621	SF4	S3-FE1	-3.24	2.31	2.33
5	A	623	PTE	C7-C12	3.23	1.45	1.41
3	B	621	SF4	S1-FE4	-3.22	2.31	2.33
3	D	621	SF4	S1-FE4	-3.21	2.31	2.33
5	B	623	PTE	C30-N31	3.10	1.37	1.33
3	D	621	SF4	S1-FE3	-3.06	2.31	2.33
3	C	621	SF4	S3-FE4	-3.05	2.31	2.33
5	A	623	PTE	C5-N6	3.02	1.49	1.45
5	B	623	PTE	C2-C3	3.01	1.56	1.51
5	A	623	PTE	C10-N11	2.94	1.37	1.33
5	B	623	PTE	C14-C5	2.89	1.58	1.53
5	C	623	PTE	C5-C4	2.76	1.54	1.50
5	C	623	PTE	C25-N26	2.76	1.49	1.45
3	D	621	SF4	S2-FE3	-2.75	2.31	2.33
3	D	621	SF4	S2-FE1	-2.72	2.31	2.33
5	A	623	PTE	C14-C5	2.69	1.58	1.53
5	C	623	PTE	C5-N6	2.68	1.49	1.45
5	B	623	PTE	C4-S4	-2.67	1.69	1.75
3	B	621	SF4	S2-FE4	-2.66	2.31	2.33
5	A	623	PTE	C34-N33	2.64	1.50	1.44
3	C	621	SF4	S1-FE2	-2.62	2.31	2.33
5	D	623	PTE	C5-C4	2.59	1.54	1.50
5	D	623	PTE	C30-N29	2.59	1.40	1.36
5	D	623	PTE	C25-C24	2.56	1.54	1.50
5	B	623	PTE	C25-N26	2.53	1.49	1.45
5	C	623	PTE	C14-C5	2.52	1.58	1.53
5	D	623	PTE	C34-C25	2.51	1.58	1.53
5	B	623	PTE	O2-C14	-2.50	1.40	1.44
3	D	621	SF4	S1-FE2	-2.50	2.31	2.33
5	D	623	PTE	C2-C3	2.48	1.55	1.51
5	A	623	PTE	C25-C24	2.48	1.54	1.50
5	D	623	PTE	C5-N6	2.42	1.49	1.45
5	A	623	PTE	O2-C14	-2.41	1.40	1.44
5	D	623	PTE	O2-C2	-2.39	1.40	1.43
5	B	623	PTE	C5-C4	2.37	1.54	1.50
5	A	623	PTE	O2-C2	-2.28	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	621	SF4	S2-FE4	-2.20	2.31	2.33
5	D	623	PTE	C14-C5	2.19	1.57	1.53
5	A	623	PTE	C5-C4	2.18	1.53	1.50
5	D	623	PTE	C22-C23	2.13	1.55	1.51
5	D	623	PTE	C30-N31	2.07	1.36	1.33
5	C	623	PTE	O2-C2	-2.00	1.40	1.43

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	623	PTE	O2-C14-N13	22.56	138.60	109.22
5	C	623	PTE	O2-C14-N13	18.34	133.10	109.22
5	A	623	PTE	C1-C2-C3	14.83	128.48	110.98
5	C	623	PTE	C14-O2-C2	14.54	140.47	112.03
5	A	623	PTE	O22-C34-N33	14.43	128.01	109.22
5	C	623	PTE	C21-C22-C23	-13.41	95.16	110.98
5	A	623	PTE	C14-O2-C2	12.14	135.79	112.03
5	B	623	PTE	O22-C34-N33	11.90	124.71	109.22
5	A	623	PTE	C34-O22-C22	10.69	132.94	112.03
5	D	623	PTE	C34-O22-C22	10.30	132.18	112.03
5	D	623	PTE	C14-O2-C2	9.17	129.97	112.03
5	D	623	PTE	N30-C30-N29	8.69	127.42	117.86
5	C	623	PTE	C34-O22-C22	8.62	128.89	112.03
5	A	623	PTE	C21-C22-C23	-8.28	101.22	110.98
5	B	623	PTE	C21-C22-C23	-8.17	101.34	110.98
5	B	623	PTE	C4-C5-N6	-7.95	94.84	111.32
5	B	623	PTE	C34-C25-N26	-7.56	98.82	108.44
5	B	623	PTE	C1-C2-C3	-7.39	102.27	110.98
