Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:36 PM BST

PDB ID	:	4A16
Title	:	Structure of mouse Acetylcholinesterase complex with Huprine derivative
Authors	:	Carletti, E.; Colletier, J.P.; Nachon, F.; Weik, M.; Ronco, C.; Jean, L.; Renard, P.Y.
Deposited on	:	2011-09-14
Resolution	:	2.65 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 ⓘ symbol.

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

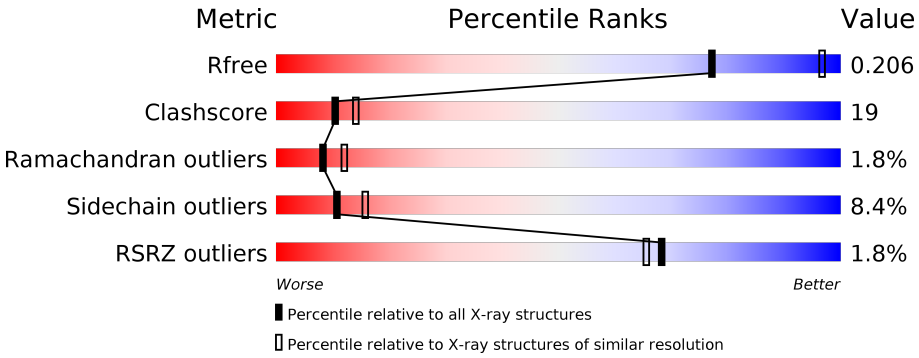
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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% 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	545	2% 76% 18%
1	B	545	2% 67% 24% 7%
1	C	545	2% 72% 23%
1	D	545	% 66% 27% 6%

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
3	SO4	A	1547	-	-	X	-
3	SO4	B	1548	-	-	-	X
3	SO4	B	1550	-	-	X	-
4	CL	B	1551	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19400 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.

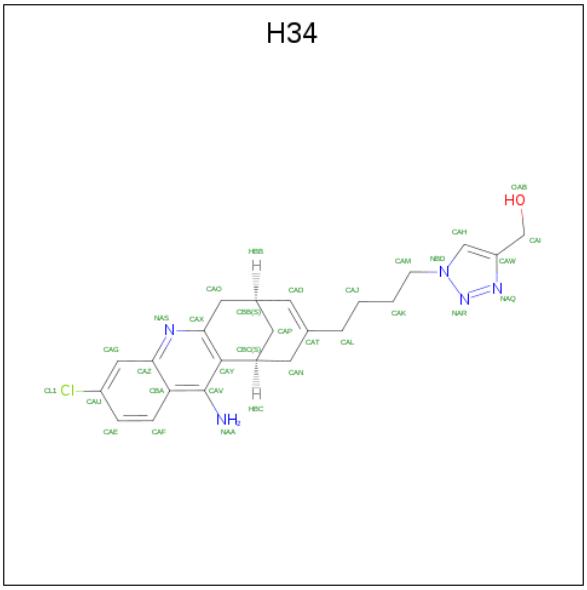
- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	6	1
			4236	2718	735	769	14			
1	B	541	Total	C	N	O	S	0	3	1
			4216	2705	732	765	14			
1	C	541	Total	C	N	O	S	0	1	1
			4202	2696	729	763	14			
1	D	541	Total	C	N	O	S	0	3	1
			4214	2704	730	766	14			

There are 20 discrepancies between the modelled and reference sequences:

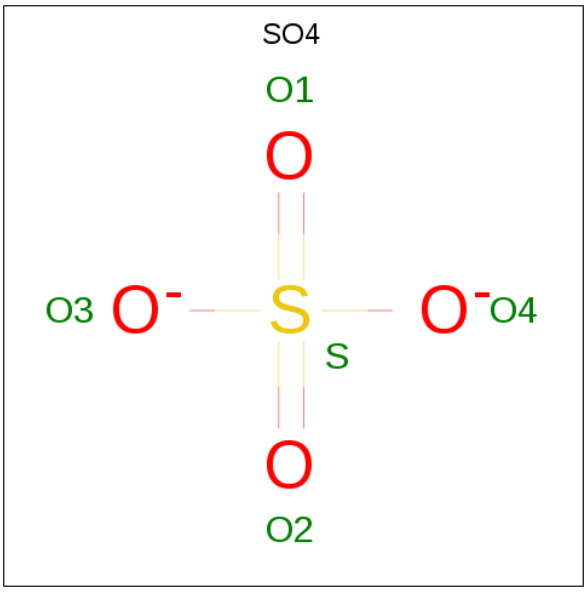
Chain	Residue	Modelled	Actual	Comment	Reference
A	544	ALA	-	expression tag	UNP P21836
A	545	THR	-	expression tag	UNP P21836
A	546	GLU	-	expression tag	UNP P21836
A	547	ALA	-	expression tag	UNP P21836
A	548	PRO	-	expression tag	UNP P21836
B	544	ALA	-	expression tag	UNP P21836
B	545	THR	-	expression tag	UNP P21836
B	546	GLU	-	expression tag	UNP P21836
B	547	ALA	-	expression tag	UNP P21836
B	548	PRO	-	expression tag	UNP P21836
C	544	ALA	-	expression tag	UNP P21836
C	545	THR	-	expression tag	UNP P21836
C	546	GLU	-	expression tag	UNP P21836
C	547	ALA	-	expression tag	UNP P21836
C	548	PRO	-	expression tag	UNP P21836
D	544	ALA	-	expression tag	UNP P21836
D	545	THR	-	expression tag	UNP P21836
D	546	GLU	-	expression tag	UNP P21836
D	547	ALA	-	expression tag	UNP P21836
D	548	PRO	-	expression tag	UNP P21836

- Molecule 2 is (1-{4-[(7S,11S)-12-AMINO-3-CHLORO-6,7,10,11-TETRAHYDRO-7,11-METHANOCYCLOOCTA[B]QUINOLIN-9-YL]BUTYL}-1H-1,2,3-TRIAZOL-4-YL)METHANOL (three-letter code: H34) (formula: $C_{23}H_{26}ClN_5O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			30	23	1	5	1		
2	B	1	Total	C	Cl	N	O	0	0
			30	23	1	5	1		
2	C	1	Total	C	Cl	N	O	0	0
			30	23	1	5	1		
2	D	1	Total	C	Cl	N	O	0	0
			30	23	1	5	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

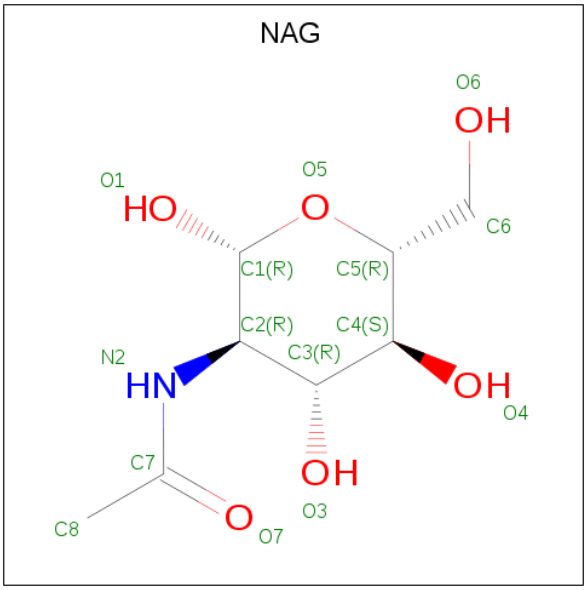


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	2	Total Cl 2 2	0	0
4	C	2	Total Cl 2 2	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

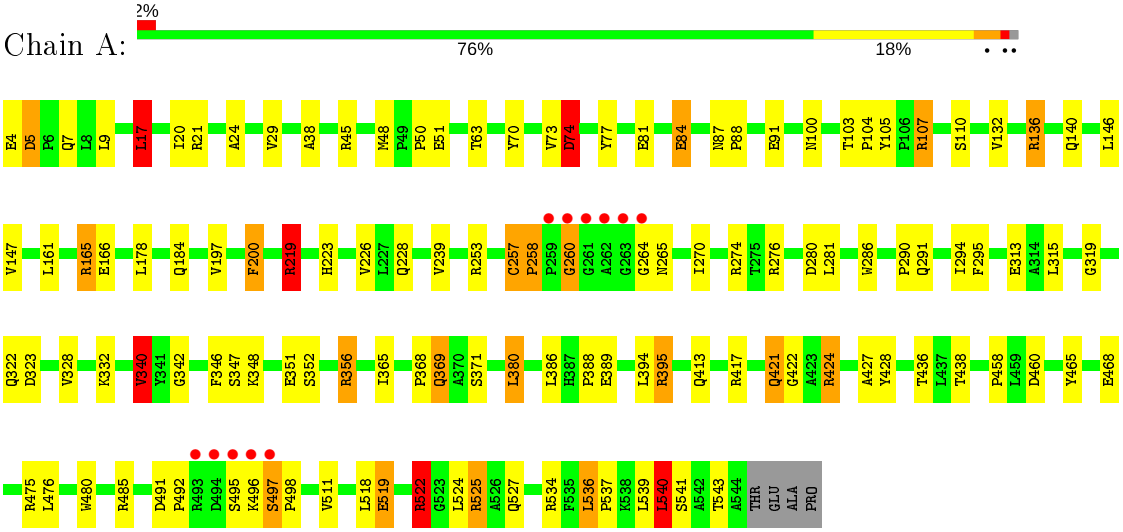
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	663	Total O 663 663	0	0
6	B	503	Total O 503 503	0	0
6	C	621	Total O 621 621	0	0
6	D	536	Total O 536 536	0	0

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 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.

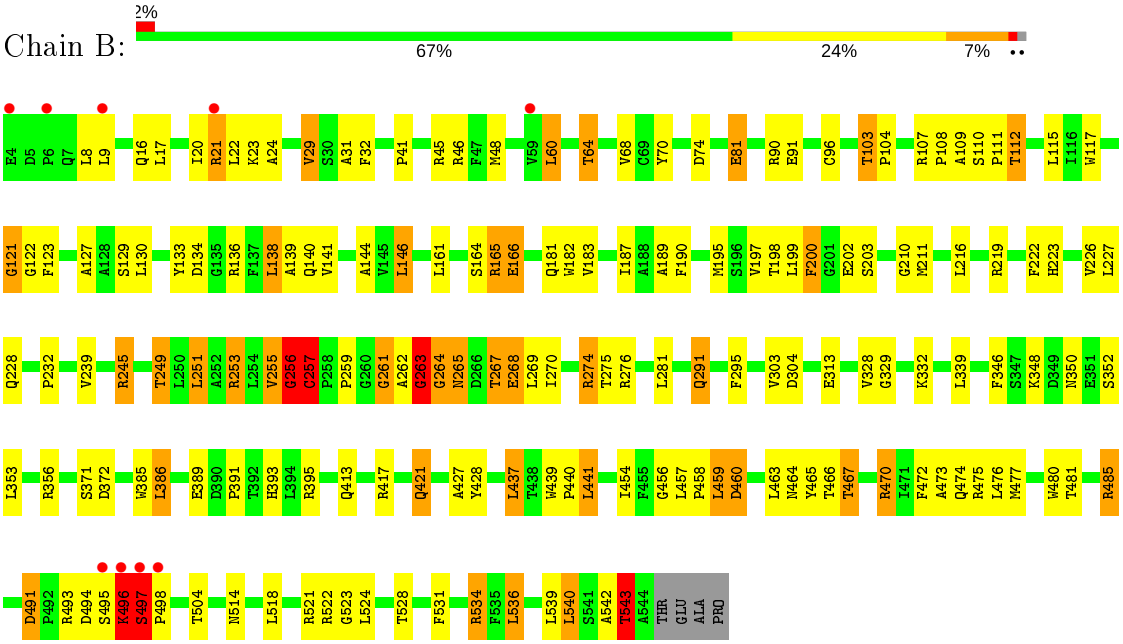
- Molecule 1: ACETYLCHOLINESTERASE

Chain A:



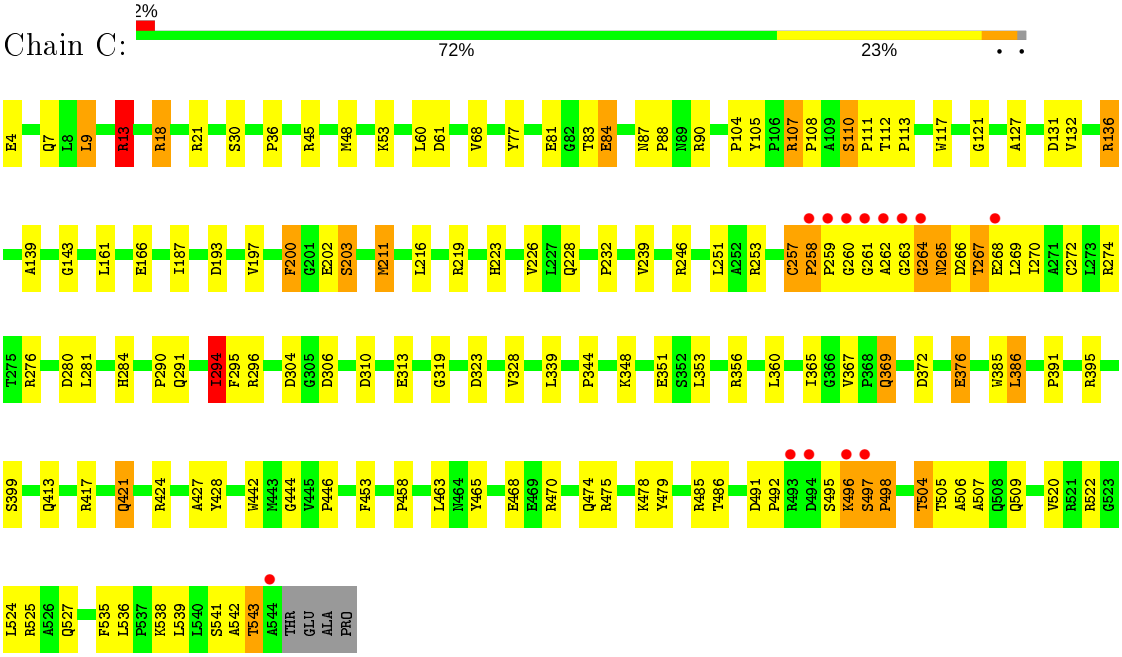
- Molecule 1: ACETYLCHOLINESTERASE

Chain B:



