Full wwPDB X-ray Structure Validation Report (i)

Jul 26, 2023 – 03:10 AM EDT

PDB ID	:	1B4N
Title	:	FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE FROM PYROCOCCUS 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

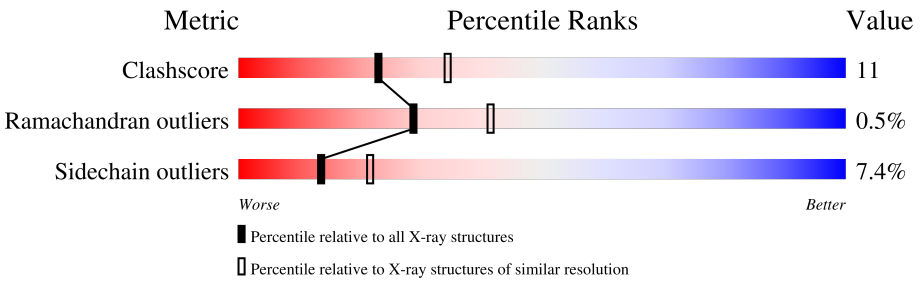
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	619	68% 28% • •
1	B	619	69% 26% • •
1	C	619	69% 26% • •
1	D	619	75% 22% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19600 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.

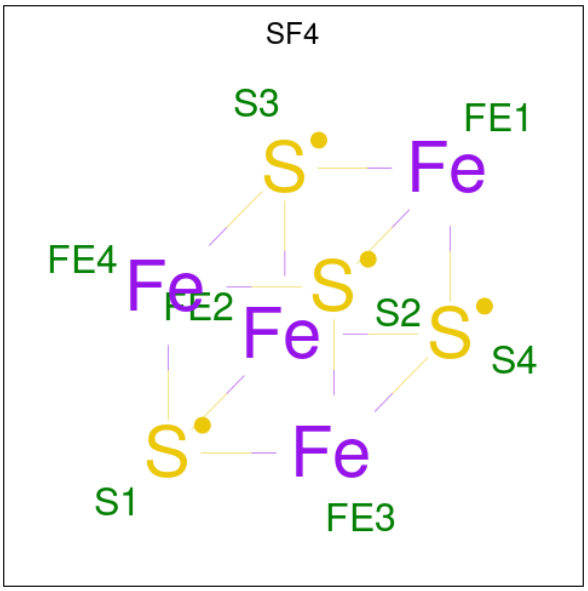
- Molecule 1 is a protein called FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE.

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

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

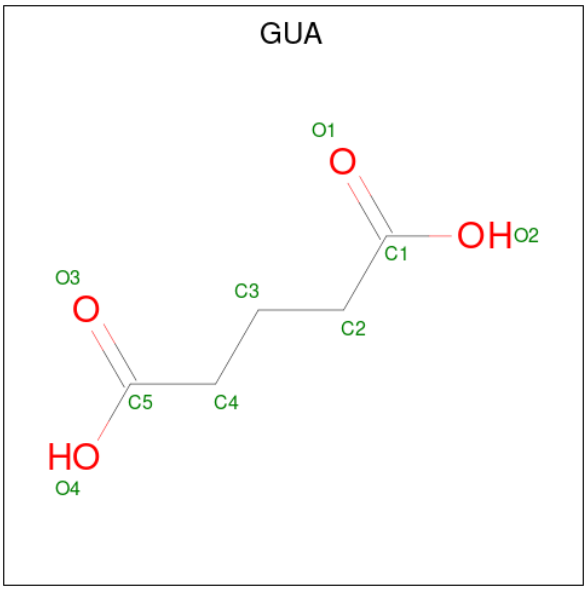
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

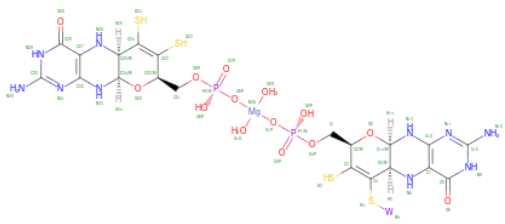
- Molecule 4 is GLUTARIC ACID (three-letter code: GUA) (formula: $C_5H_8O_4$).



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

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

PTE



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

- Molecule 6 is water.

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

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

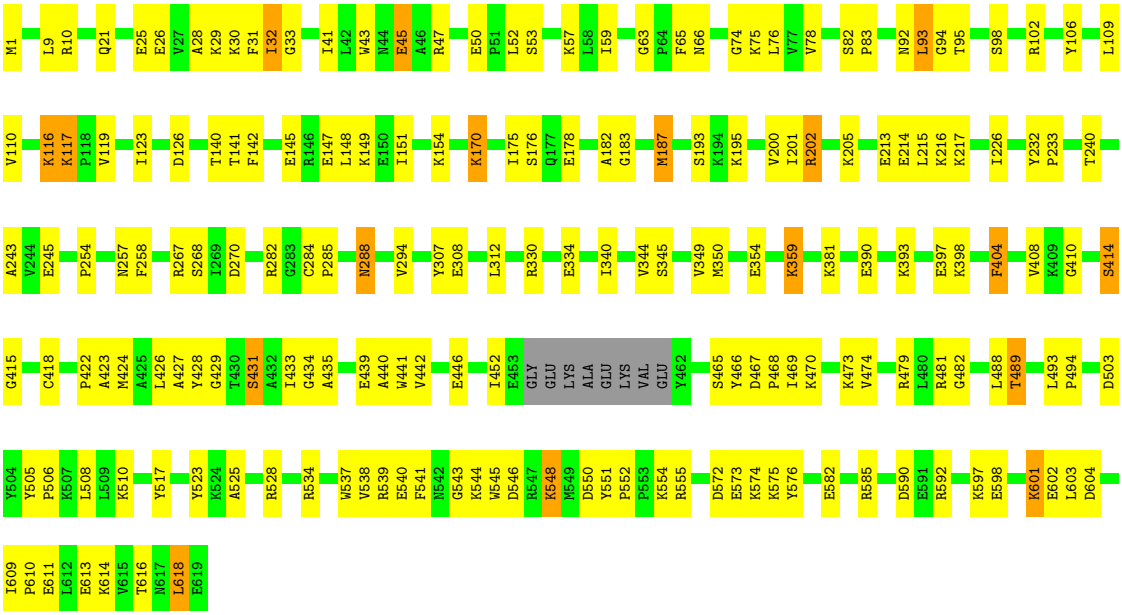
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

