



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:12 PM UTC

PDB ID : 3EIH / pdb_00003eih
Title : Crystal structure of S.cerevisiae Vps4 in the presence of ATPgammaS
Authors : Gonciarz, M.D.; Whitby, F.G.; Eckert, D.M.; Kieffer, C.; Heroux, A.; Sundquist, W.I.; Hill, C.P.
Deposited on : 2008-09-15
Resolution : 3.25 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

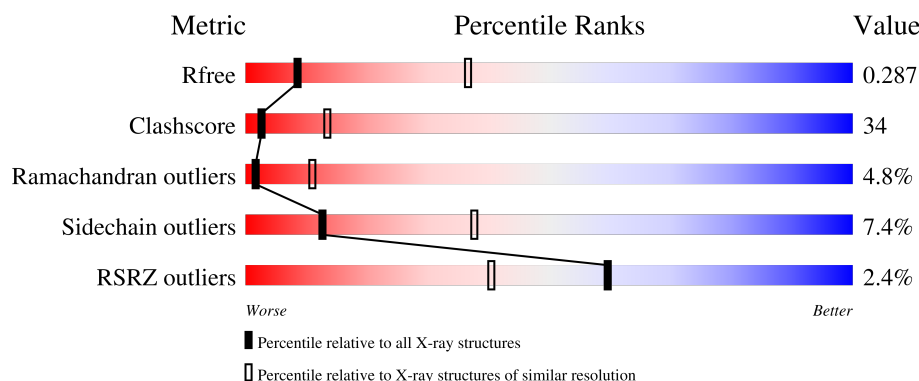
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	340	
1	B	340	
1	C	340	

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
4	EDO	C	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7396 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 Vacuolar protein sorting-associated protein 4.

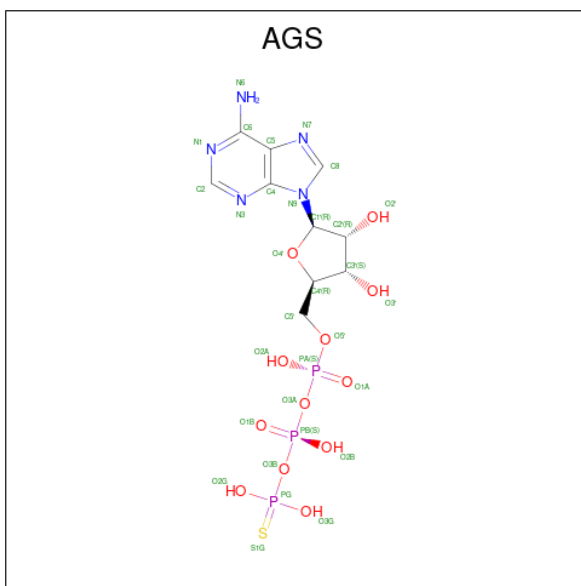
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2469	1552	419	489	9			
1	B	316	Total	C	N	O	S	0	0	0
			2449	1540	415	485	9			
1	C	310	Total	C	N	O	S	0	0	0
			2409	1518	407	475	9			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	GLY	-	expression tag	UNP P52917
A	99	ILE	-	expression tag	UNP P52917
A	100	ASP	-	expression tag	UNP P52917
A	101	PRO	-	expression tag	UNP P52917
A	102	PHE	-	expression tag	UNP P52917
A	103	THR	-	expression tag	UNP P52917
A	233	GLN	GLU	engineered mutation	UNP P52917
B	98	GLY	-	expression tag	UNP P52917
B	99	ILE	-	expression tag	UNP P52917
B	100	ASP	-	expression tag	UNP P52917
B	101	PRO	-	expression tag	UNP P52917
B	102	PHE	-	expression tag	UNP P52917
B	103	THR	-	expression tag	UNP P52917
B	233	GLN	GLU	engineered mutation	UNP P52917
C	98	GLY	-	expression tag	UNP P52917
C	99	ILE	-	expression tag	UNP P52917
C	100	ASP	-	expression tag	UNP P52917
C	101	PRO	-	expression tag	UNP P52917
C	102	PHE	-	expression tag	UNP P52917
C	103	THR	-	expression tag	UNP P52917
C	233	GLN	GLU	engineered mutation	UNP P52917

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID:

AGS) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{12}\text{P}_3\text{S}$).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).

