Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:50 PM GMT

PDB ID	:	1MAA
Title	:	MOUSE ACETYLCHOLINESTERASE CATALYTIC DOMAIN, GLYCOSYLATED PROTEIN
Authors	:	Bourne, Y.; Taylor, P.; Bougis, P.E.; Marchot, P.
Deposited on	:	1998-11-04
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

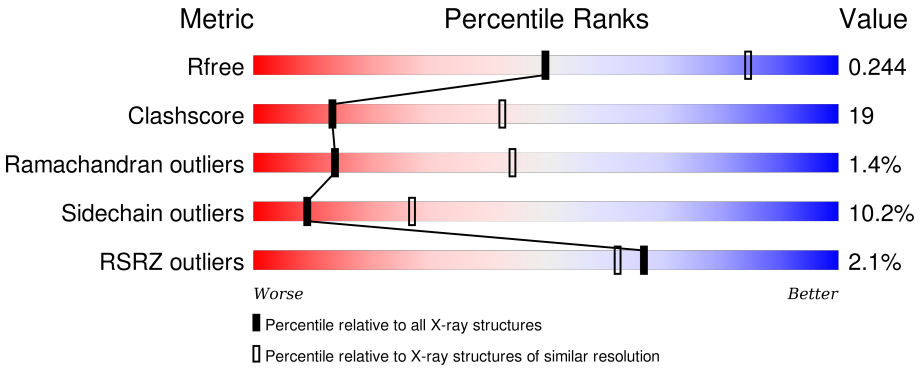
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	547	3% 56% 36% 6%
1	B	547	2% 64% 28% 5%
1	C	547	2% 62% 33%
1	D	547	2% 59% 33% 7%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	609	-	-	-	X
3	NAG	A	709	-	-	-	X
4	PO4	B	548	-	X	-	X
4	PO4	C	548	-	X	-	X
4	PO4	C	998	-	X	-	-
5	DME	A	998	-	-	-	X
5	DME	B	996	-	-	X	X
5	DME	C	997	-	-	X	X
5	DME	D	999	-	-	-	X
6	GOL	C	951	-	-	X	-
6	GOL	D	952	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17084 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 ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4187	2689	727	757	14			
1	B	536	Total	C	N	O	S	0	0	0
			4169	2678	723	754	14			
1	C	540	Total	C	N	O	S	0	0	0
			4186	2688	724	760	14			
1	D	541	Total	C	N	O	S	0	0	0
			4192	2692	728	758	14			

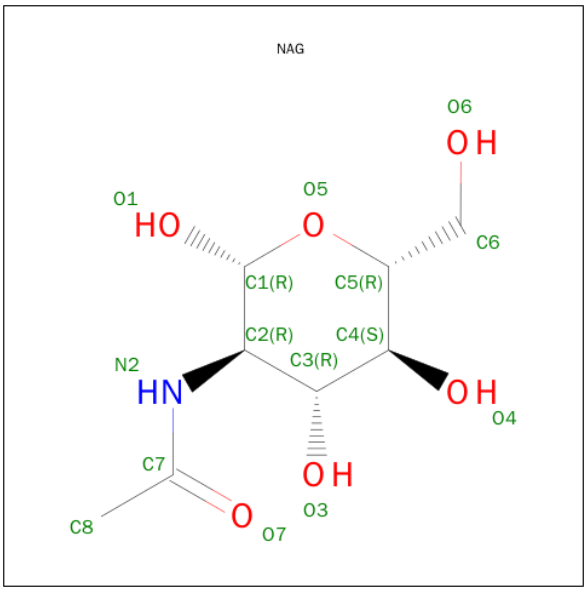
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	ARG	SER	CONFLICT	UNP P21836
B	495	ARG	SER	CONFLICT	UNP P21836
C	495	ARG	SER	CONFLICT	UNP P21836
D	495	ARG	SER	CONFLICT	UNP P21836

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

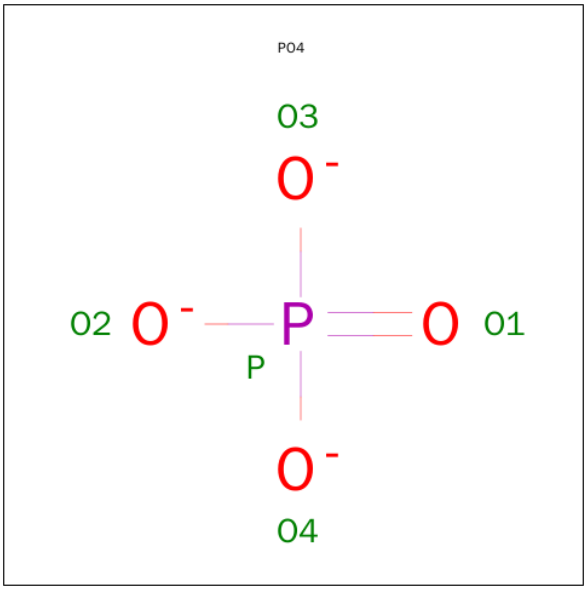
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



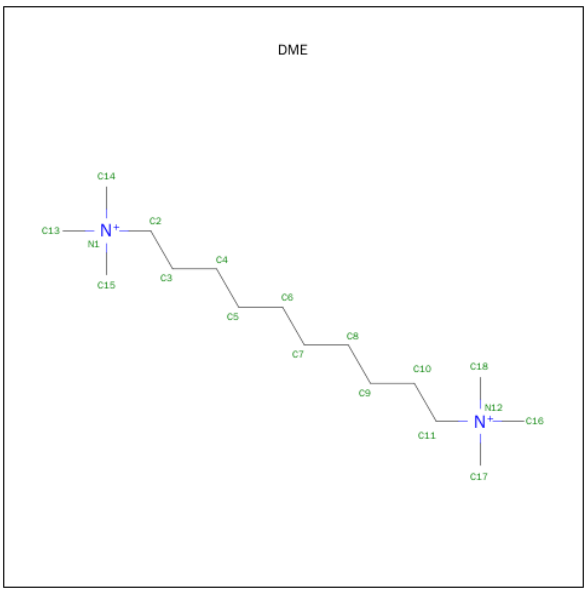
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



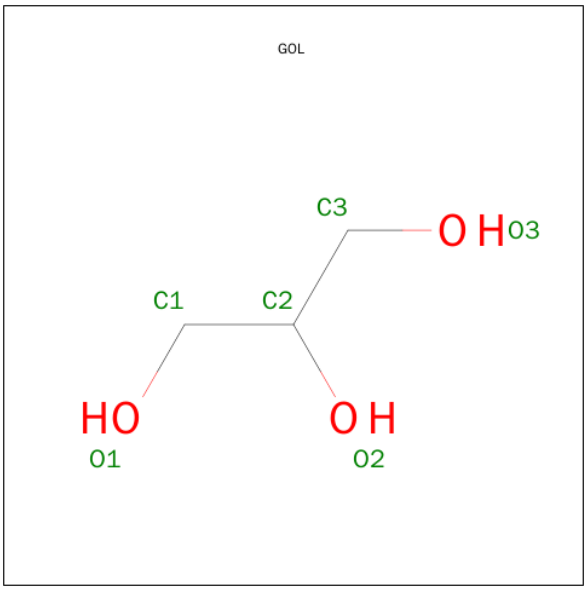
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0

- Molecule 5 is DECAMETHONIUM ION (three-letter code: DME) (formula: $C_{16}H_{38}N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N 18 16 2	0	0
5	D	1	Total C N 18 16 2	0	0
5	B	1	Total C N 18 16 2	0	0
5	A	1	Total C N 18 16 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

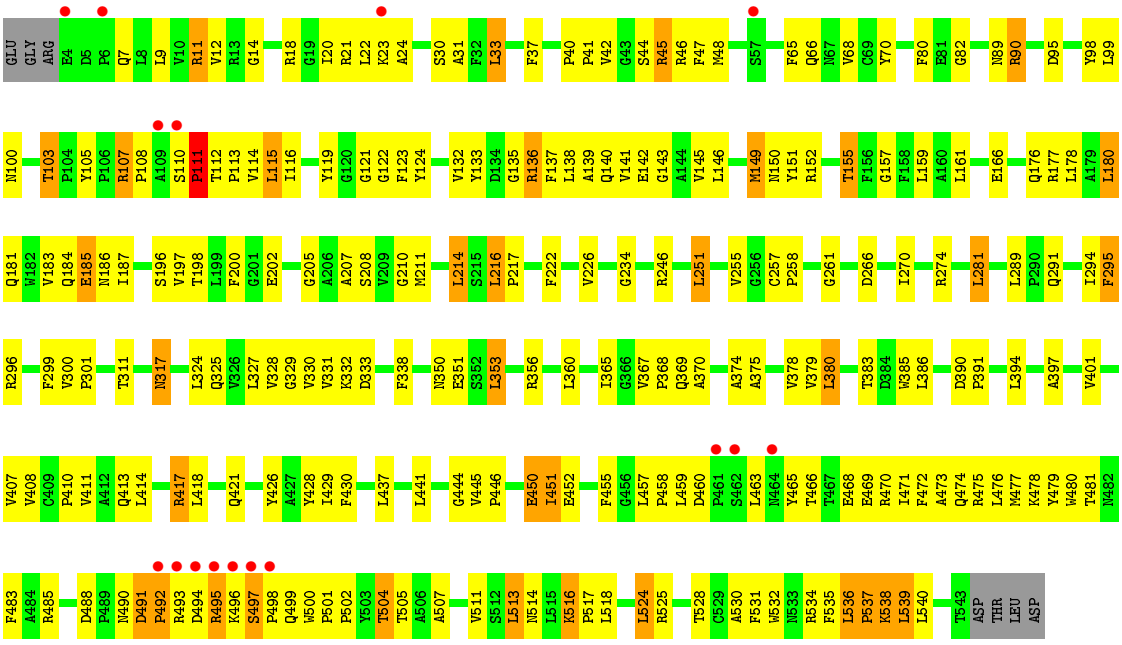
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	27	Total O 27 27	0	0
7	B	49	Total O 49 49	0	0
7	C	59	Total O 59 59	0	0
7	D	52	Total O 52 52	0	0

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.