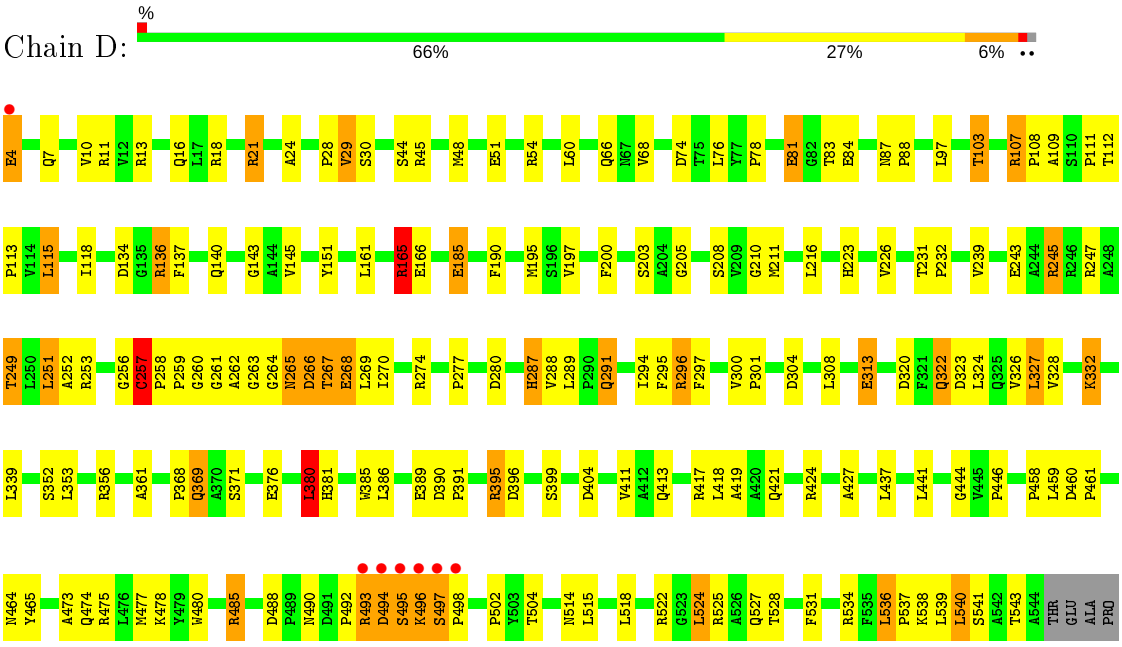
- Molecule 1: ACETYLCHOLINESTERASE

Chain C:



• Molecule 1: ACETYLCHOLINESTERASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	137.94Å 171.93Å 225.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 2.65 48.72 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.72-2.65) 99.9 (48.72-2.65)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.155 , 0.206 0.155 , 0.206	Depositor DCC
R_{free} test set	4658 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19400	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CL, SO4, H34, 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	1.09	2/4380 (0.0%)	1.02	12/5985 (0.2%)
1	B	1.06	8/4351 (0.2%)	1.05	18/5947 (0.3%)
1	C	1.12	8/4331 (0.2%)	1.06	17/5921 (0.3%)
1	D	1.11	6/4349 (0.1%)	1.06	22/5946 (0.4%)
All	All	1.10	24/17411 (0.1%)	1.05	69/23799 (0.3%)

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	B	0	1
1	C	0	3
All	All	0	5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	268	GLU	CG-CD	10.27	1.67	1.51
1	C	4	GLU	CD-OE2	9.71	1.36	1.25
1	D	81	GLU	CG-CD	7.58	1.63	1.51
1	D	81	GLU	CB-CG	7.50	1.66	1.52
1	C	268	GLU	CG-CD	7.15	1.62	1.51
1	B	96	CYS	CB-SG	6.65	1.93	1.82
1	A	340	VAL	CB-CG2	-6.57	1.39	1.52
1	C	304	ASP	CB-CG	6.24	1.64	1.51
1	C	428	TYR	CB-CG	6.16	1.60	1.51
1	C	257	CYS	CB-SG	-5.94	1.72	1.81
1	D	185	GLU	CG-CD	5.89	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	268	GLU	CB-CG	5.81	1.63	1.52
1	B	245	ARG	CZ-NH2	5.59	1.40	1.33
1	D	268	GLU	CD-OE1	5.53	1.31	1.25
1	D	151	TYR	CE1-CZ	5.53	1.45	1.38
1	C	479	TYR	CG-CD1	5.46	1.46	1.39
1	A	519	GLU	CG-CD	5.46	1.60	1.51
1	C	132	VAL	CB-CG2	-5.45	1.41	1.52
1	B	256	GLY	N-CA	5.38	1.54	1.46
1	B	81	GLU	CG-CD	5.36	1.59	1.51
1	B	81	GLU	CB-CG	5.12	1.61	1.52
1	C	117	TRP	CE3-CZ3	5.05	1.47	1.38
1	D	151	TYR	CG-CD1	5.04	1.45	1.39
1	B	256	GLY	C-O	-5.00	1.15	1.23