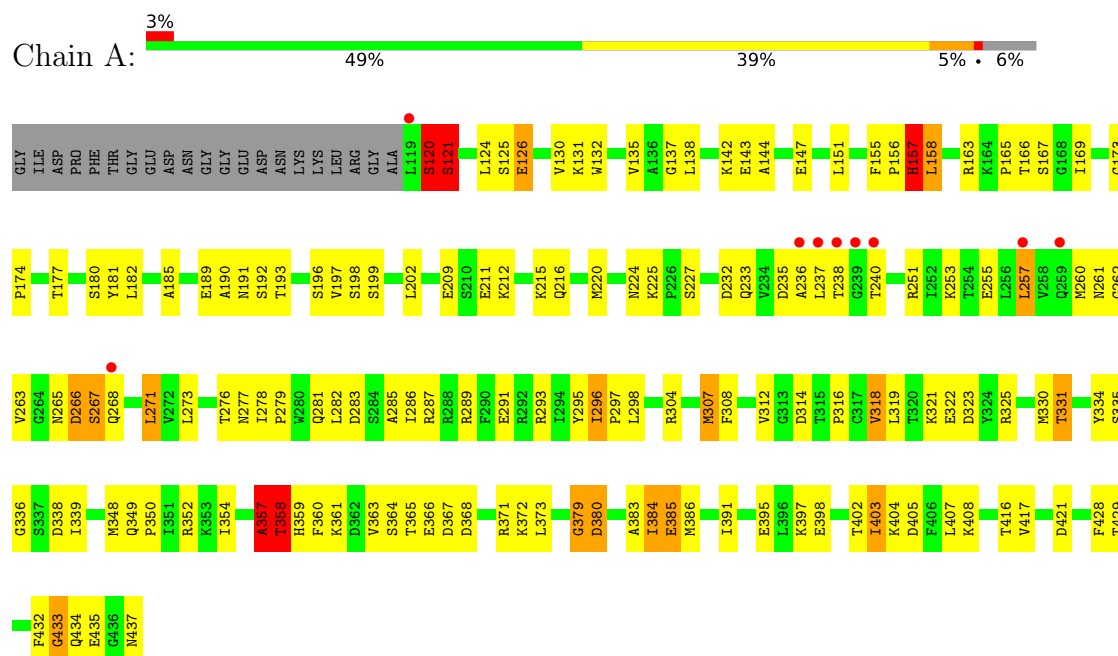


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		

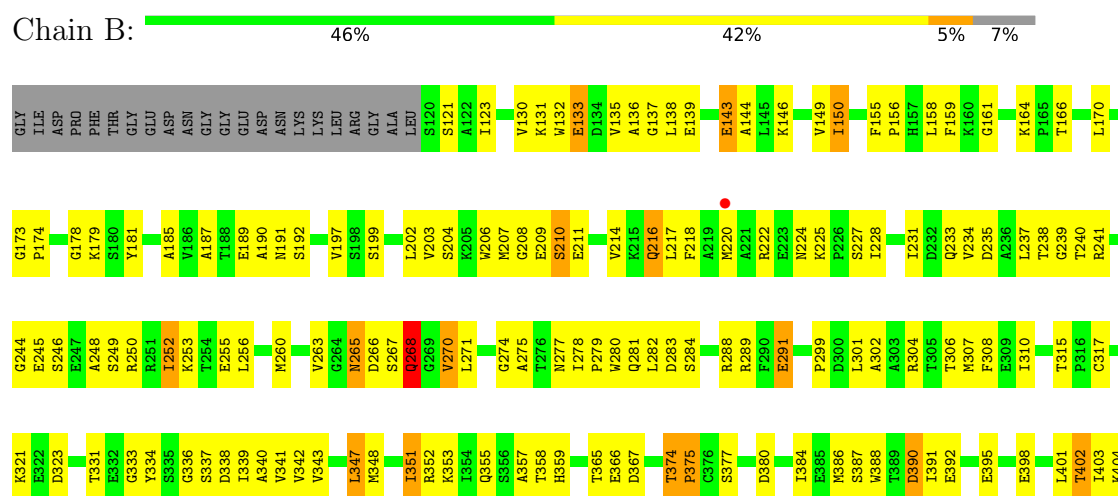
3 Residue-property plots

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: Vacuolar protein sorting-associated protein 4

