



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:28 AM EDT

PDB ID : 3KFK / pdb_00003kfk
Title : Crystal structures of a group II chaperonin from *Methanococcus maripaludis*
Authors : Pereira, J.H.; Ralston, C.Y.; Douglas, N.; Meyer, D.; Knee, K.M.; Goulet, D.R.; King, J.A.; Frydman, J.; Adams, P.D.
Deposited on : 2009-10-27
Resolution : 6.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

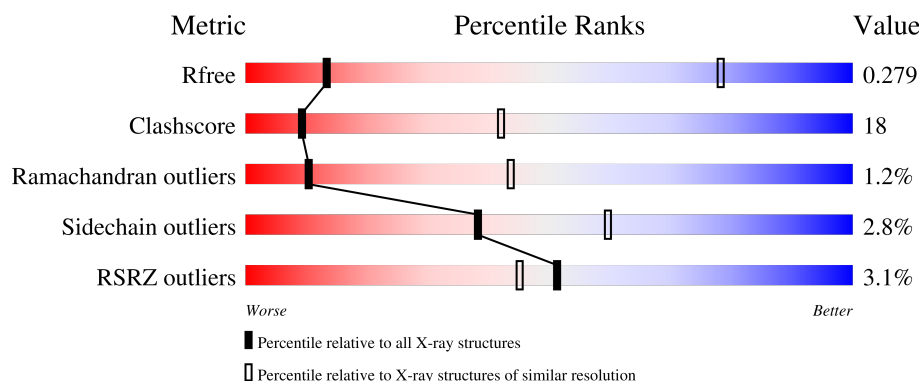
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

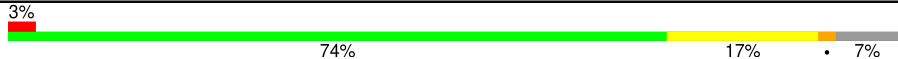
The reported resolution of this entry is 6.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	521	
1	B	521	
1	C	521	
1	D	521	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AGS	D	544	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14619 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 Chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	B	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	C	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	D	484	Total	C	N	O	S	0	0	0
			3608	2235	627	722	24			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP Q877G8
A	?	-	LYS	deletion	UNP Q877G8
A	?	-	GLU	deletion	UNP Q877G8
A	?	-	THR	deletion	UNP Q877G8
A	?	-	ASP	deletion	UNP Q877G8
A	?	-	ALA	deletion	UNP Q877G8
A	?	-	GLU	deletion	UNP Q877G8
A	?	-	ILE	deletion	UNP Q877G8
A	?	-	ARG	deletion	UNP Q877G8
A	?	-	ILE	deletion	UNP Q877G8
A	?	-	THR	deletion	UNP Q877G8
A	?	-	ASP	deletion	UNP Q877G8
A	?	-	PRO	deletion	UNP Q877G8
A	?	-	LYS	deletion	UNP Q877G8
A	?	-	LEU	deletion	UNP Q877G8
A	?	-	MET	deletion	UNP Q877G8
A	?	-	GLU	deletion	UNP Q877G8
A	?	-	PHE	deletion	UNP Q877G8
A	?	-	ILE	deletion	UNP Q877G8
A	264	THR	GLN	engineered mutation	UNP Q877G8
A	265	ALA	GLU	engineered mutation	UNP Q877G8

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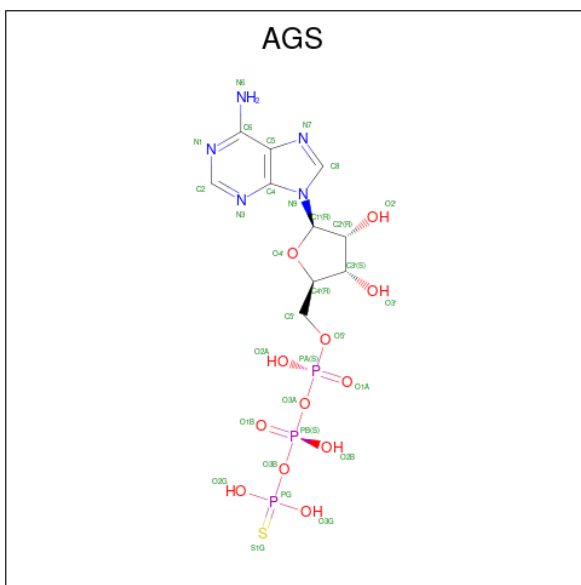
Chain	Residue	Modelled	Actual	Comment	Reference
A	266	SER	GLU	engineered mutation	UNP Q877G8
A	267	GLU	LYS	engineered mutation	UNP Q877G8
B	?	-	ILE	deletion	UNP Q877G8
B	?	-	LYS	deletion	UNP Q877G8
B	?	-	GLU	deletion	UNP Q877G8
B	?	-	THR	deletion	UNP Q877G8
B	?	-	ASP	deletion	UNP Q877G8
B	?	-	ALA	deletion	UNP Q877G8
B	?	-	GLU	deletion	UNP Q877G8
B	?	-	ILE	deletion	UNP Q877G8
B	?	-	ARG	deletion	UNP Q877G8
B	?	-	ILE	deletion	UNP Q877G8
B	?	-	THR	deletion	UNP Q877G8
B	?	-	ASP	deletion	UNP Q877G8
B	?	-	PRO	deletion	UNP Q877G8
B	?	-	LYS	deletion	UNP Q877G8
B	?	-	LEU	deletion	UNP Q877G8
B	?	-	MET	deletion	UNP Q877G8
B	?	-	GLU	deletion	UNP Q877G8
B	?	-	PHE	deletion	UNP Q877G8
B	?	-	ILE	deletion	UNP Q877G8
B	264	THR	GLN	engineered mutation	UNP Q877G8
B	265	ALA	GLU	engineered mutation	UNP Q877G8
B	266	SER	GLU	engineered mutation	UNP Q877G8
B	267	GLU	LYS	engineered mutation	UNP Q877G8
C	?	-	ILE	deletion	UNP Q877G8
C	?	-	LYS	deletion	UNP Q877G8
C	?	-	GLU	deletion	UNP Q877G8
C	?	-	THR	deletion	UNP Q877G8
C	?	-	ASP	deletion	UNP Q877G8
C	?	-	ALA	deletion	UNP Q877G8
C	?	-	GLU	deletion	UNP Q877G8
C	?	-	ILE	deletion	UNP Q877G8
C	?	-	ARG	deletion	UNP Q877G8
C	?	-	ILE	deletion	UNP Q877G8
C	?	-	THR	deletion	UNP Q877G8
C	?	-	ASP	deletion	UNP Q877G8
C	?	-	PRO	deletion	UNP Q877G8
C	?	-	LYS	deletion	UNP Q877G8
C	?	-	LEU	deletion	UNP Q877G8
C	?	-	MET	deletion	UNP Q877G8
C	?	-	GLU	deletion	UNP Q877G8

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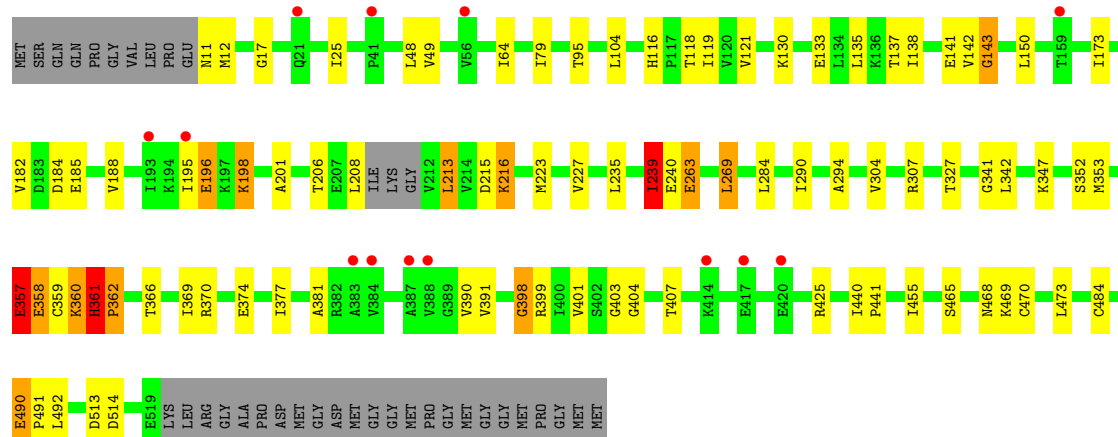
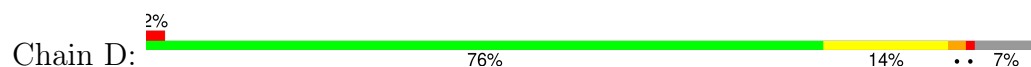
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PHE	deletion	UNP Q877G8
C	?	-	ILE	deletion	UNP Q877G8
C	264	THR	GLN	engineered mutation	UNP Q877G8
C	265	ALA	GLU	engineered mutation	UNP Q877G8
C	266	SER	GLU	engineered mutation	UNP Q877G8
C	267	GLU	LYS	engineered mutation	UNP Q877G8
D	?	-	ILE	deletion	UNP Q877G8
D	?	-	LYS	deletion	UNP Q877G8
D	?	-	GLU	deletion	UNP Q877G8
D	?	-	THR	deletion	UNP Q877G8
D	?	-	ASP	deletion	UNP Q877G8
D	?	-	ALA	deletion	UNP Q877G8
D	?	-	GLU	deletion	UNP Q877G8
D	?	-	ILE	deletion	UNP Q877G8
D	?	-	ARG	deletion	UNP Q877G8
D	?	-	ILE	deletion	UNP Q877G8
D	?	-	THR	deletion	UNP Q877G8
D	?	-	ASP	deletion	UNP Q877G8
D	?	-	PRO	deletion	UNP Q877G8
D	?	-	LYS	deletion	UNP Q877G8
D	?	-	LEU	deletion	UNP Q877G8
D	?	-	MET	deletion	UNP Q877G8
D	?	-	GLU	deletion	UNP Q877G8
D	?	-	PHE	deletion	UNP Q877G8
D	?	-	ILE	deletion	UNP Q877G8
D	264	THR	GLN	engineered mutation	UNP Q877G8
D	265	ALA	GLU	engineered mutation	UNP Q877G8
D	266	SER	GLU	engineered mutation	UNP Q877G8
D	267	GLU	LYS	engineered mutation	UNP Q877G8

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0

Chain C: 2% 72% 20% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	150.53Å 209.53Å 266.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.56 – 6.00 58.56 – 6.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (58.56-6.00) 95.4 (58.56-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 6.17Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_162)	Depositor
R, R_{free}	0.241 , 0.270 0.254 , 0.279	Depositor DCC
R_{free} test set	496 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	342.4	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 817.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	14619	wwPDB-VP
Average B, all atoms (Å ²)	555.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: AGS

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	0.47	4/3649 (0.1%)	0.79	7/4911 (0.1%)
1	B	0.47	3/3649 (0.1%)	0.79	4/4911 (0.1%)
1	C	0.49	4/3649 (0.1%)	0.82	6/4911 (0.1%)
1	D	0.48	4/3627 (0.1%)	0.80	5/4881 (0.1%)
All	All	0.48	15/14574 (0.1%)	0.80	22/19614 (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	2
1	B	0	3
1	C	0	4
1	D	0	4
All	All	0	13