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	13	ARG	NE-CZ-NH1	-12.83	113.89	120.30
1	A	540	LEU	CA-CB-CG	11.95	142.78	115.30
1	D	257	CYS	CA-CB-SG	-8.63	98.47	114.00
1	C	246	ARG	NE-CZ-NH1	-7.84	116.38	120.30
1	A	475	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	17	LEU	CA-CB-CG	7.79	133.22	115.30
1	D	245	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	B	257	CYS	N-CA-C	7.61	131.55	111.00
1	B	253	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	D	404	ASP	CB-CG-OD1	7.53	125.08	118.30
1	D	475	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	D	245	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	B	263	GLY	N-CA-C	7.31	131.37	113.10
1	D	266	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	D	475	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	C	18	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	C	269	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	522[A]	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	A	522[B]	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	C	4	GLU	OE1-CD-OE2	6.61	131.23	123.30
1	B	211	MET	CG-SD-CE	6.57	110.71	100.20
1	B	253	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	D	274	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	C	310	ASP	CB-CG-OD1	6.34	124.00	118.30
1	B	251	LEU	CA-CB-CG	-6.30	100.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	219	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	C	294	ILE	CB-CA-C	-6.16	99.29	111.60
1	B	475	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	D	380	LEU	CA-CB-CG	6.12	129.38	115.30
1	B	291	GLN	CB-CA-C	-6.00	98.40	110.40
1	D	21	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	C	211	MET	CA-CB-CG	-5.80	103.43	113.30
1	D	296	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	115	LEU	CA-CB-CG	5.79	128.61	115.30
1	C	475	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	390	ASP	CB-CG-OD1	5.66	123.40	118.30
1	B	17	LEU	CA-CB-CG	5.66	128.31	115.30
1	B	274	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	372	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	C	9	LEU	CB-CG-CD2	5.53	120.39	111.00
1	B	251	LEU	CB-CG-CD1	5.51	120.37	111.00
1	B	211	MET	CA-CB-CG	-5.49	103.96	113.30
1	C	136	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	D	395	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	46	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	246	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	D	251	LEU	CA-CB-CG	-5.40	102.87	115.30
1	A	280	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	B	60	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	380	LEU	CA-CB-CG	5.35	127.61	115.30
1	D	395	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	280	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	18	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	D	165	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	D	327	LEU	CA-CB-CG	5.20	127.27	115.30
1	C	306	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	274	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	21	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	D	296	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	380	LEU	CB-CG-CD1	5.16	119.77	111.00
1	B	134	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	395	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	74	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	C	9	LEU	CA-CB-CG	5.04	126.90	115.30
1	D	485	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	485	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	60	LEU	CB-CG-CD2	-5.03	102.45	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	131	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	534	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	CYS	Peptide
1	B	256	GLY	Peptide
1	C	257	CYS	Peptide
1	C	495	SER	Peptide
1	C	542	ALA	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	4236	0	4136	122	0
1	B	4216	0	4111	173	0
1	C	4202	0	4092	146	0
1	D	4214	0	4106	191	0
2	A	30	0	26	1	0
2	B	30	0	26	2	0
2	C	30	0	26	1	0
2	D	30	0	26	0	0
3	A	15	0	0	2	0
3	B	20	0	0	2	0
3	C	15	0	0	1	0
3	D	20	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	2	0
4	C	2	0	0	0	0
5	B	14	0	13	5	0
6	A	663	0	0	62	0
6	B	503	0	0	78	0
6	C	621	0	0	63	1
6	D	536	0	0	84	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19400	0	16562	627	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:PRO:HD2	6:C:2568:HOH:O	1.28	1.29
1:D:313:GLU:HG3	6:D:2366:HOH:O	1.30	1.28
1:D:44:SER:HB2	6:D:2064:HOH:O	1.33	1.27
1:B:262:ALA:HA	6:B:2277:HOH:O	1.20	1.27
1:D:258:PRO:HD2	6:D:2303:HOH:O	1.25	1.27
1:A:5:ASP:HB3	6:A:2012:HOH:O	1.36	1.24
6:A:2659:HOH:O	1:D:261:GLY:HA3	1.14	1.23
1:C:339:LEU:HD12	6:C:2439:HOH:O	1.37	1.22
1:C:313:GLU:HG2	6:C:2415:HOH:O	1.39	1.21
1:B:264:GLY:HA3	6:B:2282:HOH:O	1.40	1.19
1:D:502:PRO:HG3	6:D:2441:HOH:O	1.40	1.16
1:B:256:GLY:HA3	1:B:276:ARG:HH21	1.06	1.16
1:D:74:ASP:HB3	6:D:2112:HOH:O	1.42	1.15
1:A:369:GLN:HB2	6:A:2501:HOH:O	1.45	1.15
1:B:262:ALA:HB2	6:B:2274:HOH:O	1.44	1.14
1:D:258:PRO:CD	6:D:2303:HOH:O	1.81	1.12
1:D:211:MET:HB2	6:D:2261:HOH:O	1.50	1.11
1:A:540:LEU:HB3	6:A:2502:HOH:O	1.51	1.11
1:B:245:ARG:HD3	6:B:2254:HOH:O	1.49	1.09
1:B:257:CYS:N	6:B:2270:HOH:O	1.80	1.09
1:B:74:ASP:HB3	6:B:2092:HOH:O	1.54	1.08
1:A:424:ARG:HH11	1:A:424:ARG:HG3	1.11	1.07
1:C:161:LEU:HD12	1:C:270:ILE:HD11	1.33	1.06
1:C:48:MET:HE1	1:C:166:GLU:HA	1.38	1.05
1:A:313[B]:GLU:HG2	6:A:2446:HOH:O	1.58	1.03
1:D:216:LEU:HB3	6:D:2267:HOH:O	1.58	1.02
1:C:203:SER:HB3	6:C:2214:HOH:O	1.58	1.02
1:A:536:LEU:HD13	1:A:540:LEU:CD1	1.90	1.02
1:B:21:ARG:HG2	1:B:21:ARG:HH11	1.23	1.02
1:C:13:ARG:HD2	1:C:13:ARG:O	1.59	1.01
5:B:1546:NAG:H3	6:B:2498:HOH:O	1.59	1.01
1:D:197:VAL:H	1:D:223:HIS:HD2	1.10	1.00
1:B:197:VAL:H	1:B:223:HIS:HD2	1.08	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:THR:HG21	1:B:190:PHE:O	1.61	0.99
1:C:13:ARG:HH11	1:C:13:ARG:CG	1.70	0.98
1:A:17:LEU:HB2	6:A:2044:HOH:O	1.61	0.98
1:C:265:ASN:H	1:C:265:ASN:HD22	1.02	0.97
1:D:51[B]:GLU:HG3	6:D:2072:HOH:O	1.64	0.97
1:B:421:GLN:HG2	6:B:2345:HOH:O	1.65	0.96
1:B:313[B]:GLU:HG2	6:B:2235:HOH:O	1.63	0.96
1:A:394:LEU:HD23	6:A:2532:HOH:O	1.63	0.95
1:D:84:GLU:HG2	1:D:87:ASN:ND2	1.80	0.94
1:C:258:PRO:HG2	1:C:261:GLY:H	1.33	0.94
1:B:542:ALA:HB2	6:B:2494:HOH:O	1.68	0.94
1:A:265:ASN:HB3	6:A:2393:HOH:O	1.66	0.93
1:B:464:ASN:ND2	6:B:2436:HOH:O	2.00	0.93
1:D:265:ASN:HB3	1:D:268:GLU:H	1.30	0.93
1:C:267:THR:HB	6:C:2271:HOH:O	1.68	0.93
1:B:108:PRO:HG3	1:B:112:THR:HG21	1.51	0.92
1:C:543:THR:HB	6:C:2619:HOH:O	1.70	0.91
1:B:64:THR:HG21	6:B:2114:HOH:O	1.71	0.91
1:A:197:VAL:H	1:A:223:HIS:HD2	1.13	0.90
1:C:367:VAL:HG12	6:C:2470:HOH:O	1.70	0.90
4:B:1551:CL:CL	6:B:2475:HOH:O	2.26	0.90
1:C:265:ASN:HD22	1:C:265:ASN:N	1.67	0.90
1:C:265:ASN:H	1:C:265:ASN:ND2	1.68	0.90
1:B:491:ASP:HB3	1:B:494:ASP:HB2	1.53	0.90
1:C:107:ARG:NH1	6:C:2195:HOH:O	2.05	0.89
1:C:197:VAL:H	1:C:223:HIS:HD2	1.13	0.89
1:A:258:PRO:HA	6:A:2387:HOH:O	1.73	0.88
1:C:13:ARG:HG2	1:C:13:ARG:HH11	1.34	0.88
1:D:107:ARG:HG2	6:D:2168:HOH:O	1.71	0.88
1:C:161:LEU:HD12	1:C:270:ILE:CD1	2.04	0.88
1:B:256:GLY:HA3	1:B:276:ARG:NH2	1.87	0.87
6:B:2284:HOH:O	1:C:344:PRO:HA	1.75	0.87
1:C:258:PRO:HD2	1:C:259:PRO:HA	1.53	0.87
1:B:245:ARG:NH1	6:B:2254:HOH:O	1.96	0.86
1:B:467:THR:HG23	1:B:470:ARG:HH21	1.39	0.85
1:D:540:LEU:HD12	6:D:2414:HOH:O	1.76	0.85
1:D:11:ARG:NH1	6:D:2016:HOH:O	2.08	0.85
1:D:536:LEU:HD13	1:D:540:LEU:HD22	1.57	0.85
1:C:360:LEU:HB3	6:C:2234:HOH:O	1.75	0.85
1:A:48:MET:HE1	1:A:166[B]:GLU:HA	1.56	0.84
1:A:424:ARG:NH1	1:A:424:ARG:HG3	1.84	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:ASP:O	6:B:2452:HOH:O	1.96	0.83
1:A:4:GLU:HA	6:A:2001:HOH:O	1.78	0.83
1:B:48:MET:HE1	1:B:166:GLU:HA	1.58	0.83
1:C:386:LEU:HD22	1:D:522:ARG:HH21	1.44	0.83
1:B:21:ARG:NH1	1:B:21:ARG:HG2	1.93	0.82
1:B:421:GLN:CG	6:B:2345:HOH:O	2.22	0.82
1:D:66:GLN:HG2	6:D:2094:HOH:O	1.78	0.82
1:C:13:ARG:NH1	1:C:13:ARG:CG	2.41	0.82
1:B:313[B]:GLU:CG	6:B:2235:HOH:O	2.24	0.82
1:D:257:CYS:CA	6:D:2303:HOH:O	2.27	0.82
1:C:107:ARG:HD3	6:C:2011:HOH:O	1.78	0.82
1:B:259:PRO:O	6:B:2274:HOH:O	1.98	0.82
1:D:51[B]:GLU:CD	6:D:2072:HOH:O	2.18	0.82
1:A:540:LEU:CB	6:A:2502:HOH:O	2.18	0.81
1:D:103:THR:HG22	1:D:145:VAL:HG22	1.61	0.81
1:D:380:LEU:HB3	6:D:2420:HOH:O	1.78	0.81
1:A:537:PRO:HA	1:A:540:LEU:HD22	1.61	0.81
1:C:13:ARG:HD2	1:C:13:ARG:C	1.95	0.81
1:B:197:VAL:H	1:B:223:HIS:CD2	1.96	0.81
1:D:197:VAL:H	1:D:223:HIS:CD2	1.99	0.81
1:B:514:ASN:HB2	6:B:2471:HOH:O	1.81	0.80
1:B:64:THR:HG22	6:B:2070:HOH:O	1.81	0.80
1:B:493:ARG:HA	6:B:2450:HOH:O	1.81	0.80
1:D:13:ARG:HG3	6:D:2242:HOH:O	1.82	0.80
1:A:369:GLN:H	1:A:369:GLN:HE21	1.30	0.80
1:D:51[B]:GLU:CG	6:D:2072:HOH:O	2.24	0.80
1:B:256:GLY:C	6:B:2270:HOH:O	2.14	0.80
1:C:166:GLU:HG3	6:C:2271:HOH:O	1.81	0.79
1:A:17:LEU:CB	6:A:2044:HOH:O	2.23	0.79
1:A:369:GLN:H	1:A:369:GLN:NE2	1.80	0.79
1:C:413:GLN:HG3	3:C:1548:SO4:O2	1.83	0.79
1:C:262:ALA:HA	6:C:2348:HOH:O	1.83	0.79
1:D:108:PRO:O	6:D:2169:HOH:O	2.00	0.79
1:D:48:MET:HE1	1:D:166:GLU:HA	1.63	0.78
1:B:181:GLN:HG2	6:B:2206:HOH:O	1.82	0.78
1:C:258:PRO:HB3	1:C:263:GLY:H	1.47	0.78
1:C:485:ARG:NH2	6:C:2243:HOH:O	2.10	0.78
1:D:332:LYS:HE2	6:D:2376:HOH:O	1.84	0.78
1:A:536:LEU:HD13	1:A:540:LEU:HD11	1.66	0.77
1:B:352:SER:O	1:B:395:ARG:HG3	1.85	0.77
1:D:497:SER:HB2	1:D:498:PRO:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:LEU:HD12	1:D:270:ILE:HD11	1.67	0.77
1:D:539:LEU:O	1:D:543:THR:HG22	1.84	0.76
1:A:413:GLN:HG3	3:A:1547:SO4:O4	1.84	0.76
1:A:219:ARG:NE	6:A:2342:HOH:O	2.15	0.76
1:D:257:CYS:O	1:D:258:PRO:C	2.17	0.76
4:B:1551:CL:CL	6:B:2474:HOH:O	2.39	0.76
1:B:22:LEU:HD12	1:B:31:ALA:HB2	1.68	0.76
1:D:380:LEU:C	6:D:2419:HOH:O	2.23	0.76
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.21	0.76
1:C:13:ARG:NE	6:C:2027:HOH:O	2.08	0.76
1:C:166:GLU:CG	6:C:2271:HOH:O	2.34	0.76
1:A:4:GLU:HB2	6:A:2025:HOH:O	1.85	0.75
1:B:467:THR:HG23	1:B:470:ARG:NH2	2.00	0.75
1:C:258:PRO:HD2	1:C:260:GLY:H	1.52	0.75
1:D:54:ARG:NH2	6:D:2077:HOH:O	2.20	0.75
5:B:1546:NAG:H4	6:B:2501:HOH:O	1.84	0.75
1:B:265:ASN:HB3	6:B:2286:HOH:O	1.85	0.75
1:A:20:ILE:HD13	6:A:2113:HOH:O	1.86	0.74
1:A:4:GLU:N	1:A:4:GLU:OE1	2.20	0.74
1:D:103:THR:HG21	1:D:190:PHE:O	1.86	0.74
1:A:276:ARG:HD3	6:A:2400:HOH:O	1.87	0.74
1:A:219:ARG:NH2	6:A:2342:HOH:O	1.93	0.74
1:B:522:ARG:HD3	6:B:2212:HOH:O	1.87	0.74
1:A:197:VAL:H	1:A:223:HIS:CD2	2.03	0.73
1:C:274:ARG:HD3	6:C:2077:HOH:O	1.88	0.73
1:A:4:GLU:HG2	1:A:4:GLU:O	1.88	0.73
1:C:36:PRO:HB2	1:C:53:LYS:HD3	1.69	0.73