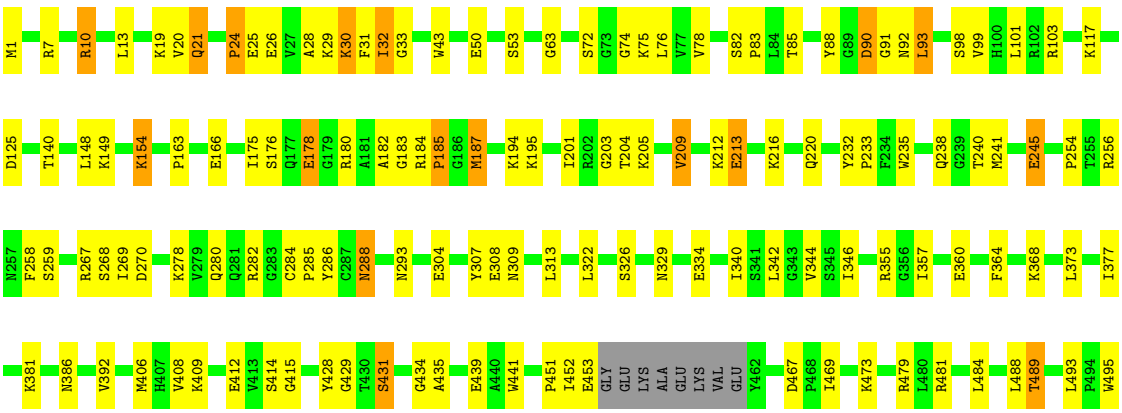
• Molecule 1: FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE

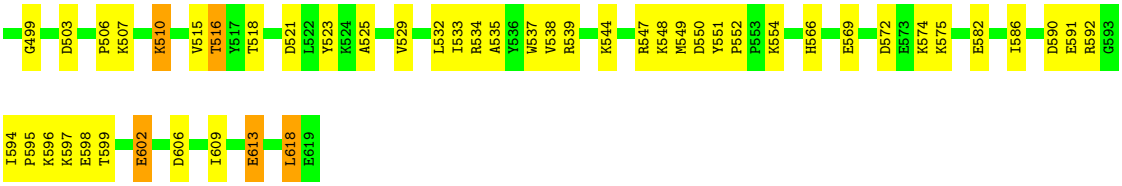
Chain A: 68% 28% • •



• Molecule 1: FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE

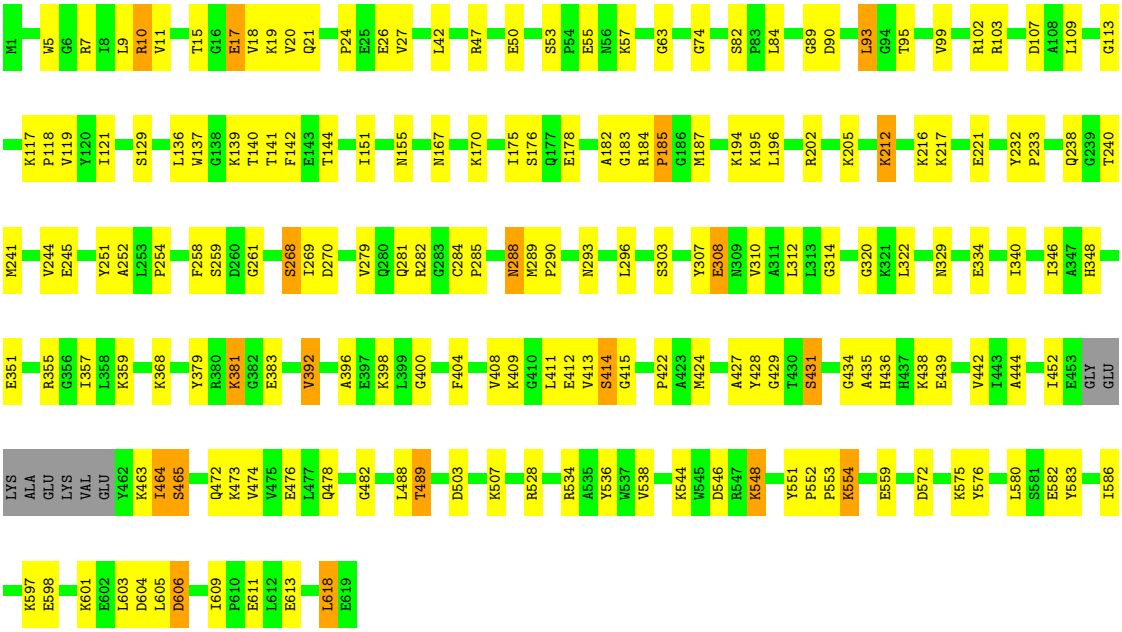
Chain B: 69% 26% • •





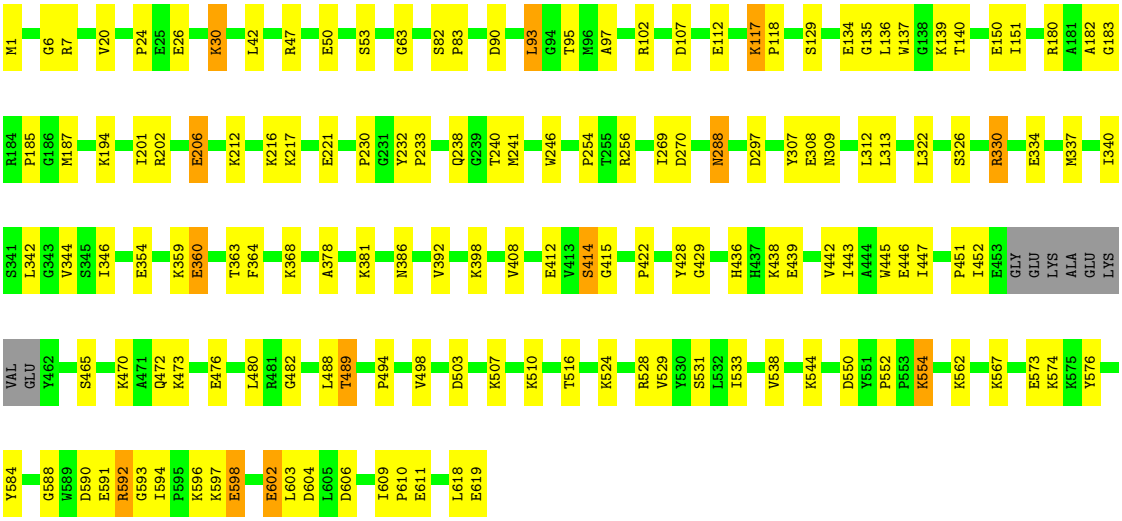
• Molecule 1: FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE

Chain C:



• Molecule 1: FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GUA, CA, PTE, 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 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	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
3	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 11.