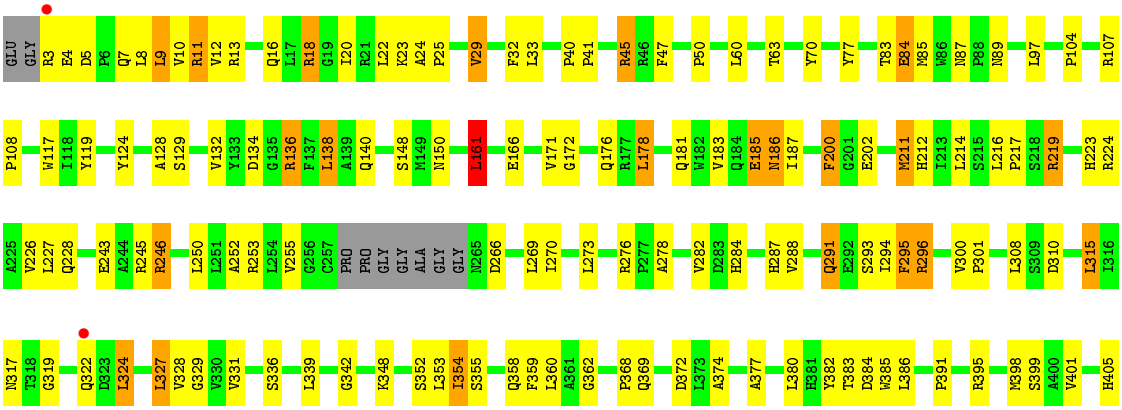
- Molecule 1: ACETYLCHOLINESTERASE

Chain A:



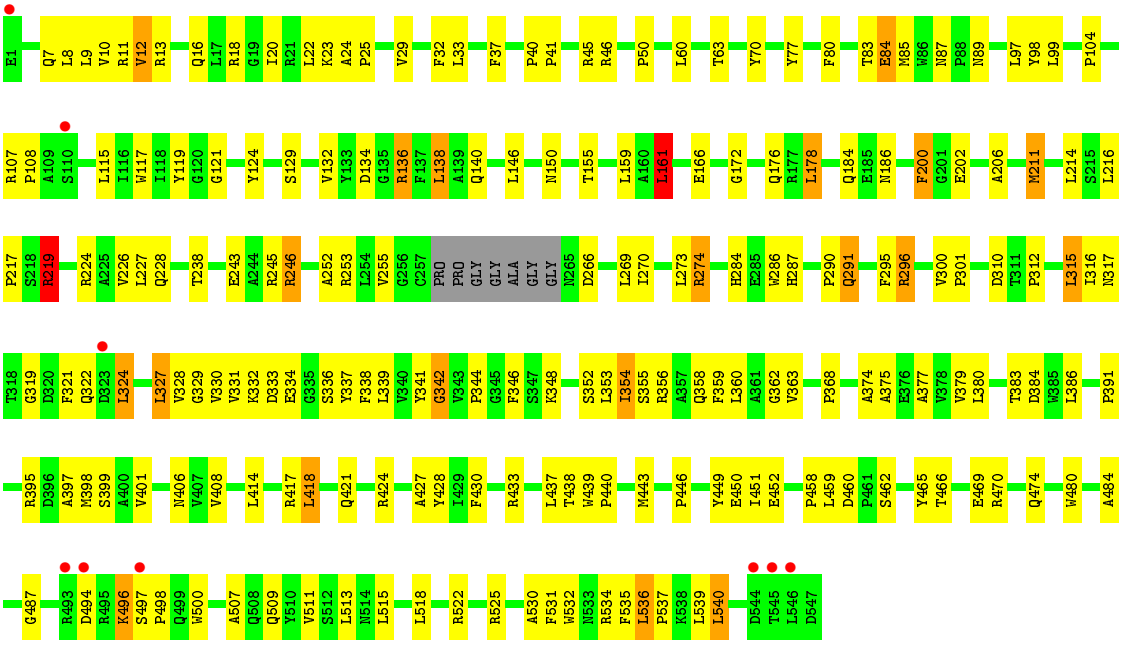
- Molecule 1: ACETYLCHOLINESTERASE

Chain B:



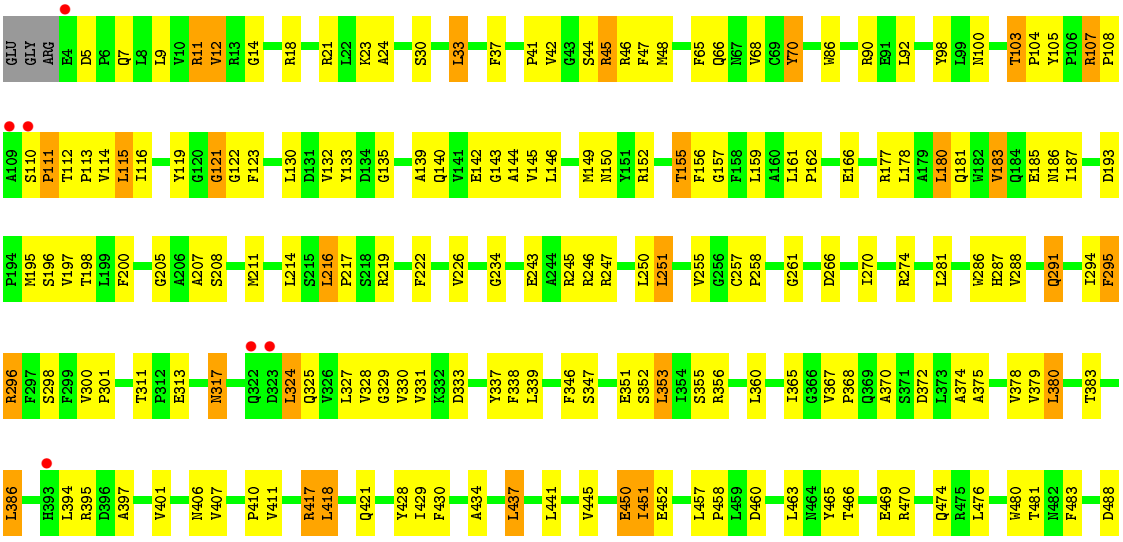
• Molecule 1: ACETYLCHOLINESTERASE

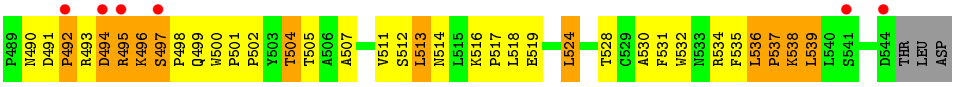
Chain C:



• Molecule 1: ACETYLCHOLINESTERASE

Chain D:




P489
N490
D491
P492
R493
D494
R495
K496
S497
P498
Q499
W500
P501
P502
Y503
T504
T505
A506
A507
V511
S512
L513
N514
L515
K516
P517
L518
E519
L524
T528
C529
A530
F531
W532
N533
R534
F535
L536
P537
K538
L539
L540
S541
D544
THR
LEU
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	136.55Å 173.13Å 224.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-2.90) 90.3 (15.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.200 , 0.248 0.202 , 0.244	Depositor DCC
R_{free} test set	2166 reflections (2.02%)	DCC
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 117431 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17084	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GOL, PO4, DME, FUL, NAG

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	0.54	0/4313	0.81	3/5898 (0.1%)
1	B	0.58	0/4292	0.82	5/5868 (0.1%)
1	C	0.58	0/4309	0.84	5/5892 (0.1%)
1	D	0.51	0/4318	0.80	1/5905 (0.0%)
All	All	0.55	0/17232	0.82	14/23563 (0.1%)

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
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	60	LEU	CA-CB-CG	6.45	130.13	115.30
1	D	18	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	18	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	C	219	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	B	18	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	274	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	C	161	LEU	N-CA-C	-5.46	96.27	111.00
1	C	60	LEU	CA-CB-CG	5.38	127.68	115.30
1	B	161	LEU	N-CA-C	-5.24	96.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	186	ASN	N-CA-C	5.20	125.04	111.00
1	B	18	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	491	ASP	C-N-CD	-5.09	109.40	120.60
1	C	246	ARG	NE-CZ-NH1	-5.07	117.77	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	TYR	Sidechain
1	C	98	TYR	Sidechain
1	D	70	TYR	Sidechain

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	4187	0	4068	159	0
1	B	4169	0	4048	139	0
1	C	4186	0	4053	154	0
1	D	4192	0	4070	168	0
2	D	38	0	34	2	0
3	A	14	0	13	1	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
5	A	18	0	38	1	0
5	B	18	0	38	13	0
5	C	18	0	38	19	0
5	D	18	0	38	7	0
6	A	6	0	8	1	0
6	B	6	0	8	2	0
6	C	6	0	8	7	0
6	D	6	0	8	1	0
7	A	27	0	0	2	0
7	B	49	0	0	1	0
7	C	59	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	52	0	0	4	0
All	All	17084	0	16470	625	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 19.