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	GLU	CA-C	6.94	1.62	1.52
1	C	263	GLU	CA-C	6.90	1.62	1.52
1	C	240	GLU	N-CA	6.71	1.53	1.45
1	D	263	GLU	CA-C	6.67	1.61	1.52
1	A	240	GLU	N-CA	6.53	1.53	1.45
1	D	240	GLU	N-CA	6.47	1.53	1.45
1	B	263	GLU	CA-C	6.30	1.61	1.52
1	B	240	GLU	N-CA	6.09	1.53	1.45
1	A	240	GLU	CA-C	5.90	1.61	1.53
1	C	240	GLU	CA-C	5.54	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	GLU	N-CA	5.53	1.53	1.46
1	C	263	GLU	N-CA	5.52	1.53	1.46
1	D	240	GLU	CA-C	5.37	1.60	1.53
1	D	263	GLU	N-CA	5.33	1.53	1.46
1	B	440	ILE	CA-CB	5.06	1.57	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	GLU	N-CA-C	10.95	126.70	110.17
1	D	240	GLU	N-CA-C	10.70	126.32	110.17
1	A	240	GLU	N-CA-C	10.59	126.77	110.36
1	B	240	GLU	N-CA-C	10.18	125.54	110.17
1	A	263	GLU	N-CA-C	8.02	127.89	110.80
1	C	263	GLU	N-CA-C	7.91	127.64	110.80
1	D	263	GLU	N-CA-C	7.84	127.51	110.80
1	B	263	GLU	N-CA-C	7.83	127.48	110.80
1	C	263	GLU	CA-C-N	7.36	131.72	121.79
1	C	263	GLU	C-N-CA	7.36	131.72	121.79
1	C	329	ILE	N-CA-C	5.90	121.60	109.34
1	B	263	GLU	CA-C-N	5.59	132.21	121.54
1	B	263	GLU	C-N-CA	5.59	132.21	121.54
1	A	239	ILE	O-C-N	-5.52	115.67	122.57
1	A	263	GLU	CA-C-N	5.49	132.03	121.54
1	A	263	GLU	C-N-CA	5.49	132.03	121.54
1	C	239	ILE	O-C-N	-5.38	115.84	122.57
1	D	263	GLU	CA-C-N	5.37	131.79	121.54
1	D	263	GLU	C-N-CA	5.37	131.79	121.54
1	D	239	ILE	O-C-N	-5.21	116.05	122.57
1	A	116	HIS	CA-C-N	5.16	125.46	119.47
1	A	116	HIS	C-N-CA	5.16	125.46	119.47

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	PHE	Peptide
1	A	398	GLY	Peptide
1	B	211	GLY	Peptide
1	B	358	GLU	Peptide
1	B	398	GLY	Peptide
1	C	143	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	210	LYS	Peptide
1	C	397	ASP	Peptide
1	C	398	GLY	Peptide
1	D	357	GLU	Peptide
1	D	360	LYS	Peptide
1	D	361	HIS	Peptide
1	D	398	GLY	Peptide

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	3629	0	3764	134	2
1	B	3629	0	3762	207	0
1	C	3629	0	3762	153	1
1	D	3608	0	3736	102	1
2	A	31	0	12	5	0
2	B	31	0	12	5	0
2	C	31	0	12	6	0
2	D	31	0	12	11	0
All	All	14619	0	15072	535	2

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 18.