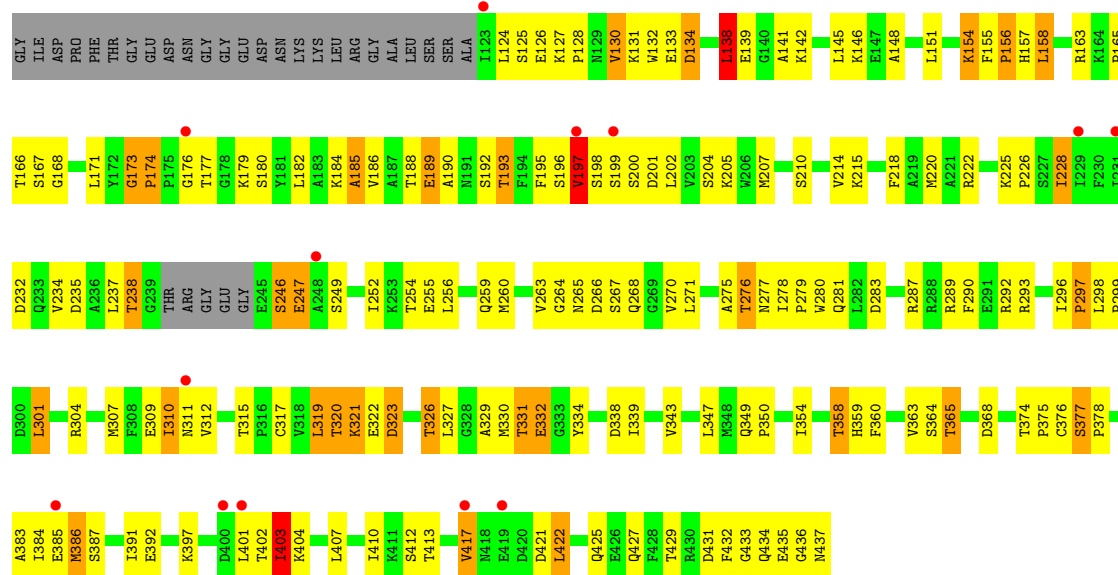


- Molecule 1: Vacuolar protein sorting-associated protein 4





• Molecule 1: Vacuolar protein sorting-associated protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.96Å 119.80Å 156.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 3.25 33.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.00-3.25) 99.8 (33.00-3.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.4.0054	Depositor
R, R_{free}	0.226 , 0.305 0.243 , 0.287	Depositor DCC
R_{free} test set	1208 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	79.8	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7396	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: EDO, MG, 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	0.80	0/2511	1.23	18/3395 (0.5%)
1	B	0.77	0/2491	1.14	15/3368 (0.4%)
1	C	0.73	1/2450 (0.0%)	1.05	6/3312 (0.2%)
All	All	0.77	1/7452 (0.0%)	1.14	39/10075 (0.4%)