1:C:197:VAL:H	1:C:223:HIS:CD2	2.03	0.73
1:D:424:ARG:HD3	6:D:2373:HOH:O	1.87	0.73
1:D:211:MET:CB	6:D:2261:HOH:O	2.22	0.72
1:B:473:ALA:O	1:B:477:MET:HG3	1.89	0.72
1:C:522:ARG:HD3	6:C:2590:HOH:O	1.89	0.72
1:B:467:THR:CG2	1:B:470:ARG:HH21	2.03	0.72
1:D:13:ARG:HD3	6:D:2022:HOH:O	1.88	0.72
1:D:112:THR:HG21	1:D:143:GLY:O	1.90	0.72
1:C:258:PRO:CD	1:C:259:PRO:HA	2.19	0.72
1:A:63:THR:O	6:A:2113:HOH:O	2.07	0.71
1:B:256:GLY:H	1:B:276:ARG:HE	1.37	0.71
1:B:130:LEU:HD12	1:B:133:TYR:CE2	2.25	0.71
1:D:495:SER:O	1:D:496:LYS:HB2	1.89	0.71
1:D:84:GLU:HG2	1:D:87:ASN:HD21	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ALA:CA	6:B:2277:HOH:O	1.96	0.71
1:C:48:MET:HE1	1:C:166:GLU:CA	2.18	0.70
1:C:121:GLY:HA2	2:C:1545:H34:HAN1	1.72	0.70
1:B:264:GLY:HA2	6:B:2284:HOH:O	1.91	0.70
1:A:84:GLU:HG3	1:A:87:ASN:ND2	2.06	0.70
1:C:108:PRO:HB3	6:C:2196:HOH:O	1.89	0.70
1:A:161:LEU:HD12	1:A:270:ILE:HD11	1.74	0.70
1:A:48:MET:HE1	1:A:165:ARG:O	1.90	0.70
1:A:540:LEU:CG	6:A:2502:HOH:O	2.37	0.70
1:C:339:LEU:CD1	6:C:2439:HOH:O	2.10	0.70
1:D:525[B]:ARG:NE	6:D:2514:HOH:O	2.25	0.70
1:C:258:PRO:HD2	1:C:260:GLY:N	2.07	0.69
1:A:253[B]:ARG:HG2	6:A:2382:HOH:O	1.93	0.69
1:D:381:HIS:N	6:D:2419:HOH:O	2.25	0.69
1:A:522[B]:ARG:CZ	6:A:2620:HOH:O	2.40	0.69
1:B:255:VAL:O	1:B:256:GLY:O	2.09	0.69
1:B:267:THR:N	6:B:2286:HOH:O	2.25	0.69
1:A:424:ARG:CG	1:A:424:ARG:HH11	1.98	0.69
1:B:166:GLU:HG3	1:B:274:ARG:HH22	1.58	0.68
1:B:256:GLY:CA	1:B:276:ARG:HH21	1.97	0.68
1:B:470:ARG:O	1:B:474:GLN:HG3	1.94	0.68
1:D:262:ALA:N	6:D:2309:HOH:O	2.25	0.68
1:C:538:LYS:HE2	1:D:376:GLU:OE1	1.93	0.68
1:A:48:MET:CE	1:A:166[B]:GLU:HA	2.23	0.68
1:D:257:CYS:O	1:D:259:PRO:N	2.26	0.68
1:C:265:ASN:OD1	6:C:2355:HOH:O	2.12	0.67
1:A:342:GLY:HA2	1:D:263:GLY:HA3	1.77	0.67
1:B:138:LEU:HD13	1:B:477:MET:HE3	1.77	0.67
1:B:303:VAL:HG12	6:B:2329:HOH:O	1.96	0.66
1:C:108:PRO:O	6:C:2194:HOH:O	2.11	0.66
1:C:365:ILE:HD11	6:C:2395:HOH:O	1.95	0.66
1:B:245:ARG:O	1:B:249:THR:HB	1.95	0.66
1:D:211:MET:HG2	1:D:308:LEU:HD21	1.77	0.66
1:B:262:ALA:CB	6:B:2277:HOH:O	2.33	0.66
1:B:350:ASN:ND2	6:B:2367:HOH:O	2.27	0.66
1:D:458:PRO:HA	1:D:465:TYR:CD2	2.30	0.66
1:A:219:ARG:NH2	1:A:323:ASP:OD1	2.29	0.66
1:D:369:GLN:HE21	1:D:369:GLN:H	1.43	0.66
1:C:296:ARG:HH21	1:C:369:GLN:NE2	1.93	0.66
1:D:211:MET:N	6:D:2261:HOH:O	2.11	0.66
1:A:17:LEU:HD13	6:A:2044:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:ARG:HD2	6:C:2602:HOH:O	1.95	0.64
1:D:10:VAL:HG22	1:D:107:ARG:HH21	1.61	0.64
1:A:258:PRO:HG3	6:A:2382:HOH:O	1.97	0.64
1:C:84:GLU:HG3	1:C:87:ASN:HD22	1.63	0.64
1:A:313[B]:GLU:CG	6:A:2446:HOH:O	2.31	0.64
1:B:45:ARG:HG3	6:B:2041:HOH:O	1.97	0.64
1:C:90:ARG:NE	6:C:2104:HOH:O	2.30	0.64
1:A:165:ARG:HD3	6:A:2288:HOH:O	1.98	0.63
1:A:74:ASP:HB2	6:A:2149:HOH:O	1.98	0.63
1:C:272:CYS:HB2	6:C:2361:HOH:O	1.98	0.63
1:D:266:ASP:O	1:D:270:ILE:HD12	1.98	0.63
1:B:108:PRO:CG	1:B:112:THR:HG21	2.26	0.63
1:A:539:LEU:O	1:A:543:THR:HG22	1.98	0.63
1:D:259:PRO:HG3	6:D:2307:HOH:O	1.97	0.63
1:C:290:PRO:C	1:C:291:GLN:HG3	2.19	0.63
5:B:1546:NAG:H5	6:B:2294:HOH:O	1.99	0.63
1:C:259:PRO:HD3	6:C:2361:HOH:O	1.99	0.63
1:A:319:GLY:O	1:A:421:GLN:HG3	1.99	0.63
1:C:507:ALA:HA	6:C:2589:HOH:O	1.98	0.63
1:D:381:HIS:CA	6:D:2419:HOH:O	2.47	0.62
1:D:84:GLU:HG2	1:D:87:ASN:HD22	1.63	0.62
1:D:245:ARG:O	1:D:249:THR:HB	1.99	0.62
1:D:249:THR:HG23	1:D:253:ARG:NH2	2.13	0.62
1:A:258:PRO:HD2	1:A:260:GLY:H	1.65	0.62
1:B:332:LYS:HE2	6:B:2154:HOH:O	2.00	0.62
1:D:323:ASP:HB2	6:D:2271:HOH:O	2.00	0.61
1:C:263:GLY:HA3	6:C:2351:HOH:O	2.00	0.61
1:D:68:VAL:HG11	1:D:88:PRO:HB3	1.81	0.61
1:B:267:THR:HG22	6:B:2191:HOH:O	1.99	0.61
1:C:376:GLU:OE2	1:D:538:LYS:HD2	1.99	0.61
1:B:91:GLU:HG3	6:B:2123:HOH:O	2.01	0.61
1:D:380:LEU:HD21	6:D:2530:HOH:O	1.99	0.61
1:D:24:ALA:HB3	1:D:140:GLN:HG3	1.82	0.60
1:B:485:ARG:NH2	6:B:2171:HOH:O	2.34	0.60
1:C:280:ASP:O	1:C:284:HIS:HD2	1.83	0.60
1:D:136:ARG:HG2	1:D:137:PHE:N	2.17	0.60
1:A:274:ARG:HD3	6:A:2093:HOH:O	2.01	0.60
1:A:351:GLU:HB2	6:A:2477:HOH:O	2.02	0.60
1:A:525[A]:ARG:HD3	6:A:2660:HOH:O	2.01	0.60
1:C:261:GLY:HA2	6:C:2347:HOH:O	2.02	0.60
1:A:348:LYS:N	6:A:2151:HOH:O	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASP:OD2	1:A:105:TYR:OH	2.13	0.59
5:B:1546:NAG:H62	6:B:2502:HOH:O	2.02	0.59
1:D:264:GLY:O	1:D:265:ASN:C	2.39	0.59
1:D:380:LEU:CD2	6:D:2530:HOH:O	2.50	0.59
1:B:265:ASN:CB	6:B:2286:HOH:O	2.45	0.59
1:B:459:LEU:O	1:B:460:ASP:C	2.41	0.59
1:A:258:PRO:HD2	1:A:260:GLY:N	2.18	0.59
1:D:369:GLN:NE2	1:D:369:GLN:H	1.99	0.59
1:D:166:GLU:HB2	1:D:270:ILE:HD13	1.85	0.59
1:D:497:SER:CB	1:D:498:PRO:HA	2.32	0.59
1:B:21:ARG:CG	1:B:21:ARG:HH11	2.03	0.58
1:D:504:THR:HB	6:D:2496:HOH:O	2.03	0.58
1:C:356:ARG:O	1:C:360:LEU:HG	2.02	0.58
1:D:473:ALA:O	1:D:477:MET:HG3	2.03	0.58
1:A:417:ARG:HD3	3:A:1547:SO4:O3	2.03	0.58
1:D:249:THR:HG23	1:D:253:ARG:HH22	1.68	0.58
1:B:249:THR:HG22	6:B:2257:HOH:O	2.04	0.57
1:C:13:ARG:O	1:C:13:ARG:CD	2.44	0.57
6:B:2314:HOH:O	1:C:253:ARG:HD3	2.04	0.57
1:B:138:LEU:HB2	1:B:146:LEU:HD12	1.86	0.57
1:C:505:THR:HA	6:C:2585:HOH:O	2.04	0.57
1:A:519:GLU:HG3	6:A:2321:HOH:O	2.03	0.57
1:A:525[B]:ARG:NH1	6:A:2646:HOH:O	2.37	0.57
1:B:261:GLY:N	6:B:2273:HOH:O	2.35	0.57
1:B:264:GLY:CA	6:B:2284:HOH:O	2.51	0.57
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.85	0.57
1:C:369:GLN:CD	6:C:2470:HOH:O	2.42	0.57
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.87	0.57
1:B:253:ARG:NE	6:B:2266:HOH:O	2.37	0.57
1:D:497:SER:CB	1:D:498:PRO:CA	2.82	0.57
1:B:41:PRO:HG2	6:B:2043:HOH:O	2.04	0.57
1:D:261:GLY:HA2	6:D:2309:HOH:O	2.05	0.57
1:D:83:THR:HG22	6:D:2382:HOH:O	2.05	0.57
1:B:121:GLY:HA2	2:B:1545:H34:CAT	2.35	0.57
1:A:107:ARG:HH11	1:A:107:ARG:HG2	1.70	0.57
1:C:211:MET:HG3	1:C:232:PRO:HB3	1.86	0.57
1:C:376:GLU:OE2	1:D:538:LYS:CD	2.53	0.57
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.86	0.56
1:B:81:GLU:HB2	6:B:2094:HOH:O	2.04	0.56
1:D:4:GLU:OE2	1:D:18:ARG:NH1	2.38	0.56
1:D:525[A]:ARG:HD2	6:D:2514:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:CD1	6:A:2044:HOH:O	2.52	0.56
1:C:265:ASN:ND2	1:C:265:ASN:N	2.39	0.56
1:D:495:SER:O	1:D:496:LYS:CB	2.52	0.56
1:D:498:PRO:HD2	1:D:518:LEU:HB2	1.88	0.56
1:A:77:TYR:OH	6:A:2151:HOH:O	1.94	0.56
1:B:265:ASN:HB3	1:B:268:GLU:H	1.70	0.56
1:B:249:THR:HG23	1:B:253:ARG:NH2	2.20	0.56
1:C:223:HIS:HE1	6:C:2312:HOH:O	1.88	0.56
1:C:424:ARG:HD2	6:C:2509:HOH:O	2.06	0.56
1:B:166:GLU:CG	1:B:274:ARG:HH22	2.19	0.56
1:D:320:ASP:OD1	1:D:322:GLN:HG2	2.06	0.56
1:C:468:GLU:HG2	6:C:2276:HOH:O	2.04	0.56
1:D:485:ARG:HD3	6:D:2233:HOH:O	2.06	0.56
1:A:48:MET:HE1	1:A:166[A]:GLU:HA	1.88	0.56
1:A:369:GLN:CB	6:A:2501:HOH:O	2.22	0.56
1:B:339:LEU:HD13	1:B:346:PHE:CE2	2.40	0.56
1:B:183:VAL:HG13	1:B:187:ILE:HB	1.88	0.55
1:C:339:LEU:HD11	1:C:399:SER:HA	1.88	0.55
1:A:534:ARG:HD3	6:A:2655:HOH:O	2.06	0.55
1:C:77:TYR:CZ	1:C:348:LYS:HG2	2.40	0.55
1:C:543:THR:C	6:C:2619:HOH:O	2.44	0.55
1:D:208:SER:HA	6:D:2261:HOH:O	2.05	0.55
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.89	0.55
1:C:113:PRO:HB2	6:C:2206:HOH:O	2.06	0.55
1:C:527:GLN:NE2	1:D:385:TRP:HD1	2.04	0.55
1:C:369:GLN:NE2	1:C:369:GLN:H	2.05	0.54
1:D:109:ALA:HB3	6:D:2172:HOH:O	2.07	0.54
1:D:165:ARG:HG3	6:D:2087:HOH:O	2.07	0.54
1:A:346:PHE:O	6:A:2465:HOH:O	2.18	0.54
1:C:60:LEU:HD12	1:C:61:ASP:N	2.21	0.54
1:C:203:SER:CB	6:C:2214:HOH:O	2.31	0.54
1:C:202:GLU:OE1	1:C:203:SER:HB2	2.08	0.54
1:A:290:PRO:C	1:A:291:GLN:HG3	2.28	0.54
1:C:442:TRP:HZ3	6:C:2439:HOH:O	1.90	0.54
1:B:458:PRO:O	1:B:459:LEU:O	2.26	0.53
6:A:2662:HOH:O	1:B:534:ARG:HD3	2.08	0.53
1:D:16:GLN:HB3	6:D:2012:HOH:O	2.07	0.53
1:D:267:THR:HG21	6:D:2159:HOH:O	2.08	0.53
1:A:322:GLN:HA	1:A:422:GLY:O	2.08	0.53
1:C:264:GLY:HA2	6:C:2353:HOH:O	2.08	0.53
1:C:84:GLU:HG3	1:C:87:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:LYS:HE3	6:D:2476:HOH:O	2.09	0.53
1:A:540:LEU:HA	1:A:543:THR:HG22	1.89	0.53
1:C:45:ARG:HG3	6:C:2080:HOH:O	2.09	0.53
1:A:184:GLN:CG	6:A:2310:HOH:O	2.57	0.53
1:B:441:LEU:HG	6:B:2430:HOH:O	2.07	0.53
1:D:304:ASP:OD2	6:D:2227:HOH:O	2.17	0.53
1:B:195:MET:HB2	6:B:2215:HOH:O	2.09	0.52
1:B:256:GLY:N	1:B:276:ARG:HE	2.07	0.52
1:B:22:LEU:HD22	1:B:136:ARG:HH12	1.73	0.52
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.91	0.52
1:D:165:ARG:CD	6:D:2223:HOH:O	2.56	0.52
1:B:107:ARG:HD2	6:B:2139:HOH:O	2.10	0.52
1:D:107:ARG:HD3	6:D:2005:HOH:O	2.08	0.52
1:A:313[A]:GLU:OE2	6:A:2352:HOH:O	2.19	0.52
1:C:470:ARG:O	1:C:474:GLN:HG3	2.09	0.52
1:A:286:TRP:CD1	1:D:260:GLY:HA2	2.45	0.52
1:D:200:PHE:HB2	1:D:226:VAL:HB	1.92	0.52
1:B:536:LEU:HD13	1:B:540:LEU:CD2	2.39	0.52
1:B:48:MET:HE1	1:B:165:ARG:O	2.10	0.52
1:D:195:MET:HG2	6:D:2252:HOH:O	2.08	0.52
1:A:73:VAL:O	6:A:2142:HOH:O	2.19	0.52
1:B:328:VAL:O	1:B:328:VAL:HG23	2.08	0.52
1:A:319:GLY:O	1:A:421:GLN:CG	2.58	0.51
1:B:371:SER:OG	1:B:543:THR:HG23	2.09	0.51
1:C:353:LEU:HB3	1:C:391:PRO:HB2	1.91	0.51
1:B:182:TRP:HA	6:B:2207:HOH:O	2.09	0.51
1:B:200:PHE:CB	1:B:226:VAL:HB	2.40	0.51
1:C:284:HIS:CE1	6:C:2345:HOH:O	2.63	0.51
1:D:83:THR:CG2	6:D:2382:HOH:O	2.57	0.51
1:A:540:LEU:HG	6:A:2502:HOH:O	2.06	0.51
1:B:129:SER:HB3	6:B:2071:HOH:O	2.10	0.51
1:B:371:SER:OG	1:B:543:THR:CG2	2.59	0.51
1:D:257:CYS:C	6:D:2303:HOH:O	2.39	0.51
1:A:328:VAL:O	1:A:427:ALA:HA	2.11	0.51
1:B:197:VAL:N	1:B:223:HIS:HD2	1.91	0.51
1:D:28:PRO:HD2	6:D:2043:HOH:O	2.11	0.51
1:D:328:VAL:O	1:D:427:ALA:HA	2.11	0.51
1:D:78:PRO:HG3	6:D:2115:HOH:O	2.09	0.51
1:B:227:LEU:N	1:B:227:LEU:HD12	2.26	0.51
1:B:464:ASN:HB2	6:B:2435:HOH:O	2.11	0.51
1:D:297:PHE:HA	6:D:2352:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:ALA:O	6:D:2437:HOH:O	2.19	0.51
1:A:536:LEU:HD13	1:A:540:LEU:HD12	1.88	0.51
1:C:444:GLY:O	1:C:446:PRO:HD3	2.11	0.51
1:C:485:ARG:HB3	1:C:486:THR:HG23	1.92	0.51
1:A:436:THR:HG22	6:A:2565:HOH:O	2.10	0.51
1:B:259:PRO:HA	6:B:2275:HOH:O	2.11	0.51
1:C:458:PRO:HA	1:C:465:TYR:CD2	2.46	0.51
1:D:113:PRO:HB2	6:D:2176:HOH:O	2.10	0.51
1:A:45:ARG:HG2	6:A:2051:HOH:O	2.11	0.50
1:B:117:TRP:HA	1:B:200:PHE:O	2.11	0.50
1:D:165:ARG:HD2	6:D:2223:HOH:O	2.10	0.50
1:D:376:GLU:HG2	1:D:380:LEU:HG	1.92	0.50
1:B:249:THR:HG23	1:B:253:ARG:HH22	1.77	0.50
1:B:68:VAL:HG13	1:B:127:ALA:HB2	1.94	0.50
1:D:488:ASP:OD1	1:D:490:ASN:HB2	2.12	0.50
1:A:522[B]:ARG:NH1	6:A:2620:HOH:O	2.44	0.50
1:A:527:GLN:NE2	1:B:385:TRP:HD1	2.09	0.50
1:C:284:HIS:HE1	6:C:2345:HOH:O	1.93	0.50
1:C:535:PHE:HB2	1:D:380:LEU:HD12	1.94	0.50
1:D:118:ILE:O	1:D:205:GLY:HA3	2.11	0.50
1:D:459:LEU:N	1:D:459:LEU:CD1	2.75	0.50
1:D:459:LEU:N	1:D:459:LEU:HD12	2.27	0.50
1:B:9:LEU:HD22	6:B:2008:HOH:O	2.12	0.49
1:C:13:ARG:NH2	6:C:2027:HOH:O	2.45	0.49
1:D:534:ARG:HD3	6:D:2522:HOH:O	2.10	0.49