All (535) 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:A:210:LYS:CB	1:A:358:GLU:H	1.13	1.53
2:D:544:AGS:PG	2:D:544:AGS:S1G	1.49	1.49
2:B:544:AGS:PG	2:B:544:AGS:S1G	1.49	1.48
2:A:544:AGS:PG	2:A:544:AGS:S1G	1.49	1.47
2:C:544:AGS:PG	2:C:544:AGS:S1G	1.49	1.47
1:A:210:LYS:HB2	1:A:358:GLU:N	1.17	1.42
1:A:210:LYS:CB	1:A:358:GLU:N	1.78	1.32
1:C:142:VAL:CG2	1:C:149:ILE:HG21	1.61	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:VAL:HG21	1:C:149:ILE:CG2	1.66	1.24
1:D:263:GLU:CB	1:D:269:LEU:HD11	1.68	1.24
1:B:390:VAL:HG12	1:B:491:PRO:CG	1.69	1.22
1:C:196:GLU:OE1	1:C:316:LYS:HE2	1.40	1.22
1:B:490:GLU:OE1	1:B:495:LYS:HE2	1.42	1.20
1:C:263:GLU:CB	1:C:269:LEU:HD11	1.71	1.20
1:B:349:SER:HB2	1:B:370:ARG:NH2	1.55	1.19
1:C:399:ARG:HD2	1:C:492:LEU:HD22	1.26	1.18
1:A:218:ARG:NH1	1:A:225:LYS:HE2	1.59	1.18
1:A:263:GLU:CB	1:A:269:LEU:HD11	1.72	1.17
1:A:210:LYS:CD	1:A:358:GLU:HA	1.77	1.15
1:B:194:LYS:HB2	1:B:316:LYS:CE	1.80	1.12
1:C:142:VAL:HG22	1:C:149:ILE:HD13	1.22	1.12
1:B:341:GLY:HA3	1:B:358:GLU:HG2	1.16	1.11
1:B:348:ILE:HG23	1:B:370:ARG:NH2	1.64	1.11
1:B:194:LYS:N	1:B:316:LYS:HZ2	1.49	1.11
1:A:210:LYS:HD2	1:A:358:GLU:HA	1.13	1.10
1:C:142:VAL:HG11	1:C:149:ILE:HB	1.20	1.10
1:A:218:ARG:HH12	1:A:225:LYS:HE2	1.06	1.09
1:B:42:LYS:HB3	1:C:118:THR:HG21	1.30	1.09
1:A:210:LYS:HB2	1:A:358:GLU:CA	1.83	1.09
1:B:390:VAL:CG1	1:B:491:PRO:HG2	1.81	1.09
1:B:348:ILE:HG23	1:B:370:ARG:HH22	0.95	1.07
1:B:341:GLY:HA3	1:B:358:GLU:CG	1.82	1.07
1:A:210:LYS:CB	1:A:358:GLU:CA	2.30	1.07
1:B:69:SER:HB3	1:C:11:ASN:ND2	1.69	1.07
1:D:269:LEU:HD23	1:D:294:ALA:CB	1.83	1.07
1:B:194:LYS:HB2	1:B:316:LYS:HE3	1.14	1.06
1:C:269:LEU:HD23	1:C:294:ALA:HB2	1.06	1.06
1:C:269:LEU:HD23	1:C:294:ALA:CB	1.85	1.05
1:A:269:LEU:HD23	1:A:294:ALA:CB	1.86	1.05
1:B:42:LYS:HD2	1:C:118:THR:HB	1.36	1.03
1:D:269:LEU:HD23	1:D:294:ALA:HB2	1.03	1.03
1:A:210:LYS:HB3	1:A:358:GLU:N	1.71	1.03
1:C:42:LYS:HD2	1:D:118:THR:HB	1.35	1.02
1:B:210:LYS:HB3	1:B:359:CYS:HB3	1.40	1.01
1:A:269:LEU:HD23	1:A:294:ALA:HB2	1.05	1.01
1:A:194:LYS:HD2	1:A:316:LYS:CD	1.92	0.99
1:B:399:ARG:HD2	1:B:492:LEU:HD22	1.45	0.98
1:B:142:VAL:HG21	1:B:153:ILE:HD11	1.46	0.97
1:C:209:ILE:CG2	1:C:211:GLY:CA	2.41	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ARG:HD2	1:A:492:LEU:HD22	1.45	0.97
1:B:399:ARG:HD2	1:B:492:LEU:CD2	1.94	0.97
1:D:360:LYS:O	1:D:362:PRO:HG3	1.64	0.96
1:A:194:LYS:CD	1:A:316:LYS:HD3	1.94	0.96
1:C:142:VAL:HG13	1:C:149:ILE:HD12	1.48	0.96
1:B:240:GLU:O	1:B:269:LEU:HD11	1.66	0.96
1:C:142:VAL:CG2	1:C:149:ILE:HD13	1.97	0.95
1:C:209:ILE:CG2	1:C:211:GLY:C	2.40	0.93
1:A:42:LYS:HE3	1:B:118:THR:HB	1.50	0.93
1:A:194:LYS:HD2	1:A:316:LYS:HD3	0.98	0.93
1:A:207:GLU:HG3	1:A:209:ILE:HD13	1.48	0.93
1:B:69:SER:HB3	1:C:11:ASN:HD22	1.27	0.93
1:B:390:VAL:HG12	1:B:491:PRO:HG2	0.94	0.93
1:B:194:LYS:N	1:B:316:LYS:NZ	2.15	0.93
1:C:399:ARG:HD2	1:C:492:LEU:CD2	2.00	0.92
1:B:194:LYS:CB	1:B:316:LYS:HE3	1.99	0.92
1:C:209:ILE:HG22	1:C:211:GLY:CA	2.00	0.92
1:C:142:VAL:HG11	1:C:149:ILE:CB	1.98	0.92
1:D:269:LEU:CD2	1:D:294:ALA:HB2	1.98	0.92
1:C:490:GLU:OE1	1:C:495:LYS:HE2	1.68	0.92
1:C:209:ILE:HG23	1:C:211:GLY:HA3	1.52	0.91
1:B:341:GLY:CA	1:B:358:GLU:HG2	1.99	0.91
1:B:210:LYS:HB3	1:B:359:CYS:CB	2.02	0.90
1:A:269:LEU:CD2	1:A:294:ALA:HB2	1.99	0.90
1:B:348:ILE:CG2	1:B:370:ARG:HH22	1.84	0.90
1:B:142:VAL:HB	1:B:394:THR:CG2	2.02	0.89
1:A:210:LYS:CG	1:A:358:GLU:HA	2.02	0.89
1:B:46:LYS:HZ2	1:C:514:ASP:HB2	1.36	0.89
1:D:357:GLU:HG2	1:D:358:GLU:HB2	1.55	0.89
1:B:490:GLU:OE1	1:B:495:LYS:CE	2.21	0.88
1:C:156:THR:HG21	1:C:489:VAL:O	1.74	0.88
1:B:142:VAL:HG12	1:B:142:VAL:O	1.72	0.87
1:C:142:VAL:CG1	1:C:149:ILE:HB	2.04	0.87
1:D:196:GLU:OE2	1:D:213:LEU:HB2	1.75	0.87
1:B:156:THR:HG21	1:B:489:VAL:N	1.89	0.87
1:B:349:SER:HB2	1:B:370:ARG:HH21	1.37	0.86
1:A:210:LYS:HD2	1:A:358:GLU:CA	2.04	0.86
1:B:50:ASP:C	1:C:518:ALA:HB3	2.00	0.86
1:A:449:GLY:HA2	1:B:116:HIS:CG	2.11	0.85
1:D:399:ARG:HD2	1:D:492:LEU:HD22	1.56	0.85
1:A:399:ARG:HD2	1:A:492:LEU:CD2	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:SER:HB2	1:B:370:ARG:CZ	2.05	0.85
1:B:50:ASP:HA	1:C:518:ALA:CB	2.07	0.85
1:B:50:ASP:HA	1:C:518:ALA:HB3	1.59	0.85
1:B:218:ARG:NH1	1:B:223:MET:O	2.08	0.85
1:A:207:GLU:HG3	1:A:209:ILE:CD1	2.07	0.85
1:A:343:VAL:HA	1:A:355:PHE:O	1.77	0.85
1:C:209:ILE:HG22	1:C:211:GLY:N	1.92	0.84
1:B:341:GLY:HA3	1:B:358:GLU:CB	2.06	0.84
1:B:390:VAL:CG1	1:B:491:PRO:CG	2.46	0.84
1:C:213:LEU:HD22	1:C:368:LEU:CD2	2.06	0.84
1:B:50:ASP:CA	1:C:518:ALA:HB3	2.07	0.84
1:C:213:LEU:HD22	1:C:368:LEU:HD21	1.58	0.84
1:C:449:GLY:HA2	1:D:116:HIS:CG	2.13	0.83
1:A:42:LYS:HB3	1:B:118:THR:HG21	1.61	0.83
1:C:269:LEU:CD2	1:C:294:ALA:HB2	2.01	0.82
1:A:211:GLY:CA	1:A:357:GLU:HA	2.08	0.82
1:B:42:LYS:HD2	1:C:118:THR:CB	2.09	0.82
1:C:209:ILE:CG2	1:C:211:GLY:HA3	2.08	0.82
1:B:194:LYS:HE3	1:B:313:ASP:OD1	1.80	0.82
1:A:218:ARG:NH1	1:A:225:LYS:CE	2.43	0.81
1:B:49:VAL:O	1:C:518:ALA:N	2.11	0.81
1:A:218:ARG:NH2	1:A:225:LYS:HZ1	1.79	0.81
1:D:360:LYS:O	1:D:362:PRO:HD3	1.79	0.81
1:B:48:LEU:CD1	1:C:516:ILE:HD12	2.11	0.81
1:D:263:GLU:CB	1:D:269:LEU:CD1	2.54	0.81
1:D:342:LEU:HB2	1:D:358:GLU:CG	2.10	0.80
1:D:360:LYS:O	1:D:362:PRO:CG	2.28	0.80
1:B:46:LYS:NZ	1:C:514:ASP:HB2	1.96	0.80
1:D:357:GLU:HB2	1:D:366:THR:OG1	1.81	0.80
1:A:218:ARG:NH2	1:A:225:LYS:NZ	2.30	0.80
1:D:342:LEU:CB	1:D:358:GLU:CB	2.59	0.80
1:C:276:ILE:HA	1:C:332:LEU:HD23	1.64	0.80
1:D:341:GLY:HA3	1:D:358:GLU:O	1.81	0.79
1:C:209:ILE:HG22	1:C:211:GLY:C	2.06	0.79
1:C:263:GLU:CB	1:C:269:LEU:CD1	2.57	0.79
1:A:263:GLU:CB	1:A:269:LEU:CD1	2.57	0.79
1:B:142:VAL:N	1:B:398:GLY:O	2.17	0.78
1:A:341:GLY:HA3	1:A:358:GLU:O	1.83	0.78
1:A:210:LYS:CB	1:A:358:GLU:HA	2.11	0.78
1:B:263:GLU:CB	1:B:269:LEU:HD21	2.13	0.78
1:A:42:LYS:CE	1:B:118:THR:HB	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:544:AGS:S1G	2:C:544:AGS:O3G	2.42	0.77
2:A:544:AGS:S1G	2:A:544:AGS:O3G	2.42	0.77
1:D:360:LYS:O	1:D:362:PRO:CD	2.31	0.77
1:A:218:ARG:CZ	1:A:225:LYS:NZ	2.47	0.77
1:D:198:LYS:HE3	1:D:213:LEU:CD2	2.14	0.76
1:A:211:GLY:N	1:A:357:GLU:HA	2.01	0.76
1:B:46:LYS:HZ2	1:C:514:ASP:CB	1.98	0.75
1:A:209:ILE:HD11	1:A:368:LEU:HB3	1.66	0.75
1:A:211:GLY:HA3	1:A:357:GLU:HA	1.67	0.75
1:D:399:ARG:HD2	1:D:492:LEU:CD2	2.15	0.75
1:B:358:GLU:O	1:B:358:GLU:CD	2.30	0.75
1:B:357:GLU:O	1:B:358:GLU:CB	2.33	0.75
1:A:42:LYS:HE3	1:B:118:THR:CB	2.16	0.74
1:A:218:ARG:CZ	1:A:225:LYS:HE2	2.17	0.74
1:A:210:LYS:HB2	1:A:358:GLU:H	0.58	0.74
1:C:209:ILE:HG21	1:C:211:GLY:C	2.14	0.73
1:B:358:GLU:OE2	1:B:358:GLU:HA	1.88	0.73
2:B:544:AGS:S1G	2:B:544:AGS:O3G	2.42	0.73
1:C:60:ASP:HA	2:C:544:AGS:S1G	2.28	0.73
2:D:544:AGS:S1G	2:D:544:AGS:O3G	2.42	0.73
1:C:156:THR:CG2	1:C:489:VAL:O	2.37	0.73
1:B:213:LEU:CD2	1:B:368:LEU:HD13	2.19	0.72
1:D:142:VAL:N	1:D:398:GLY:O	2.18	0.72
1:D:342:LEU:HB2	1:D:358:GLU:CB	2.17	0.72
1:B:390:VAL:HG12	1:B:491:PRO:CD	2.19	0.72
1:A:142:VAL:HG22	1:A:149:ILE:HG21	1.72	0.71
1:D:342:LEU:CB	1:D:358:GLU:HB3	2.20	0.71
1:D:342:LEU:HD13	1:D:358:GLU:HG2	1.73	0.71
1:B:156:THR:HG21	1:B:489:VAL:H	1.54	0.71
1:D:342:LEU:HB3	1:D:358:GLU:CB	2.21	0.71
1:B:42:LYS:HB3	1:C:118:THR:CG2	2.15	0.71
1:C:209:ILE:HG22	1:C:211:GLY:O	1.91	0.71
1:B:69:SER:CB	1:C:11:ASN:ND2	2.51	0.71
1:D:342:LEU:N	1:D:358:GLU:HB3	2.05	0.71
1:A:390:VAL:HG12	1:A:491:PRO:HG2	1.73	0.70
1:C:42:LYS:HB3	1:D:118:THR:HG21	1.72	0.70
1:C:142:VAL:HG22	1:C:149:ILE:CD1	2.11	0.70
1:C:156:THR:HG21	1:C:489:VAL:C	2.16	0.70
1:D:342:LEU:HB2	1:D:358:GLU:HB3	1.72	0.70
1:B:240:GLU:O	1:B:269:LEU:CD1	2.39	0.70
1:A:209:ILE:HD12	1:A:368:LEU:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:GLU:O	1:D:359:CYS:SG	2.49	0.70
1:A:209:ILE:CD1	1:A:368:LEU:HB2	2.21	0.70
1:B:341:GLY:HA3	1:B:358:GLU:HB2	1.72	0.69
1:B:358:GLU:OE2	1:B:358:GLU:CA	2.39	0.69