All (625) 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:428:TYR:HB2	1:D:513:LEU:HD23	1.33	1.10
1:A:261:GLY:HA3	5:C:997:DME:H152	1.29	1.09
1:B:219:ARG:HG3	1:B:219:ARG:HH11	1.23	0.99
1:A:428:TYR:HB2	1:A:513:LEU:HD23	1.44	0.98
1:B:84:GLU:HA	1:B:87:ASN:HD22	1.31	0.96
1:A:261:GLY:HA3	5:C:997:DME:C15	1.95	0.95
1:D:45:ARG:HG3	1:D:45:ARG:HH11	1.31	0.95
1:D:429:ILE:HD11	1:D:524:LEU:HD21	1.45	0.95
1:C:84:GLU:HA	1:C:87:ASN:HD22	1.34	0.93
1:A:429:ILE:HD11	1:A:524:LEU:HD21	1.53	0.91
1:C:219:ARG:HG2	1:C:219:ARG:HH11	1.37	0.89
1:B:498:PRO:HB2	1:B:518:LEU:HB2	1.55	0.88
1:D:329:GLY:HA3	1:D:428:TYR:CZ	2.08	0.88
1:D:329:GLY:HA3	1:D:428:TYR:CE2	2.10	0.87
1:D:11:ARG:HB2	1:D:11:ARG:HH11	1.41	0.85
1:A:45:ARG:HH11	1:A:45:ARG:HG3	1.40	0.85
1:C:341:TYR:CD2	5:C:997:DME:H22	2.11	0.84
1:D:107:ARG:HG3	1:D:107:ARG:HH11	1.42	0.84
1:B:219:ARG:HG3	1:B:219:ARG:NH1	1.91	0.83
1:B:319:GLY:H	1:B:421:GLN:HE22	1.25	0.83
1:D:534:ARG:HG3	1:D:534:ARG:HH11	1.44	0.83
1:A:30:SER:HB2	1:A:103:THR:HG22	1.60	0.81
1:B:161:LEU:HD22	1:B:270:ILE:HD11	1.62	0.80
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.43	0.80
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.16	0.80
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.62	0.80
1:C:286:TRP:CH2	5:C:997:DME:C15	2.65	0.80
1:C:286:TRP:CH2	5:C:997:DME:H151	2.16	0.79
1:C:498:PRO:HB2	1:C:518:LEU:HB2	1.63	0.79
1:A:226:VAL:HG11	1:A:480:TRP:HE1	1.48	0.79
1:B:41:PRO:HD3	1:B:97:LEU:HD12	1.66	0.78
1:C:286:TRP:CZ2	5:C:997:DME:H151	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:ASP:O	1:D:270:ILE:HG12	1.85	0.77
1:A:534:ARG:HG3	1:A:534:ARG:HH11	1.49	0.77
1:B:124:TYR:OH	5:B:996:DME:H82	1.84	0.77
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.68	0.76
1:B:136:ARG:HH11	1:B:136:ARG:HG2	1.50	0.75
1:C:161:LEU:HD22	1:C:270:ILE:HD11	1.68	0.74
7:A:1009:HOH:O	1:B:527:GLN:HG3	1.88	0.74
1:C:219:ARG:NH1	1:C:219:ARG:HG2	2.02	0.73
1:B:291:GLN:HE21	1:B:368:PRO:HB2	1.53	0.73
1:B:319:GLY:H	1:B:421:GLN:NE2	1.86	0.72
1:D:528:THR:O	1:D:531:PHE:HB3	1.88	0.72
1:C:329:GLY:HA3	1:C:428:TYR:CE2	2.25	0.72
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.25	0.71
1:C:104:PRO:HD2	1:C:108:PRO:HD3	1.71	0.71
1:D:45:ARG:HG3	1:D:45:ARG:NH1	1.98	0.71
1:D:367:VAL:HG12	1:D:370:ALA:HB2	1.73	0.71
1:D:460:ASP:HB3	1:D:463:LEU:HD12	1.72	0.71
1:C:7:GLN:NE2	1:C:107:ARG:H	1.88	0.71
1:D:535:PHE:O	1:D:538:LYS:HG2	1.90	0.70
1:A:528:THR:O	1:A:531:PHE:HB3	1.92	0.70
1:A:45:ARG:NH1	1:A:45:ARG:HG3	2.05	0.70
1:D:161:LEU:HD22	1:D:270:ILE:HD11	1.74	0.70
1:C:362:GLY:HA3	1:C:398:MET:HE3	1.73	0.70
1:D:65:PHE:HB2	1:D:90:ARG:HH11	1.55	0.69
1:A:180:LEU:O	1:A:183:VAL:HG12	1.92	0.69
1:C:338:PHE:HE2	5:C:997:DME:H71	1.56	0.69
1:C:291:GLN:HE21	1:C:368:PRO:HB2	1.58	0.69
1:D:428:TYR:CB	1:D:513:LEU:HD23	2.18	0.69
1:A:535:PHE:O	1:A:538:LYS:HG2	1.92	0.69
1:D:30:SER:HB2	1:D:103:THR:HG22	1.73	0.69
1:B:362:GLY:HA3	1:B:398:MET:HE3	1.75	0.68
5:B:996:DME:H153	1:D:261:GLY:HA2	1.76	0.67
1:A:116:ILE:HD11	1:A:183:VAL:HG11	1.75	0.67
1:C:319:GLY:H	1:C:421:GLN:HE22	1.42	0.67
1:D:337:TYR:HE2	5:D:999:DME:H71	1.60	0.67
1:C:310:ASP:HB3	1:C:315:LEU:HD13	1.77	0.66
1:D:347:SER:HB2	2:D:609:NAG:H62	1.76	0.66
1:D:250:LEU:HD23	1:D:288:VAL:HG12	1.78	0.66
1:D:44:SER:HA	1:D:274:ARG:HD2	1.78	0.66
1:D:24:ALA:HB3	1:D:140:GLN:HG3	1.77	0.66
1:A:261:GLY:CA	5:C:997:DME:H152	2.17	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:534:ARG:NH1	1:D:534:ARG:HG3	2.11	0.66
1:B:104:PRO:HD2	1:B:108:PRO:HD3	1.76	0.66
1:A:397:ALA:O	1:A:401:VAL:HG23	1.96	0.66
1:C:286:TRP:CH2	5:C:997:DME:H153	2.31	0.65
1:A:266:ASP:O	1:A:270:ILE:HG12	1.97	0.65
1:B:459:LEU:HD23	1:B:470:ARG:HG2	1.79	0.65
1:C:226:VAL:HG13	1:C:327:LEU:HB3	1.79	0.65
1:A:44:SER:HA	1:A:274:ARG:HD2	1.79	0.65
1:A:365:ILE:O	1:A:368:PRO:HD3	1.96	0.65
1:D:245:ARG:HD2	7:D:1000:HOH:O	1.97	0.64
1:D:452:GLU:OE2	6:D:952:GOL:O1	2.12	0.64
1:C:440:PRO:HG2	1:C:443:MET:HG3	1.78	0.64
1:A:294:ILE:HG12	1:A:365:ILE:HG22	1.79	0.64
1:A:460:ASP:HB3	1:A:463:LEU:HD12	1.80	0.64
1:A:497:SER:CB	1:A:498:PRO:HD3	2.27	0.64
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.32	0.64
1:B:310:ASP:HB3	1:B:315:LEU:HD13	1.79	0.64
1:B:252:ALA:HA	1:B:273:LEU:HD21	1.80	0.63
1:C:117:TRP:HB2	1:C:200:PHE:CE1	2.33	0.63
1:B:294:ILE:HA	5:B:996:DME:C3	2.28	0.63
1:C:494:ASP:C	1:C:496:LYS:H	2.00	0.63
1:A:450:GLU:HG2	1:A:451:ILE:N	2.12	0.63
1:D:417:ARG:HH11	1:D:417:ARG:HG3	1.62	0.63
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.32	0.63
1:B:136:ARG:CG	1:B:136:ARG:HH11	2.12	0.63
1:C:219:ARG:NH2	1:C:324:LEU:HG	2.13	0.62
1:A:452:GLU:OE2	6:A:954:GOL:O1	2.17	0.62
1:A:114:VAL:HG23	1:A:197:VAL:HA	1.80	0.62
1:B:226:VAL:HG13	1:B:327:LEU:HB3	1.80	0.62
1:B:317:ASN:ND2	1:B:417:ARG:HE	1.97	0.62
1:B:348:LYS:HA	1:B:440:PRO:HG3	1.81	0.62
1:A:534:ARG:NH1	1:A:534:ARG:HG3	2.14	0.62
1:A:207:ALA:O	1:A:211:MET:HG2	1.99	0.62
1:A:11:ARG:HB2	1:A:11:ARG:HH11	1.65	0.62
1:D:497:SER:CB	1:D:498:PRO:HD3	2.30	0.62
1:D:450:GLU:HG2	1:D:451:ILE:N	2.14	0.62
1:B:77:TYR:CD2	1:B:348:LYS:HD3	2.35	0.61
1:D:498:PRO:HB2	1:D:518:LEU:HB2	1.80	0.61
1:D:12:VAL:HG12	1:D:14:GLY:H	1.65	0.61
1:B:494:ASP:C	1:B:496:LYS:H	2.03	0.61
1:B:446:PRO:HG2	1:B:449:TYR:CD2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:GLY:HA3	1:C:428:TYR:CZ	2.36	0.61
1:B:352:SER:O	1:B:395:ARG:HG3	2.01	0.60
1:A:155:THR:HG22	1:A:159:LEU:HD12	1.83	0.60
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.36	0.60
1:B:50:PRO:HB2	1:B:178:LEU:HD12	1.83	0.60
1:B:117:TRP:HB2	1:B:200:PHE:CE1	2.37	0.60
5:D:999:DME:H92	5:D:999:DME:H182	1.83	0.60
1:B:317:ASN:HD22	1:B:417:ARG:HH21	1.49	0.60
1:D:470:ARG:O	1:D:474:GLN:HG3	2.01	0.60
1:D:300:VAL:HB	1:D:301:PRO:HD2	1.84	0.60
1:D:356:ARG:HA	1:D:394:LEU:HD13	1.84	0.60
1:A:197:VAL:HB	1:A:222:PHE:HA	1.84	0.59
1:C:337:TYR:CE1	5:C:997:DME:H61	2.36	0.59
1:A:37:PHE:HD1	1:A:178:LEU:HD12	1.66	0.59
1:C:224:ARG:HH11	1:C:224:ARG:HG3	1.67	0.59
1:A:532:TRP:O	1:A:537:PRO:HD3	2.02	0.59
1:A:113:PRO:HA	1:A:196:SER:OG	2.02	0.59
1:B:293:SER:O	5:B:996:DME:H132	2.01	0.59
1:D:113:PRO:HA	1:D:196:SER:OG	2.03	0.59
1:A:473:ALA:O	1:A:477:MET:HG3	2.02	0.59
1:B:211:MET:HG3	1:B:308:LEU:HD21	1.84	0.59
1:D:114:VAL:HG11	1:D:187:ILE:HG12	1.85	0.59
1:C:20:ILE:HB	1:C:63:THR:HG22	1.83	0.59
1:C:319:GLY:H	1:C:421:GLN:NE2	2.00	0.59
1:D:287:HIS:HB3	7:D:1034:HOH:O	2.02	0.59
1:A:135:GLY:HA3	1:A:146:LEU:HD22	1.83	0.59
1:C:77:TYR:CD2	1:C:348:LYS:HD3	2.37	0.59
1:D:374:ALA:HA	1:D:539:LEU:HD13	1.85	0.59
1:C:266:ASP:O	1:C:270:ILE:HG12	2.02	0.59
1:D:162:PRO:HG2	7:D:1000:HOH:O	2.03	0.59
1:B:470:ARG:O	1:B:474:GLN:HG3	2.03	0.59
1:C:337:TYR:HE1	5:C:997:DME:H61	1.67	0.58
1:D:45:ARG:CG	1:D:45:ARG:HH11	2.12	0.58
1:B:339:LEU:HD11	1:B:399:SER:HA	1.86	0.58
1:D:504:THR:OG1	1:D:507:ALA:HB3	2.03	0.58
1:B:328:VAL:O	1:B:427:ALA:HA	2.03	0.58
1:C:85:MET:CE	6:C:951:GOL:HO1	2.16	0.58
1:A:12:VAL:HG12	1:A:14:GLY:H	1.67	0.58
1:A:470:ARG:O	1:A:474:GLN:HG3	2.03	0.58
1:C:353:LEU:HB3	1:C:391:PRO:HB2	1.85	0.58