1:B:165:ARG:HD2	6:B:2193:HOH:O	2.12	0.49
1:C:13:ARG:CZ	6:C:2027:HOH:O	2.54	0.49
1:C:104:PRO:HD2	1:C:108:PRO:HD3	1.93	0.49
1:C:351:GLU:HB2	6:C:2451:HOH:O	2.12	0.49
1:C:21:ARG:HD3	1:C:105:TYR:CZ	2.46	0.49
1:D:265:ASN:ND2	6:D:2313:HOH:O	2.46	0.49
1:B:202:GLU:HA	1:B:228:GLN:O	2.12	0.49
1:B:454:ILE:HD12	1:B:480:TRP:CE2	2.48	0.49
1:C:284:HIS:HE1	6:C:2380:HOH:O	1.95	0.49
1:A:340:VAL:HA	6:A:2465:HOH:O	2.12	0.49
1:A:371:SER:OG	1:A:543:THR:HG23	2.13	0.49
1:D:13:ARG:HD2	6:D:2020:HOH:O	2.12	0.49
1:D:525[B]:ARG:CZ	6:D:2514:HOH:O	2.59	0.49
1:B:108:PRO:HG3	1:B:112:THR:CG2	2.34	0.49
1:B:536:LEU:HD13	1:B:540:LEU:HD22	1.94	0.49
1:C:18:ARG:HD3	6:C:2004:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:LEU:HB3	1:D:537:PRO:HD3	1.94	0.49
5:B:1546:NAG:C1	6:B:2499:HOH:O	2.61	0.48
1:C:87:ASN:O	1:C:88:PRO:C	2.51	0.48
1:A:537:PRO:HA	1:A:540:LEU:CD2	2.37	0.48
1:A:84:GLU:HG3	1:A:87:ASN:HD22	1.76	0.48
1:B:8:LEU:HD11	1:B:21:ARG:HB2	1.95	0.48
1:A:332:LYS:HE3	6:A:2461:HOH:O	2.12	0.48
1:B:459:LEU:C	6:B:2433:HOH:O	2.51	0.48
1:A:313[A]:GLU:OE1	6:A:2443:HOH:O	2.18	0.48
1:C:319:GLY:O	1:C:421:GLN:HG2	2.14	0.48
1:D:107:ARG:CG	1:D:107:ARG:HH11	2.27	0.48
1:D:391:PRO:HG3	6:D:2395:HOH:O	2.12	0.48
1:A:522[B]:ARG:NH2	6:A:2620:HOH:O	2.46	0.48
1:B:29:VAL:HG12	1:B:104:PRO:HA	1.96	0.48
1:C:219:ARG:HA	1:C:219:ARG:HD2	1.68	0.48
1:C:36:PRO:CD	1:C:60:LEU:HD21	2.44	0.48
1:A:219:ARG:HD2	1:A:219:ARG:HA	1.58	0.48
1:A:291:GLN:NE2	6:A:2422:HOH:O	2.43	0.48
1:B:22:LEU:CD1	1:B:31:ALA:HB2	2.42	0.48
1:D:48:MET:HE1	1:D:165:ARG:O	2.13	0.48
1:D:444:GLY:O	1:D:446:PRO:HD3	2.13	0.48
1:B:262:ALA:O	1:B:264:GLY:N	2.46	0.47
1:D:165:ARG:HH11	1:D:165:ARG:HB2	1.79	0.47
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.96	0.47
1:C:294:ILE:HG12	1:C:365:ILE:HG22	1.95	0.47
1:D:326:VAL:HG21	1:D:418:LEU:HD13	1.96	0.47
1:D:45:ARG:HA	1:D:48:MET:HG3	1.96	0.47
1:B:542:ALA:O	1:B:543:THR:HB	2.14	0.47
1:B:539:LEU:O	1:B:543:THR:HB	2.14	0.47
1:C:504:THR:HG22	6:C:2252:HOH:O	2.13	0.47
1:C:84:GLU:HG2	6:C:2148:HOH:O	2.15	0.47
1:B:48:MET:CE	1:B:166:GLU:HA	2.37	0.47
1:B:197:VAL:HB	1:B:222:PHE:HA	1.96	0.47
1:B:348:LYS:O	1:B:440:PRO:HG3	2.15	0.47
1:D:109:ALA:N	6:D:2171:HOH:O	2.47	0.47
1:D:161:LEU:HD12	1:D:270:ILE:CD1	2.43	0.47
1:B:542:ALA:HA	6:B:2219:HOH:O	2.14	0.47
1:C:258:PRO:HD2	1:C:259:PRO:CA	2.35	0.47
1:D:223:HIS:HE1	6:D:2254:HOH:O	1.97	0.47
1:D:522:ARG:HE	1:D:522:ARG:HB3	1.54	0.47
1:C:258:PRO:CB	1:C:263:GLY:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:LEU:HB2	6:C:2439:HOH:O	2.14	0.47
1:C:328:VAL:O	1:C:427:ALA:HA	2.15	0.47
1:C:485:ARG:HB2	6:C:2560:HOH:O	2.14	0.47
1:D:256:GLY:O	1:D:257:CYS:O	2.32	0.47
1:D:300:VAL:HB	1:D:301:PRO:HD2	1.97	0.47
1:A:87:ASN:HB3	1:A:88:PRO:HD2	1.97	0.46
1:B:265:ASN:HB2	1:B:268:GLU:HG3	1.97	0.46
1:D:103:THR:CG2	1:D:145:VAL:HG22	2.38	0.46
1:A:38:ALA:HB2	1:A:178:LEU:HD23	1.97	0.46
1:D:495:SER:HA	6:D:2485:HOH:O	2.15	0.46
1:A:352:SER:O	1:A:395:ARG:HG3	2.15	0.46
1:C:200:PHE:CB	1:C:226:VAL:HB	2.45	0.46
1:D:492:PRO:O	1:D:494:ASP:N	2.44	0.46
1:C:68:VAL:HG23	1:C:90:ARG:HB2	1.97	0.46
1:D:497:SER:HB3	1:D:498:PRO:C	2.36	0.46
1:A:497:SER:H	1:A:498:PRO:HA	1.80	0.46
1:B:108:PRO:CG	1:B:112:THR:CG2	2.92	0.46
1:C:84:GLU:CG	6:C:2148:HOH:O	2.64	0.46
1:B:210:GLY:HA3	1:B:232:PRO:HD3	1.97	0.46
1:B:460:ASP:N	6:B:2433:HOH:O	2.48	0.46
1:D:200:PHE:CB	1:D:226:VAL:HB	2.45	0.46
1:A:458:PRO:HA	1:A:465:TYR:CD1	2.50	0.46
1:B:166:GLU:HB2	6:B:2191:HOH:O	2.15	0.46
1:C:68:VAL:HG13	1:C:127:ALA:HB2	1.97	0.46
1:D:265:ASN:HB2	1:D:268:GLU:HB2	1.97	0.46
1:D:528:THR:O	1:D:531:PHE:HB3	2.15	0.46
1:A:365:ILE:O	1:A:368:PRO:HD3	2.16	0.45
1:D:496:LYS:HB3	1:D:497:SER:H	1.50	0.45
1:B:263:GLY:HA3	6:B:2279:HOH:O	2.16	0.45
1:B:498:PRO:HG2	6:B:2455:HOH:O	2.16	0.45
1:C:266:ASP:O	1:C:270:ILE:HD12	2.15	0.45
1:D:339:LEU:HD11	1:D:399:SER:HA	1.99	0.45
1:A:460:ASP:C	1:A:460:ASP:OD1	2.55	0.45
1:A:485:ARG:NH1	6:A:2603:HOH:O	2.41	0.45
1:A:184:GLN:HG3	6:A:2310:HOH:O	2.14	0.45
1:C:258:PRO:N	1:C:259:PRO:HA	2.30	0.45
1:D:7:GLN:HG2	6:D:2003:HOH:O	2.16	0.45
1:A:228:GLN:HG2	1:A:428:TYR:OH	2.17	0.45
1:B:138:LEU:HB2	1:B:146:LEU:CD1	2.46	0.45
1:B:386:LEU:HA	1:B:386:LEU:HD23	1.75	0.45
1:D:265:ASN:HB3	1:D:268:GLU:N	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:PRO:HD2	6:A:2099:HOH:O	2.17	0.45
1:C:339:LEU:HD11	1:C:399:SER:CA	2.46	0.45
1:D:498:PRO:HB2	6:D:2489:HOH:O	2.17	0.45
1:B:504:THR:HB	6:B:2463:HOH:O	2.16	0.45
1:C:497:SER:H	1:C:498:PRO:HA	1.82	0.45
1:D:247:ARG:HB3	1:D:288:VAL:HG21	1.99	0.45
1:A:100:ASN:O	1:A:147:VAL:HA	2.16	0.45
1:A:539:LEU:O	1:A:543:THR:CG2	2.65	0.45
1:A:540:LEU:HD12	6:A:2502:HOH:O	2.17	0.45
1:D:231:THR:HG21	1:D:411:VAL:HA	1.99	0.45
1:A:4:GLU:CB	6:A:2025:HOH:O	2.52	0.44
1:C:107:ARG:HG2	1:C:107:ARG:HH11	1.82	0.44
1:D:352:SER:O	1:D:395:ARG:HG3	2.17	0.44
1:B:463:LEU:O	1:B:464:ASN:HB2	2.18	0.44
1:C:395:ARG:NH2	6:C:2496:HOH:O	2.47	0.44
1:C:541:SER:HB3	6:C:2618:HOH:O	2.18	0.44
1:D:464:ASN:ND2	6:D:2460:HOH:O	2.49	0.44
1:D:536:LEU:HD13	1:D:540:LEU:CD2	2.37	0.44
1:B:32:PHE:CG	1:B:190:PHE:HE2	2.35	0.44
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.52	0.44
1:B:477:MET:O	1:B:481:THR:OG1	2.29	0.44
1:D:165:ARG:HG2	6:D:2225:HOH:O	2.16	0.44
1:D:324:LEU:N	6:D:2372:HOH:O	2.50	0.44
1:B:441:LEU:HG	1:B:441:LEU:H	1.75	0.44
1:B:371:SER:CB	1:B:543:THR:HG23	2.47	0.44
1:C:110:SER:C	6:C:2197:HOH:O	2.55	0.44
1:D:361:ALA:HA	6:D:2196:HOH:O	2.18	0.44
1:D:353:LEU:HB3	1:D:391:PRO:HB2	1.98	0.44
1:A:81[B]:GLU:HG3	1:A:438:THR:HG21	1.99	0.44
1:D:493:ARG:CB	6:D:2238:HOH:O	2.66	0.44
1:B:304:ASP:N	1:B:304:ASP:OD1	2.46	0.44
1:D:243:GLU:O	1:D:247:ARG:HG3	2.16	0.44
1:D:264:GLY:HA3	6:D:2312:HOH:O	2.17	0.44
1:D:514:ASN:HB2	6:D:2507:HOH:O	2.17	0.44
1:A:107:ARG:HD3	6:A:2014:HOH:O	2.16	0.44
1:D:29:VAL:HG21	1:D:136:ARG:HB2	1.99	0.44
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.99	0.44
1:C:161:LEU:HD12	1:C:270:ILE:CG1	2.47	0.44
1:D:245:ARG:HH22	1:D:266:ASP:CG	2.21	0.44
1:B:165:ARG:HG3	6:B:2195:HOH:O	2.18	0.43
1:C:442:TRP:CZ3	6:C:2439:HOH:O	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:ASP:HA	1:D:461:PRO:HD3	1.91	0.43
1:D:371:SER:OG	1:D:543:THR:HG21	2.18	0.43
1:A:541:SER:HB2	6:A:2658:HOH:O	2.18	0.43
1:B:276:ARG:HD2	6:B:2298:HOH:O	2.18	0.43
1:D:76:LEU:HD12	6:D:2046:HOH:O	2.17	0.43
1:B:70:TYR:N	6:B:2082:HOH:O	2.51	0.43
1:D:107:ARG:HG2	1:D:107:ARG:HH11	1.83	0.43
1:D:424:ARG:HD3	6:D:2443:HOH:O	2.18	0.43
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.89	0.43
1:A:536:LEU:O	1:A:540:LEU:HD13	2.18	0.43
1:B:457:LEU:N	1:B:458:PRO:CD	2.82	0.43
1:C:478:LYS:HE2	6:C:2562:HOH:O	2.18	0.43
1:D:48:MET:CE	1:D:166:GLU:HA	2.42	0.43
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.92	0.43
1:B:219:ARG:HA	1:B:219:ARG:HD2	1.74	0.43
1:B:456:GLY:O	1:B:459:LEU:HB2	2.18	0.43
1:C:369:GLN:H	1:C:369:GLN:HE21	1.66	0.43
1:D:252:ALA:CB	1:D:269:LEU:HD21	2.48	0.43
1:D:258:PRO:HD3	1:D:269:LEU:HG	2.01	0.43
1:D:515:LEU:HA	1:D:515:LEU:HD23	1.77	0.43
1:D:211:MET:CA	6:D:2261:HOH:O	2.52	0.43
1:D:107:ARG:HG2	1:D:107:ARG:NH1	2.33	0.43
1:B:45:ARG:HD3	6:B:2051:HOH:O	2.19	0.43
1:C:112:THR:HG22	1:C:113:PRO:N	2.34	0.43
1:C:7:GLN:HG3	6:C:2190:HOH:O	2.19	0.43
1:D:289:LEU:HD23	1:D:289:LEU:HA	1.85	0.43
1:B:328:VAL:O	1:B:427:ALA:HA	2.19	0.42
1:A:45:ARG:HE	1:A:51:GLU:CD	2.22	0.42
1:D:45:ARG:HB3	6:D:2066:HOH:O	2.19	0.42
1:B:164:SER:HB2	6:B:2191:HOH:O	2.19	0.42
1:D:210:GLY:HA3	1:D:232:PRO:HD3	2.00	0.42
6:A:2193:HOH:O	1:D:287:HIS:HB3	2.18	0.42
1:A:84:GLU:HG2	6:A:2077:HOH:O	2.17	0.42
1:C:386:LEU:HD22	1:D:522:ARG:NH2	2.23	0.42
1:D:413:GLN:NE2	6:D:2279:HOH:O	2.51	0.42
1:B:122:GLY:O	1:B:123:PHE:HB2	2.19	0.42
1:D:185:GLU:HG2	6:D:2023:HOH:O	2.18	0.42
1:B:130:LEU:HB2	1:B:133:TYR:CD2	2.55	0.42
1:D:81:GLU:HB3	6:D:2121:HOH:O	2.19	0.42
1:B:107:ARG:CD	6:B:2139:HOH:O	2.66	0.42
1:D:11:ARG:NE	6:D:2015:HOH:O	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PHE:CB	1:A:226:VAL:HB	2.50	0.42
1:D:252:ALA:HB2	1:D:269:LEU:HD21	2.01	0.42
1:D:291:GLN:NE2	1:D:368:PRO:HB2	2.34	0.42
1:A:107:ARG:NH1	6:A:2219:HOH:O	2.52	0.42
1:B:437:LEU:HD23	1:B:439:TRP:H	1.85	0.42
1:C:187:ILE:HD12	1:C:187:ILE:HA	1.86	0.41
1:A:103:THR:HB	1:A:104:PRO:HD2	2.03	0.41
1:C:376:GLU:HG3	6:C:2477:HOH:O	2.19	0.41
1:B:139:ALA:HA	1:B:144:ALA:O	2.19	0.41
1:B:439:TRP:CZ2	2:B:1545:H34:HAE	2.55	0.41
1:B:199:LEU:O	1:B:200:PHE:HB3	2.20	0.41
1:C:506:ALA:HB3	6:C:2588:HOH:O	2.19	0.41
1:D:267:THR:HG22	6:D:2160:HOH:O	2.19	0.41
1:D:277:PRO:HD2	1:D:280:ASP:OD2	2.20	0.41
1:C:202:GLU:HA	1:C:228:GLN:O	2.20	0.41
1:B:437:LEU:HD21	1:B:439:TRP:HB2	2.02	0.41
1:B:45:ARG:HD2	1:B:45:ARG:HA	1.78	0.41
1:B:528:THR:O	1:B:531:PHE:HB3	2.21	0.41
1:A:476:LEU:HA	1:A:476:LEU:HD23	1.79	0.41
1:C:112:THR:O	1:C:193:ASP:N	2.49	0.41
1:C:386:LEU:CD2	1:D:522:ARG:HH21	2.24	0.41
1:A:286:TRP:CZ3	2:A:1545:H34:HAI1	2.55	0.41
1:A:356:ARG:HD2	1:A:388:PRO:O	2.21	0.41
1:A:91:GLU:HG3	6:A:2126:HOH:O	2.20	0.41
1:B:393:HIS:CD2	6:B:2397:HOH:O	2.73	0.41
1:C:13:ARG:NH1	1:C:13:ARG:HG3	2.30	0.41
1:D:245:ARG:NH2	1:D:266:ASP:OD2	2.54	0.41
1:D:395:ARG:HD2	1:D:396:ASP:OD1	2.20	0.41
1:B:261:GLY:CA	6:B:2273:HOH:O	2.69	0.41
1:C:453:PHE:HE1	6:C:2531:HOH:O	2.03	0.41
1:D:296:ARG:HH21	1:D:369:GLN:NE2	2.18	0.41
1:B:413:GLN:HG3	3:B:1550:SO4:O2	2.21	0.41
1:B:115:LEU:HD23	1:B:198:THR:HB	2.01	0.41
1:B:472:PHE:CZ	1:B:476:LEU:HD11	2.56	0.41
1:C:139:ALA:O	1:C:143:GLY:HA2	2.21	0.41
1:D:502:PRO:CG	6:D:2441:HOH:O	2.26	0.41
1:A:29:VAL:HG21	1:A:136:ARG:HB2	2.01	0.41
1:B:249:THR:CG2	6:B:2257:HOH:O	2.64	0.41
1:D:494:ASP:O	1:D:495:SER:CB	2.68	0.41
1:D:524:LEU:HA	1:D:524:LEU:HD23	1.91	0.41
1:D:97:LEU:HD23	1:D:97:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:CD1	6:A:2113:HOH:O	2.57	0.40
1:B:9:LEU:HD21	1:B:16:GLN:NE2	2.36	0.40
1:C:385:TRP:HD1	1:D:527:GLN:NE2	2.19	0.40
1:C:509:GLN:HE21	1:C:520:VAL:HG11	1.86	0.40
1:C:83:THR:HG22	6:C:2134:HOH:O	2.21	0.40
1:B:141:VAL:HG21	1:B:459:LEU:HD23	2.03	0.40
1:B:496:LYS:HA	6:B:2454:HOH:O	2.22	0.40
1:B:497:SER:HB2	1:B:498:PRO:O	2.20	0.40
1:A:511:VAL:HB	1:A:518:LEU:HD22	2.02	0.40
1:A:5:ASP:HB3	1:A:7:GLN:H	1.86	0.40
1:B:521:ARG:HD3	6:B:2474:HOH:O	2.21	0.40
1:C:413:GLN:O	1:C:417:ARG:HG2	2.22	0.40
1:D:371:SER:OG	1:D:543:THR:CG2	2.69	0.40
1:B:417:ARG:HD3	3:B:1550:SO4:O4	2.21	0.40
1:C:200:PHE:HB2	1:C:226:VAL:HB	2.03	0.40
1:B:265:ASN:HA	1:B:265:ASN:HD22	1.76	0.40
1:B:498:PRO:CG	6:B:2455:HOH:O	2.69	0.40
1:C:107:ARG:HB2	6:C:2012:HOH:O	2.21	0.40
1:C:463:LEU:HA	1:C:463:LEU:HD23	1.77	0.40
1:D:134:ASP:OD2	1:D:136:ARG:HD2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:2024:HOH:O	6:D:2077:HOH:O[2_554]	2.19	0.01