1:D:342:LEU:CB	1:D:358:GLU:CG	2.70	0.69
1:D:342:LEU:CB	1:D:358:GLU:HG2	2.22	0.69
1:A:210:LYS:CA	1:A:358:GLU:H	2.00	0.68
1:B:194:LYS:H	1:B:316:LYS:HZ2	1.41	0.68
1:B:42:LYS:CD	1:C:118:THR:HB	2.19	0.67
1:A:447:ASN:O	1:B:116:HIS:CE1	2.47	0.67
1:A:218:ARG:CZ	1:A:225:LYS:CE	2.73	0.67
1:A:210:LYS:CG	1:A:358:GLU:CA	2.69	0.67
1:A:209:ILE:HD11	1:A:368:LEU:CB	2.25	0.66
1:A:210:LYS:C	1:A:357:GLU:HA	2.21	0.66
1:B:156:THR:CG2	1:B:489:VAL:H	2.08	0.66
1:C:156:THR:CB	1:C:489:VAL:O	2.44	0.66
1:B:349:SER:CB	1:B:370:ARG:HH21	2.09	0.66
1:A:342:LEU:HB3	1:A:357:GLU:HG3	1.78	0.65
1:B:142:VAL:O	1:B:143:GLY:C	2.38	0.65
1:B:341:GLY:CA	1:B:358:GLU:CG	2.67	0.65
1:A:209:ILE:CD1	1:A:368:LEU:CB	2.74	0.65
1:B:60:ASP:HA	2:B:544:AGS:S1G	2.37	0.65
1:C:209:ILE:CG2	1:C:211:GLY:O	2.43	0.65
1:D:390:VAL:HG12	1:D:491:PRO:HG2	1.78	0.65
1:C:393:CYS:SG	1:C:493:ARG:NH1	2.70	0.64
1:B:397:ASP:HB3	1:B:399:ARG:HG3	1.79	0.64
1:C:399:ARG:CD	1:C:492:LEU:HD22	2.16	0.64
1:A:218:ARG:CZ	1:A:225:LYS:HZ3	2.10	0.64
1:A:142:VAL:CG2	1:A:149:ILE:HG21	2.28	0.64
1:A:142:VAL:HG12	1:A:142:VAL:O	1.97	0.64
1:A:218:ARG:NH2	1:A:225:LYS:CE	2.61	0.64
1:D:142:VAL:O	1:D:142:VAL:HG12	1.98	0.64
1:B:193:ILE:C	1:B:316:LYS:NZ	2.56	0.63
1:D:360:LYS:HD2	1:D:361:HIS:H	1.63	0.63
1:B:209:ILE:HD13	1:B:213:LEU:HD13	1.81	0.63
1:B:156:THR:HG21	1:B:489:VAL:O	1.98	0.63
1:B:447:ASN:O	1:C:116:HIS:CE1	2.51	0.63
1:B:341:GLY:CA	1:B:358:GLU:CB	2.77	0.63
1:B:399:ARG:HD2	1:B:492:LEU:HD23	1.78	0.63
1:C:142:VAL:CG1	1:C:146:ASP:HB3	2.29	0.63
1:C:327:THR:O	1:C:328:ASN:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:O	1:A:143:GLY:C	2.42	0.62
1:D:357:GLU:CG	1:D:358:GLU:HB2	2.29	0.62
1:C:142:VAL:HG13	1:C:149:ILE:CD1	2.25	0.62
1:A:210:LYS:HG2	1:A:359:CYS:N	2.15	0.62
1:A:449:GLY:HA2	1:B:116:HIS:CD2	2.33	0.62
1:B:46:LYS:HD2	1:C:514:ASP:HB3	1.80	0.62
1:A:210:LYS:HB3	1:A:358:GLU:CA	2.22	0.62
1:A:46:LYS:NZ	1:B:514:ASP:CB	2.63	0.62
1:A:449:GLY:HA2	1:B:116:HIS:CB	2.30	0.62
1:B:193:ILE:C	1:B:316:LYS:HZ1	2.07	0.62
1:B:194:LYS:CA	1:B:316:LYS:HZ2	2.12	0.62
1:A:46:LYS:NZ	1:B:514:ASP:HB2	2.15	0.61
1:C:209:ILE:HG22	1:C:211:GLY:H	1.64	0.61
1:D:342:LEU:HB3	1:D:358:GLU:HB2	1.82	0.61
1:B:153:ILE:HG12	1:B:400:ILE:HG21	1.83	0.61
1:C:449:GLY:HA2	1:D:116:HIS:CB	2.30	0.61
1:B:37:SER:OG	1:C:513:ASP:OD2	2.19	0.61
1:A:211:GLY:HA3	1:A:357:GLU:CA	2.31	0.60
1:B:198:LYS:NZ	1:B:215:ASP:OD2	2.33	0.60
1:C:95:THR:HG23	2:C:544:AGS:O2B	2.01	0.60
1:C:213:LEU:HD22	1:C:368:LEU:HD22	1.83	0.60
1:D:357:GLU:HG3	1:D:358:GLU:OE1	2.01	0.60
1:C:470:CYS:SG	1:C:484:CYS:N	2.75	0.60
1:B:46:LYS:NZ	1:C:514:ASP:CB	2.60	0.60
1:D:374:GLU:HA	1:D:377:ILE:HD12	1.83	0.60
1:B:218:ARG:NH2	1:B:221:ALA:O	2.35	0.60
1:B:341:GLY:H	1:B:358:GLU:HB3	1.67	0.60
1:B:156:THR:CG2	1:B:489:VAL:O	2.51	0.59
1:C:390:VAL:HG12	1:C:491:PRO:HG2	1.83	0.59
1:B:156:THR:CG2	1:B:489:VAL:N	2.65	0.59
1:B:390:VAL:CG1	1:B:491:PRO:CD	2.78	0.59
1:C:153:ILE:HG12	1:C:400:ILE:HG21	1.84	0.59
1:B:210:LYS:CB	1:B:359:CYS:CB	2.77	0.59
1:B:194:LYS:HD3	1:B:366:THR:HG23	1.85	0.58
1:C:328:ASN:O	1:C:330:LYS:N	2.37	0.58
1:A:374:GLU:HA	1:A:377:ILE:HD12	1.85	0.58
1:B:46:LYS:CD	1:C:514:ASP:HB3	2.33	0.58
1:B:357:GLU:O	1:B:358:GLU:HB3	2.03	0.58
1:B:194:LYS:CB	1:B:316:LYS:CE	2.67	0.58
1:B:194:LYS:HD3	1:B:366:THR:CG2	2.34	0.58
1:B:357:GLU:O	1:B:358:GLU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HD22	1:A:368:LEU:HD11	1.86	0.58
1:B:25:ILE:HG23	1:B:104:LEU:HB3	1.86	0.57
1:B:213:LEU:HD22	1:B:368:LEU:HD13	1.86	0.57
1:B:374:GLU:HA	1:B:377:ILE:HD12	1.86	0.57
1:B:194:LYS:CE	1:B:313:ASP:OD1	2.51	0.57
1:C:46:LYS:HZ2	1:D:514:ASP:CB	2.17	0.57
1:C:374:GLU:HA	1:C:377:ILE:HD12	1.86	0.57
1:B:390:VAL:CB	1:B:491:PRO:CG	2.81	0.57
1:A:37:SER:OG	1:B:513:ASP:OD2	2.15	0.57
1:A:173:ILE:HG23	1:A:208:LEU:HB2	1.86	0.57
1:B:341:GLY:CA	1:B:358:GLU:HB2	2.34	0.57
1:C:25:ILE:HG23	1:C:104:LEU:HB3	1.86	0.57
1:C:42:LYS:HD2	1:D:118:THR:CB	2.24	0.57
1:A:211:GLY:HA3	1:A:356:VAL:C	2.30	0.57
1:D:142:VAL:O	1:D:143:GLY:C	2.48	0.57
1:B:358:GLU:CG	1:B:358:GLU:O	2.52	0.57
1:B:142:VAL:CB	1:B:394:THR:CG2	2.81	0.56
1:A:60:ASP:HA	2:A:544:AGS:S1G	2.45	0.56
1:A:95:THR:HG23	2:A:544:AGS:O2B	2.04	0.56
1:A:470:CYS:HG	1:A:484:CYS:HG	0.58	0.56
1:C:142:VAL:HG11	1:C:149:ILE:CG2	2.35	0.56
1:C:42:LYS:HB3	1:D:118:THR:CG2	2.35	0.56
1:B:48:LEU:HD12	1:C:516:ILE:HD12	1.85	0.56
1:A:449:GLY:CA	1:B:116:HIS:CG	2.87	0.56
1:D:135:LEU:HD23	1:D:138:ILE:HD11	1.87	0.56
1:B:48:LEU:HD11	1:C:516:ILE:HD12	1.89	0.55
1:D:490:GLU:OE2	2:D:544:AGS:C2'	2.54	0.55
1:B:142:VAL:HG21	1:B:153:ILE:CD1	2.31	0.55
1:B:368:LEU:HD23	1:B:370:ARG:NH1	2.20	0.55
1:B:156:THR:HG21	1:B:489:VAL:C	2.30	0.55
1:A:25:ILE:HG23	1:A:104:LEU:HB3	1.89	0.55
1:B:390:VAL:HB	1:B:491:PRO:HG3	1.89	0.55
1:A:194:LYS:HE3	1:A:316:LYS:HA	1.89	0.55
1:A:349:SER:HB2	1:A:370:ARG:HH22	1.71	0.55
1:C:48:LEU:HD11	1:C:64:ILE:HG23	1.89	0.55
1:A:447:ASN:O	1:B:116:HIS:HE1	1.87	0.54
1:B:368:LEU:HD21	1:B:370:ARG:CZ	2.36	0.54
1:A:349:SER:HB2	1:A:370:ARG:NH2	2.22	0.54
1:B:194:LYS:CA	1:B:316:LYS:NZ	2.71	0.54
1:B:210:LYS:O	1:B:359:CYS:HB2	2.07	0.54
1:D:342:LEU:CD1	1:D:358:GLU:HG2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:HD2	1:A:358:GLU:HG2	1.89	0.54
1:C:393:CYS:SG	1:C:493:ARG:CZ	2.96	0.54
1:B:142:VAL:HG11	1:B:394:THR:HG21	1.89	0.54
1:D:269:LEU:HD22	1:D:294:ALA:N	2.23	0.54
1:B:344:GLU:OE1	1:B:346:ARG:NE	2.24	0.54
1:B:196:GLU:OE2	1:B:215:ASP:HB2	2.09	0.53
1:B:368:LEU:CD2	1:B:370:ARG:NH1	2.71	0.53
1:C:269:LEU:HD22	1:C:294:ALA:N	2.23	0.53
1:D:25:ILE:HG23	1:D:104:LEU:HB3	1.90	0.53
1:D:95:THR:HG23	2:D:544:AGS:O2B	2.07	0.53
1:B:240:GLU:C	1:B:269:LEU:HD11	2.33	0.53
1:B:142:VAL:HG22	1:B:149:ILE:HG21	1.91	0.53
1:D:48:LEU:HD11	1:D:64:ILE:HG23	1.91	0.53
1:D:119:ILE:HG21	1:D:425:ARG:HB3	1.90	0.53
1:A:239:ILE:HD12	1:A:290:ILE:HG12	1.91	0.53
1:B:156:THR:HB	1:B:489:VAL:O	2.08	0.53
1:C:142:VAL:CG2	1:C:149:ILE:CD1	2.79	0.53
1:D:490:GLU:OE2	2:D:544:AGS:H3'	2.09	0.52
1:B:210:LYS:C	1:B:359:CYS:SG	2.92	0.52
1:B:213:LEU:HD23	1:B:368:LEU:HD13	1.89	0.52
1:C:341:GLY:HA3	1:C:358:GLU:O	2.09	0.52
1:C:490:GLU:CD	1:C:495:LYS:HE2	2.32	0.52
1:A:46:LYS:NZ	1:B:514:ASP:HB3	2.25	0.52
1:B:349:SER:CB	1:B:370:ARG:NH2	2.48	0.52
1:A:320:ALA:HA	1:A:364:ALA:CB	2.40	0.52
1:B:50:ASP:HA	1:C:518:ALA:HB2	1.89	0.52
1:B:142:VAL:O	1:B:142:VAL:CG1	2.46	0.52
1:C:46:LYS:NZ	1:D:514:ASP:HB2	2.25	0.52
1:D:195:ILE:HG23	1:D:369:ILE:HD12	1.93	0.52
1:C:142:VAL:HG12	1:C:146:ASP:HB3	1.91	0.51
1:C:156:THR:HB	1:C:489:VAL:O	2.10	0.51
1:C:449:GLY:CA	1:D:116:HIS:CG	2.92	0.51
2:C:544:AGS:S1G	2:C:544:AGS:O3B	2.58	0.51
1:D:216:LYS:HD2	1:D:307:ARG:O	2.10	0.51
2:D:544:AGS:S1G	2:D:544:AGS:O3B	2.58	0.51
1:B:142:VAL:HB	1:B:394:THR:HG23	1.88	0.51
1:C:46:LYS:NZ	1:D:514:ASP:CB	2.73	0.51
1:A:119:ILE:HG21	1:A:425:ARG:HB3	1.91	0.51
1:C:446:GLU:O	1:D:116:HIS:NE2	2.44	0.51
1:B:369:ILE:HD13	1:B:381:ALA:HA	1.92	0.51
2:B:544:AGS:S1G	2:B:544:AGS:O3B	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:HG23	1:B:369:ILE:HD12	1.92	0.51
1:A:218:ARG:HH22	1:A:225:LYS:CE	2.24	0.51
1:A:46:LYS:HZ2	1:B:514:ASP:CB	2.23	0.50
1:C:195:ILE:HG23	1:C:369:ILE:HD12	1.92	0.50
1:D:239:ILE:HD12	1:D:290:ILE:HG12	1.93	0.50
1:D:490:GLU:CD	2:D:544:AGS:O2'	2.54	0.50
1:A:235:LEU:HD12	1:A:284:LEU:HD11	1.92	0.50
1:C:398:GLY:O	1:C:399:ARG:HG3	2.12	0.50
1:B:358:GLU:CD	1:B:358:GLU:C	2.76	0.50
1:C:239:ILE:HD12	1:C:290:ILE:HG12	1.92	0.50
1:C:210:LYS:HG2	1:C:362:PRO:HG2	1.93	0.50
1:D:404:GLY:HA2	2:D:544:AGS:N3	2.27	0.50
1:B:216:LYS:HD2	1:B:307:ARG:O	2.12	0.50
1:A:369:ILE:HD13	1:A:381:ALA:HA	1.92	0.50
1:B:390:VAL:CB	1:B:491:PRO:HG2	2.38	0.50
1:A:195:ILE:HG23	1:A:369:ILE:HD12	1.92	0.50
1:C:269:LEU:CD2	1:C:294:ALA:N	2.75	0.50
1:C:399:ARG:CD	1:C:492:LEU:CD2	2.81	0.50
1:D:360:LYS:CD	1:D:361:HIS:H	2.24	0.49