1:C:332:LYS:HG2	1:C:333:ASP:OD1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:PRO:CB	1:B:518:LEU:HB2	2.31	0.58
1:C:134:ASP:OD1	1:C:136:ARG:HB3	2.03	0.58
1:C:341:TYR:CD2	5:C:997:DME:C2	2.84	0.57
1:D:197:VAL:HB	1:D:222:PHE:HA	1.86	0.57
1:A:66:GLN:HG3	1:A:98:TYR:CG	2.38	0.57
1:B:354:ILE:HB	1:B:358:GLN:OE1	2.04	0.57
1:C:216:LEU:HB3	1:C:217:PRO:HD3	1.86	0.57
1:C:338:PHE:CE2	5:C:997:DME:H71	2.38	0.57
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.85	0.57
1:A:374:ALA:HA	1:A:539:LEU:HD13	1.86	0.57
1:B:84:GLU:HA	1:B:87:ASN:ND2	2.11	0.57
1:C:355:SER:OG	1:C:358:GLN:HG3	2.05	0.57
1:A:114:VAL:HG12	1:A:145:VAL:HB	1.87	0.57
1:D:114:VAL:HG23	1:D:197:VAL:HA	1.87	0.57
1:C:414:LEU:HG	1:C:418:LEU:HD22	1.85	0.57
1:C:437:LEU:HA	6:C:951:GOL:H32	1.87	0.57
1:D:365:ILE:O	1:D:368:PRO:HD3	2.05	0.57
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.87	0.57
1:D:226:VAL:HG11	1:D:480:TRP:HE1	1.70	0.57
1:D:155:THR:HG22	1:D:159:LEU:HB2	1.86	0.56
1:D:532:TRP:O	1:D:537:PRO:HD3	2.05	0.56
1:C:300:VAL:HB	1:C:301:PRO:CD	2.35	0.56
1:B:293:SER:O	5:B:996:DME:C13	2.53	0.56
1:B:211:MET:HE2	1:B:301:PRO:HG2	1.88	0.56
1:A:181:GLN:O	1:A:185:GLU:HG2	2.04	0.56
1:B:176:GLN:OE1	1:B:212:HIS:HE1	1.88	0.56
1:A:375:ALA:O	1:A:379:VAL:HG23	2.06	0.56
1:A:119:TYR:CE1	1:A:151:TYR:CE1	2.94	0.56
1:D:114:VAL:HG12	1:D:145:VAL:HB	1.88	0.56
1:C:202:GLU:HA	1:C:228:GLN:O	2.06	0.56
1:C:328:VAL:O	1:C:427:ALA:HA	2.06	0.56
1:C:460:ASP:OD1	1:C:462:SER:HB3	2.05	0.56
1:C:535:PHE:CE2	1:C:539:LEU:HD12	2.40	0.56
1:C:41:PRO:HD3	1:C:97:LEU:HD12	1.87	0.55
1:A:65:PHE:HE1	1:A:100:ASN:ND2	2.04	0.55
1:A:417:ARG:HH11	1:A:417:ARG:HG3	1.71	0.55
1:B:266:ASP:O	1:B:270:ILE:HG12	2.06	0.55
1:C:252:ALA:HA	1:C:273:LEU:HD21	1.88	0.55
1:A:139:ALA:O	1:A:143:GLY:HA2	2.06	0.55
1:A:498:PRO:HB2	1:A:518:LEU:HB2	1.88	0.55
1:A:511:VAL:HB	1:A:518:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:PRO:CB	1:C:518:LEU:HB2	2.32	0.55
1:D:65:PHE:HB2	1:D:90:ARG:NH1	2.21	0.55
1:B:433:ARG:NH2	1:B:439:TRP:O	2.33	0.55
1:B:300:VAL:HB	1:B:301:PRO:CD	2.36	0.55
5:B:996:DME:H41	5:B:996:DME:H142	1.87	0.55
1:C:252:ALA:CB	1:C:269:LEU:HD21	2.37	0.55
1:A:119:TYR:HE2	1:A:150:ASN:HA	1.72	0.55
1:A:132:VAL:HG23	1:A:133:TYR:CD1	2.42	0.55
1:A:516:LYS:HA	1:A:516:LYS:HE3	1.89	0.55
1:B:161:LEU:HD21	1:B:269:LEU:HD13	1.89	0.55
1:D:207:ALA:O	1:D:211:MET:HG2	2.07	0.54
1:C:211:MET:HE2	1:C:301:PRO:HG2	1.89	0.54
1:C:458:PRO:HA	1:C:465:TYR:CD2	2.43	0.54
1:D:329:GLY:O	1:D:330:VAL:HG23	2.07	0.54
1:B:11:ARG:HG3	1:B:16:GLN:HG2	1.89	0.54
1:D:397:ALA:O	1:D:401:VAL:HG23	2.07	0.54
1:D:458:PRO:HA	1:D:465:TYR:CD2	2.42	0.54
1:C:452:GLU:CD	6:C:951:GOL:H11	2.28	0.54
1:D:132:VAL:HG23	1:D:133:TYR:CD1	2.42	0.54
1:D:112:THR:HG23	1:D:113:PRO:HD2	1.90	0.54
1:D:116:ILE:HD11	1:D:183:VAL:HG11	1.90	0.54
1:C:459:LEU:HD23	1:C:470:ARG:HG2	1.88	0.54
1:D:155:THR:HG22	1:D:159:LEU:HD12	1.89	0.54
1:D:123:PHE:HB2	1:D:300:VAL:HG12	1.88	0.54
1:C:317:ASN:ND2	1:C:417:ARG:HE	2.05	0.54
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.43	0.54
1:C:224:ARG:NH1	1:C:224:ARG:HG3	2.22	0.54
1:C:84:GLU:HA	1:C:87:ASN:ND2	2.15	0.53
1:D:300:VAL:HB	1:D:301:PRO:CD	2.38	0.53
1:C:77:TYR:CE2	1:C:348:LYS:HD3	2.44	0.53
1:A:112:THR:HG23	1:A:113:PRO:HD2	1.90	0.53
1:A:123:PHE:HB2	1:A:300:VAL:HG12	1.91	0.53
1:D:107:ARG:HG3	1:D:107:ARG:NH1	2.18	0.53
1:D:66:GLN:HG3	1:D:98:TYR:CG	2.44	0.53
1:A:45:ARG:CG	1:A:45:ARG:HH11	2.15	0.53
1:A:205:GLY:O	1:A:208:SER:HB2	2.08	0.53
1:C:433:ARG:NH2	1:C:439:TRP:O	2.37	0.53
1:C:184:GLN:HE21	1:C:184:GLN:HA	1.73	0.53
1:D:200:PHE:HB2	1:D:226:VAL:HB	1.91	0.53
1:A:141:VAL:HG21	1:A:459:LEU:CD2	2.39	0.53
1:D:251:LEU:O	1:D:251:LEU:HG	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:HA	1:B:228:GLN:O	2.09	0.52
1:D:119:TYR:HE2	1:D:150:ASN:HA	1.73	0.52
1:A:468:GLU:HA	1:A:471:ILE:HD12	1.89	0.52
1:A:475:ARG:O	1:A:478:LYS:HB2	2.09	0.52
1:B:8:LEU:O	1:B:18:ARG:HA	2.08	0.52
1:C:341:TYR:CE2	5:C:997:DME:H22	2.45	0.52
1:A:488:ASP:OD1	1:A:490:ASN:HB2	2.10	0.52
1:A:504:THR:OG1	1:A:507:ALA:HB3	2.10	0.52
1:A:152:ARG:O	1:A:157:GLY:HA3	2.10	0.52
1:C:85:MET:CE	6:C:951:GOL:O1	2.58	0.52
1:B:414:LEU:HG	1:B:418:LEU:HD22	1.92	0.52
1:C:348:LYS:HA	1:C:440:PRO:HG3	1.91	0.52
1:A:444:GLY:O	1:A:446:PRO:HD3	2.10	0.52
1:A:407:VAL:O	1:A:411:VAL:HG23	2.10	0.51
1:D:251:LEU:HD21	1:D:281:LEU:HD12	1.92	0.51
1:C:172:GLY:O	1:C:176:GLN:HG3	2.10	0.51
1:D:115:LEU:HD12	1:D:198:THR:HB	1.92	0.51
1:A:331:VAL:HB	1:A:445:VAL:HG12	1.91	0.51
5:B:996:DME:C15	1:D:261:GLY:HA2	2.39	0.51
1:B:291:GLN:NE2	1:B:368:PRO:HB2	2.22	0.51
1:C:536:LEU:HD13	1:C:540:LEU:CD2	2.40	0.51
1:A:80:PHE:CE2	1:A:82:GLY:HA3	2.46	0.51
1:B:252:ALA:CB	1:B:269:LEU:HD21	2.40	0.51
1:C:452:GLU:OE2	6:C:951:GOL:H11	2.09	0.51
1:D:243:GLU:O	1:D:247:ARG:HG3	2.10	0.51
1:C:227:LEU:HB2	1:C:328:VAL:HG12	1.93	0.51
1:B:7:GLN:NE2	1:B:107:ARG:H	2.08	0.51
1:B:20:ILE:HB	1:B:63:THR:HG22	1.93	0.51
1:B:531:PHE:CZ	1:B:536:LEU:HG	2.45	0.51
1:C:80:PHE:CE1	1:C:438:THR:HB	2.46	0.51
1:A:107:ARG:HH11	1:A:107:ARG:CG	2.20	0.51
1:D:488:ASP:OD1	1:D:490:ASN:HB2	2.11	0.51
1:D:375:ALA:O	1:D:379:VAL:HG23	2.11	0.51
1:D:356:ARG:HH12	1:D:383:THR:HG23	1.76	0.51
1:D:139:ALA:O	1:D:143:GLY:HA2	2.10	0.51
1:B:460:ASP:OD1	1:B:462:SER:HB3	2.11	0.51
1:D:511:VAL:HB	1:D:518:LEU:HD22	1.92	0.51
1:B:536:LEU:HD13	1:B:540:LEU:CD2	2.41	0.51
1:A:356:ARG:HH12	1:A:383:THR:HG23	1.75	0.51
1:A:89:ASN:O	1:A:90:ARG:HD3	2.11	0.50
5:D:999:DME:H173	5:D:999:DME:C9	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:GLU:OE1	6:C:951:GOL:H11	2.10	0.50
1:C:136:ARG:HH11	1:C:136:ARG:HB3	1.75	0.50
1:D:110:SER:HB2	1:D:111:PRO:HD2	1.93	0.50
1:A:328:VAL:HG12	1:A:329:GLY:N	2.26	0.50
1:D:294:ILE:HG12	1:D:365:ILE:HG22	1.94	0.50
1:B:310:ASP:HB3	1:B:315:LEU:CD1	2.40	0.50
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.94	0.50
1:C:466:THR:OG1	1:C:469:GLU:HG3	2.11	0.50
1:D:205:GLY:O	1:D:208:SER:HB2	2.11	0.50
1:A:41:PRO:HA	1:A:45:ARG:HB3	1.93	0.50
1:A:466:THR:OG1	1:A:469:GLU:HG3	2.10	0.50
1:A:7:GLN:CB	1:A:105:TYR:HE1	2.25	0.50
1:C:89:ASN:OD1	1:C:129:SER:HB2	2.12	0.50
1:D:135:GLY:HA3	1:D:146:LEU:HD22	1.93	0.50
1:A:21:ARG:HH21	1:A:23:LYS:NZ	2.10	0.50
1:B:535:PHE:CE2	1:B:539:LEU:HD12	2.47	0.50
1:A:367:VAL:HG12	1:A:370:ALA:HB2	1.94	0.49
1:D:166:GLU:HB2	1:D:274:ARG:HH12	1.77	0.49
1:C:339:LEU:HD11	1:C:399:SER:HA	1.94	0.49
1:A:251:LEU:HD21	1:A:281:LEU:HD12	1.94	0.49
1:C:166:GLU:CD	1:C:166:GLU:H	2.15	0.49
1:B:161:LEU:HD22	1:B:270:ILE:CD1	2.39	0.49
1:C:536:LEU:N	1:C:537:PRO:HD2	2.27	0.49
1:C:12:VAL:HG22	1:C:186:ASN:HB3	1.94	0.49
1:A:407:VAL:O	1:A:410:PRO:HD2	2.12	0.49
1:C:352:SER:O	1:C:395:ARG:HG3	2.13	0.49
1:D:11:ARG:CB	1:D:11:ARG:HH11	2.20	0.49
1:B:124:TYR:OH	5:B:996:DME:C8	2.57	0.49
1:B:355:SER:OG	1:B:358:GLN:HG3	2.12	0.49
1:B:250:LEU:HD23	1:B:288:VAL:HG12	1.95	0.49
1:D:466:THR:OG1	1:D:469:GLU:HG3	2.12	0.49
1:B:331:VAL:HG12	1:B:430:PHE:HB3	1.95	0.49
1:D:327:LEU:HD23	1:D:328:VAL:N	2.27	0.49
1:B:216:LEU:HB3	1:B:217:PRO:HD3	1.94	0.49