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	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	PRO	CA-C	6.79	1.55	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	HIS	N-CA-C	-17.49	85.06	110.06
1	A	156	PRO	N-CA-C	16.99	147.47	112.47
1	B	216	GLN	N-CA-C	10.99	127.87	112.04
1	B	375	PRO	CA-N-CD	-9.79	98.29	112.00
1	A	156	PRO	CB-CA-C	-8.68	97.23	111.56
1	B	137	GLY	N-CA-C	-7.71	98.97	112.53
1	A	158	LEU	N-CA-C	-7.56	104.06	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	ASP	N-CA-C	7.16	119.95	111.71
1	A	395	GLU	N-CA-C	7.06	120.77	112.72
1	B	266	ASP	N-CA-C	6.91	120.16	111.24
1	B	252	ILE	N-CA-C	-6.86	106.36	112.12
1	B	174	PRO	CA-C-N	6.77	126.73	119.76
1	B	174	PRO	C-N-CA	6.77	126.73	119.76
1	C	256	LEU	N-CA-C	-6.70	105.73	114.04
1	A	240	THR	N-CA-C	6.41	119.57	109.96
1	A	120	SER	N-CA-C	6.37	115.81	108.49
1	A	357	ALA	N-CA-C	-6.37	99.32	109.76
1	A	379	GLY	N-CA-C	-6.30	99.02	111.31
1	A	318	VAL	N-CA-C	6.27	122.39	109.34
1	B	422	LEU	N-CA-C	-5.92	107.04	114.56
1	B	331	THR	N-CA-C	5.81	119.57	111.56
1	A	357	ALA	CA-C-N	5.79	132.13	121.70
1	A	357	ALA	C-N-CA	5.79	132.13	121.70
1	A	296	ILE	CA-C-N	5.78	126.24	120.52
1	A	296	ILE	C-N-CA	5.78	126.24	120.52
1	B	333	GLY	N-CA-C	-5.54	106.89	114.64
1	A	383	ALA	CA-C-N	-5.51	115.92	123.14
1	A	383	ALA	C-N-CA	-5.51	115.92	123.14
1	B	321	LYS	N-CA-C	-5.45	104.74	111.33
1	C	377	SER	CA-C-N	5.43	124.88	119.24
1	C	377	SER	C-N-CA	5.43	124.88	119.24
1	A	196	SER	N-CA-C	5.42	118.27	109.06
1	C	173	GLY	CA-C-N	5.26	123.50	119.66
1	C	173	GLY	C-N-CA	5.26	123.50	119.66
1	B	317	CYS	N-CA-C	5.21	114.48	108.49
1	C	146	LYS	N-CA-C	-5.16	105.34	110.97
1	B	341	VAL	CB-CA-C	-5.10	105.45	111.97
1	B	216	GLN	CA-C-N	5.05	130.41	123.04
1	B	216	GLN	C-N-CA	5.05	130.41	123.04