1:B:141:GLU:HA	1:B:398:GLY:O	2.11	0.49
1:B:194:LYS:HB2	1:B:316:LYS:CD	2.40	0.49
1:A:182:VAL:HG22	1:A:188:VAL:HG22	1.94	0.49
1:B:156:THR:CB	1:B:489:VAL:O	2.61	0.49
1:D:369:ILE:HD13	1:D:381:ALA:HA	1.94	0.49
1:B:210:LYS:CB	1:B:359:CYS:HB2	2.42	0.49
1:B:393:CYS:SG	1:B:493:ARG:CZ	3.00	0.49
1:A:269:LEU:HD22	1:A:294:ALA:N	2.27	0.49
1:C:206:THR:HG22	1:C:370:ARG:H	1.78	0.49
1:A:320:ALA:HA	1:A:364:ALA:HB3	1.94	0.49
1:C:119:ILE:HG21	1:C:425:ARG:HB3	1.95	0.49
1:C:135:LEU:HD23	1:C:138:ILE:HD11	1.95	0.49
1:A:211:GLY:HA3	1:A:356:VAL:O	2.13	0.49
1:D:269:LEU:CD2	1:D:294:ALA:N	2.76	0.49
2:A:544:AGS:S1G	2:A:544:AGS:O3B	2.58	0.49
1:C:182:VAL:HG22	1:C:188:VAL:HG22	1.95	0.49
1:B:173:ILE:HG23	1:B:208:LEU:HB2	1.95	0.49
1:B:182:VAL:HG22	1:B:188:VAL:HG22	1.95	0.49
1:D:173:ILE:HG23	1:D:208:LEU:HB2	1.94	0.49
1:B:235:LEU:HD12	1:B:284:LEU:HD11	1.95	0.48
1:C:46:LYS:HZ2	1:D:514:ASP:HB3	1.77	0.48
1:C:216:LYS:HD2	1:C:307:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ILE:HD13	1:C:381:ALA:HA	1.93	0.48
1:A:46:LYS:HZ3	1:B:514:ASP:CB	2.24	0.48
1:B:119:ILE:HG21	1:B:425:ARG:HB3	1.94	0.48
1:A:213:LEU:HD11	1:A:355:PHE:CZ	2.49	0.48
1:D:206:THR:HG22	1:D:370:ARG:H	1.78	0.48
1:A:118:THR:HA	1:A:121:VAL:HG12	1.95	0.48
1:B:142:VAL:CG1	1:B:394:THR:HG21	2.43	0.48
1:D:198:LYS:HA	1:D:198:LYS:HD3	1.57	0.48
1:A:449:GLY:HA2	1:B:116:HIS:HB2	1.96	0.48
1:C:142:VAL:CG1	1:C:149:ILE:HD12	2.32	0.48
1:A:48:LEU:HD11	1:A:64:ILE:HG23	1.95	0.48
1:B:118:THR:HA	1:B:121:VAL:HG12	1.95	0.48
1:A:206:THR:HG22	1:A:370:ARG:H	1.79	0.48
1:A:455:ILE:HG21	1:A:473:LEU:HD13	1.96	0.48
1:B:206:THR:HG22	1:B:370:ARG:H	1.78	0.48
1:C:142:VAL:CG1	1:C:149:ILE:CD1	2.90	0.48
1:A:228:THR:HG22	1:A:229:ASP:CG	2.39	0.47
1:B:135:LEU:HD23	1:B:138:ILE:HD11	1.96	0.47
1:B:239:ILE:HD12	1:B:290:ILE:HG12	1.95	0.47
1:D:360:LYS:CD	1:D:361:HIS:N	2.77	0.47
1:B:142:VAL:HB	1:B:394:THR:HG22	1.92	0.47
1:D:223:MET:HB3	1:D:304:VAL:HG22	1.95	0.47
1:D:404:GLY:CA	2:D:544:AGS:N3	2.78	0.47
1:A:135:LEU:HD23	1:A:138:ILE:HD11	1.96	0.47
1:B:194:LYS:CB	1:B:316:LYS:HZ2	2.25	0.47
1:C:173:ILE:HG23	1:C:208:LEU:HB2	1.96	0.47
1:B:341:GLY:H	1:B:358:GLU:CB	2.28	0.47
1:C:142:VAL:HG21	1:C:149:ILE:HG21	0.69	0.47
1:B:358:GLU:OE2	1:B:358:GLU:C	2.58	0.47
1:C:118:THR:HA	1:C:121:VAL:HG12	1.97	0.47
1:C:327:THR:O	1:C:328:ASN:CB	2.61	0.47
1:B:91:ASP:HB2	1:B:386:ASP:OD2	2.15	0.47
1:C:449:GLY:HA2	1:D:116:HIS:CD2	2.48	0.47
1:C:142:VAL:CG1	1:C:149:ILE:CB	2.78	0.47
1:B:143:GLY:O	1:B:145:GLN:N	2.48	0.46
1:D:182:VAL:HG22	1:D:188:VAL:HG22	1.97	0.46
1:B:11:ASN:HA	1:B:12:MET:HA	1.50	0.46
1:B:95:THR:HG23	2:B:544:AGS:O2B	2.15	0.46
1:B:215:ASP:HA	1:B:353:MET:HG2	1.97	0.46
1:D:403:GLY:HA3	2:D:544:AGS:O2'	2.15	0.46
1:A:341:GLY:CA	1:A:358:GLU:O	2.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:CYS:SG	1:D:484:CYS:N	2.89	0.46
1:A:184:ASP:HA	1:A:185:GLU:HA	1.61	0.46
1:A:356:VAL:O	1:A:357:GLU:HB3	2.16	0.46
1:B:48:LEU:HD11	1:B:64:ILE:HG23	1.97	0.46
1:B:399:ARG:CD	1:B:492:LEU:CD2	2.83	0.46
1:A:209:ILE:HG13	1:A:368:LEU:H	1.80	0.46
1:B:347:LYS:HG2	1:B:352:SER:HB3	1.97	0.46
1:C:184:ASP:HA	1:C:185:GLU:HA	1.60	0.46
1:D:11:ASN:HA	1:D:12:MET:HA	1.51	0.46
1:D:141:GLU:HA	1:D:398:GLY:O	2.15	0.46
1:A:150:LEU:HD22	1:A:391:VAL:HG13	1.97	0.46
1:B:49:VAL:O	1:C:518:ALA:CB	2.64	0.46
1:C:404:GLY:HA2	2:C:544:AGS:N3	2.30	0.46
1:A:216:LYS:HD2	1:A:307:ARG:O	2.16	0.46
1:D:468:ASN:O	1:D:469:LYS:HB3	2.16	0.46
1:A:344:GLU:N	1:A:355:PHE:O	2.46	0.45
1:A:470:CYS:HG	1:A:484:CYS:CB	2.22	0.45
1:C:210:LYS:HG2	1:C:362:PRO:CG	2.47	0.45
1:B:142:VAL:HG23	1:B:400:ILE:HG12	1.98	0.45
1:C:213:LEU:CD2	1:C:368:LEU:HD21	2.40	0.45
1:A:210:LYS:HB3	1:A:358:GLU:C	2.40	0.45
1:C:209:ILE:HG21	1:C:211:GLY:O	2.15	0.45
1:C:357:GLU:O	1:C:358:GLU:HB2	2.16	0.45
1:C:401:VAL:HB	1:C:407:THR:HG21	1.99	0.45
1:B:449:GLY:HA2	1:C:116:HIS:HB2	1.97	0.45
1:A:213:LEU:HD22	1:A:368:LEU:CD1	2.46	0.45
1:C:69:SER:HB3	1:D:11:ASN:ND2	2.32	0.45
1:C:150:LEU:HD22	1:C:391:VAL:HG13	1.99	0.45
1:B:150:LEU:HD22	1:B:391:VAL:HG13	1.98	0.45
1:B:455:ILE:HG21	1:B:473:LEU:HD13	1.98	0.45
1:D:401:VAL:HB	1:D:407:THR:HG21	1.97	0.45
1:B:198:LYS:HA	1:B:198:LYS:HD3	1.59	0.45
1:D:215:ASP:HA	1:D:353:MET:HG2	1.98	0.45
1:D:150:LEU:HD22	1:D:391:VAL:HG13	1.99	0.44
1:D:118:THR:HA	1:D:121:VAL:HG12	1.99	0.44
1:A:46:LYS:HZ2	1:B:514:ASP:HB2	1.79	0.44
1:B:50:ASP:C	1:C:518:ALA:CB	2.84	0.44
1:D:347:LYS:HG2	1:D:352:SER:HB3	1.98	0.44
1:A:401:VAL:HB	1:A:407:THR:HG21	1.98	0.44
1:C:46:LYS:HZ2	1:D:514:ASP:HB2	1.81	0.44
1:C:269:LEU:CD2	1:C:294:ALA:H	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:HA	1:C:516:ILE:HB	2.00	0.44
1:B:449:GLY:HA2	1:C:116:HIS:CB	2.47	0.44
1:A:447:ASN:C	1:B:116:HIS:CE1	2.96	0.44
1:B:470:CYS:SG	1:B:484:CYS:N	2.91	0.44
1:D:342:LEU:HB3	1:D:358:GLU:HG2	1.98	0.44
1:B:449:GLY:HA2	1:C:116:HIS:CG	2.52	0.44
1:A:470:CYS:SG	1:A:484:CYS:N	2.91	0.43
1:B:341:GLY:N	1:B:358:GLU:CB	2.81	0.43
1:D:490:GLU:OE2	2:D:544:AGS:C3'	2.66	0.43
1:C:447:ASN:O	1:D:118:THR:HG21	2.19	0.43
1:D:470:CYS:SG	1:D:484:CYS:CB	3.05	0.43
1:A:228:THR:HG22	1:A:229:ASP:OD1	2.18	0.43
1:A:440:ILE:HB	1:A:441:PRO:HD3	2.00	0.43
1:B:198:LYS:NZ	1:B:215:ASP:CG	2.75	0.43
1:D:235:LEU:HD12	1:D:284:LEU:HD11	1.99	0.43
1:B:48:LEU:HG	1:C:516:ILE:CD1	2.48	0.43
1:B:142:VAL:CB	1:B:394:THR:HG21	2.48	0.43
1:A:470:CYS:SG	1:A:484:CYS:CB	3.05	0.43
1:B:144:ALA:HB1	1:B:395:ILE:HG23	2.01	0.43
1:C:37:SER:OG	1:D:513:ASP:OD2	2.26	0.43
1:D:198:LYS:NZ	1:D:353:MET:HE1	2.33	0.43
1:A:37:SER:CB	1:B:513:ASP:OD2	2.67	0.43
1:A:213:LEU:HD11	1:A:355:PHE:CE1	2.54	0.42
1:D:184:ASP:HA	1:D:185:GLU:HA	1.61	0.42
1:B:390:VAL:CB	1:B:491:PRO:HG3	2.47	0.42
1:A:449:GLY:CA	1:B:116:HIS:CB	2.95	0.42
1:C:79:ILE:HG22	1:C:79:ILE:O	2.20	0.42
1:C:268:MET:C	1:C:269:LEU:HD12	2.45	0.42
1:A:207:GLU:O	1:A:209:ILE:HG12	2.20	0.42
1:B:324:ASN:HB2	1:B:336:ASP:HB3	2.00	0.42
1:B:440:ILE:HB	1:B:441:PRO:HD3	2.01	0.42
1:C:11:ASN:HA	1:C:12:MET:HA	1.51	0.42
1:D:468:ASN:C	1:D:470:CYS:H	2.28	0.42
1:B:184:ASP:HA	1:B:185:GLU:HA	1.61	0.42
1:B:202:SER:C	1:B:204:ASP:H	2.26	0.42
1:B:399:ARG:CD	1:B:492:LEU:HD23	2.47	0.42
1:B:194:LYS:CB	1:B:316:LYS:NZ	2.83	0.42
1:B:236:ASN:HB2	1:B:325:VAL:HG12	2.02	0.42
1:C:202:SER:C	1:C:204:ASP:H	2.28	0.42
1:D:130:LYS:HA	1:D:133:GLU:HG2	2.01	0.42
1:D:455:ILE:HG21	1:D:473:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:HD2	1:A:358:GLU:CG	2.50	0.42
1:D:440:ILE:HB	1:D:441:PRO:HD3	2.02	0.41
1:B:79:ILE:HG22	1:B:79:ILE:O	2.20	0.41
1:B:390:VAL:HB	1:B:491:PRO:CG	2.48	0.41
1:C:440:ILE:HB	1:C:441:PRO:HD3	2.02	0.41
1:C:468:ASN:O	1:C:469:LYS:HB3	2.20	0.41
1:A:72:HIS:HA	1:A:73:PRO:HD3	1.94	0.41
1:D:79:ILE:O	1:D:79:ILE:HG22	2.20	0.41
1:A:419:ALA:HA	1:A:422:ILE:HD12	2.02	0.41
1:B:194:LYS:HB2	1:B:316:LYS:NZ	2.33	0.41
1:B:419:ALA:HA	1:B:422:ILE:HD12	2.03	0.41
1:C:390:VAL:CG1	1:C:491:PRO:HG2	2.49	0.41
1:C:398:GLY:O	1:C:399:ARG:CG	2.69	0.41
1:A:342:LEU:N	1:A:357:GLU:O	2.52	0.41
1:B:192:LEU:O	1:B:316:LYS:NZ	2.47	0.41
1:B:198:LYS:HZ1	1:B:215:ASP:CG	2.29	0.41
1:B:401:VAL:HB	1:B:407:THR:HG21	2.02	0.41
1:C:185:GLU:HA	1:C:186:GLY:HA2	1.94	0.41
1:C:347:LYS:HG2	1:C:352:SER:HB3	2.02	0.41
1:C:449:GLY:HA2	1:D:116:HIS:HB2	2.02	0.41
1:C:69:SER:HB3	1:D:11:ASN:HD22	1.86	0.41
1:C:72:HIS:HA	1:C:73:PRO:HD3	1.96	0.41
1:D:269:LEU:CD2	1:D:294:ALA:H	2.33	0.41
1:A:202:SER:C	1:A:204:ASP:H	2.30	0.40
1:A:207:GLU:HG3	1:A:209:ILE:HD11	1.96	0.40
1:B:468:ASN:O	1:B:469:LYS:HB3	2.22	0.40
1:A:269:LEU:HD21	1:A:291:ASP:HB3	2.02	0.40
1:C:419:ALA:HA	1:C:422:ILE:HD12	2.04	0.40
1:C:455:ILE:HG21	1:C:473:LEU:HD13	2.03	0.40
1:A:268:MET:C	1:A:269:LEU:HD12	2.47	0.40
1:A:347:LYS:HG2	1:A:352:SER:HB3	2.03	0.40
1:B:49:VAL:HB	1:C:517:ALA:HA	2.04	0.40
1:D:361:HIS:HA	1:D:362:PRO:HD3	1.80	0.40
1:A:269:LEU:CD2	1:A:294:ALA:N	2.84	0.40
1:C:398:GLY:O	1:C:399:ARG:CB	2.70	0.40