1:C:219:ARG:HH21	1:C:324:LEU:HG	1.77	0.49
1:A:22:LEU:HD13	1:A:31:ALA:HB3	1.95	0.49
1:B:89:ASN:OD1	1:B:129:SER:HB2	2.13	0.49
1:A:122:GLY:O	1:A:123:PHE:HB2	2.13	0.49
1:C:32:PHE:N	1:C:32:PHE:CD1	2.80	0.49
1:B:293:SER:O	5:B:996:DME:H22	2.13	0.49
1:C:535:PHE:CB	1:D:380:LEU:HD12	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:GLU:HB2	7:D:1046:HOH:O	2.12	0.49
1:C:446:PRO:HG2	1:C:449:TYR:CD1	2.47	0.49
1:D:33:LEU:HD12	1:D:100:ASN:HB3	1.95	0.49
1:A:327:LEU:HD23	1:A:328:VAL:N	2.28	0.48
1:B:255:VAL:HG12	1:B:284:HIS:ND1	2.27	0.48
1:D:352:SER:O	1:D:395:ARG:HG3	2.13	0.48
1:C:80:PHE:O	1:C:84:GLU:HG2	2.13	0.48
1:A:42:VAL:O	1:A:45:ARG:HB2	2.13	0.48
1:C:354:ILE:HB	1:C:358:GLN:OE1	2.13	0.48
1:C:470:ARG:O	1:C:474:GLN:HG3	2.13	0.48
1:B:246:ARG:HG3	1:B:246:ARG:HH11	1.78	0.48
1:D:86:TRP:CZ3	5:D:999:DME:H161	2.48	0.48
1:D:530:ALA:O	1:D:534:ARG:HB2	2.13	0.48
1:C:37:PHE:CD1	1:C:99:LEU:HD23	2.49	0.48
1:B:294:ILE:HA	5:B:996:DME:H31	1.94	0.48
5:C:997:DME:H42	5:C:997:DME:C14	2.43	0.48
1:C:211:MET:CE	1:C:301:PRO:HG2	2.44	0.48
1:C:375:ALA:O	1:C:379:VAL:HG23	2.13	0.48
1:A:493:ARG:O	1:A:495:ARG:N	2.47	0.48
1:C:219:ARG:HH11	1:C:219:ARG:CG	2.18	0.48
1:B:440:PRO:HG2	1:B:443:MET:HG3	1.96	0.48
1:B:536:LEU:N	1:B:537:PRO:HD2	2.28	0.48
1:D:494:ASP:O	1:D:496:LYS:N	2.40	0.48
1:A:107:ARG:NH1	1:A:107:ARG:HG3	2.20	0.48
1:C:269:LEU:O	1:C:269:LEU:HD23	2.13	0.48
1:D:142:GLU:CB	1:D:481:THR:HG21	2.44	0.48
1:C:184:GLN:NE2	1:C:184:GLN:HA	2.29	0.47
1:C:255:VAL:HG12	1:C:284:HIS:ND1	2.28	0.47
1:A:200:PHE:HB2	1:A:226:VAL:HB	1.95	0.47
1:C:374:ALA:O	1:C:377:ALA:HB3	2.13	0.47
1:C:243:GLU:HA	1:C:243:GLU:OE1	2.14	0.47
1:B:47:PHE:O	1:B:171:VAL:HG11	2.14	0.47
1:A:110:SER:HB2	1:A:111:PRO:HD2	1.96	0.47
1:A:329:GLY:HA3	1:A:428:TYR:CD2	2.49	0.47
1:B:329:GLY:HA3	1:B:428:TYR:CE1	2.49	0.47
1:B:172:GLY:O	1:B:176:GLN:HG3	2.15	0.47
1:D:347:SER:HB2	2:D:609:NAG:C6	2.43	0.47
1:A:317:ASN:HB2	1:A:417:ARG:NH1	2.29	0.47
1:A:300:VAL:HB	1:A:301:PRO:HD2	1.95	0.47
1:B:362:GLY:HA3	1:B:398:MET:CE	2.43	0.47
1:C:300:VAL:HB	1:C:301:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:VAL:CG1	1:D:411:VAL:HG13	2.44	0.47
1:C:296:ARG:NH2	1:C:406:ASN:OD1	2.47	0.47
1:C:331:VAL:HG22	1:C:334:GLU:OE2	2.15	0.47
1:D:37:PHE:HD1	1:D:178:LEU:HD12	1.79	0.47
1:C:511:VAL:HB	1:C:518:LEU:HD22	1.95	0.47
1:A:142:GLU:CB	1:A:481:THR:HG21	2.44	0.47
1:C:8:LEU:O	1:C:18:ARG:HA	2.14	0.47
1:B:119:TYR:HE2	1:B:150:ASN:HA	1.79	0.47
1:A:210:GLY:O	1:A:214:LEU:HD22	2.14	0.47
1:D:516:LYS:HE2	1:D:516:LYS:HA	1.96	0.47
1:C:531:PHE:CZ	1:C:536:LEU:HG	2.49	0.47
1:B:536:LEU:HD13	1:B:540:LEU:HD23	1.97	0.47
1:A:138:LEU:HD11	1:A:455:PHE:HA	1.97	0.47
1:C:119:TYR:HE2	1:C:150:ASN:HA	1.80	0.47
1:D:418:LEU:HA	1:D:418:LEU:HD12	1.69	0.47
1:D:317:ASN:HB2	1:D:417:ARG:NH1	2.30	0.47
1:D:374:ALA:O	1:D:378:VAL:HG23	2.15	0.47
1:B:29:VAL:CG2	1:B:140:GLN:HB2	2.45	0.47
1:C:346:PHE:HA	1:C:352:SER:OG	2.15	0.47
1:D:70:TYR:HB3	1:D:156:PHE:CE2	2.50	0.47
1:A:331:VAL:HG12	1:A:430:PHE:HB3	1.97	0.46
1:D:45:ARG:O	1:D:48:MET:HB2	2.14	0.46
1:A:374:ALA:O	1:A:378:VAL:HG23	2.15	0.46
1:D:339:LEU:HD13	1:D:346:PHE:CE2	2.50	0.46
1:C:29:VAL:CG2	1:C:140:GLN:HB2	2.45	0.46
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.47	0.46
1:C:245:ARG:NH2	1:C:266:ASP:OD2	2.49	0.46
1:A:451:ILE:HG12	1:A:451:ILE:H	1.49	0.46
1:B:128:ALA:HB1	7:B:1021:HOH:O	2.15	0.46
1:D:121:GLY:HA2	5:D:999:DME:H101	1.97	0.46
1:C:161:LEU:HD21	1:C:269:LEU:HD13	1.98	0.46
1:C:331:VAL:HG12	1:C:430:PHE:HB3	1.98	0.46
1:C:138:LEU:HD23	1:C:146:LEU:CD1	2.46	0.46
1:B:432:HIS:CE1	1:B:515:LEU:HD11	2.51	0.46
1:D:181:GLN:O	1:D:185:GLU:HG2	2.15	0.46
1:D:429:ILE:CD1	1:D:524:LEU:HD21	2.33	0.46
1:A:37:PHE:CD1	1:A:178:LEU:HD12	2.48	0.46
1:A:114:VAL:HG11	1:A:187:ILE:HG12	1.98	0.46
1:B:317:ASN:ND2	1:B:417:ARG:HH21	2.12	0.46
1:B:369:GLN:HE22	1:B:405:HIS:CE1	2.34	0.46
1:B:278:ALA:O	1:B:282:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:GLY:HA3	1:D:428:TYR:CD2	2.50	0.46
1:C:362:GLY:HA3	1:C:398:MET:CE	2.43	0.46
1:A:300:VAL:HB	1:A:301:PRO:CD	2.46	0.46
1:C:24:ALA:HB3	1:C:140:GLN:HG3	1.97	0.46
1:C:530:ALA:O	1:C:534:ARG:HB2	2.16	0.46
1:C:329:GLY:HA3	1:C:428:TYR:CD2	2.50	0.45
1:A:115:LEU:HD12	1:A:198:THR:HB	1.98	0.45
1:D:331:VAL:HG12	1:D:430:PHE:HB3	1.98	0.45
1:B:4:GLU:HG2	1:B:9:LEU:HB2	1.97	0.45
1:B:161:LEU:CD2	1:B:270:ILE:HD11	2.39	0.45
1:B:295:PHE:H	5:B:996:DME:H31	1.80	0.45
1:B:243:GLU:HA	1:B:243:GLU:OE1	2.16	0.45
1:D:329:GLY:HA3	1:D:428:TYR:CE1	2.48	0.45
1:C:161:LEU:HD22	1:C:270:ILE:CD1	2.44	0.45
1:A:457:LEU:N	1:A:458:PRO:CD	2.80	0.45
1:B:532:TRP:O	1:B:537:PRO:HD3	2.16	0.45
1:B:128:ALA:HB1	1:B:148:SER:OG	2.16	0.45
1:A:33:LEU:CD1	1:A:33:LEU:N	2.79	0.45
1:A:408:VAL:O	1:A:411:VAL:HB	2.17	0.45
1:C:494:ASP:C	1:C:496:LYS:N	2.67	0.45
1:C:85:MET:SD	6:C:951:GOL:O1	2.73	0.45
1:D:21:ARG:HH21	1:D:23:LYS:NZ	2.14	0.45
1:C:50:PRO:HB2	1:C:178:LEU:HD12	1.97	0.45
1:D:42:VAL:O	1:D:45:ARG:HB2	2.16	0.45
1:A:530:ALA:O	1:A:534:ARG:HB2	2.17	0.45
1:B:10:VAL:HG22	1:B:107:ARG:NH1	2.32	0.45
1:C:29:VAL:HG21	1:C:140:GLN:HB2	1.99	0.45
1:B:219:ARG:NH2	1:B:324:LEU:HG	2.32	0.45
1:A:33:LEU:HD13	1:A:33:LEU:N	2.32	0.45
1:A:136:ARG:HG2	1:A:137:PHE:N	2.32	0.45
1:A:112:THR:HG21	1:A:143:GLY:O	2.17	0.44
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.52	0.44
1:C:40:PRO:HA	1:C:41:PRO:HD2	1.74	0.44
1:C:515:LEU:HD23	1:C:515:LEU:HA	1.81	0.44
1:A:501:PRO:HA	1:A:502:PRO:HD3	1.92	0.44
1:D:112:THR:HG21	1:D:143:GLY:O	2.17	0.44
1:B:29:VAL:HG21	1:B:140:GLN:HB2	1.99	0.44
1:D:180:LEU:O	1:D:183:VAL:HG12	2.16	0.44
1:C:536:LEU:HD23	1:C:536:LEU:HA	1.79	0.44
1:C:252:ALA:HB2	1:C:269:LEU:HD21	2.00	0.44
5:C:997:DME:H102	5:C:997:DME:H182	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:O	1:A:48:MET:HB2	2.18	0.44
1:D:417:ARG:HH11	1:D:417:ARG:CG	2.30	0.44
1:B:77:TYR:CE2	1:B:348:LYS:HD3	2.51	0.44
1:C:380:LEU:HD22	1:D:535:PHE:CB	2.47	0.44
1:B:459:LEU:HD21	1:B:474:GLN:HG2	1.98	0.44
1:A:166:GLU:HB2	1:A:274:ARG:HH12	1.82	0.44
1:A:497:SER:CB	1:A:498:PRO:CD	2.94	0.44
1:D:356:ARG:HG2	1:D:360:LEU:CD2	2.48	0.44
1:C:224:ARG:HD3	1:C:487:GLY:HA2	1.99	0.44
1:B:300:VAL:HB	1:B:301:PRO:HD2	2.00	0.44
1:C:507:ALA:HA	1:C:522:ARG:HH21	1.82	0.44
1:D:512:SER:HB3	1:D:519:GLU:HB3	2.00	0.44
1:C:11:ARG:NH1	1:C:11:ARG:HG3	2.32	0.44
1:C:7:GLN:HE22	1:C:107:ARG:H	1.65	0.44
1:D:155:THR:HG22	1:D:159:LEU:CD1	2.48	0.44
1:D:372:ASP:O	1:D:375:ALA:HB3	2.18	0.44
1:D:177:ARG:CZ	1:D:217:PRO:HB2	2.48	0.44
1:D:152:ARG:O	1:D:157:GLY:HA3	2.18	0.44
1:D:104:PRO:HG2	1:D:108:PRO:HD3	2.00	0.44
1:D:41:PRO:HA	1:D:45:ARG:HB3	1.99	0.43
1:C:206:ALA:O	1:C:227:LEU:HD23	2.18	0.43
1:A:491:ASP:HA	1:A:492:PRO:HD2	1.56	0.43
1:A:216:LEU:HA	1:A:216:LEU:HD12	1.80	0.43
1:D:291:GLN:HE21	1:D:291:GLN:HB2	1.60	0.43
1:D:524:LEU:HD23	1:D:524:LEU:HA	1.73	0.43
1:B:4:GLU:HG3	1:B:5:ASP:N	2.34	0.43
1:A:124:TYR:CD1	1:A:124:TYR:C	2.91	0.43
1:B:287:HIS:N	1:B:287:HIS:CD2	2.86	0.43
1:D:11:ARG:HB2	1:D:11:ARG:NH1	2.21	0.43
1:A:226:VAL:HG11	1:A:480:TRP:NE1	2.25	0.43