All (441) 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: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:HZ2	1:B:510:LYS:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:LEU:HD23	1:C:109:LEU:HD13	1.68	0.76
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:A:330:ARG:O	1:A:334:GLU:HG2	1.92	0.70
1:A:414:SER:HB2	1:A:428:TYR:OH	1.91	0.70
1:C:11:VAL:HG22	1:C:18:VAL:HG22	1.74	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:HD22	1:C:288:ASN:H	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:HD22	1:B:288:ASN:N	1.90	0.62
1:C:183:GLY:HA3	1:C:187:MET:HB2	1.80	0.62
1:C:431:SER:HB3	1:C:434:GLY:O	1.99	0.62
1:D:232:TYR:HB3	1:D:233:PRO:HD3	1.79	0.62
1:A:288:ASN:HD22	1:A:288:ASN:H	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:63:GLY:HA3	1:A:488:LEU:O	2.02	0.60
1:B:148:LEU:HD23	1:C:151:ILE:HD12	1.82	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: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:B:342:LEU:O	1:B:346:ILE:HG13	2.03	0.58
1:C:355:ARG:CB	1:C:357:ILE:HD12	2.34	0.58
1:A:543:GLY:HA3	1:A:616:THR:HG23	1.84	0.57
1:B:431:SER:HB3	1:B:434:GLY:O	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:142:PHE:CE1	1:C:178:GLU:HA	2.41	0.55
1:D:308:GLU:CG	1:D:340:ILE:HD11	2.36	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:A:597:LYS:NZ	1:A:618:LEU:HB3	2.22	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: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:A:503:ASP:O	1:A:506:PRO:HD2	2.06	0.54
1:D:312:LEU:HG	1:D:340:ILE:HG23	1.89	0.54
1:A:52:LEU:HD22	1:A:193:SER:HB3	1.89	0.54
1:D:240:THR:O	1:D:307:TYR:HB2	2.07	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: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:D:26:GLU:CD	1:D:26:GLU:H	2.12	0.53
1:A:140:THR:HB	1:A:334:GLU:HB2	1.91	0.53
1:B:288:ASN:H	1:B:288:ASN:ND2	1.95	0.53
1:B:232:TYR:HB3	1:B:233:PRO:HD3	1.89	0.53
1:D:445:TRP:CD1	1:D:473:LYS:HE2	2.44	0.53
1:B:259:SER:HB2	6:B:656:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:GLY:HA3	1:B:187:MET:HB2	1.90	0.52
1:D:93:LEU:HA	5:D:623:PTE:O5P	2.09	0.52
1:D:185:PRO:HD2	1:D:187:MET:HE2	1.90	0.52
1:A:404:PHE:N	1:A:404:PHE:CD1	2.78	0.52
1:A:468:PRO:HB2	1:A:582:GLU:HG2	1.90	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:C:251:TYR:HA	1:C:261:GLY:O	2.09	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:A:202:ARG:NH1	1:A:202:ARG:HG3	2.25	0.51
1:B:180:ARG:HD2	1:B:180:ARG:N	2.26	0.51
1:D:494:PRO:O	1:D:498:VAL:HG22	2.11	0.51
1:A:340:ILE:O	1:A:344:VAL:HG23	2.10	0.51
1:B:1:MET:SD	1:B:25:GLU:HG3	2.49	0.51
1:B:245:GLU:OE1	1:B:270:ASP:OD2	2.29	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:HG13	1:D:452:ILE:O	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:C:580:LEU:O	1:C:583:TYR:HB3	2.11	0.50
1:D:439:GLU:HG2	1:D:482:GLY:HA3	1.93	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:28:ALA:O	1:A:32:ILE:N	2.41	0.50
1:A:47:ARG:NH1	1:A:611:GLU:OE2	2.44	0.50
1:C:442:VAL:HG22	1:C:442:VAL:O	2.11	0.50
1:D:140:THR:HB	1:D:334:GLU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:598:GLU:OE1	1:C:598:GLU:HA	2.12	0.50
1:D:256:ARG:HG2	1:D:364:PHE:CG	2.47	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
1:B:596:LYS:O	1:B:599:THR:HB	2.12	0.50
1:C:414:SER:HB2	1:C:428:TYR:CE1	2.46	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:B:479:ARG:HD3	1:B:523:TYR:HB3	1.94	0.49
1:D:308:GLU:OE2	1:D:415:GLY:N	2.36	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:26:GLU:O	1:A:30:LYS:HB2	2.12	0.49
1:A:47:ARG:HG3	1:A:539:ARG:CZ	2.43	0.49
1:A:308:GLU:OE2	1:A:414:SER:HB3	2.13	0.49
1:C:554:LYS:O	1:C:554:LYS:HG2	2.12	0.49
1:D:97:ALA:HB1	1:D:201:ILE:HD12	1.95	0.49
1:A:175:ILE:HG22	1:A:176:SER:N	2.28	0.49
1:A:597:LYS:HZ3	1:A:618:LEU:HB3	1.78	0.49
1:B:88:TYR:HB3	1:B:533:ILE:HG23	1.95	0.49
1:A:145:GLU:O	1:A:149:LYS:HG3	2.12	0.49
1:B:74:GLY:HA3	1:B:285:PRO:HG2	1.95	0.49
1:D:288:ASN:HD22	1:D:288:ASN:N	2.10	0.49
1:C:408:VAL:O	1:C:409:LYS:HB2	2.13	0.48
1:A:31:PHE:O	1:A:33:GLY:N	2.42	0.48
1:C:597:LYS:O	1:C:601:LYS:HG3	2.13	0.48
4:D:622:GUA:C4	4:D:622:GUA:O1	2.66	0.48
1:B:344:VAL:HG12	1:B:392:VAL:HG11	1.95	0.48
1:C:184:ARG:HB2	1:C:185:PRO:HD3	1.95	0.48
1:A:488:LEU:N	1:A:489:THR:HA	2.28	0.48
1:B:254:PRO:HG2	1:B:415:GLY:HA2	1.95	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
1:A:183:GLY:HA3	1:A:187:MET:HB2	1.96	0.48
1:C:452:ILE:HG13	1:C:452:ILE:O	2.13	0.48
4:C:622:GUA:O1	4:C:622:GUA:C4	2.66	0.48
1:B:28:ALA:O	1:B:32:ILE:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:72:SER:HB3	3:B:621:SF4:S3	2.53	0.47
1:B:85:THR:HB	1:B:537:TRP:HH2	1.79	0.47
1:C:270:ASP:HB2	6:C:644:HOH:O	2.14	0.47
1:D:524:LYS:HE3	1:D:528:ARG:HH22	1.78	0.47
1:A:423:ALA:HB2	1:A:470:LYS:HD3	1.96	0.47
1:B:439:GLU:O	1:B:481:ARG:HB2	2.15	0.47
1:B:525:ALA:O	1:B:529:VAL:HG23	2.15	0.47
1:C:288:ASN:HD22	1:C:288:ASN:N	2.10	0.47
1:D:552:PRO:HD3	1:D:576:TYR:CZ	2.49	0.47
4:A:622:GUA:C4	4:A:622:GUA:O1	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:7:ARG:NH1	1:C:20:VAL:HG11	2.29	0.47
1:C:289:MET:N	1:C:290:PRO:CD	2.77	0.47
1:C:312:LEU:HG	1:C:340:ILE:HG23	1.96	0.47
1:B:140:THR:HB	1:B:334:GLU:HB2	1.95	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:D:429:GLY:O	1:D:550:ASP:HA	2.14	0.47
1:A:202:ARG:HG3	1:A:202:ARG:HH11	1.80	0.47
1:A:215:LEU:HD12	1:A:508:LEU:CD2	2.45	0.47
1:B:414:SER:HB2	1:B:428:TYR:OH	2.15	0.47
1:B:582:GLU:O	1:B:586:ILE:HG13	2.15	0.47
1:C:310:VAL:O	1:C:314:GLY:N	2.47	0.47
1:A:408:VAL:HB	1:A:435:ALA:HB2	1.96	0.47
1:B:510:LYS:HZ2	1:B:510:LYS:CB	2.22	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:O1	4:B:622:GUA:C4	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:C:582:GLU:O	1:C:586:ILE:HG13	2.15	0.46
1:D:597:LYS:HG2	1:D:618:LEU:HD23	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ILE:O	1:A:452:ILE:HG13	2.14	0.46
1:A:466:TYR:O	1:A:467:ASP:C	2.51	0.46
1:A:479:ARG:HD3	1:A:523:TYR:HB3	1.98	0.46
1:C:10:ARG:HD3	1:C:21:GLN:OE1	2.15	0.46
1:C:175:ILE:CG2	1:C:176:SER:N	2.78	0.46
1:C:472:GLN:O	1:C:476:GLU:HG3	2.15	0.46
1:D:270:ASP:OD1	1:D:270:ASP:C	2.53	0.46
1:A:116:LYS:H	1:A:116:LYS:HG2	1.44	0.46
1:A:240:THR:O	1:A:307:TYR:HB2	2.15	0.46
1:C:439:GLU:HG2	1:C:482:GLY:CA	2.45	0.46