5	C	623	PTE	C1-C2-C3	7.19	119.45	110.98
5	B	623	PTE	O2-C14-N13	-6.77	100.40	109.22
5	A	623	PTE	C14-C5-N6	-6.49	100.17	108.44
5	B	623	PTE	C34-O22-C22	6.45	124.64	112.03
5	D	623	PTE	N10-C10-N9	6.42	124.92	117.86
5	C	623	PTE	C28-C27-N26	6.27	128.21	119.10
5	C	623	PTE	C8-C7-N6	6.04	127.89	119.10
5	C	623	PTE	O2-C2-C1	5.90	124.03	108.81
5	B	623	PTE	C28-C27-N26	5.84	127.60	119.10
5	D	623	PTE	C34-C25-N26	-5.81	101.05	108.44
5	A	623	PTE	C8-C7-N6	5.67	127.34	119.10
5	A	623	PTE	C4-C5-N6	5.50	122.72	111.32
5	D	623	PTE	C8-C7-N6	5.41	126.96	119.10
5	C	623	PTE	C14-C5-C4	5.27	118.04	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	623	PTE	O2-C2-C1	5.14	122.06	108.81
5	A	623	PTE	N10-C10-N9	5.10	123.47	117.86
5	D	623	PTE	O22-C22-C21	5.06	121.85	108.81
5	D	623	PTE	O6P-P2-O5P	4.97	123.75	108.83
5	C	623	PTE	O2-C14-C5	-4.94	102.78	109.50
5	B	623	PTE	C14-O2-C2	4.88	121.58	112.03
5	B	623	PTE	C27-C32-N33	-4.81	113.64	119.12
5	D	623	PTE	C28-C27-N26	4.77	126.04	119.10
5	C	623	PTE	N10-C10-N9	4.72	123.06	117.86
5	C	623	PTE	C14-C5-N6	-4.71	102.45	108.44
5	B	623	PTE	N10-C10-N9	4.59	122.92	117.86
5	C	623	PTE	C24-C25-N26	-4.55	103.11	111.70
5	C	623	PTE	O22-C34-N33	4.54	115.13	109.22
5	B	623	PTE	N33-C32-N31	4.46	123.50	116.51
5	A	623	PTE	C14-C5-C4	4.36	116.51	109.14
5	A	623	PTE	N33-C32-N31	4.36	123.34	116.51
5	D	623	PTE	O2-C14-N13	4.33	114.86	109.22
5	A	623	PTE	O2-C14-C5	-4.27	103.69	109.50
5	B	623	PTE	C8-C7-N6	4.22	125.23	119.10
5	C	623	PTE	O22-C22-C21	4.13	119.46	108.81
5	D	623	PTE	N30-C30-N31	-4.11	114.76	120.31
5	A	623	PTE	C28-C27-N26	4.08	125.03	119.10
5	B	623	PTE	C5-C14-N13	4.06	115.55	110.01
5	C	623	PTE	C4-C5-N6	4.03	119.69	111.32
5	C	623	PTE	C34-C25-N26	-3.89	103.48	108.44
5	B	623	PTE	O2P-P1-O1P	3.87	120.43	108.83
5	D	623	PTE	O2-C14-C5	-3.86	104.25	109.50
5	B	623	PTE	C28-N29-C30	3.83	126.21	119.51
5	C	623	PTE	N13-C12-N11	3.83	122.51	116.51
5	C	623	PTE	N9-C10-N11	-3.77	116.50	121.78
5	A	623	PTE	C27-C32-N33	-3.65	114.97	119.12
5	A	623	PTE	O22-C34-C25	-3.60	104.60	109.50
5	D	623	PTE	O22-C34-N33	3.52	113.80	109.22
5	A	623	PTE	C34-C25-N26	-3.51	103.96	108.44
5	B	623	PTE	C25-C24-C23	3.44	128.73	116.27
5	B	623	PTE	O22-C22-C23	3.42	118.26	109.81
5	D	623	PTE	C14-C5-C4	3.35	114.80	109.14
5	B	623	PTE	O6P-P2-O5P	3.35	118.88	108.83
5	A	623	PTE	C28-N29-C30	3.33	125.33	119.51