1:B:40:PRO:HA	1:B:41:PRO:HD2	1.80	0.43
1:B:211:MET:CE	1:B:301:PRO:HG2	2.49	0.43
1:B:382:TYR:CD2	1:B:401:VAL:HG22	2.53	0.43
1:C:466:THR:HG23	1:C:469:GLU:OE1	2.18	0.43
1:D:311:THR:HG22	1:D:313:GLU:H	1.82	0.43
1:A:407:VAL:C	1:A:410:PRO:HD2	2.38	0.43
1:D:112:THR:HG21	1:D:144:ALA:HA	2.00	0.43
1:A:356:ARG:O	1:A:360:LEU:HD22	2.19	0.43
1:A:426:TYR:HD2	1:A:500:TRP:CD1	2.36	0.43
1:D:367:VAL:CG1	1:D:370:ALA:HB2	2.45	0.43
1:C:9:LEU:HD11	1:C:16:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:TRP:CE3	5:D:999:DME:H161	2.54	0.43
1:D:518:LEU:HA	1:D:518:LEU:HD23	1.79	0.43
1:B:183:VAL:HG13	1:B:187:ILE:HB	2.01	0.43
1:B:32:PHE:N	1:B:32:PHE:CD1	2.86	0.43
1:B:359:PHE:O	1:B:398:MET:HE1	2.19	0.43
1:A:202:GLU:O	1:A:205:GLY:N	2.52	0.43
1:D:328:VAL:HG11	1:D:411:VAL:HG13	1.99	0.43
1:D:407:VAL:O	1:D:411:VAL:HG23	2.19	0.43
1:C:246:ARG:HD3	1:C:246:ARG:HH11	1.61	0.43
1:A:295:PHE:CE2	1:A:338:PHE:CZ	3.07	0.43
1:C:321:PHE:CD2	1:C:418:LEU:HD12	2.54	0.43
1:A:356:ARG:HA	1:A:394:LEU:HD13	2.00	0.43
1:A:472:PHE:CE1	1:A:476:LEU:HD11	2.54	0.43
1:B:223:HIS:CD2	1:B:223:HIS:N	2.87	0.43
1:D:250:LEU:HD23	1:D:288:VAL:HA	2.00	0.43
1:D:12:VAL:HG13	1:D:186:ASN:OD1	2.19	0.43
1:A:12:VAL:HG13	1:A:186:ASN:OD1	2.19	0.43
1:C:532:TRP:O	1:C:537:PRO:HD3	2.18	0.42
1:D:33:LEU:N	1:D:33:LEU:HD13	2.34	0.42
1:D:493:ARG:O	1:D:495:ARG:N	2.52	0.42
1:D:386:LEU:HD23	1:D:386:LEU:HA	1.94	0.42
1:A:540:LEU:HD23	1:A:540:LEU:HA	1.78	0.42
1:D:351:GLU:HB2	1:D:353:LEU:HD22	2.01	0.42
1:C:226:VAL:HA	1:C:327:LEU:O	2.19	0.42
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.49	0.42
1:C:450:GLU:HG2	1:C:451:ILE:N	2.35	0.42
1:B:134:ASP:OD1	1:B:136:ARG:NH1	2.53	0.42
1:D:46:ARG:HB3	1:D:274:ARG:HG2	2.00	0.42
1:C:327:LEU:HD21	1:C:500:TRP:CH2	2.55	0.42
1:D:331:VAL:HB	1:D:445:VAL:HG12	2.01	0.42
1:A:40:PRO:HG3	1:A:95:ASP:OD1	2.19	0.42
1:D:193:ASP:OD1	1:D:195:MET:HB2	2.19	0.42
1:A:418:LEU:HA	1:A:418:LEU:HD12	1.83	0.42
1:C:121:GLY:CA	5:C:997:DME:H91	2.49	0.42
1:C:291:GLN:NE2	1:C:368:PRO:HB2	2.31	0.42
1:D:46:ARG:HD3	1:D:47:PHE:CZ	2.54	0.42
1:C:397:ALA:O	1:C:401:VAL:HG23	2.19	0.42
1:B:138:LEU:HD13	1:B:477:MET:HG2	2.00	0.42
1:D:286:TRP:CZ2	5:D:999:DME:H142	2.55	0.42
1:A:476:LEU:HA	1:A:479:TYR:HD2	1.85	0.42
1:D:495:ARG:O	1:D:496:LYS:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:PRO:O	1:C:316:ILE:HG12	2.20	0.42
1:B:185:GLU:HB2	1:B:186:ASN:H	1.66	0.42
1:B:224:ARG:HH11	1:B:224:ARG:HG3	1.85	0.42
1:B:166:GLU:H	1:B:166:GLU:CD	2.21	0.42
1:C:80:PHE:HE1	1:C:438:THR:HB	1.84	0.42
1:D:107:ARG:CG	1:D:107:ARG:NH1	2.82	0.42
1:D:132:VAL:HA	1:D:457:LEU:HD21	2.02	0.42
1:B:383:THR:HG22	1:B:384:ASP:N	2.34	0.42
1:C:540:LEU:HA	1:C:540:LEU:HD13	1.78	0.42
1:B:224:ARG:HG3	1:B:224:ARG:NH1	2.35	0.42
1:D:296:ARG:NH2	1:D:406:ASN:OD1	2.53	0.42
1:A:380:LEU:HA	1:A:385:TRP:HZ2	1.84	0.42
1:C:359:PHE:O	1:C:363:VAL:HG23	2.20	0.42
1:D:130:LEU:HA	1:D:130:LEU:HD23	1.92	0.42
1:B:535:PHE:HE2	1:B:539:LEU:HD12	1.83	0.42
1:A:46:ARG:HD3	1:A:47:PHE:CZ	2.54	0.42
1:D:434:ALA:O	1:D:437:LEU:HB2	2.19	0.42
1:D:476:LEU:HD21	1:D:513:LEU:HD12	2.02	0.42
1:B:494:ASP:C	1:B:496:LYS:N	2.71	0.42
1:D:491:ASP:HA	1:D:492:PRO:HD2	1.58	0.42
1:B:374:ALA:O	1:B:377:ALA:HB3	2.20	0.42
1:C:124:TYR:OH	5:C:997:DME:H42	2.19	0.42
1:A:524:LEU:HD23	1:A:524:LEU:HA	1.82	0.42
1:D:122:GLY:O	1:D:123:PHE:HB2	2.20	0.42
1:B:536:LEU:HA	1:B:536:LEU:HD23	1.87	0.42
1:D:501:PRO:HA	1:D:502:PRO:HD3	1.90	0.42
1:D:325:GLN:O	1:D:483:PHE:HZ	2.03	0.42
1:A:328:VAL:CG1	1:A:411:VAL:HG13	2.50	0.41
1:C:10:VAL:HG22	1:C:107:ARG:NH1	2.35	0.41
1:D:538:LYS:HE3	1:D:538:LYS:HB3	1.94	0.41
1:D:250:LEU:CD2	1:D:288:VAL:HG12	2.49	0.41
1:D:457:LEU:N	1:D:458:PRO:CD	2.83	0.41
1:A:414:LEU:O	1:A:418:LEU:HB2	2.20	0.41
1:D:324:LEU:HD23	1:D:325:GLN:H	1.85	0.41
1:A:330:VAL:CG1	1:A:331:VAL:N	2.83	0.41
1:C:342:GLY:O	1:C:344:PRO:HD3	2.21	0.41
1:D:295:PHE:CE2	1:D:338:PHE:CZ	3.07	0.41
1:A:516:LYS:CA	1:A:516:LYS:HE3	2.50	0.41
1:D:119:TYR:CE2	1:D:150:ASN:HA	2.53	0.41
1:B:243:GLU:OE1	1:B:246:ARG:NH1	2.53	0.41
1:C:155:THR:HG22	1:C:159:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ILE:HA	5:B:996:DME:H22	2.03	0.41
1:A:113:PRO:HA	1:A:196:SER:HG	1.85	0.41
1:B:418:LEU:HD12	1:B:418:LEU:HA	1.91	0.41
1:A:351:GLU:HB2	1:A:353:LEU:HD22	2.02	0.41
1:A:390:ASP:HA	1:A:391:PRO:HD2	1.80	0.41
1:A:289:LEU:HA	1:A:289:LEU:HD23	1.89	0.41
1:A:536:LEU:HB3	1:A:537:PRO:HD3	2.03	0.41
1:A:20:ILE:HG12	1:A:21:ARG:N	2.35	0.41
1:C:383:THR:HG22	1:C:384:ASP:N	2.35	0.41
1:B:85:MET:SD	6:B:953:GOL:O1	2.72	0.41
1:B:85:MET:CE	6:B:953:GOL:HO1	2.33	0.41
1:D:534:ARG:NH1	1:D:534:ARG:CG	2.80	0.41
1:B:41:PRO:HA	1:B:45:ARG:HB3	2.03	0.41
1:D:536:LEU:HB3	1:D:537:PRO:HD3	2.02	0.41
1:D:142:GLU:HG3	1:D:481:THR:HG21	2.03	0.41
1:D:70:TYR:CD1	1:D:92:LEU:HB3	2.55	0.41
1:A:350:ASN:ND2	3:A:709:NAG:C7	2.83	0.41
1:A:149:MET:HE2	1:A:176:GLN:HA	2.02	0.41
1:B:518:LEU:HD23	1:B:518:LEU:HA	1.94	0.41
1:B:255:VAL:HG21	1:B:276:ARG:HG3	2.02	0.41
1:C:356:ARG:NH2	1:C:383:THR:CG2	2.84	0.41
1:C:287:HIS:CD2	1:C:287:HIS:N	2.89	0.41
1:A:513:LEU:HA	1:A:513:LEU:HD13	1.87	0.41
1:A:159:LEU:HA	1:A:299:PHE:CD1	2.56	0.41
1:A:413:GLN:O	1:A:417:ARG:HB2	2.20	0.41
1:C:243:GLU:OE1	1:C:246:ARG:NH1	2.54	0.41
1:B:13:ARG:NE	1:B:185:GLU:HB3	2.35	0.41
1:B:511:VAL:HB	1:B:518:LEU:HD22	2.02	0.41
1:D:407:VAL:O	1:D:410:PRO:HD2	2.21	0.41
1:A:257:CYS:HA	1:A:258:PRO:HA	1.80	0.41
1:D:257:CYS:HA	1:D:258:PRO:HA	1.73	0.41
1:C:115:LEU:HD21	1:C:484:ALA:HB2	2.02	0.41
1:D:216:LEU:HA	1:D:219:ARG:HG2	2.03	0.41
1:C:46:ARG:HB3	1:C:274:ARG:HG2	2.02	0.41
1:D:500:TRP:HA	1:D:501:PRO:HD2	1.89	0.41
1:A:325:GLN:O	1:A:483:PHE:HZ	2.04	0.41
1:B:41:PRO:CD	1:B:97:LEU:HD12	2.43	0.40
1:D:68:VAL:HG23	1:D:90:ARG:HB2	2.03	0.40
1:A:187:ILE:HA	1:A:187:ILE:HD12	1.94	0.40
1:A:155:THR:HG22	1:A:159:LEU:CD1	2.51	0.40
5:A:998:DME:H102	5:A:998:DME:H173	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:GLU:O	1:A:472:PHE:HB3	2.21	0.40
1:B:380:LEU:HA	1:B:385:TRP:HZ2	1.87	0.40
1:A:107:ARG:HG2	1:A:108:PRO:HD2	2.03	0.40
1:C:330:VAL:HG21	1:C:408:VAL:HG22	2.04	0.40
1:C:290:PRO:HA	7:C:1010:HOH:O	2.20	0.40
5:C:997:DME:H72	5:C:997:DME:H101	1.54	0.40
1:C:80:PHE:CZ	1:C:438:THR:O	2.74	0.40
1:B:245:ARG:NH2	1:B:266:ASP:OD2	2.55	0.40
1:B:124:TYR:HH	5:B:996:DME:H82	1.82	0.40
1:A:161:LEU:HD22	1:A:270:ILE:HD11	2.04	0.40
1:B:317:ASN:ND2	1:B:417:ARG:NE	2.67	0.40
1:A:208:SER:O	1:A:211:MET:N	2.55	0.40
1:A:99:LEU:HA	1:A:149:MET:HA	2.03	0.40
1:C:317:ASN:HD22	1:C:417:ARG:HH21	1.70	0.40
1:B:181:GLN:O	1:B:185:GLU:HG3	2.22	0.40
1:A:369:GLN:HB3	7:A:1000:HOH:O	2.21	0.40
1:B:492:PRO:HB2	1:B:493:ARG:H	1.78	0.40
1:D:7:GLN:CB	1:D:105:TYR:HE1	2.33	0.40
1:B:501:PRO:HA	1:B:502:PRO:HD3	1.78	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	538/547 (98%)	482 (90%)	45 (8%)	11 (2%)	9 33
1	B	532/547 (97%)	493 (93%)	33 (6%)	6 (1%)	17 51
1	C	536/547 (98%)	497 (93%)	36 (7%)	3 (1%)	30 67
1	D	539/547 (98%)	486 (90%)	43 (8%)	10 (2%)	10 35
All	All	2145/2188 (98%)	1958 (91%)	157 (7%)	30 (1%)	14 44