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	HIS	Peptide
1	A	357	ALA	Peptide
1	B	216	GLN	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	2469	0	2476	128	0
1	B	2449	0	2457	155	0
1	C	2409	0	2417	226	0
2	A	31	0	12	1	0
2	B	31	0	12	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	C	4	0	6	10	0
All	All	7396	0	7380	501	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (501) 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:154:LYS:HD3	1:C:155:PHE:CE1	1.61	1.34
1:B:386:MET:CE	1:B:391:ILE:HG13	1.63	1.27
1:B:374:THR:HG23	1:B:375:PRO:CD	1.68	1.24
1:C:154:LYS:HE3	1:C:155:PHE:CZ	1.75	1.21
1:C:218:PHE:CD1	1:C:259:GLN:HG2	1.75	1.21
1:C:218:PHE:CD1	1:C:259:GLN:CG	2.24	1.20
1:B:386:MET:HE2	1:B:391:ILE:CG1	1.73	1.18
1:C:287:ARG:HG2	1:C:293:ARG:HH21	1.04	1.15
1:A:147:GLU:HB2	1:B:355:GLN:OE1	1.49	1.10
1:C:154:LYS:CD	1:C:155:PHE:CE1	2.34	1.09
1:B:374:THR:HG23	1:B:375:PRO:HD3	1.32	1.07
1:C:154:LYS:CE	1:C:155:PHE:CZ	2.38	1.06
1:C:218:PHE:CE1	1:C:259:GLN:HG2	1.90	1.05
1:B:386:MET:CE	1:B:391:ILE:CG1	2.29	1.04
1:B:374:THR:CG2	1:B:375:PRO:CD	2.36	1.04
1:B:386:MET:HE2	1:B:391:ILE:CD1	1.88	1.03
1:C:263:VAL:HB	1:C:289:ARG:NH2	1.73	1.02
1:C:287:ARG:HG2	1:C:293:ARG:NH2	1.71	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:THR:HG23	1:B:375:PRO:HD2	1.40	1.00
1:B:374:THR:CG2	1:B:375:PRO:HD2	1.91	1.00
1:A:307:MET:HE3	1:A:336:GLY:HA2	1.44	0.99
1:C:154:LYS:HD3	1:C:155:PHE:HE1	1.19	0.99
1:C:287:ARG:CG	1:C:293:ARG:HH21	1.75	0.99
1:A:319:LEU:CD2	1:A:403:ILE:HD13	1.94	0.97
1:C:154:LYS:O	1:C:156:PRO:HD3	1.62	0.97
1:C:218:PHE:CG	1:C:259:GLN:CD	2.43	0.96
1:A:151:LEU:HD21	1:B:351:ILE:HG23	1.46	0.95
1:C:264:GLY:HA2	1:C:265:ASN:HB3	1.46	0.94
1:A:287:ARG:NH1	1:A:437:ASN:O	2.01	0.92
1:A:319:LEU:HD22	1:A:323:ASP:HB3	1.51	0.92
1:C:298:LEU:HD12	1:C:298:LEU:O	1.67	0.92
1:A:304:ARG:HG2	1:A:339:ILE:HD11	1.49	0.92
1:A:307:MET:CE	1:A:336:GLY:HA2	2.00	0.92
1:C:280:TRP:CZ3	1:C:425:GLN:NE2	2.38	0.92
1:C:195:PHE:CE2	1:C:220:MET:HB3	2.05	0.91
1:B:386:MET:HE2	1:B:391:ILE:HG13	1.35	0.91
1:C:218:PHE:CE1	1:C:259:GLN:CG	2.51	0.91
1:B:386:MET:HE2	1:B:391:ILE:HD11	1.53	0.90
1:B:386:MET:HE1	1:B:391:ILE:HG13	1.52	0.90
1:B:413:THR:HG22	1:B:414:ARG:N	1.83	0.90
1:C:218:PHE:CG	1:C:259:GLN:CG	2.53	0.90
1:C:127:LYS:HG2	1:C:193:THR:HA	1.54	0.89
1:C:403:ILE:O	1:C:407:LEU:HG	1.73	0.88
1:C:141:ALA:O	1:C:145:LEU:HD12	1.76	0.86
1:C:218:PHE:CB	1:C:259:GLN:OE1	2.23	0.86
1:B:375:PRO:HD2	1:B:375:PRO:O	1.75	0.86
1:A:357:ALA:HA	1:A:358:THR:OG1	1.76	0.86