5	B	623	PTE	C25-C34-N33	-3.32	105.48	110.01
5	D	623	PTE	C14-C5-N6	-3.29	104.25	108.44
5	A	623	PTE	N29-C30-N31	-3.29	117.18	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	623	PTE	O22-C34-C25	3.18	113.84	109.50
5	B	623	PTE	C14-C5-C4	3.16	114.48	109.14
5	A	623	PTE	O4P-C1-C2	3.02	116.36	108.53
5	D	623	PTE	N29-C30-N31	-2.95	117.64	121.78
5	C	623	PTE	C10-N11-C12	2.93	121.77	117.61
5	A	623	PTE	N30-C30-N31	2.91	124.23	120.31
5	C	623	PTE	N33-C32-N31	2.87	121.02	116.51
5	A	623	PTE	C25-C24-C23	2.85	126.60	116.27
5	D	623	PTE	N9-C10-N11	-2.84	117.80	121.78
5	C	623	PTE	N30-C30-N29	2.83	120.97	117.86
5	D	623	PTE	C8-N9-C10	2.79	124.38	119.51
5	A	623	PTE	C5-C14-N13	-2.70	106.31	110.01
5	D	623	PTE	O6P-P2-O8P	-2.68	94.97	108.51
5	A	623	PTE	C10-N11-C12	2.64	121.36	117.61
5	B	623	PTE	N29-C30-N31	-2.64	118.08	121.78
5	D	623	PTE	N33-C32-N31	2.62	120.62	116.51
5	D	623	PTE	O22-C34-C25	-2.60	105.96	109.50
5	D	623	PTE	C10-N11-C12	2.58	121.28	117.61
5	B	623	PTE	N13-C12-N11	2.57	120.54	116.51
5	C	623	PTE	C8-N9-C10	2.57	124.01	119.51
5	A	623	PTE	O5P-P2-O7P	-2.56	105.92	112.87
5	A	623	PTE	C27-N26-C25	2.56	125.27	118.60
5	C	623	PTE	C25-C24-C23	2.54	125.49	116.27
5	D	623	PTE	N13-C12-N11	2.49	120.41	116.51
5	D	623	PTE	C21-C22-C23	-2.43	108.11	110.98
5	A	623	PTE	O2P-P1-O1P	2.42	116.09	108.83
5	D	623	PTE	C27-C32-N33	-2.41	116.37	119.12
5	A	623	PTE	C7-C12-N13	-2.40	116.39	119.12
5	A	623	PTE	C7-C8-N9	2.38	120.16	114.06
5	D	623	PTE	N10-C10-N11	-2.36	117.11	120.31
5	B	623	PTE	N30-C30-N31	2.34	123.47	120.31
5	C	623	PTE	C7-C12-N13	-2.30	116.50	119.12
5	D	623	PTE	C7-C12-N13	-2.30	116.50	119.12
5	A	623	PTE	N13-C12-N11	2.28	120.08	116.51
5	B	623	PTE	C10-N11-C12	2.26	120.82	117.61
5	D	623	PTE	C28-N29-C30	2.26	123.46	119.51
5	B	623	PTE	O2P-P1-O4P	-2.23	97.29	108.51
5	C	623	PTE	C27-N26-C25	2.18	124.28	118.60
5	C	623	PTE	C27-C32-N33	-2.17	116.64	119.12
5	A	623	PTE	N9-C10-N11	-2.11	118.83	121.78
5	C	623	PTE	C27-C28-N29	2.10	119.46	114.06
5	B	623	PTE	C5-C4-C3	2.09	125.34	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	623	PTE	O6P-P2-O5P	2.09	115.11	108.83
5	C	623	PTE	O8P-C21-C22	-2.09	103.13	108.53
5	B	623	PTE	N10-C10-N11	-2.06	117.52	120.31
5	D	623	PTE	C30-N31-C32	2.05	120.53	117.61
5	A	623	PTE	N10-C10-N11	-2.00	117.60	120.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.