All (2) 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)
1:A:225:LYS:CB	1:C:335:GLN:CG[8_444]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ALA:N	1:D:49:VAL:O[2_545]	2.15	0.05

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	485/521 (93%)	454 (94%)	26 (5%)	5 (1%)	12	48
1	B	485/521 (93%)	449 (93%)	30 (6%)	6 (1%)	10	44
1	C	485/521 (93%)	446 (92%)	34 (7%)	5 (1%)	12	48
1	D	480/521 (92%)	442 (92%)	31 (6%)	7 (2%)	8	39
All	All	1935/2084 (93%)	1791 (93%)	121 (6%)	23 (1%)	10	44

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	GLU
1	C	328	ASN
1	C	329	ILE
1	D	358	GLU
1	D	361	HIS
1	A	17	GLY
1	A	143	GLY
1	B	17	GLY
1	B	143	GLY
1	C	17	GLY
1	D	17	GLY
1	D	143	GLY
1	C	465	SER
1	D	465	SER
1	A	465	SER
1	B	465	SER

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Mol	Chain	Res	Type
1	A	201	ALA
1	A	358	GLU
1	B	201	ALA
1	B	263	GLU
1	C	201	ALA
1	D	201	ALA
1	D	362	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	388/413 (94%)	373 (96%)	15 (4%)	28	49
1	B	388/413 (94%)	378 (97%)	10 (3%)	40	61
1	C	388/413 (94%)	380 (98%)	8 (2%)	47	65
1	D	386/413 (94%)	375 (97%)	11 (3%)	38	60
All	All	1550/1652 (94%)	1506 (97%)	44 (3%)	38	60

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	39	LEU
1	A	209	ILE
1	A	210	LYS
1	A	216	LYS
1	A	225	LYS
1	A	229	ASP
1	A	239	ILE
1	A	269	LEU
1	A	300	LYS
1	A	327	THR
1	A	342	LEU
1	A	356	VAL
1	A	358	GLU

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Mol	Chain	Res	Type
1	A	453	ILE
1	B	39	LEU
1	B	216	LYS
1	B	218	ARG
1	B	239	ILE
1	B	269	LEU
1	B	327	THR
1	B	335	GLN
1	B	342	LEU
1	B	349	SER
1	B	358	GLU
1	C	194	LYS
1	C	213	LEU
1	C	216	LYS
1	C	239	ILE
1	C	269	LEU
1	C	327	THR
1	C	342	LEU
1	C	453	ILE
1	D	137	THR
1	D	196	GLU
1	D	198	LYS
1	D	213	LEU
1	D	216	LYS
1	D	227	VAL
1	D	239	ILE
1	D	269	LEU
1	D	327	THR
1	D	357	GLU
1	D	490	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	GLN
1	A	500	GLN
1	B	11	ASN
1	B	236	ASN
1	B	361	HIS
1	B	500	GLN
1	C	11	ASN
1	C	59	ASN

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Mol	Chain	Res	Type
1	C	236	ASN
1	C	474	ASN
1	C	500	GLN
1	D	11	ASN
1	D	287	GLN
1	D	500	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AGS	C	544	-	32,33,33	3.64	5 (15%)	45,52,52	0.93	0
2	AGS	A	544	-	32,33,33	3.63	5 (15%)	45,52,52	0.93	0
2	AGS	D	544	-	32,33,33	3.63	5 (15%)	45,52,52	0.93	0
2	AGS	B	544	-	32,33,33	3.63	5 (15%)	45,52,52	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	C	544	-	-	4/21/38/38	0/3/3/3
2	AGS	A	544	-	-	4/21/38/38	0/3/3/3
2	AGS	D	544	-	-	4/21/38/38	0/3/3/3
2	AGS	B	544	-	-	4/21/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	544	AGS	PG-S1G	-18.93	1.49	1.90
2	A	544	AGS	PG-S1G	-18.92	1.49	1.90
2	D	544	AGS	PG-S1G	-18.92	1.49	1.90
2	B	544	AGS	PG-S1G	-18.89	1.49	1.90
2	A	544	AGS	PB-O3A	3.95	1.63	1.59
2	C	544	AGS	PB-O3A	3.95	1.63	1.59
2	B	544	AGS	PB-O3A	3.91	1.63	1.59
2	D	544	AGS	PB-O3A	3.87	1.63	1.59
2	C	544	AGS	PA-O3A	3.43	1.63	1.59
2	A	544	AGS	PA-O3A	3.41	1.63	1.59
2	D	544	AGS	PA-O3A	3.41	1.63	1.59
2	B	544	AGS	PA-O3A	3.34	1.63	1.59
2	C	544	AGS	PB-O3B	3.03	1.62	1.59
2	B	544	AGS	PB-O3B	2.98	1.62	1.59
2	D	544	AGS	PB-O3B	2.94	1.62	1.59
2	A	544	AGS	PB-O3B	2.89	1.62	1.59
2	C	544	AGS	C4-N3	2.28	1.38	1.34
2	B	544	AGS	C4-N3	2.27	1.38	1.34
2	D	544	AGS	C4-N3	2.26	1.38	1.34
2	A	544	AGS	C4-N3	2.24	1.38	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	544	AGS	PB-O3B-PG-O2G
2	A	544	AGS	PB-O3B-PG-O3G
2	B	544	AGS	PB-O3B-PG-O2G
2	B	544	AGS	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
2	C	544	AGS	PB-O3B-PG-O2G
2	C	544	AGS	PB-O3B-PG-O3G
2	D	544	AGS	PB-O3B-PG-O2G
2	D	544	AGS	PB-O3B-PG-O3G
2	A	544	AGS	PA-O3A-PB-O1B
2	B	544	AGS	PA-O3A-PB-O1B
2	C	544	AGS	PA-O3A-PB-O1B
2	D	544	AGS	PA-O3A-PB-O1B
2	A	544	AGS	PA-O3A-PB-O2B
2	B	544	AGS	PA-O3A-PB-O2B
2	C	544	AGS	PA-O3A-PB-O2B
2	D	544	AGS	PA-O3A-PB-O2B