1:C:244:VAL:HB	6:C:644:HOH:O	2.15	0.46
1:C:308:GLU:HG2	1:C:340:ILE:CD1	2.45	0.46
1:A:170:LYS:HD2	1:A:170:LYS:HA	1.68	0.46
1:B:10:ARG:HD3	1:B:21:GLN:OE1	2.15	0.46
1:B:101:LEU:HA	1:B:201:ILE:HG21	1.98	0.46
1:B:355:ARG:HB2	1:B:357:ILE:HD12	1.98	0.46
1:B:452:ILE:O	1:B:452:ILE:HG13	2.16	0.46
1:D:117:LYS:HB3	1:D:117:LYS:HZ2	1.81	0.46
1:B:235:TRP:CH2	1:B:493:LEU:HD13	2.51	0.45
1:C:74:GLY:CA	1:C:285:PRO:HG2	2.36	0.45
1:A:359:LYS:HA	1:A:359:LYS:HD3	1.52	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: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:82:SER:HA	1:A:83:PRO:HD3	1.78	0.45
1:A:422:PRO:HD2	1:A:446:GLU:OE2	2.16	0.45
1:A:148:LEU:HD13	1:A:200:VAL:CG2	2.47	0.45
1:B:43:TRP:O	1:B:539:ARG:NH2	2.46	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:D:538:VAL:HG21	1:D:594:ILE:HG23	1.98	0.45
1:A:270:ASP:OD1	1:A:270:ASP:C	2.55	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:546:ASP:C	1:A:546:ASP:OD1	2.54	0.45
1:C:240:THR:O	1:C:307:TYR:HB2	2.16	0.45
1:A:418:CYS:SG	1:A:424:MET:HB3	2.57	0.45
1:B:373:LEU:O	1:B:377:ILE:HG13	2.16	0.45
1:B:518:THR:O	1:B:521:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:609:ILE:HG23	1:C:618:LEU:HD23	1.99	0.45
1:A:117:LYS:O	1:A:119:VAL:HG13	2.16	0.44
1:A:546:ASP:OD1	1:A:548:LYS:HB2	2.17	0.44
1:C:102:ARG:NH1	1:C:107:ASP:OD1	2.50	0.44
1:A:350:MET:O	1:A:354:GLU:HG3	2.17	0.44
1:A:423:ALA:HB1	1:A:442:VAL:HG21	2.00	0.44
1:B:163:PRO:HA	1:B:166:GLU:HB2	1.99	0.44
1:B:548:LYS:HD2	1:B:548:LYS:HA	1.75	0.44
1:C:396:ALA:O	1:C:400:GLY:N	2.49	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:B:597:LYS:HG3	1:B:618:LEU:HB3	2.00	0.44
1:C:351:GLU:HG2	1:C:404:PHE:CE2	2.53	0.44
1:D:503:ASP:O	1:D:507:LYS:HG3	2.18	0.44
1:C:548:LYS:HE2	1:C:551:TYR:CE2	2.53	0.44
1:D:183:GLY:HA3	1:D:187:MET:HB2	2.00	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:B:90:ASP:OD1	1:B:90:ASP:C	2.56	0.44
1:B:125:ASP:OD2	1:B:204:THR:OG1	2.36	0.44
1:B:551:TYR:HA	1:B:552:PRO:HD3	1.85	0.44
1:C:141:THR:OG1	1:C:334:GLU:HA	2.18	0.44
1:D:246:TRP:CD2	1:D:451:PRO:HG3	2.52	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:HD3	1:C:359:LYS:HA	1.78	0.43
1:A:148:LEU:HD13	1:A:200:VAL:HG22	2.00	0.43
1:A:534:ARG:HA	1:A:534:ARG:HD3	1.78	0.43
1:B:484:LEU:O	1:B:488:LEU:HG	2.17	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:A:142:PHE:N	1:A:142:PHE:CD1	2.86	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:312:LEU:N	1:A:312:LEU:HD22	2.33	0.43
1:D:47:ARG:NH1	1:D:611:GLU:OE2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:PRO:HD2	1:D:446:GLU:OE2	2.19	0.43
1:D:554:LYS:O	1:D:554:LYS:HG2	2.18	0.43
1:A:78:VAL:HG12	1:A:187:MET:HG3	2.00	0.43
1:A:493:LEU:N	1:A:494:PRO:CD	2.82	0.43
1:B:185:PRO:HD2	1:B:187:MET:CE	2.48	0.43
1:A:141:THR:OG1	1:A:334:GLU:HA	2.17	0.43
1:B:284:CYS:HB3	1:B:285:PRO:HD2	2.00	0.43
1:D:26:GLU:O	1:D:30:LYS:HB2	2.19	0.43
1:A:50:GLU:CB	1:A:53:SER:HB3	2.46	0.43
1:B:414:SER:HB2	1:B:428:TYR:HE1	1.84	0.43
1:C:546:ASP:OD1	1:C:546:ASP:C	2.57	0.43
1:A:25:GLU:HG2	1:A:29:LYS:HE3	2.00	0.43
1:A:102:ARG:HA	1:A:106:TYR:O	2.18	0.43
1:B:26:GLU:CD	1:B:26:GLU:H	2.22	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:A:312:LEU:HD13	1:A:312:LEU:HA	1.77	0.42
1:B:408:VAL:HG11	1:B:429:GLY:HA2	2.01	0.42
1:D:42:LEU:HD23	1:D:42:LEU:HA	1.88	0.42
1:A:202:ARG:NH2	1:D:134:GLU:OE2	2.52	0.42
1:B:178:GLU:O	1:B:282:ARG:NH1	2.52	0.42
1:C:24:PRO:HD2	1:C:27:VAL:CG2	2.47	0.42
1:D:82:SER:HA	1:D:83:PRO:HD3	1.78	0.42
1:D:117:LYS:HB3	1:D:117:LYS:NZ	2.33	0.42
1:A:29:LYS:HA	1:A:517:TYR:OH	2.19	0.42
1:D:93:LEU:HB3	1:D:182:ALA:CB	2.25	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:OD1	1:D:90:ASP:C	2.58	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:183:GLY:HA2	1:C:187:MET:HE3	2.01	0.42
1:C:552:PRO:HD3	1:C:576:TYR:CZ	2.55	0.42
1:A:466:TYR:N	1:A:466:TYR:CD1	2.87	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:B:467:ASP:CG	1:B:469:ILE:HG22	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:597:LYS:N	1:D:619:GLU:O	2.38	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:B:392:VAL:HG22	1:B:412:GLU:HG3	2.01	0.41
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:D:139:LYS:HA	6:D:660:HOH:O	2.19	0.41
1:C:251:TYR:O	1:C:261:GLY:HA3	2.21	0.41
1:C:413:VAL:HG21	1:C:553:PRO:HG2	2.02	0.41
1:D:442:VAL:HG22	1:D:442:VAL:O	2.20	0.41
1:B:479:ARG:HD3	1:B:523:TYR:CB	2.50	0.41
1:A:257:ASN:ND2	1:A:404:PHE:HB2	2.35	0.41
1:A:505:TYR:HB2	1:A:506:PRO:HD3	2.02	0.41
1:A:525:ALA:O	1:A:528:ARG:HB3	2.20	0.41
1:D:529:VAL:HG12	1:D:533:ILE:HD12	2.02	0.41
1:A:552:PRO:HD3	1:A:576:TYR:CZ	2.55	0.41
1:D:63:GLY:HA3	1:D:488:LEU:O	2.20	0.41
1:A:282:ARG:CZ	1:A:294:VAL:HG21	2.51	0.41
1:A:597:LYS:O	1:A:601:LYS:HG3	2.20	0.41
1:B:82:SER:HB3	1:B:85:THR:OG1	2.20	0.41
1:A:9:LEU:HD23	1:A:109:LEU:HD13	2.02	0.41
1:A:10:ARG:HD3	1:A:21:GLN:OE1	2.19	0.41
1:A:94:GLY:HA3	1:A:284:CYS:SG	2.61	0.41
1:A:126:ASP:OD2	1:A:205:LYS:NZ	2.54	0.41
1:A:585:ARG:NH1	1:A:585:ARG:HG2	2.36	0.41
1:B:72:SER:N	1:B:286:TYR:O	2.49	0.41
1:B:409:LYS:HG2	1:B:549:MET:HE3	2.03	0.41
1:C:252:ALA:O	1:C:254:PRO:HD3	2.21	0.41
1:C:279:VAL:HG11	1:C:296:LEU:HG	2.03	0.41
1:B:213:GLU:OE1	1:B:213:GLU:HA	2.16	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:C:254:PRO:HG2	1:C:415:GLY:HA2	2.03	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:A:123:ILE:O	1:A:201:ILE:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:GLU:OE1	4:C:622:GUA:O3	2.39	0.40
1:A:288:ASN:HD22	1:A:288:ASN:N	2.14	0.40
1:A:582:GLU:OE1	1:A:582:GLU:HA	2.21	0.40
1:B:82:SER:HA	1:B:83:PRO:HD3	1.68	0.40
1:B:326:SER:O	1:B:329:ASN:HB3	2.22	0.40
1:B:516:THR:O	1:B:516:THR:HG22	2.20	0.40
1:D:443:ILE:O	1:D:447:ILE:HG13	2.21	0.40
1:A:537:TRP:O	1:A:541:PHE:HB2	2.21	0.40
1:C:290:PRO:HA	3:C:621:SF4:S2	2.62	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
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 (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	607/619 (98%)	570 (94%)	34 (6%)	3 (0%)	29	41
1	B	607/619 (98%)	572 (94%)	31 (5%)	4 (1%)	22	32
1	C	607/619 (98%)	569 (94%)	35 (6%)	3 (0%)	29	41
1	D	607/619 (98%)	572 (94%)	34 (6%)	1 (0%)	47	62
All	All	2428/2476 (98%)	2283 (94%)	134 (6%)	11 (0%)	29	41