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	545/545 (100%)	518 (95%)	21 (4%)	6 (1%)	14	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	542/545 (99%)	491 (91%)	34 (6%)	17 (3%)	4 5
1	C	540/545 (99%)	512 (95%)	21 (4%)	7 (1%)	12 18
1	D	542/545 (99%)	505 (93%)	28 (5%)	9 (2%)	9 13
All	All	2169/2180 (100%)	2026 (93%)	104 (5%)	39 (2%)	8 12

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	ALA
1	B	256	GLY
1	B	263	GLY
1	B	459	LEU
1	C	264	GLY
1	D	257	CYS
1	D	493	ARG
1	D	496	LYS
1	D	497	SER
1	B	261	GLY
1	B	264	GLY
1	B	466	THR
1	B	543	THR
1	D	265	ASN
1	D	322	GLN
1	D	494	ASP
1	A	258	PRO
1	B	121	GLY
1	B	497	SER
1	C	258	PRO
1	C	497	SER
1	B	189	ALA
1	B	460	ASP
1	B	496	LYS
1	C	110	SER
1	C	496	LYS
1	A	492	PRO
1	B	111	PRO
1	B	255	VAL
1	B	257	CYS
1	D	495	SER
1	A	257	CYS
1	A	497	SER

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Mol	Chain	Res	Type
1	A	264	GLY
1	C	111	PRO
1	B	523	GLY
1	D	111	PRO
1	A	260	GLY
1	C	498	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	446/444 (100%)	407 (91%)	39 (9%)	10 15
1	B	443/444 (100%)	400 (90%)	43 (10%)	8 11
1	C	441/444 (99%)	409 (93%)	32 (7%)	14 21
1	D	443/444 (100%)	407 (92%)	36 (8%)	11 17
All	All	1773/1776 (100%)	1623 (92%)	150 (8%)	11 15

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	9	LEU
1	A	17	LEU
1	A	70	TYR
1	A	74	ASP
1	A	84	GLU
1	A	107	ARG
1	A	110	SER
1	A	132	VAL
1	A	136	ARG
1	A	146	LEU
1	A	165	ARG
1	A	200	PHE
1	A	219	ARG
1	A	239	VAL

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Mol	Chain	Res	Type
1	A	281	LEU
1	A	294	ILE
1	A	295	PHE
1	A	340	VAL
1	A	347	SER
1	A	356	ARG
1	A	369	GLN
1	A	380	LEU
1	A	386	LEU
1	A	389	GLU
1	A	421	GLN
1	A	424	ARG
1	A	468	GLU
1	A	480	TRP
1	A	491	ASP
1	A	495	SER
1	A	496	LYS
1	A	522[A]	ARG
1	A	522[B]	ARG
1	A	524	LEU
1	A	525[A]	ARG
1	A	525[B]	ARG
1	A	536	LEU
1	A	540	LEU
1	B	20	ILE
1	B	21	ARG
1	B	23	LYS
1	B	29	VAL
1	B	60	LEU
1	B	64	THR
1	B	103	THR
1	B	110	SER
1	B	112	THR
1	B	138	LEU
1	B	146	LEU
1	B	165	ARG
1	B	166	GLU
1	B	200	PHE
1	B	203	SER
1	B	216	LEU
1	B	239	VAL
1	B	249	THR

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Mol	Chain	Res	Type
1	B	251	LEU
1	B	265	ASN
1	B	267	THR
1	B	275	THR
1	B	281	LEU
1	B	291	GLN
1	B	295	PHE
1	B	356	ARG
1	B	372	ASP
1	B	386	LEU
1	B	389	GLU
1	B	421	GLN
1	B	437	LEU
1	B	441	LEU
1	B	467	THR
1	B	470	ARG
1	B	491	ASP
1	B	495	SER
1	B	496	LYS
1	B	497	SER
1	B	518	LEU
1	B	524	LEU
1	B	536	LEU
1	B	540	LEU
1	B	543	THR
1	C	9	LEU
1	C	13	ARG
1	C	30	SER
1	C	81	GLU
1	C	84	GLU
1	C	107	ARG
1	C	136	ARG
1	C	200	PHE
1	C	203	SER
1	C	216	LEU
1	C	239	VAL
1	C	251	LEU
1	C	265	ASN
1	C	267	THR
1	C	276	ARG
1	C	281	LEU
1	C	294	ILE

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Mol	Chain	Res	Type
1	C	295	PHE
1	C	323	ASP
1	C	369	GLN
1	C	376	GLU
1	C	386	LEU
1	C	421	GLN
1	C	491	ASP
1	C	496	LYS
1	C	504	THR
1	C	524	LEU
1	C	525[A]	ARG
1	C	525[B]	ARG
1	C	536	LEU
1	C	539	LEU
1	C	543	THR
1	D	4	GLU
1	D	21	ARG
1	D	29	VAL
1	D	30	SER
1	D	103	THR
1	D	107	ARG
1	D	115	LEU
1	D	136	ARG
1	D	165	ARG
1	D	203	SER
1	D	239	VAL
1	D	249	THR
1	D	251	LEU
1	D	267	THR
1	D	287	HIS
1	D	291	GLN
1	D	294	ILE
1	D	295	PHE
1	D	313	GLU
1	D	327	LEU
1	D	332	LYS
1	D	356	ARG
1	D	369	GLN
1	D	380	LEU
1	D	386	LEU
1	D	389	GLU
1	D	417	ARG

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Mol	Chain	Res	Type
1	D	421	GLN
1	D	437	LEU
1	D	441	LEU
1	D	474	GLN
1	D	480	TRP
1	D	524	LEU
1	D	536	LEU
1	D	540	LEU
1	D	541	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	87	ASN
1	A	184	GLN
1	A	223	HIS
1	A	369	GLN
1	A	393	HIS
1	B	16	GLN
1	B	223	HIS
1	B	291	GLN
1	B	421	GLN
1	C	87	ASN
1	C	223	HIS
1	C	265	ASN
1	C	284	HIS
1	C	369	GLN
1	C	509	GLN
1	D	87	ASN
1	D	223	HIS
1	D	265	ASN
1	D	291	GLN
1	D	369	GLN
1	D	413	GLN
1	D	421	GLN
1	D	509	GLN

5.3.3 RNA

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 24 ligands modelled in this entry, 5 are monoatomic - leaving 19 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	SO4	A	1548	-	4,4,4	0.23	0	6,6,6	0.23	0
5	NAG	B	1546	-	14,14,15	1.13	1 (7%)	17,19,21	2.60	7 (41%)
3	SO4	B	1548	-	4,4,4	0.17	0	6,6,6	0.20	0
3	SO4	C	1547	-	4,4,4	0.23	0	6,6,6	0.55	0
3	SO4	A	1547	-	4,4,4	0.13	0	6,6,6	0.37	0
3	SO4	B	1547	-	4,4,4	0.34	0	6,6,6	0.54	0
3	SO4	D	1548	-	4,4,4	0.11	0	6,6,6	0.42	0
3	SO4	D	1546	-	4,4,4	0.21	0	6,6,6	1.06	1 (16%)
3	SO4	D	1549	-	4,4,4	0.16	0	6,6,6	0.47	0
3	SO4	B	1549	-	4,4,4	0.35	0	6,6,6	0.37	0
2	H34	B	1545	-	34,34,34	3.06	14 (41%)	33,49,49	3.03	9 (27%)
2	H34	A	1545	-	34,34,34	2.45	14 (41%)	33,49,49	2.56	8 (24%)
3	SO4	A	1546	-	4,4,4	0.15	0	6,6,6	0.78	0
3	SO4	B	1550	-	4,4,4	0.23	0	6,6,6	0.56	0
2	H34	D	1545	-	34,34,34	2.66	14 (41%)	33,49,49	2.41	10 (30%)
3	SO4	D	1547	-	4,4,4	0.21	0	6,6,6	0.57	0
3	SO4	C	1546	-	4,4,4	0.08	0	6,6,6	0.66	0
3	SO4	C	1548	-	4,4,4	0.18	0	6,6,6	0.45	0
2	H34	C	1545	-	34,34,34	3.44	14 (41%)	33,49,49	2.60	11 (33%)

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
5	NAG	B	1546	-	-	4/6/23/26	0/1/1/1
2	H34	B	1545	-	-	0/7/29/29	0/6/5/5
2	H34	A	1545	-	-	0/7/29/29	0/6/5/5
2	H34	D	1545	-	-	0/7/29/29	0/6/5/5
2	H34	C	1545	-	-	0/7/29/29	0/6/5/5

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1545	H34	CAO-CAX	-12.97	1.36	1.51
2	C	1545	H34	NAQ-NAR	-10.15	1.16	1.34
2	D	1545	H34	CAO-CAX	-8.71	1.41	1.51
2	B	1545	H34	CAO-CAX	-8.41	1.41	1.51
2	A	1545	H34	CAY-CBC	-6.88	1.40	1.51
2	B	1545	H34	CAY-CBC	-6.26	1.41	1.51
2	B	1545	H34	NAQ-NAR	-5.77	1.24	1.34
2	B	1545	H34	CAU-CL1	5.61	1.86	1.74
2	A	1545	H34	CAP-CBC	5.49	1.60	1.53
2	D	1545	H34	CAL-CAT	-5.48	1.42	1.51
2	A	1545	H34	CAO-CAX	-5.45	1.45	1.51
2	B	1545	H34	NAR-NBD	-5.15	1.24	1.34
2	B	1545	H34	CAL-CAT	-5.04	1.43	1.51
2	B	1545	H34	CAM-NBD	4.46	1.55	1.47
2	C	1545	H34	CAL-CAT	-4.43	1.44	1.51
2	C	1545	H34	CAV-CBA	-4.27	1.38	1.44
2	D	1545	H34	CAV-CBA	-4.26	1.38	1.44
2	D	1545	H34	CAN-CAT	-3.98	1.42	1.50
2	D	1545	H34	CAY-CBC	-3.96	1.45	1.51
2	C	1545	H34	CAN-CAT	-3.75	1.43	1.50
2	D	1545	H34	CAU-CL1	3.70	1.82	1.74
2	C	1545	H34	CAY-CBC	-3.58	1.45	1.51
2	B	1545	H34	CAD-CAT	3.27	1.44	1.33
2	B	1545	H34	CAV-CBA	-3.25	1.40	1.44
2	A	1545	H34	CAV-CBA	-3.17	1.40	1.44
2	D	1545	H34	CAG-CAZ	-3.13	1.37	1.41
2	A	1545	H34	CAL-CAT	-2.98	1.46	1.51
2	D	1545	H34	CAX-NAS	2.94	1.36	1.32
2	C	1545	H34	CAE-CAU	2.88	1.43	1.38
2	C	1545	H34	CAU-CL1	2.88	1.80	1.74
2	A	1545	H34	CAX-NAS	2.81	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1545	H34	CBB-CAD	-2.81	1.43	1.51
2	A	1545	H34	CAG-CAU	2.66	1.41	1.36
2	B	1545	H34	CAG-CAU	2.59	1.41	1.36
5	B	1546	NAG	C1-C2	2.57	1.56	1.52
2	B	1545	H34	CAF-CAE	2.55	1.42	1.36
2	A	1545	H34	CAN-CAT	-2.54	1.45	1.50
2	A	1545	H34	CAF-CAE	2.52	1.41	1.36
2	C	1545	H34	CAD-CAT	2.52	1.41	1.33
2	C	1545	H34	CAP-CBB	-2.49	1.50	1.53
2	A	1545	H34	CAP-CBB	-2.39	1.50	1.53
2	A	1545	H34	CAJ-CAL	2.35	1.60	1.52
2	C	1545	H34	CBB-CAD	-2.34	1.44	1.51
2	D	1545	H34	CAD-CAT	2.34	1.41	1.33
2	B	1545	H34	CAP-CBC	2.34	1.56	1.53
2	D	1545	H34	CBB-CAD	-2.30	1.45	1.51
2	A	1545	H34	CAE-CAU	2.28	1.42	1.38
2	D	1545	H34	CBA-CAZ	-2.26	1.38	1.42
2	C	1545	H34	CAH-CAW	-2.25	1.32	1.36
2	C	1545	H34	CAF-CAE	2.19	1.41	1.36
2	D	1545	H34	CAG-CAU	2.17	1.40	1.36
2	A	1545	H34	CAD-CAT	2.17	1.40	1.33
2	D	1545	H34	CAM-NBD	2.17	1.51	1.47
2	B	1545	H34	CAH-CAW	-2.12	1.33	1.36
2	C	1545	H34	NAR-NBD	-2.07	1.30	1.34
2	D	1545	H34	CAZ-NAS	-2.07	1.34	1.37
2	B	1545	H34	CAX-NAS	2.03	1.34	1.32