1:A:403:ILE:HG22	1:A:407:LEU:HD11	1.57	0.85
1:A:384:ILE:HD12	1:A:386:MET:CE	2.05	0.85
1:C:192:SER:OG	1:C:226:PRO:HB2	1.74	0.84
1:C:218:PHE:HB2	1:C:259:GLN:CD	2.02	0.84
1:C:334:TYR:HD2	1:C:338:ASP:HB3	1.41	0.83
1:A:319:LEU:HD23	1:A:403:ILE:HD13	1.61	0.82
1:C:276:THR:HG22	1:C:278:ILE:H	1.43	0.82
1:C:218:PHE:CB	1:C:259:GLN:CD	2.54	0.81
1:A:308:PHE:O	1:A:312:VAL:HG23	1.80	0.80
1:B:413:THR:CG2	1:B:414:ARG:N	2.45	0.80
1:C:280:TRP:CH2	1:C:425:GLN:NE2	2.50	0.79
1:A:368:ASP:OD2	1:A:372:LYS:HD3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:LEU:CD2	1:C:422:LEU:HD11	2.12	0.79
1:B:323:ASP:OD1	1:B:403:ILE:HG21	1.83	0.78
1:B:250:ARG:HG2	1:B:253:LYS:HE2	1.66	0.77
1:C:154:LYS:CE	1:C:155:PHE:CE1	2.66	0.77
1:B:337:SER:O	1:B:340:ALA:HB3	1.84	0.77
1:A:216:GLN:O	1:A:220:MET:HG3	1.85	0.76
1:A:322:GLU:HA	1:A:325:ARG:HD2	1.68	0.76
1:B:185:ALA:O	1:B:189:GLU:HG2	1.85	0.76
1:A:158:LEU:HD22	1:B:398:GLU:OE1	1.85	0.76
1:B:132:TRP:CE2	1:B:189:GLU:HG3	2.20	0.76
1:B:245:GLU:HA	1:B:249:SER:HB2	1.68	0.76
1:C:260:MET:SD	1:C:289:ARG:HG2	2.26	0.76
1:C:218:PHE:CG	1:C:259:GLN:HG3	2.21	0.75
1:B:149:VAL:HG13	1:B:271:LEU:HD13	1.67	0.75
1:B:386:MET:HE1	1:B:391:ILE:CG1	2.12	0.75
1:C:365:THR:HG23	1:C:368:ASP:HB2	1.69	0.74
1:C:263:VAL:HB	1:C:289:ARG:HH22	1.53	0.74
1:C:218:PHE:CD1	1:C:259:GLN:CD	2.62	0.74
1:C:218:PHE:CD1	1:C:259:GLN:HG3	2.22	0.74
1:C:260:MET:HB3	1:C:289:ARG:HE	1.52	0.74
1:B:241:ARG:O	1:B:246:SER:HB2	1.87	0.74
1:C:158:LEU:O	1:C:163:ARG:NH1	2.20	0.74
1:C:360:PHE:HE2	1:C:387:SER:HA	1.53	0.74
1:A:257:LEU:HD23	1:A:289:ARG:HH11	1.51	0.74
1:C:350:PRO:HD3	1:C:401:LEU:CD2	2.18	0.74
1:C:218:PHE:CD2	1:C:259:GLN:HG3	2.23	0.73
1:C:317:CYS:CB	1:C:401:LEU:HB2	2.18	0.73
1:C:391:ILE:HG22	1:C:392:GLU:O	1.88	0.73
1:C:263:VAL:HB	1:C:289:ARG:HH21	1.51	0.73
1:A:429:THR:O	1:A:433:GLY:HA3	1.88	0.73
1:C:260:MET:HA	1:C:263:VAL:HG23	1.68	0.73
1:C:334:TYR:CD2	1:C:338:ASP:HB3	2.22	0.73
1:A:151:LEU:CD2	1:B:351:ILE:HG23	2.18	0.72
1:B:222:ARG:HD3	1:B:267:SER:HB2	1.70	0.72
1:C:350:PRO:HD3	1:C:401:LEU:HD21	1.71	0.72
1:C:197:VAL:HG13	1:C:198:SER:H	1.55	0.72
1:C:197:VAL:CG1	1:C:198:SER:N	2.52	0.72
1:B:235:ASP:HA	1:B:282:LEU:HD13	1.72	0.72
1:C:265:ASN:HD22	1:C:268:GLN:N	1.88	0.72
1:C:156:PRO:C	1:C:158:LEU:H	1.98	0.71
1:A:322:GLU:O	1:A:325:ARG:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD22	1:A:323:ASP:CB	2.20	0.71
1:C:154:LYS:CE	1:C:155:PHE:HZ	2.02	0.71
1:A:163:ARG:NH1	1:B:351:ILE:HD11	2.06	0.70
1:C:225:LYS:NZ	1:C:266:ASP:O	2.24	0.70