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	492	PRO
1	A	494	ASP
1	A	497	SER
1	B	496	LYS
1	B	497	SER
1	C	496	LYS
1	D	494	ASP
1	D	495	ARG
1	D	497	SER
1	A	111	PRO
1	A	184	GLN
1	A	495	ARG
1	B	492	PRO
1	B	494	ASP
1	C	497	SER
1	D	111	PRO
1	D	234	GLY
1	D	492	PRO
1	A	234	GLY
1	A	517	PRO
1	B	185	GLU
1	D	517	PRO
1	A	185	GLU
1	A	496	LYS
1	C	342	GLY
1	A	121	GLY
1	D	121	GLY
1	D	496	LYS
1	B	342	GLY
1	D	5	ASP

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	436/447 (98%)	388 (89%)	48 (11%)	8 23
1	B	435/447 (97%)	391 (90%)	44 (10%)	9 28
1	C	435/447 (97%)	395 (91%)	40 (9%)	11 33
1	D	436/447 (98%)	391 (90%)	45 (10%)	9 26
All	All	1742/1788 (97%)	1565 (90%)	177 (10%)	9 27

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	ARG
1	A	33	LEU
1	A	45	ARG
1	A	103	THR
1	A	107	ARG
1	A	111	PRO
1	A	115	LEU
1	A	136	ARG
1	A	149	MET
1	A	155	THR
1	A	180	LEU
1	A	214	LEU
1	A	216	LEU
1	A	246	ARG
1	A	251	LEU
1	A	255	VAL
1	A	281	LEU
1	A	291	GLN
1	A	295	PHE
1	A	296	ARG
1	A	311	THR
1	A	317	ASN
1	A	324	LEU
1	A	332	LYS
1	A	333	ASP
1	A	353	LEU
1	A	380	LEU
1	A	386	LEU
1	A	417	ARG