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	B	24	PRO

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Mol	Chain	Res	Type
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 (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	493/499 (99%)	454 (92%)	39 (8%)	12 19
1	B	493/499 (99%)	456 (92%)	37 (8%)	13 21
1	C	493/499 (99%)	453 (92%)	40 (8%)	11 18
1	D	493/499 (99%)	464 (94%)	29 (6%)	19 32
All	All	1972/1996 (99%)	1827 (93%)	145 (7%)	13 22

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Sometimes 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
1	B	288	ASN
1	C	280	GLN
1	C	288	ASN
1	D	288	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	0,12,12	-	-	-		
3	SF4	B	621	1	0,12,12	-	-	-		
4	GUA	B	622	5	8,8,8	1.05	0	9,9,9	0.93	0
5	PTE	C	623	4,2,1,6	42,55,57	2.79	16 (38%)	35,84,89	5.57	15 (42%)
4	GUA	C	622	5	8,8,8	0.97	0	9,9,9	1.04	0
3	SF4	C	621	1	0,12,12	-	-	-		
5	PTE	B	623	4,2,1,6	42,55,57	2.96	15 (35%)	35,84,89	4.54	18 (51%)
3	SF4	D	621	1	0,12,12	-	-	-		
4	GUA	D	622	5	8,8,8	1.02	0	9,9,9	0.96	0
4	GUA	A	622	5	8,8,8	0.98	0	9,9,9	1.01	0
5	PTE	A	623	4,2,1,6	42,55,57	2.59	14 (33%)	35,84,89	6.87	16 (45%)
5	PTE	D	623	4,2,1,6	42,55,57	2.68	14 (33%)	35,84,89	3.79	16 (45%)