1:C:429:THR:O	1:C:433:GLY:CA	2.38	0.70
1:A:253:LYS:HG3	1:A:286:ILE:HD11	1.73	0.70
1:C:312:VAL:HG13	1:C:315:THR:HB	1.72	0.70
1:A:361:LYS:O	1:A:373:LEU:HA	1.92	0.70
1:B:225:LYS:NZ	1:B:267:SER:O	2.24	0.70
1:C:196:SER:O	1:C:197:VAL:HG23	1.91	0.69
1:C:180:SER:H	4:C:501:EDO:H12	1.57	0.69
1:A:349:GLN:HB2	1:A:350:PRO:HD3	1.72	0.69
1:C:197:VAL:CG1	1:C:198:SER:H	2.05	0.69
1:C:167:SER:HA	1:C:271:LEU:HD12	1.73	0.69
1:A:319:LEU:HD23	1:A:403:ILE:CD1	2.23	0.69
1:B:136:ALA:O	2:B:501:AGS:N6	2.26	0.69
1:C:218:PHE:CE1	1:C:259:GLN:HG3	2.28	0.69
1:A:348:MET:O	1:A:352:ARG:HG3	1.93	0.69
1:A:130:VAL:O	1:A:185:ALA:HA	1.93	0.68
1:A:304:ARG:CG	1:A:339:ILE:HD11	2.23	0.68
1:A:147:GLU:CB	1:B:355:GLN:OE1	2.35	0.68
1:B:431:ASP:O	1:B:432:PHE:CG	2.47	0.68
1:C:218:PHE:CE2	1:C:259:GLN:HG3	2.29	0.68
1:B:403:ILE:HG13	1:B:404:LYS:N	2.07	0.68
1:C:260:MET:HB3	1:C:289:ARG:NE	2.08	0.68
1:C:298:LEU:CD2	1:C:422:LEU:CD1	2.72	0.68
1:B:374:THR:HG22	1:B:375:PRO:HD2	1.74	0.67
1:A:304:ARG:HG2	1:A:339:ILE:CD1	2.20	0.67
1:A:262:GLY:O	1:A:266:ASP:HB2	1.95	0.67
1:B:365:THR:C	1:B:367:ASP:H	2.02	0.67
1:B:203:VAL:O	1:B:207:MET:HG3	1.95	0.67
1:B:323:ASP:OD1	1:B:403:ILE:CG2	2.43	0.66
1:C:315:THR:HG21	1:C:347:LEU:HD22	1.76	0.66
1:C:218:PHE:HB2	1:C:259:GLN:OE1	1.92	0.66
1:A:215:LYS:HE3	1:A:255:GLU:OE2	1.96	0.66
1:C:317:CYS:HB2	1:C:401:LEU:HB2	1.76	0.66
1:C:167:SER:HB2	1:C:263:VAL:HG12	1.78	0.65
1:A:357:ALA:HB1	1:A:359:HIS:H	1.61	0.65
1:B:203:VAL:HG13	1:B:249:SER:OG	1.96	0.65
1:C:154:LYS:HE3	1:C:155:PHE:HZ	1.49	0.65
1:B:158:LEU:HD23	1:B:158:LEU:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:PHE:CZ	1:C:259:GLN:HG3	2.32	0.65
1:A:261:ASN:N	1:A:289:ARG:HH22	1.95	0.65
1:C:228:ILE:O	1:C:228:ILE:HG22	1.97	0.65
1:C:156:PRO:O	1:C:158:LEU:N	2.23	0.64
1:C:375:PRO:O	1:C:376:CYS:HB3	1.98	0.64
1:B:413:THR:HG22	1:B:414:ARG:O	1.98	0.64
1:C:179:LYS:CB	4:C:501:EDO:H22	2.28	0.64
1:C:218:PHE:CG	1:C:259:GLN:OE1	2.49	0.64
1:C:235:ASP:OD2	1:C:276:THR:HG23	1.98	0.64
1:C:323:ASP:O	1:C:327:LEU:HG	1.97	0.63
1:C:350:PRO:CD	1:C:401:LEU:HD21	2.28	0.63
1:C:326:THR:HG22	1:C:330:MET:HE2	1.79	0.63
1:A:185:ALA:O	1:A:189:GLU:HG2	1.99	0.63
1:A:211:GLU:OE2	1:A:251:ARG:HB3	1.99	0.63
1:C:280:TRP:HH2	1:C:425:GLN:HE21	1.47	0.63
1:C:429:THR:O	1:C:433:GLY:HA3	1.97	0.62
1:C:202:LEU:HD22	1:C:210:SER:OG	2.00	0.62
1:B:413:THR:CG2	1:B:414:ARG:H	2.11	0.62
1:B:351:ILE:N	1:B:351:ILE:HD12	2.14	0.62
1:C:184:LYS:C	1:C:186:VAL:H	2.07	0.61
1:A:232:ASP:CG	1:A:233:GLN:HE21	2.08	0.61
1:A:282:LEU:HD23	1:A:287:ARG:HG3	1.80	0.61