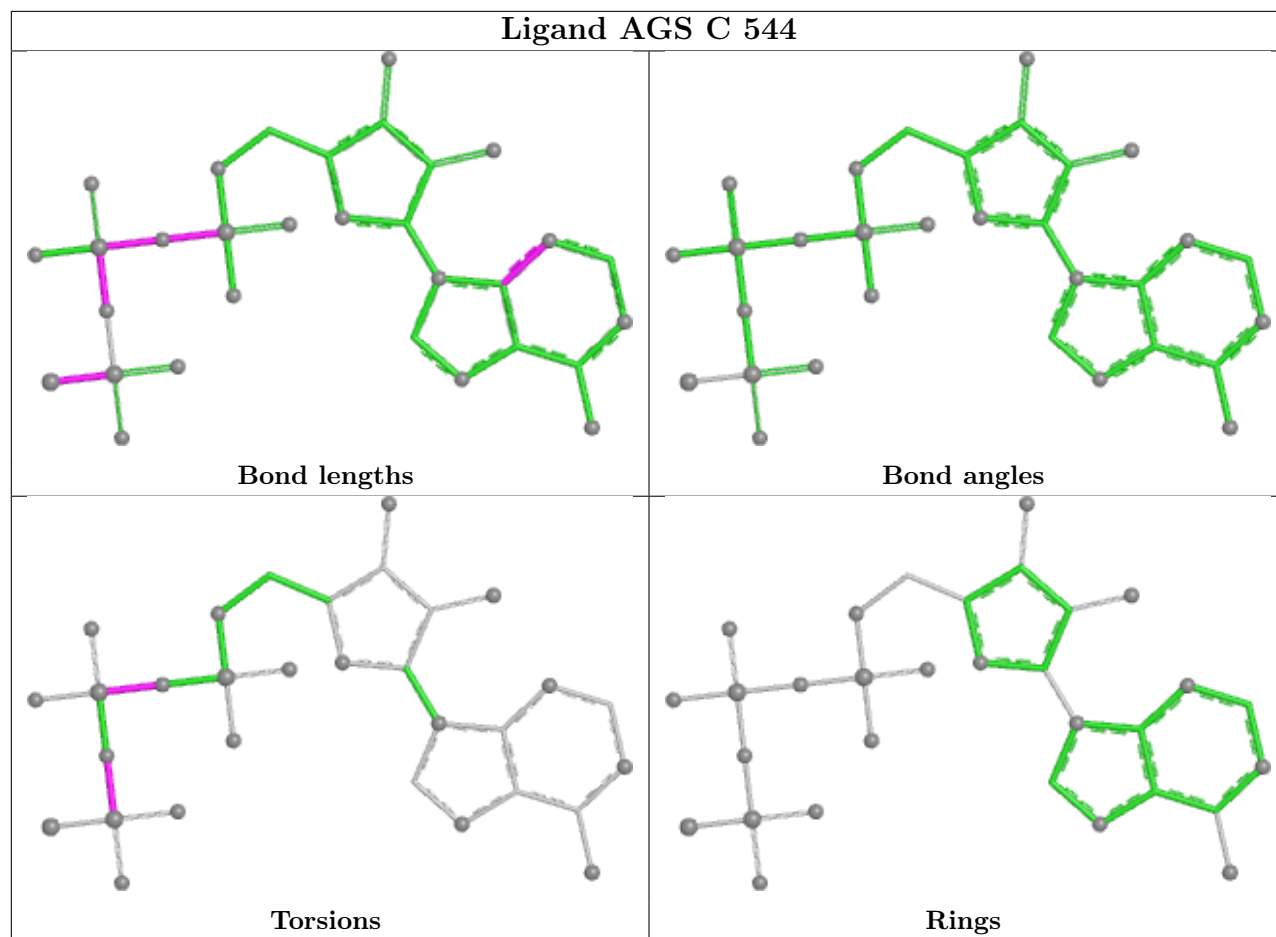
There are no ring outliers.

4 monomers are involved in 27 short contacts:

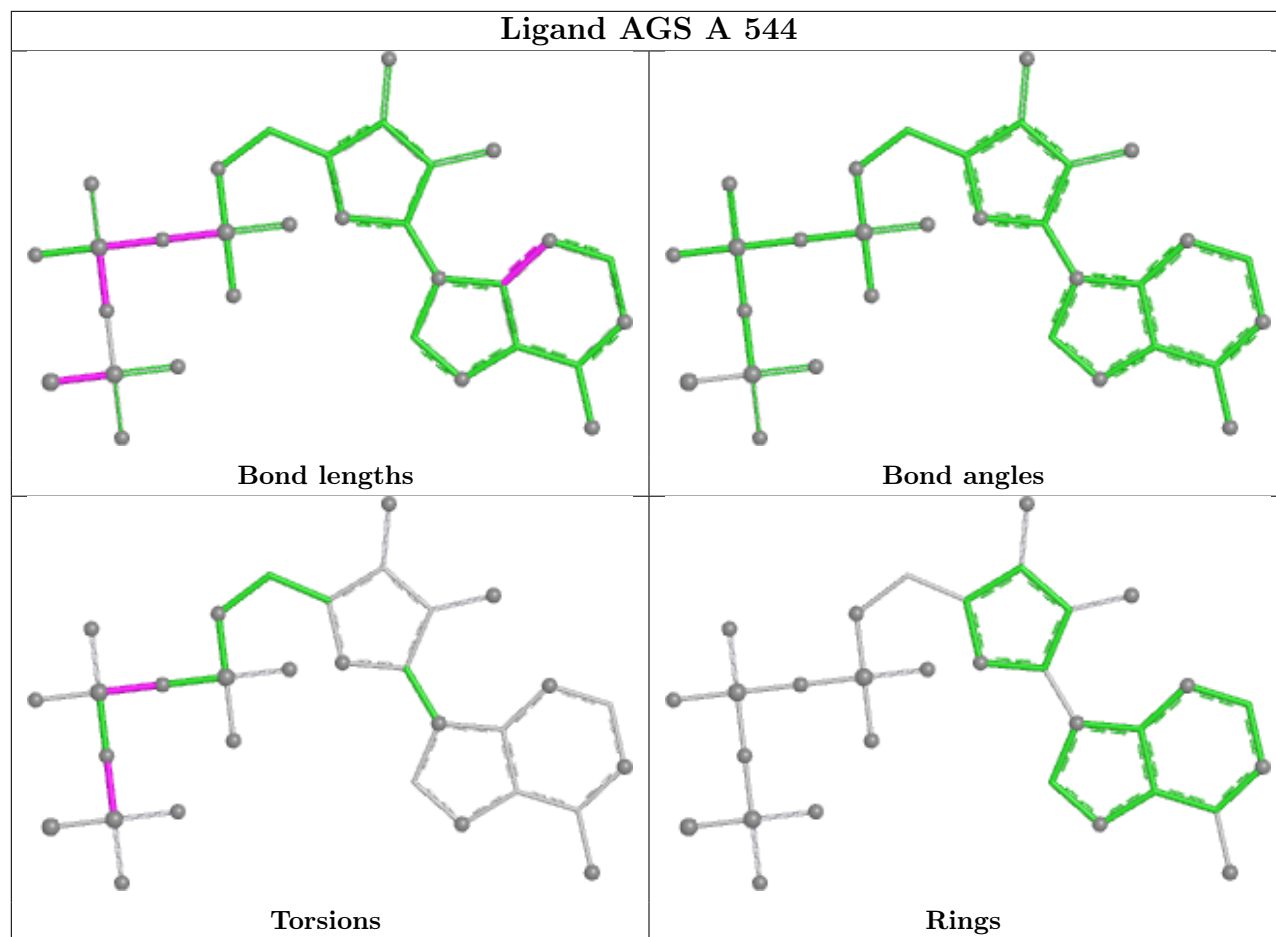
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	544	AGS	6	0
2	A	544	AGS	5	0
2	D	544	AGS	11	0
2	B	544	AGS	5	0

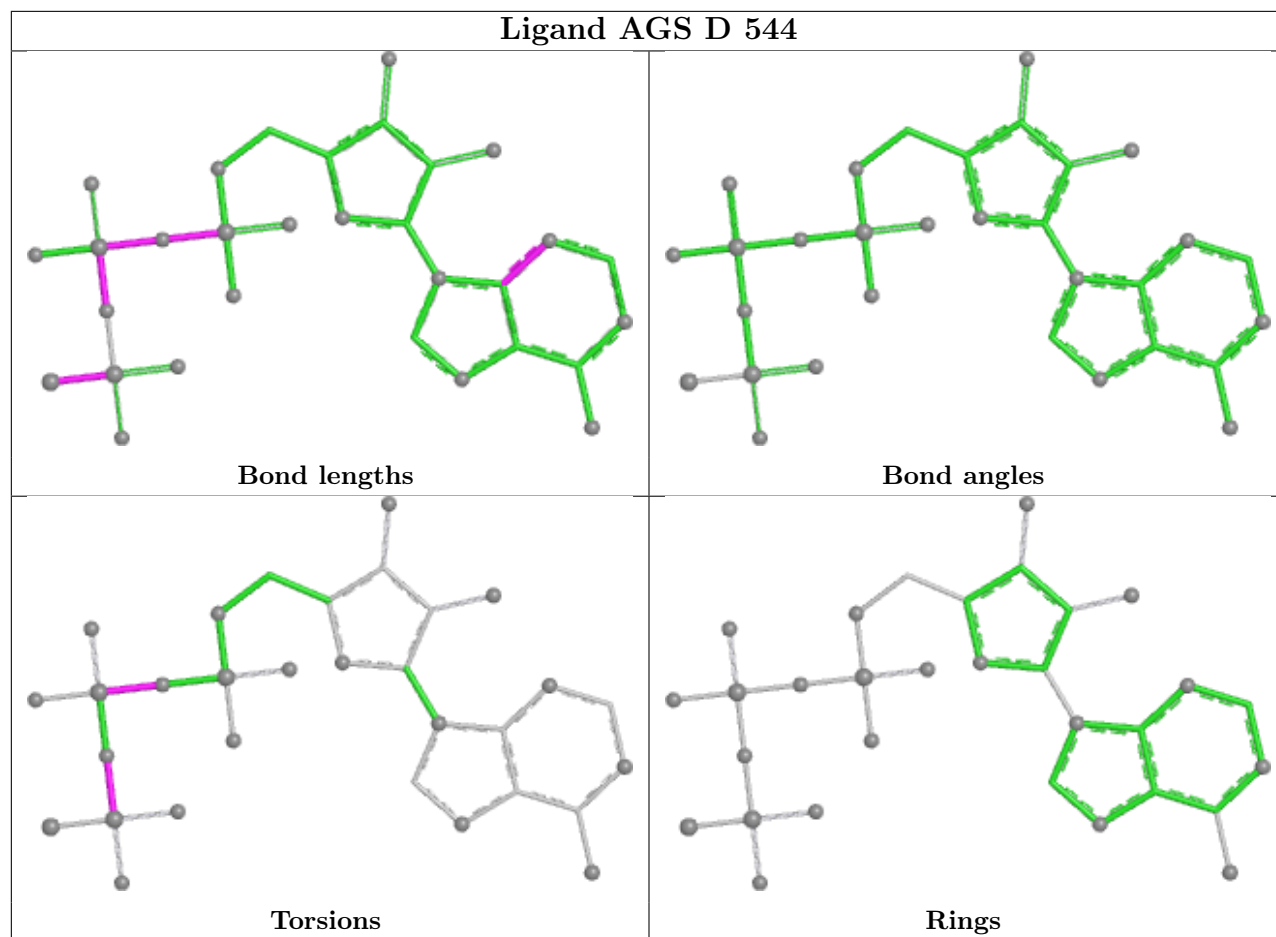
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