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

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	623	PTE	P1-O1P	7.49	1.62	1.50
5	B	623	PTE	O28-C28	7.11	1.42	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	623	PTE	P2-O5P	7.00	1.61	1.50
5	B	623	PTE	C4-S4	-6.98	1.69	1.75
5	C	623	PTE	P2-O5P	6.92	1.61	1.50
5	C	623	PTE	O8-C8	6.58	1.41	1.24
5	B	623	PTE	C14-C5	6.53	1.58	1.53
5	B	623	PTE	P1-O1P	6.51	1.60	1.50
5	B	623	PTE	O8-C8	6.50	1.40	1.24
5	D	623	PTE	P2-O5P	6.26	1.60	1.50
5	C	623	PTE	O28-C28	6.25	1.40	1.24
5	A	623	PTE	C14-C5	6.09	1.58	1.53
5	D	623	PTE	O28-C28	6.08	1.39	1.24
5	D	623	PTE	O8-C8	6.05	1.39	1.24
5	D	623	PTE	P1-O1P	5.94	1.60	1.50
5	A	623	PTE	P2-O5P	5.79	1.59	1.50
5	A	623	PTE	O28-C28	5.72	1.38	1.24
5	C	623	PTE	C14-C5	5.71	1.58	1.53
5	D	623	PTE	C34-C25	5.68	1.58	1.53
5	C	623	PTE	P1-O1P	5.60	1.59	1.50
5	A	623	PTE	O8-C8	5.12	1.37	1.24
5	D	623	PTE	C14-C5	4.98	1.57	1.53
5	D	623	PTE	C8-N9	3.71	1.39	1.33
5	B	623	PTE	C34-C25	3.56	1.56	1.53
5	D	623	PTE	C25-N26	3.55	1.50	1.45
5	C	623	PTE	C34-C25	3.50	1.56	1.53
5	C	623	PTE	C8-N9	3.33	1.38	1.33
5	A	623	PTE	C5-N6	3.30	1.49	1.45
5	C	623	PTE	C27-C32	3.29	1.47	1.41
5	C	623	PTE	O2-C14	-3.24	1.39	1.43
5	C	623	PTE	C28-N29	3.21	1.38	1.33
5	D	623	PTE	C30-N29	3.08	1.40	1.35
5	C	623	PTE	C25-N26	3.04	1.49	1.45
5	C	623	PTE	C5-N6	2.95	1.49	1.45
5	A	623	PTE	C27-C32	2.88	1.46	1.41
5	B	623	PTE	C27-C32	2.87	1.46	1.41
5	D	623	PTE	C7-C12	2.86	1.46	1.41
5	B	623	PTE	C25-N26	2.80	1.49	1.45
5	A	623	PTE	C34-N33	2.79	1.50	1.44
5	B	623	PTE	C28-N29	2.76	1.37	1.33
5	B	623	PTE	C8-N9	2.76	1.37	1.33
5	B	623	PTE	C7-C12	2.75	1.46	1.41
5	D	623	PTE	O2-C2	-2.74	1.40	1.43
5	D	623	PTE	C5-N6	2.69	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	623	PTE	O2-C2	-2.62	1.40	1.43
5	D	623	PTE	C28-N29	2.60	1.37	1.33
5	D	623	PTE	C27-C32	2.58	1.46	1.41
5	A	623	PTE	C8-N9	2.57	1.37	1.33
5	C	623	PTE	C4-S4	-2.51	1.73	1.75
5	C	623	PTE	C7-C12	2.41	1.46	1.41
5	A	623	PTE	C7-C12	2.36	1.45	1.41
5	B	623	PTE	O2-C14	-2.36	1.40	1.43
5	A	623	PTE	C34-C25	2.35	1.55	1.53
5	C	623	PTE	O2-C2	-2.30	1.40	1.43
5	A	623	PTE	O2-C14	-2.27	1.40	1.43
5	B	623	PTE	C5-N6	2.25	1.48	1.45
5	C	623	PTE	C28-C27	2.13	1.44	1.41
5	B	623	PTE	C32-N31	2.07	1.38	1.34
5	A	623	PTE	C32-N31	2.02	1.38	1.34

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	623	PTE	O2-C14-N13	29.23	138.60	108.57
5	C	623	PTE	O2-C14-N13	23.87	133.10	108.57
5	A	623	PTE	O22-C34-N33	18.92	128.01	108.57
5	B	623	PTE	O22-C34-N33	15.71	124.71	108.57
5	C	623	PTE	C28-C27-N26	10.83	128.21	119.12
5	C	623	PTE	C8-C7-N6	10.45	127.89	119.12
5	B	623	PTE	C28-C27-N26	10.10	127.60	119.12
5	A	623	PTE	C8-C7-N6	9.79	127.34	119.12
5	D	623	PTE	C8-C7-N6	9.34	126.96	119.12
5	C	623	PTE	O2-C14-C5	-9.26	102.78	108.96
5	D	623	PTE	C28-C27-N26	8.24	126.04	119.12
5	B	623	PTE	O2-C14-N13	-7.94	100.40	108.57
5	A	623	PTE	O2-C14-C5	-7.91	103.69	108.96
5	B	623	PTE	O22-C34-C25	7.31	113.84	108.96
5	B	623	PTE	C8-C7-N6	7.28	125.23	119.12
5	D	623	PTE	O2-C14-C5	-7.07	104.25	108.96
5	A	623	PTE	C28-C27-N26	7.04	125.03	119.12
5	A	623	PTE	O22-C34-C25	-6.54	104.60	108.96
5	D	623	PTE	N30-C30-N29	6.54	127.42	117.25
5	B	623	PTE	C28-N29-C30	6.47	126.21	115.93
5	C	623	PTE	O22-C34-N33	6.38	115.13	108.57
5	D	623	PTE	O2-C14-N13	6.13	114.86	108.57
5	A	623	PTE	C28-N29-C30	5.92	125.33	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	623	PTE	N11-C10-N9	-5.69	116.50	125.42
5	D	623	PTE	C10-N9-C8	5.32	124.38	115.93
5	A	623	PTE	N29-C30-N31	-5.26	117.18	125.42
5	D	623	PTE	O22-C34-N33	5.09	113.80	108.57
5	C	623	PTE	C10-N9-C8	5.09	124.01	115.93
5	D	623	PTE	N29-C30-N31	-4.96	117.64	125.42
5	D	623	PTE	N10-C10-N9	4.93	124.92	117.25
5	B	623	PTE	C27-C32-N33	-4.91	113.64	118.13
5	D	623	PTE	N11-C10-N9	-4.86	117.80	125.42
5	D	623	PTE	C28-N29-C30	4.74	123.46	115.93
5	B	623	PTE	N29-C30-N31	-4.68	118.08	125.42
5	D	623	PTE	O22-C34-C25	-4.50	105.96	108.96
5	A	623	PTE	N30-C30-N31	4.49	124.23	117.25
5	B	623	PTE	C10-N9-C8	4.39	122.90	115.93
5	C	623	PTE	C28-N29-C30	4.37	122.88	115.93
5	A	623	PTE	N11-C10-N9	-4.20	118.83	125.42
5	A	623	PTE	C10-N9-C8	4.13	122.50	115.93
5	B	623	PTE	N30-C30-N31	4.00	123.47	117.25
5	A	623	PTE	N10-C10-N9	4.00	123.47	117.25
5	B	623	PTE	N11-C10-N9	-3.88	119.33	125.42
5	C	623	PTE	N10-C10-N9	3.73	123.06	117.25
5	B	623	PTE	N10-C10-N9	3.64	122.92	117.25
5	C	623	PTE	N29-C30-N31	-3.49	119.94	125.42
5	A	623	PTE	C27-C32-N33	-3.46	114.97	118.13
5	C	623	PTE	C10-N11-C12	3.23	121.77	114.54
5	B	623	PTE	O2-C14-C5	3.21	111.10	108.96
5	A	623	PTE	C10-N11-C12	3.04	121.36	114.54
5	D	623	PTE	C10-N11-C12	3.01	121.28	114.54
5	B	623	PTE	C10-N11-C12	2.80	120.82	114.54
5	D	623	PTE	O6P-P2-O8P	-2.75	94.97	107.75
5	D	623	PTE	C30-N31-C32	2.67	120.53	114.54
5	C	623	PTE	C30-N31-C32	2.60	120.36	114.54
5	C	623	PTE	C7-C8-N9	-2.42	117.12	124.01
5	B	623	PTE	C27-C28-N29	-2.41	117.15	124.01
5	C	623	PTE	N30-C30-N29	2.39	120.97	117.25
5	A	623	PTE	C30-N31-C32	2.27	119.62	114.54
5	B	623	PTE	O2P-P1-O4P	-2.25	97.29	107.75
5	B	623	PTE	C30-N31-C32	2.16	119.38	114.54
5	B	623	PTE	C7-C8-N9	-2.12	117.98	124.01
5	D	623	PTE	C7-C8-N9	-2.08	118.09	124.01
5	A	623	PTE	O4P-P1-O3P	2.04	117.05	109.07
5	C	623	PTE	N10-C10-N11	2.03	120.41	117.25