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1545	H34	CAY-CAX-NAS	-10.63	118.91	123.66
2	B	1545	H34	NAQ-NAR-NBD	9.63	114.57	107.31
2	B	1545	H34	CAY-CAX-NAS	-9.60	119.37	123.66
2	C	1545	H34	NAQ-NAR-NBD	8.36	113.62	107.31
2	D	1545	H34	CAY-CAX-NAS	-7.54	120.29	123.66
2	D	1545	H34	NAQ-NAR-NBD	6.56	112.26	107.31
2	C	1545	H34	CAY-CAX-NAS	-5.53	121.19	123.66
2	C	1545	H34	CAG-CAU-CL1	-5.46	112.81	119.64
5	B	1546	NAG	C1-O5-C5	5.17	119.19	112.19
2	B	1545	H34	CAX-NAS-CAZ	4.96	123.79	117.67
2	B	1545	H34	CAN-CBC-CAY	-4.92	106.17	111.33
2	A	1545	H34	CAN-CBC-CAY	-4.72	106.39	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1546	NAG	C8-C7-N2	4.20	123.22	116.10
5	B	1546	NAG	C2-N2-C7	4.09	128.73	122.90
2	A	1545	H34	NAQ-NAR-NBD	3.96	110.30	107.31
2	D	1545	H34	CAF-CBA-CAZ	3.82	122.60	118.33
5	B	1546	NAG	O3-C3-C2	3.80	117.33	109.47
2	D	1545	H34	CAX-NAS-CAZ	3.73	122.27	117.67
2	B	1545	H34	CAU-CAG-CAZ	3.59	122.52	119.50
2	C	1545	H34	CAF-CBA-CAZ	3.54	122.29	118.33
2	A	1545	H34	CAX-NAS-CAZ	3.51	122.00	117.67
2	C	1545	H34	CBC-CAP-CBB	-3.46	103.76	111.03
2	C	1545	H34	CAE-CAU-CL1	3.43	124.72	119.35
2	B	1545	H34	CBA-CAZ-NAS	-3.21	119.41	122.81
5	B	1546	NAG	C1-C2-N2	3.17	115.90	110.49
2	A	1545	H34	CAF-CBA-CAZ	3.04	121.72	118.33
2	D	1545	H34	CBC-CAP-CBB	-3.03	104.67	111.03
2	A	1545	H34	CAG-CAU-CL1	-3.02	115.86	119.64
2	C	1545	H34	CAX-NAS-CAZ	3.01	121.38	117.67
2	A	1545	H34	OAB-CAI-CAW	-3.00	105.49	112.10
2	C	1545	H34	OAB-CAI-CAW	-2.87	105.77	112.10
2	D	1545	H34	CAL-CAT-CAD	-2.79	116.97	122.84
2	D	1545	H34	CAL-CAT-CAN	2.70	121.94	116.08
5	B	1546	NAG	O5-C1-C2	2.57	115.35	111.29
2	D	1545	H34	CAX-CAO-CBB	-2.57	110.51	113.96
2	B	1545	H34	CAG-CAZ-NAS	2.56	122.62	118.72
2	C	1545	H34	CAX-CAO-CBB	-2.48	110.63	113.96
5	B	1546	NAG	O7-C7-C8	-2.38	117.64	122.06
2	C	1545	H34	CAH-CAW-NAQ	-2.37	107.82	111.34
2	D	1545	H34	OAB-CAI-CAW	-2.34	106.95	112.10
2	D	1545	H34	CAN-CBC-CAY	-2.25	108.98	111.33
2	B	1545	H34	CAH-CAW-NAQ	-2.24	108.01	111.34
2	B	1545	H34	CAE-CAU-CAG	-2.12	119.48	121.99
2	A	1545	H34	CBC-CAP-CBB	-2.11	106.59	111.03
3	D	1546	SO4	O3-S-O2	-2.07	98.52	109.31
2	C	1545	H34	CAL-CAT-CAN	2.02	120.47	116.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1546	NAG	C8-C7-N2-C2
5	B	1546	NAG	O7-C7-N2-C2
5	B	1546	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1546	NAG	C3-C2-N2-C7

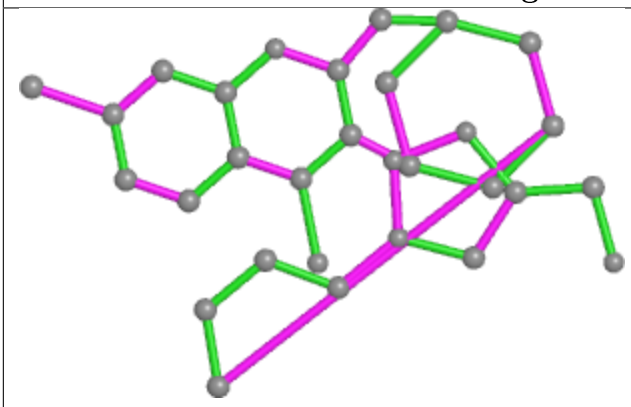
There are no ring outliers.

7 monomers are involved in 14 short contacts:

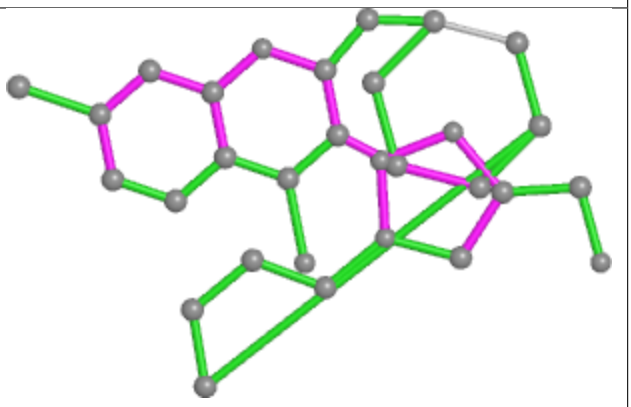
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1546	NAG	5	0
3	A	1547	SO4	2	0
2	B	1545	H34	2	0
2	A	1545	H34	1	0
3	B	1550	SO4	2	0
3	C	1548	SO4	1	0
2	C	1545	H34	1	0

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.