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Mol	Chain	Res	Type
1	A	421	GLN
1	A	437	LEU
1	A	441	LEU
1	A	450	GLU
1	A	451	ILE
1	A	485	ARG
1	A	499	GLN
1	A	504	THR
1	A	505	THR
1	A	513	LEU
1	A	514	ASN
1	A	516	LYS
1	A	524	LEU
1	A	525	ARG
1	A	536	LEU
1	A	537	PRO
1	A	538	LYS
1	A	539	LEU
1	B	3	ARG
1	B	9	LEU
1	B	11	ARG
1	B	12	VAL
1	B	22	LEU
1	B	23	LYS
1	B	25	PRO
1	B	29	VAL
1	B	33	LEU
1	B	45	ARG
1	B	70	TYR
1	B	83	THR
1	B	84	GLU
1	B	132	VAL
1	B	136	ARG
1	B	138	LEU
1	B	161	LEU
1	B	178	LEU
1	B	200	PHE
1	B	211	MET
1	B	214	LEU
1	B	219	ARG
1	B	246	ARG
1	B	253	ARG

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Mol	Chain	Res	Type
1	B	291	GLN
1	B	295	PHE
1	B	296	ARG
1	B	315	LEU
1	B	322	GLN
1	B	324	LEU
1	B	327	LEU
1	B	336	SER
1	B	354	ILE
1	B	360	LEU
1	B	372	ASP
1	B	386	LEU
1	B	418	LEU
1	B	424	ARG
1	B	480	TRP
1	B	509	GLN
1	B	513	LEU
1	B	536	LEU
1	B	539	LEU
1	B	540	LEU
1	C	12	VAL
1	C	13	ARG
1	C	22	LEU
1	C	23	LYS
1	C	25	PRO
1	C	33	LEU
1	C	45	ARG
1	C	70	TYR
1	C	83	THR
1	C	84	GLU
1	C	132	VAL
1	C	136	ARG
1	C	138	LEU
1	C	161	LEU
1	C	178	LEU
1	C	200	PHE
1	C	211	MET
1	C	214	LEU
1	C	219	ARG
1	C	238	THR
1	C	253	ARG
1	C	291	GLN

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Mol	Chain	Res	Type
1	C	295	PHE
1	C	296	ARG
1	C	315	LEU
1	C	322	GLN
1	C	324	LEU
1	C	327	LEU
1	C	336	SER
1	C	354	ILE
1	C	360	LEU
1	C	386	LEU
1	C	418	LEU
1	C	424	ARG
1	C	480	TRP
1	C	509	GLN
1	C	513	LEU
1	C	525	ARG
1	C	536	LEU
1	C	540	LEU
1	D	9	LEU
1	D	11	ARG
1	D	12	VAL
1	D	33	LEU
1	D	45	ARG
1	D	103	THR
1	D	107	ARG
1	D	115	LEU
1	D	149	MET
1	D	155	THR
1	D	180	LEU
1	D	183	VAL
1	D	214	LEU
1	D	216	LEU
1	D	246	ARG
1	D	251	LEU
1	D	255	VAL
1	D	291	GLN
1	D	295	PHE
1	D	296	ARG
1	D	298	SER
1	D	317	ASN
1	D	324	LEU
1	D	333	ASP

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Mol	Chain	Res	Type
1	D	353	LEU
1	D	355	SER
1	D	380	LEU
1	D	386	LEU
1	D	417	ARG
1	D	418	LEU
1	D	421	GLN
1	D	437	LEU
1	D	441	LEU
1	D	450	GLU
1	D	451	ILE
1	D	499	GLN
1	D	504	THR
1	D	505	THR
1	D	513	LEU
1	D	514	ASN
1	D	524	LEU
1	D	536	LEU
1	D	537	PRO
1	D	538	LYS
1	D	539	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	66	GLN
1	A	212	HIS
1	A	228	GLN
1	A	291	GLN
1	A	317	ASN
1	A	482	ASN
1	A	499	GLN
1	A	514	ASN
1	B	7	GLN
1	B	212	HIS
1	B	223	HIS
1	B	291	GLN
1	B	317	ASN
1	B	405	HIS
1	B	421	GLN
1	B	509	GLN

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Mol	Chain	Res	Type
1	C	7	GLN
1	C	16	GLN
1	C	184	GLN
1	C	287	HIS
1	C	291	GLN
1	C	317	ASN
1	C	325	GLN
1	C	421	GLN
1	C	474	GLN
1	C	509	GLN
1	D	16	GLN
1	D	228	GLN
1	D	291	GLN
1	D	317	ASN
1	D	482	ASN
1	D	499	GLN
1	D	514	ASN

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

3 carbohydrates 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	NAG	D	608	2	14,14,15	0.56	0	15,19,21	0.50	0
2	NAG	D	609	1,2	14,14,15	0.73	0	15,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FUL	D	610	2	10,10,11	0.58	0	14,14,16	0.99	1 (7%)

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	NAG	D	608	2	-	0/6/23/26	0/1/1/1
2	NAG	D	609	1,2	-	0/6/23/26	0/1/1/1
2	FUL	D	610	2	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	610	FUL	C1-O5-C5	2.62	116.43	112.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	609	NAG	2	0

5.6 Ligand geometry (i)

12 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	$\#\|Z\|>2$
3	NAG	A	709	1	14,14,15	0.93	0	15,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	A	954	-	5,5,5	0.60	0	5,5,5	0.59	0
5	DME	A	998	-	17,17,17	0.53	0	22,22,22	0.75	1 (4%)
4	PO4	B	548	-	4,4,4	3.01	4 (100%)	6,6,6	0.28	0
6	GOL	B	953	-	5,5,5	0.80	0	5,5,5	0.59	0
5	DME	B	996	-	17,17,17	0.73	0	22,22,22	0.88	2 (9%)
4	PO4	C	548	-	4,4,4	2.69	4 (100%)	6,6,6	0.29	0
6	GOL	C	951	-	5,5,5	0.68	0	5,5,5	0.49	0
5	DME	C	997	-	17,17,17	0.64	0	22,22,22	0.72	0
4	PO4	C	998	-	4,4,4	3.46	4 (100%)	6,6,6	0.29	0
6	GOL	D	952	-	5,5,5	0.69	0	5,5,5	0.64	0
5	DME	D	999	-	17,17,17	0.58	0	22,22,22	0.86	2 (9%)

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	NAG	A	709	1	-	0/6/23/26	0/1/1/1
6	GOL	A	954	-	-	0/4/4/4	0/0/0/0
5	DME	A	998	-	-	0/15/15/15	0/0/0/0
4	PO4	B	548	-	-	0/0/0/0	0/0/0/0
6	GOL	B	953	-	-	0/4/4/4	0/0/0/0
5	DME	B	996	-	-	0/15/15/15	0/0/0/0
4	PO4	C	548	-	-	0/0/0/0	0/0/0/0
6	GOL	C	951	-	-	0/4/4/4	0/0/0/0
5	DME	C	997	-	-	0/15/15/15	0/0/0/0
4	PO4	C	998	-	-	0/0/0/0	0/0/0/0
6	GOL	D	952	-	-	0/4/4/4	0/0/0/0
5	DME	D	999	-	-	0/15/15/15	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	548	PO4	P-O3	2.52	1.62	1.53
4	B	548	PO4	P-O1	2.65	1.64	1.52
4	C	548	PO4	P-O1	2.70	1.64	1.52
4	C	548	PO4	P-O4	2.71	1.63	1.53
4	C	548	PO4	P-O2	2.84	1.63	1.53
4	B	548	PO4	P-O2	3.02	1.64	1.53
4	B	548	PO4	P-O4	3.03	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	998	PO4	P-O4	3.11	1.64	1.53
4	B	548	PO4	P-O3	3.30	1.65	1.53
4	C	998	PO4	P-O3	3.46	1.65	1.53
4	C	998	PO4	P-O1	3.48	1.67	1.52
4	C	998	PO4	P-O2	3.76	1.66	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	998	DME	C2-C3-C4	2.08	118.97	110.64
5	B	996	DME	C11-C10-C9	2.14	119.21	110.64
5	D	999	DME	C2-C3-C4	2.32	119.91	110.64
5	B	996	DME	C2-C3-C4	2.42	120.32	110.64
5	D	999	DME	C11-C10-C9	2.44	120.41	110.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	709	NAG	1	0
6	A	954	GOL	1	0
5	A	998	DME	1	0
6	B	953	GOL	2	0
5	B	996	DME	13	0
6	C	951	GOL	7	0
5	C	997	DME	19	0
6	D	952	GOL	1	0
5	D	999	DME	7	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	540/547 (98%)	-0.48	16 (2%) 54 47	20, 50, 79, 80	0
1	B	536/547 (97%)	-0.82	9 (1%) 73 70	13, 35, 61, 80	0
1	C	540/547 (98%)	-0.83	9 (1%) 73 70	11, 34, 64, 80	0
1	D	541/547 (98%)	-0.63	12 (2%) 65 60	16, 44, 79, 80	0
All	All	2157/2188 (98%)	-0.69	46 (2%) 67 62	11, 40, 75, 80	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	546	LEU	5.8
1	C	545	THR	5.6
1	B	545	THR	5.2
1	A	497	SER	5.0
1	B	494	ASP	4.7
1	A	4	GLU	4.4
1	B	493	ARG	4.1
1	C	497	SER	3.9
1	D	544	ASP	3.8
1	D	4	GLU	3.7
1	B	497	SER	3.7
1	A	494	ASP	3.5
1	A	110	SER	3.5
1	D	497	SER	3.4
1	C	494	ASP	3.4
1	A	6	PRO	3.2
1	D	492	PRO	3.2
1	D	494	ASP	3.2
1	A	493	ARG	3.2
1	D	495	ARG	3.1
1	B	544	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	544	ASP	2.9
1	C	1	GLU	2.9
1	A	495	ARG	2.9
1	A	492	PRO	2.8
1	B	3	ARG	2.7
1	C	110	SER	2.7
1	C	323	ASP	2.7
1	A	462	SER	2.7
1	A	496	LYS	2.6
1	B	322	GLN	2.6
1	D	323	ASP	2.6
1	C	493	ARG	2.4
1	D	110	SER	2.4
1	D	322	GLN	2.3
1	A	109	ALA	2.3
1	A	23	LYS	2.2
1	D	541	SER	2.2
1	D	109	ALA	2.2
1	A	57	SER	2.2
1	A	464	ASN	2.2
1	A	461	PRO	2.1
1	B	492	PRO	2.1
1	D	393	HIS	2.1
1	A	498	PRO	2.1
1	B	495	ARG	2.0

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

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

6.3 Carbohydrates (i)

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
2	NAG	D	609	14/15	0.89	0.25	2.82	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	D	608	14/15	0.80	0.49	-	80,80,80,80	0
2	FUL	D	610	10/11	0.89	0.43	-	80,80,80,80	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	DME	A	998	18/18	0.85	0.31	7.06	70,79,80,80	0
5	DME	D	999	18/18	0.85	0.27	6.28	40,68,80,80	0
4	PO4	B	548	5/5	0.93	0.34	6.21	80,80,80,80	0
5	DME	C	997	18/18	0.82	0.34	5.87	53,77,80,80	0
3	NAG	A	709	14/15	0.74	0.34	5.26	75,80,80,80	0
4	PO4	C	548	5/5	0.91	0.34	4.68	80,80,80,80	0
5	DME	B	996	18/18	0.81	0.30	3.86	44,65,80,80	0
6	GOL	D	952	6/6	0.90	0.23	2.65	48,54,55,61	0
6	GOL	B	953	6/6	0.94	0.17	1.85	33,36,48,53	0
6	GOL	A	954	6/6	0.86	0.25	1.27	66,74,75,76	0
6	GOL	C	951	6/6	0.97	0.11	-0.09	31,36,38,42	0
4	PO4	C	998	5/5	0.90	0.49	-	80,80,80,80	0

6.5 Other polymers (i)

There are no such residues in this entry.