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	623	PTE	O4P-C1-C2-O2
4	A	622	GUA	C3-C4-C5-O3
4	B	622	GUA	C3-C4-C5-O3
4	D	622	GUA	C3-C4-C5-O3
5	A	623	PTE	O4P-C1-C2-O2
5	B	623	PTE	O4P-C1-C2-O2
4	C	622	GUA	C3-C4-C5-O3
4	A	622	GUA	C3-C4-C5-O4
4	B	622	GUA	C3-C4-C5-O4
4	D	622	GUA	C3-C4-C5-O4
4	C	622	GUA	C3-C4-C5-O4
5	D	623	PTE	C1-O4P-P1-O3P
4	C	622	GUA	O2-C1-C2-C3
4	A	622	GUA	O2-C1-C2-C3
4	C	622	GUA	O1-C1-C2-C3

There are no ring outliers.

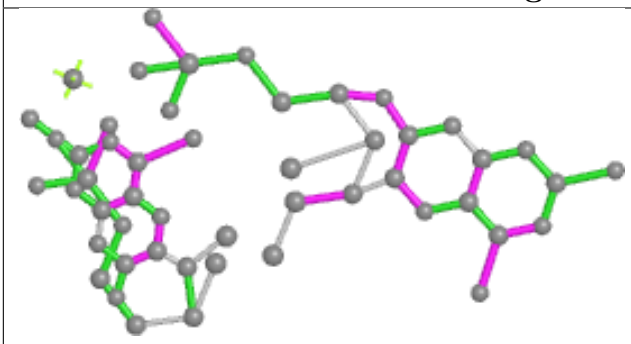
10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	621	SF4	1	0
4	B	622	GUA	3	0
5	C	623	PTE	1	0
4	C	622	GUA	2	0
3	C	621	SF4	1	0
5	B	623	PTE	1	0
4	D	622	GUA	1	0
4	A	622	GUA	2	0
5	A	623	PTE	1	0
5	D	623	PTE	1	0

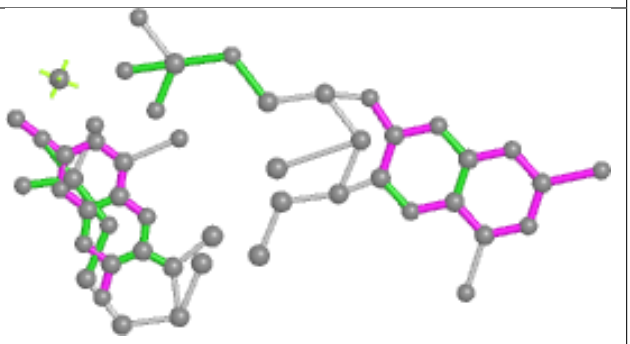
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