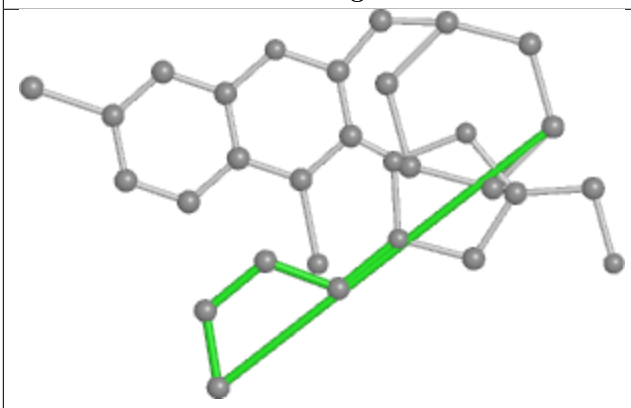
Ligand H34 B 1545



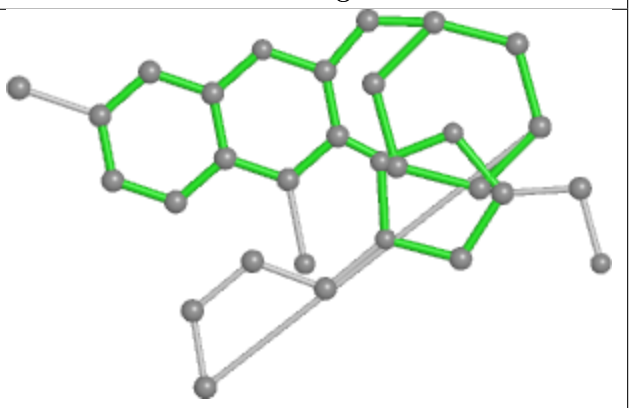
Bond lengths



Bond angles

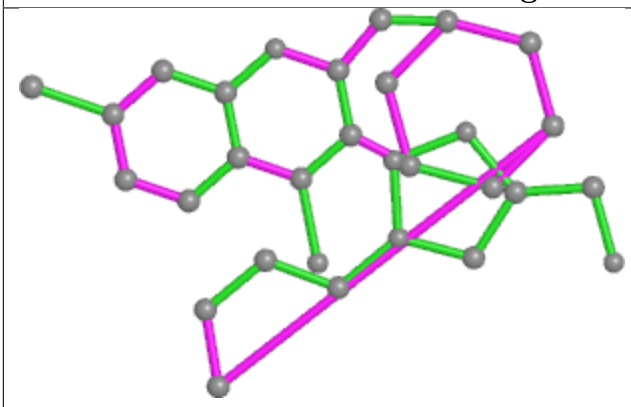


Torsions

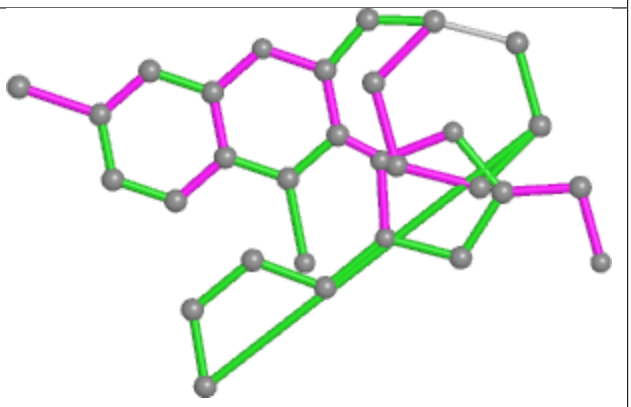


Rings

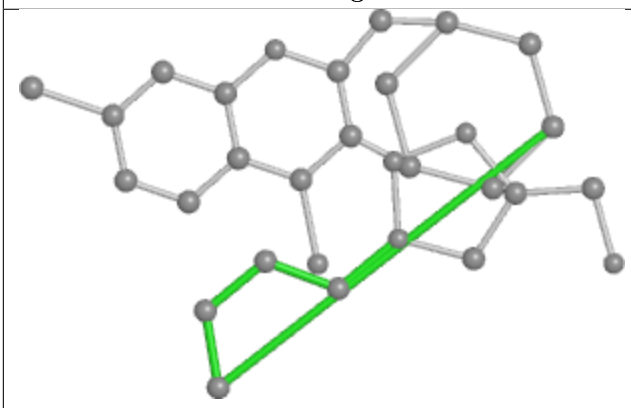
Ligand H34 A 1545



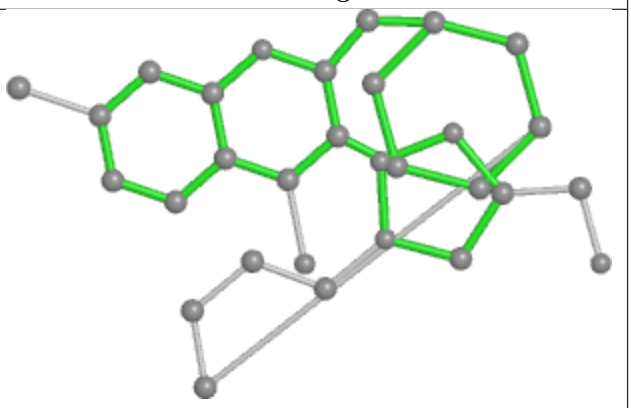
Bond lengths



Bond angles

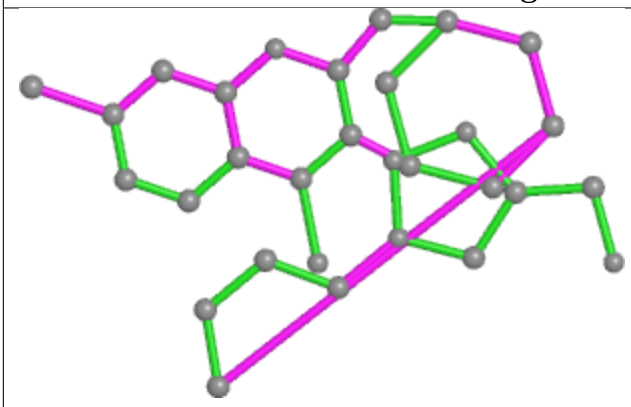


Torsions

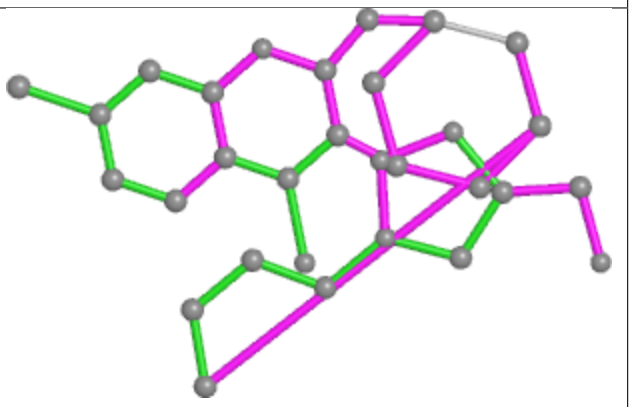


Rings

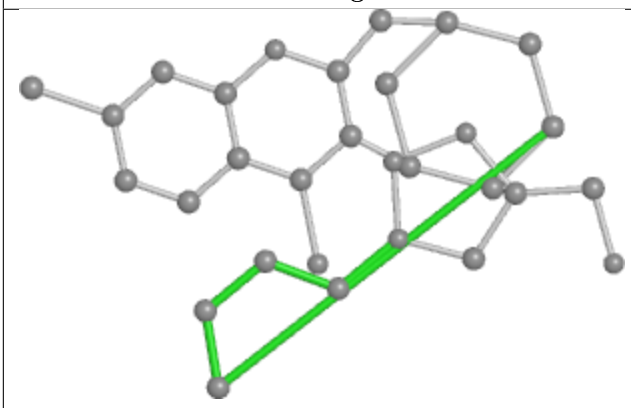
Ligand H34 D 1545



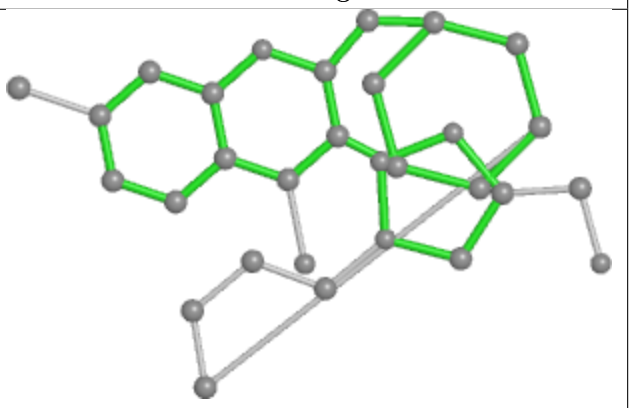
Bond lengths



Bond angles

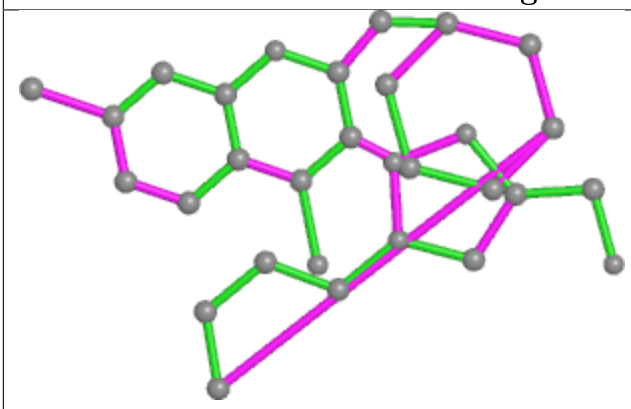


Torsions

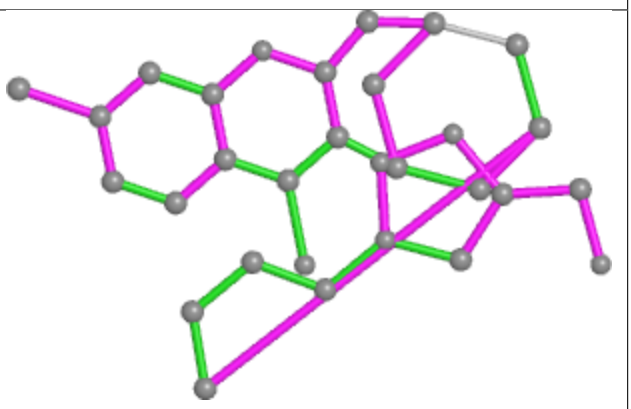


Rings

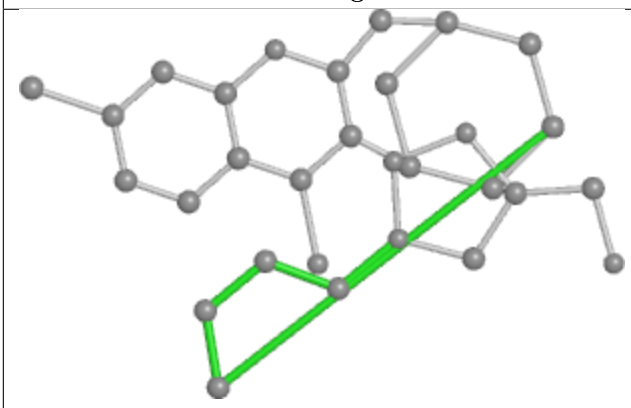
Ligand H34 C 1545



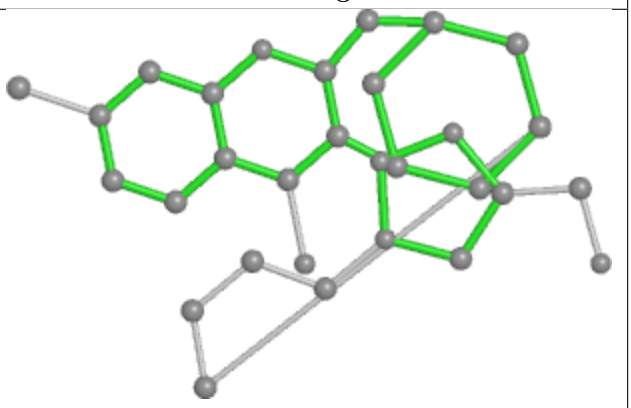
Bond lengths



Bond angles



Torsions



Rings

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	541/545 (99%)	-0.51	11 (2%) 65 60	32, 45, 68, 117	1 (0%)
1	B	541/545 (99%)	-0.35	9 (1%) 70 67	35, 59, 94, 128	0
1	C	541/545 (99%)	-0.51	13 (2%) 59 54	31, 45, 72, 115	1 (0%)
1	D	541/545 (99%)	-0.44	7 (1%) 77 75	30, 51, 81, 122	0
All	All	2164/2180 (99%)	-0.45	40 (1%) 68 65	30, 49, 84, 128	2 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	PRO	7.4
1	C	260	GLY	7.4
1	C	259	PRO	6.7
1	A	261	GLY	6.2
1	A	260	GLY	6.0
1	A	496	LYS	5.2
1	C	544	ALA	4.9
1	D	497	SER	4.8
1	A	262	ALA	4.7
1	C	262	ALA	4.6
1	C	261	GLY	4.6
1	C	264	GLY	4.3
1	B	4	GLU	4.1
1	D	493	ARG	4.0
1	D	496	LYS	3.9
1	B	496	LYS	3.9
1	B	495	SER	3.8
1	C	496	LYS	3.8
1	C	263	GLY	3.6
1	A	497	SER	3.5
1	A	264	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	493	ARG	3.4
1	B	59	VAL	3.3
1	D	495	SER	3.2
1	C	493	ARG	3.1
1	A	494	ASP	3.0
1	D	4	GLU	2.8
1	B	6	PRO	2.6
1	A	263	GLY	2.5
1	B	9	LEU	2.5
1	C	258	PRO	2.5
1	A	495	SER	2.5
1	C	497	SER	2.5
1	B	498	PRO	2.4
1	B	497	SER	2.3
1	C	268	GLU	2.3
1	B	21	ARG	2.1
1	D	494	ASP	2.1
1	D	498	PRO	2.1
1	C	494	ASP	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å^2)	Q<0.9
3	SO4	B	1548	5/5	0.64	0.60	211,211,211,211	0
5	NAG	B	1546	14/15	0.82	0.17	123,126,128,128	0
3	SO4	D	1549	5/5	0.86	0.23	138,138,139,140	0
4	CL	A	1550	1/1	0.89	0.13	103,103,103,103	0

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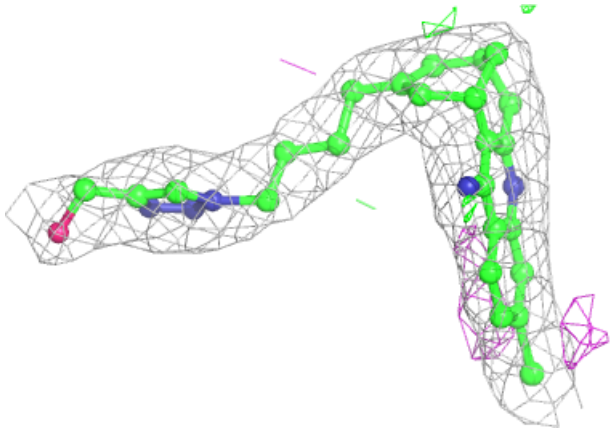
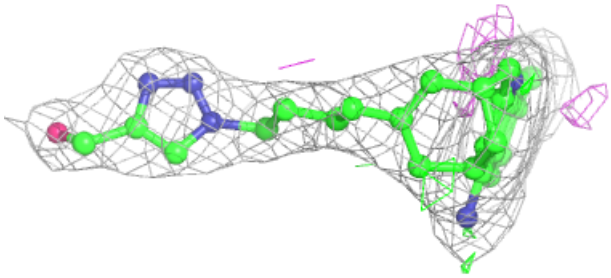
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	C	1547	5/5	0.91	0.26	119,120,121,121	0
4	CL	C	1549	1/1	0.91	0.11	100,100,100,100	0
4	CL	B	1551	1/1	0.92	0.10	94,94,94,94	0
4	CL	C	1550	1/1	0.92	0.05	69,69,69,69	0
3	SO4	A	1548	5/5	0.93	0.17	114,115,116,117	0
3	SO4	B	1550	5/5	0.93	0.12	110,110,112,113	0
3	SO4	C	1548	5/5	0.93	0.11	124,125,126,126	0
3	SO4	D	1547	5/5	0.94	0.24	96,97,99,100	0
3	SO4	D	1548	5/5	0.94	0.15	114,115,116,116	0
3	SO4	B	1549	5/5	0.95	0.15	100,101,102,103	0
2	H34	B	1545	30/30	0.95	0.14	45,50,60,61	0
2	H34	D	1545	30/30	0.97	0.16	40,49,56,64	0
4	CL	A	1549	1/1	0.97	0.05	75,75,75,75	0
3	SO4	A	1547	5/5	0.97	0.13	110,110,111,113	0
3	SO4	C	1546	5/5	0.98	0.10	73,76,78,79	0
3	SO4	B	1547	5/5	0.98	0.09	81,82,83,83	0
2	H34	C	1545	30/30	0.98	0.15	40,44,47,52	0
3	SO4	D	1546	5/5	0.98	0.09	70,72,73,74	0
3	SO4	A	1546	5/5	0.99	0.09	69,70,71,75	0
2	H34	A	1545	30/30	0.99	0.12	34,39,43,48	0

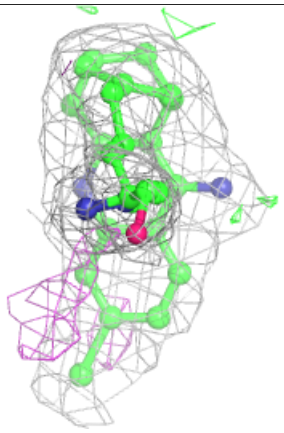
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around H34 B 1545:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

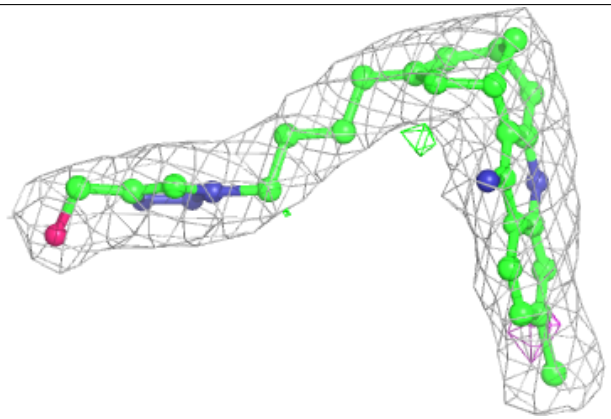


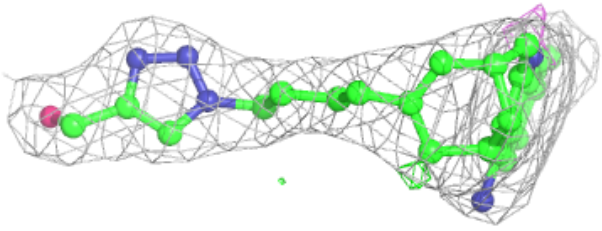


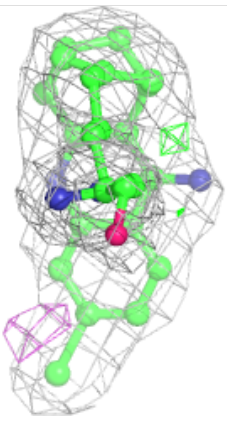


Electron density around H34 D 1545:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

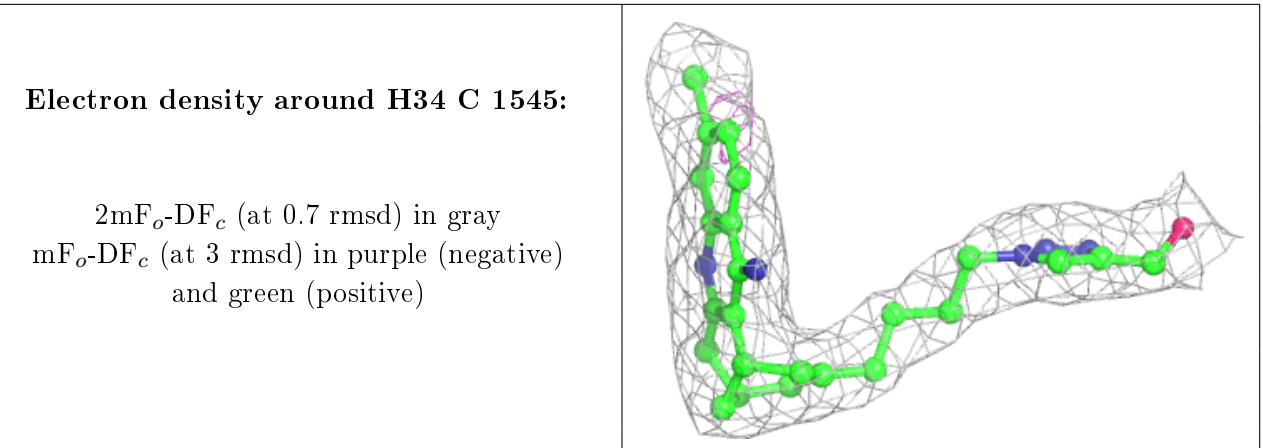






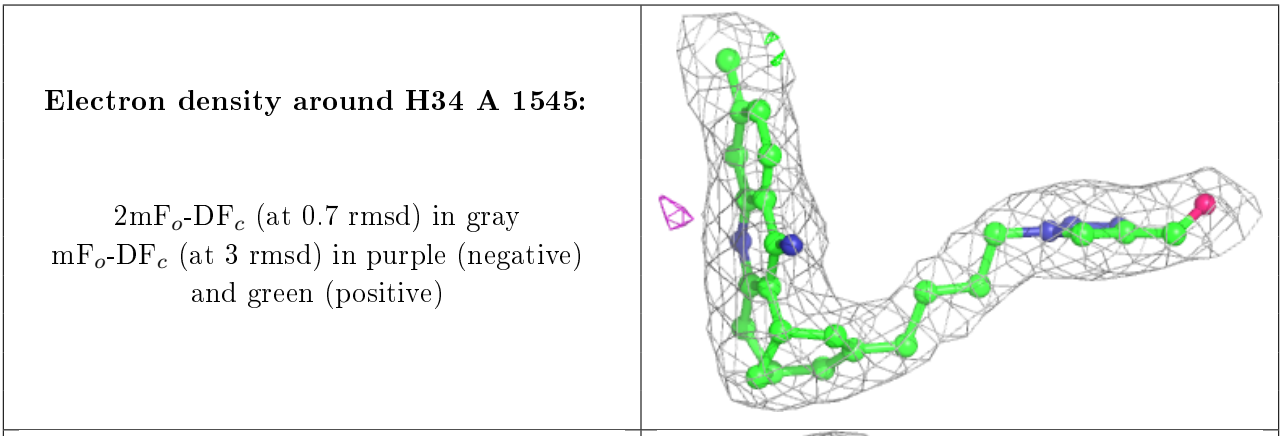
Electron density around H34 C 1545:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around H34 A 1545:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.