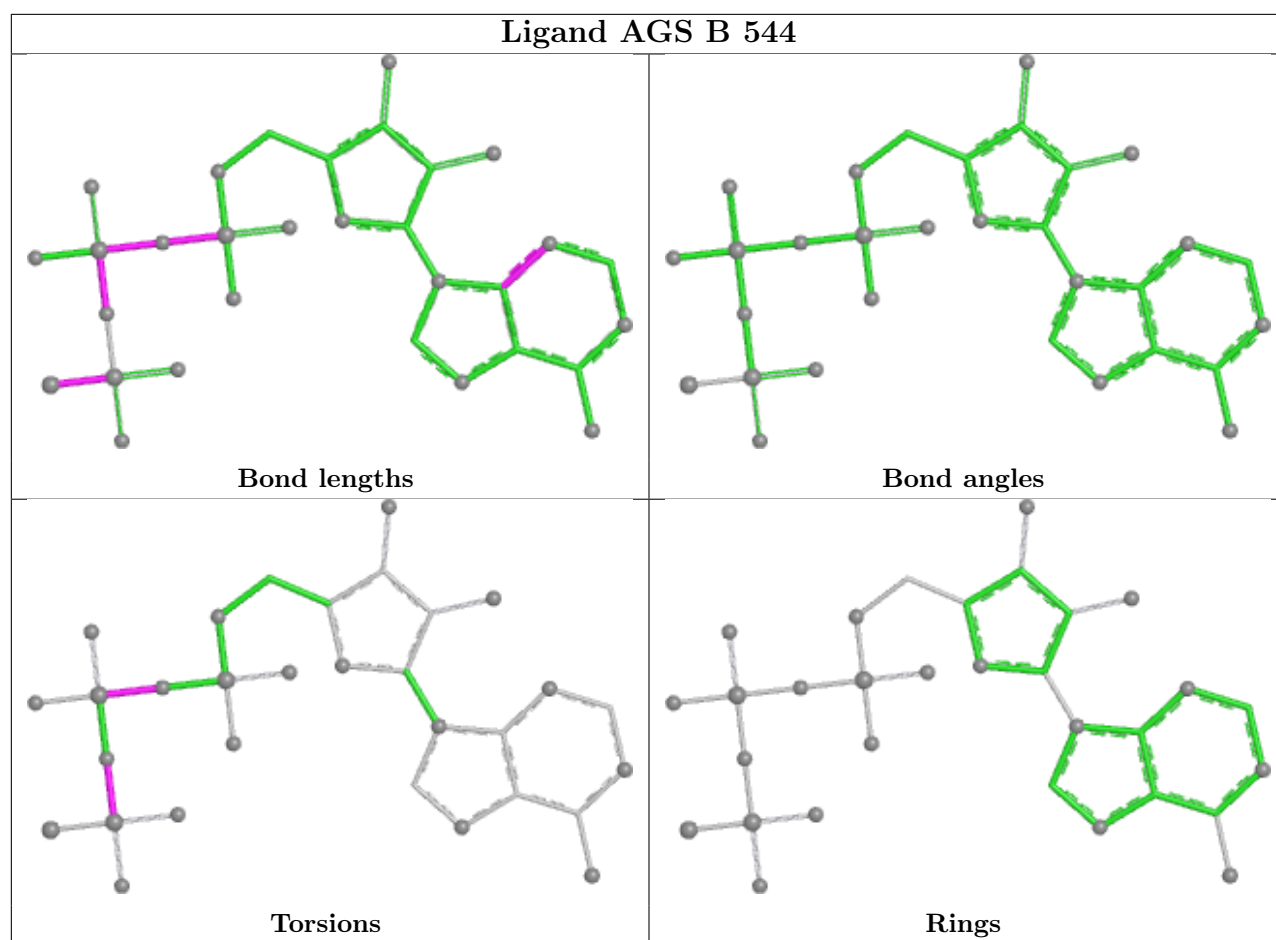
Ligand AGS C 544



Ligand AGS A 544







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th 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	487/521 (93%)	-0.02	15 (3%) 51 45	283, 526, 830, 912	0
1	B	487/521 (93%)	0.13	22 (4%) 38 38	246, 522, 794, 846	0
1	C	487/521 (93%)	-0.09	10 (2%) 63 54	294, 527, 844, 901	0
1	D	484/521 (92%)	0.03	13 (2%) 56 48	303, 528, 839, 939	0
All	All	1945/2084 (93%)	0.01	60 (3%) 51 45	246, 526, 824, 939	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	494	VAL	7.9
1	B	495	LYS	7.7
1	D	384	VAL	5.4
1	B	388	VAL	4.8
1	D	388	VAL	4.7
1	D	414	LYS	4.4
1	D	41	PRO	4.3
1	D	387	ALA	4.2
1	C	494	VAL	4.0
1	B	490	GLU	3.9
1	A	285	PHE	3.8
1	A	420	GLU	3.7
1	B	460	ARG	3.7
1	C	495	LYS	3.7
1	B	387	ALA	3.5
1	B	400	ILE	3.5
1	C	388	VAL	3.4
1	A	305	ALA	3.4
1	C	158	ILE	3.2
1	B	491	PRO	3.1
1	B	489	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	284	LEU	3.1
1	B	411	LEU	3.0
1	A	159	THR	3.0
1	B	401	VAL	2.9
1	B	135	LEU	2.9
1	A	48	LEU	2.9
1	D	417	GLU	2.9
1	C	178	VAL	2.9
1	D	56	VAL	2.8
1	B	431	ARG	2.8
1	B	410	GLU	2.8
1	A	384	VAL	2.7
1	D	420	GLU	2.6
1	B	239	ILE	2.5
1	B	407	THR	2.5
1	C	391	VAL	2.5
1	D	195	ILE	2.5
1	B	416	ARG	2.4
1	A	276	ILE	2.4
1	C	384	VAL	2.4
1	A	388	VAL	2.4
1	A	51	ASP	2.4
1	B	384	VAL	2.4
1	C	135	LEU	2.4
1	A	158	ILE	2.3
1	B	101	GLY	2.3
1	A	495	LYS	2.3
1	D	21	GLN	2.2
1	B	517	ALA	2.2
1	A	91	ASP	2.2
1	C	387	ALA	2.1
1	A	332	LEU	2.1
1	D	383	ALA	2.1
1	B	391	VAL	2.1
1	B	420	GLU	2.1
1	C	285	PHE	2.0
1	D	193	ILE	2.0
1	A	494	VAL	2.0
1	D	159	THR	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

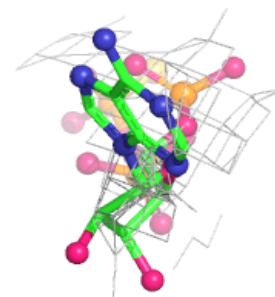
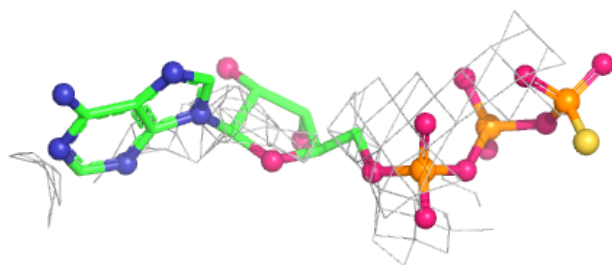
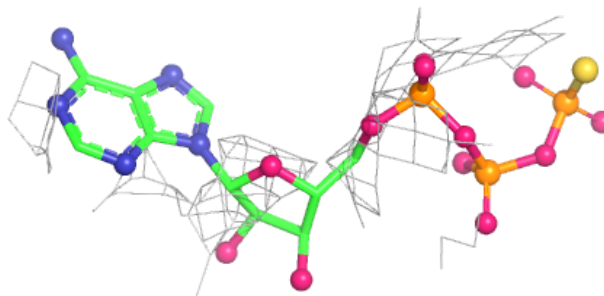
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AGS	C	544	31/31	0.90	0.11	209,414,549,549	0
2	AGS	A	544	31/31	0.94	0.11	260,437,549,549	0
2	AGS	D	544	31/31	0.94	0.11	209,409,549,549	0
2	AGS	B	544	31/31	0.95	0.10	255,382,549,549	0

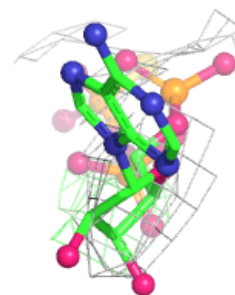
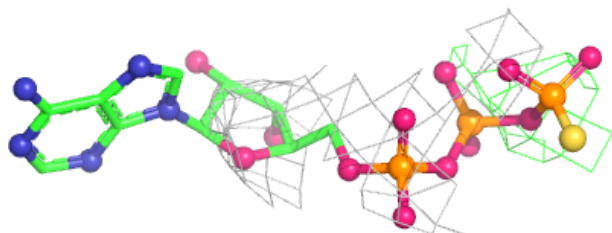
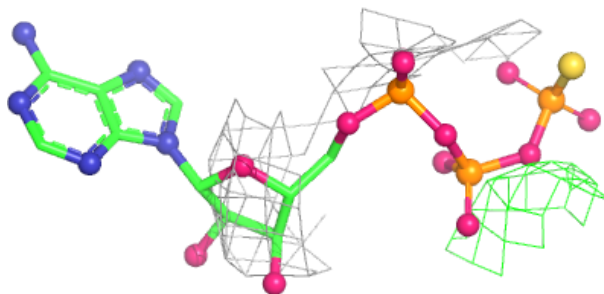
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS C 544:

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

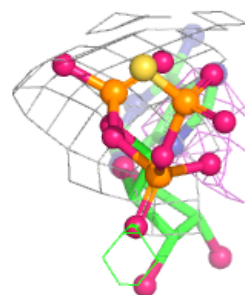
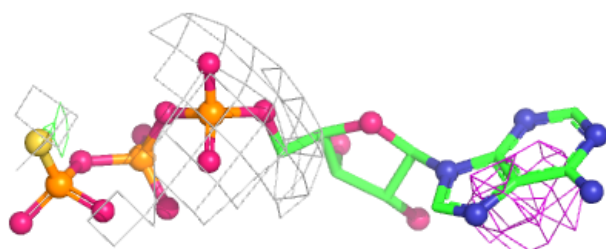
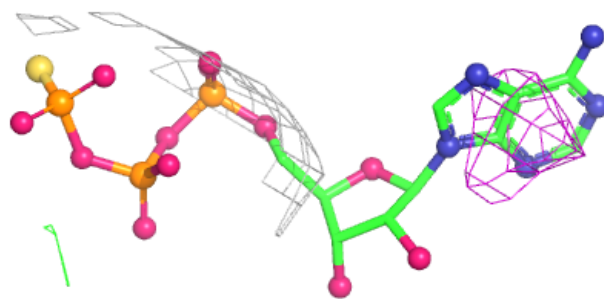
**Electron density around AGS A 544:**

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

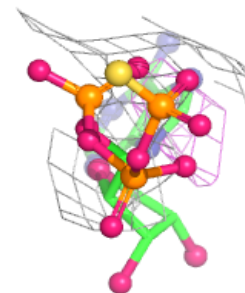
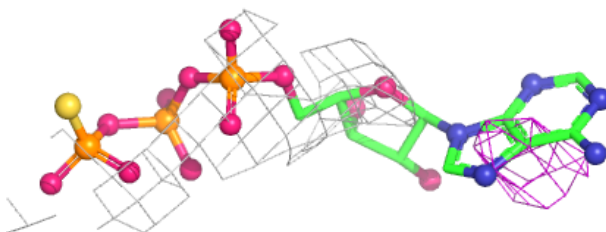
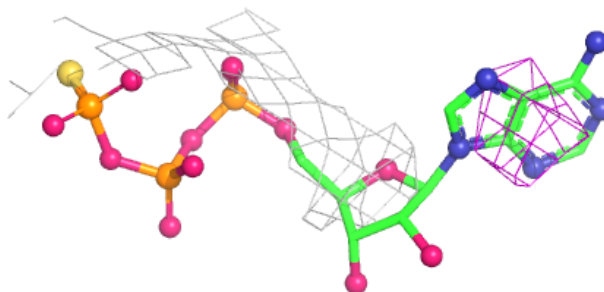


Electron density around AGS D 544:

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

**Electron density around AGS B 544:**

$2mF_o-DF_c$ (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.