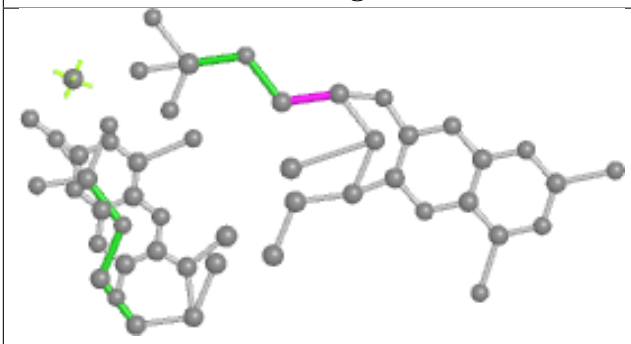
Ligand PTE C 623



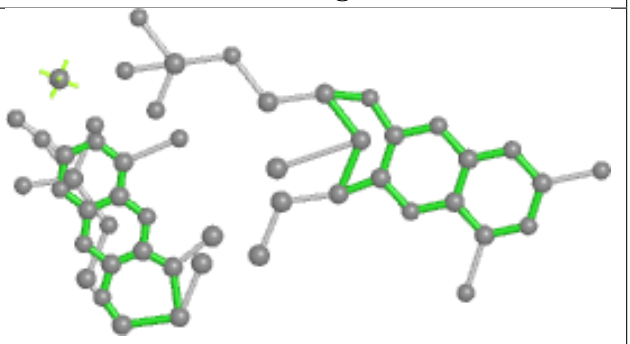
Bond lengths



Bond angles

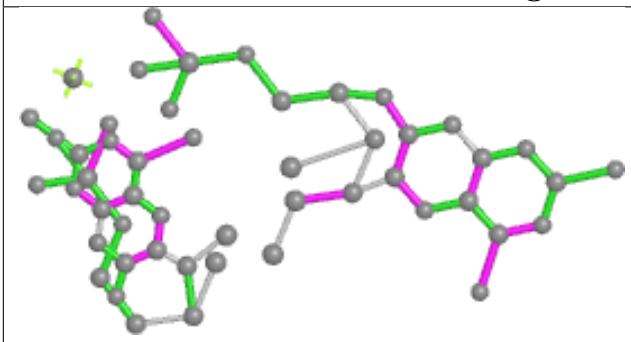


Torsions

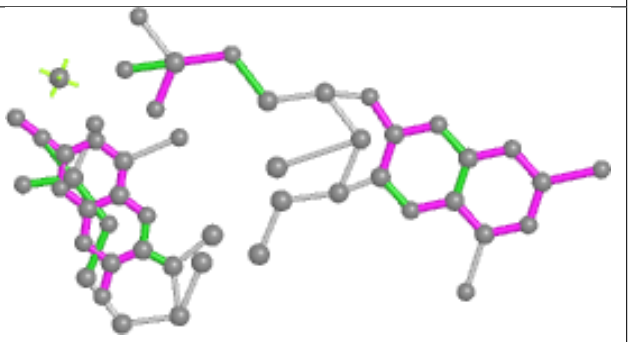


Rings

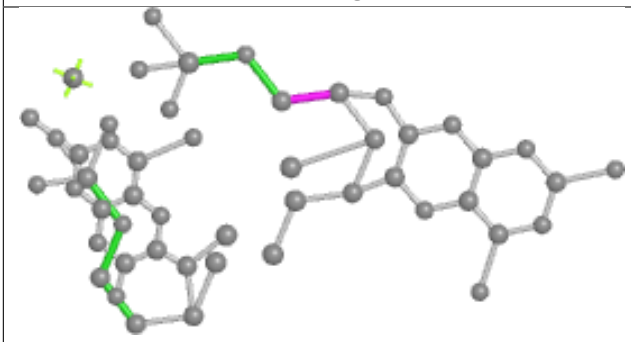
Ligand PTE B 623



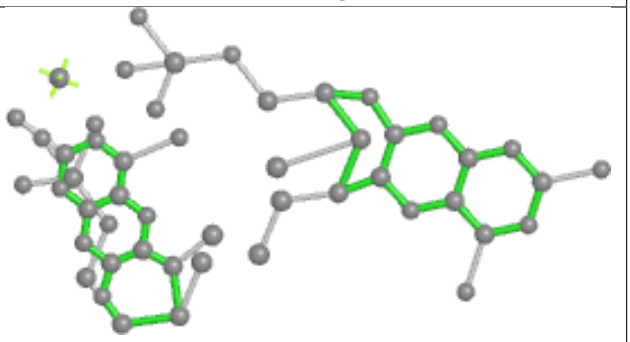
Bond lengths



Bond angles

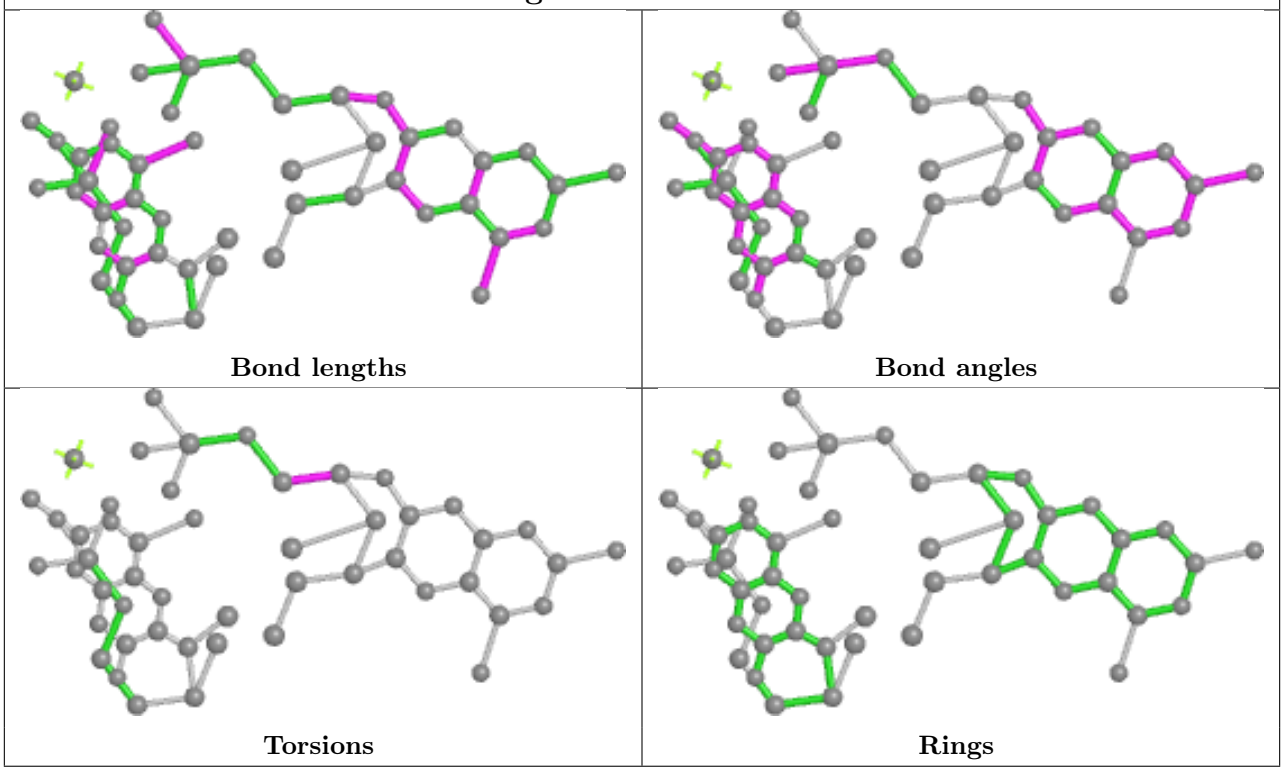


Torsions

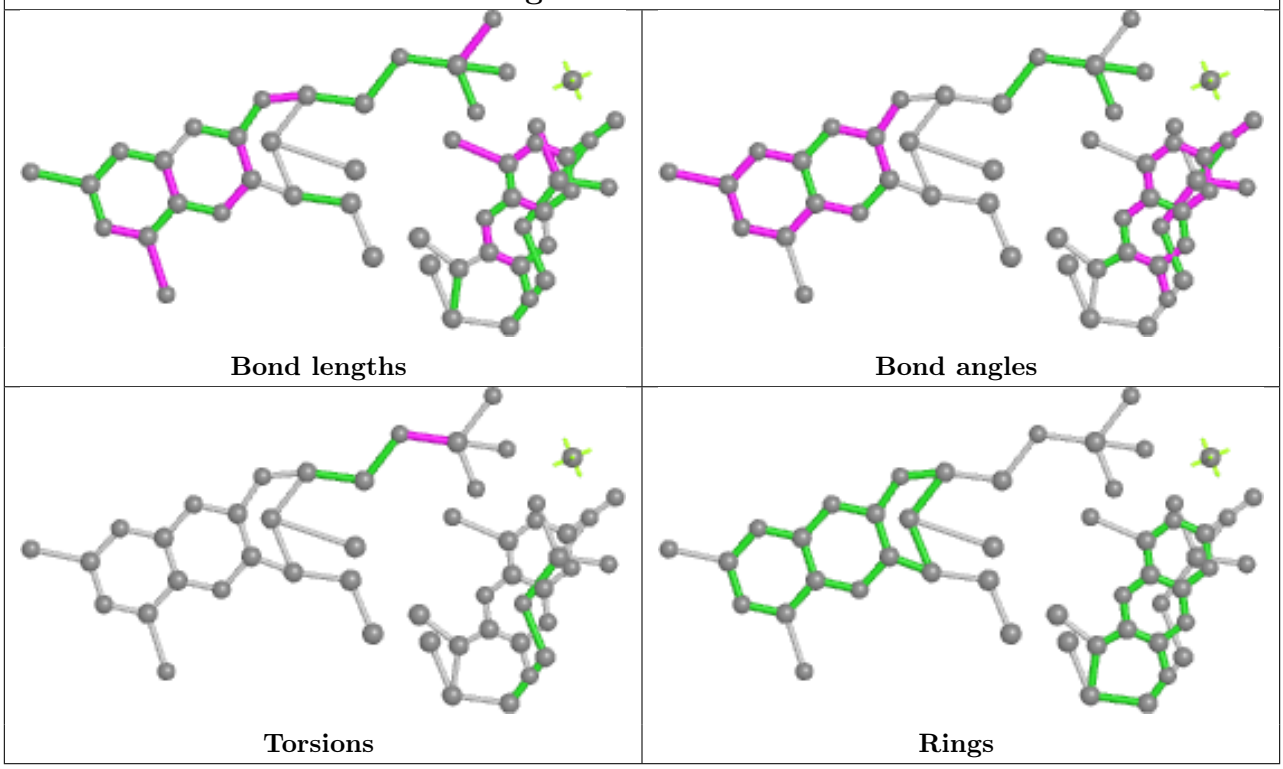


Rings

Ligand PTE A 623



Ligand PTE D 623



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.