1:B:244:GLY:O	1:B:248:ALA:HB3	2.01	0.61
1:C:317:CYS:HB3	1:C:401:LEU:HB2	1.82	0.61
1:B:428:PHE:O	1:B:432:PHE:HB2	2.01	0.61
1:C:171:LEU:HG	1:C:296:ILE:HD11	1.81	0.61
1:C:339:ILE:O	1:C:343:VAL:HG23	2.01	0.60
1:A:125:SER:O	1:A:126:GLU:HB3	2.01	0.60
1:B:365:THR:C	1:B:367:ASP:N	2.59	0.60
1:A:132:TRP:CE2	1:A:189:GLU:HG3	2.37	0.60
1:C:432:PHE:HD1	1:C:437:ASN:HB3	1.66	0.60
1:A:384:ILE:HD12	1:A:386:MET:HE2	1.82	0.60
1:B:388:TRP:HA	1:B:391:ILE:HD12	1.83	0.60
1:A:235:ASP:OD1	1:A:236:ALA:N	2.35	0.60
1:B:278:ILE:HG22	1:B:281:GLN:HB3	1.83	0.60
1:A:151:LEU:HD21	1:B:351:ILE:CG2	2.28	0.60
1:A:151:LEU:CD2	1:B:351:ILE:CG2	2.79	0.60
1:C:374:THR:HG23	1:C:375:PRO:HD2	1.83	0.60
1:A:372:LYS:HE2	1:A:397:LYS:HD3	1.84	0.59
1:C:307:MET:HA	1:C:310:ILE:HD12	1.83	0.59
1:B:211:GLU:HB2	1:B:255:GLU:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:MET:SD	1:C:289:ARG:CG	2.90	0.59
1:A:192:SER:OG	1:A:227:SER:HA	2.02	0.59
1:A:316:PRO:CG	1:A:398:GLU:OE2	2.51	0.59
1:B:343:VAL:O	1:B:347:LEU:HG	2.02	0.59
1:A:287:ARG:CD	1:A:293:ARG:HH12	2.16	0.59
1:C:127:LYS:CG	1:C:193:THR:HA	2.30	0.59
1:C:197:VAL:HG12	1:C:198:SER:N	2.18	0.59
1:C:280:TRP:HZ3	1:C:425:GLN:NE2	1.99	0.58
1:B:217:LEU:O	1:B:218:PHE:C	2.45	0.58
1:A:278:ILE:HG21	1:A:281:GLN:OE1	2.02	0.58
1:B:187:ALA:HA	1:B:228:ILE:HD12	1.83	0.58
1:C:249:SER:HA	1:C:252:ILE:HD13	1.84	0.58
1:A:307:MET:HE1	1:A:336:GLY:HA2	1.85	0.58
1:A:257:LEU:HD23	1:A:289:ARG:NH1	2.18	0.58
1:A:403:ILE:HG22	1:A:407:LEU:CD1	2.33	0.58
1:A:132:TRP:CD2	1:A:189:GLU:HG3	2.39	0.58
1:B:375:PRO:CD	1:B:375:PRO:O	2.47	0.58
1:C:173:GLY:O	1:C:277:ASN:HA	2.04	0.58
1:C:326:THR:O	1:C:329:ALA:HB3	2.03	0.58
1:B:279:PRO:HD2	1:B:280:TRP:CE3	2.39	0.58
1:B:199:SER:HB3	1:B:233:GLN:O	2.03	0.57
1:A:404:LYS:HA	1:A:407:LEU:HD12	1.86	0.57
1:C:179:LYS:HB2	4:C:501:EDO:H22	1.86	0.57
1:A:173:GLY:O	1:A:277:ASN:HA	2.05	0.57
1:B:211:GLU:OE1	1:B:255:GLU:HB2	2.05	0.57
1:C:167:SER:HB3	1:C:268:GLN:HE22	1.67	0.57
1:C:265:ASN:HD22	1:C:268:GLN:HB2	1.70	0.57
1:C:218:PHE:HB2	1:C:259:GLN:NE2	2.19	0.57
1:C:360:PHE:HE2	1:C:387:SER:CA	2.16	0.57
1:A:215:LYS:CG	1:A:255:GLU:OE2	2.52	0.57
1:C:331:THR:HG21	1:C:339:ILE:HD13	1.85	0.57
1:B:146:LYS:HA	1:B:150:ILE:HD13	1.87	0.56
1:B:279:PRO:HD2	1:B:280:TRP:CZ3	2.40	0.56
1:A:283:ASP:HB3	1:A:286:ILE:HD12	1.88	0.56
1:A:287:ARG:HD3	1:A:293:ARG:HH12	1.70	0.56
1:A:363:VAL:HG12	1:A:363:VAL:O	2.06	0.56
1:C:179:LYS:H	4:C:501:EDO:H11	1.70	0.56
1:C:320:THR:HG22	1:C:322:GLU:H	1.70	0.56
1:B:158:LEU:HD22	1:B:159:PHE:CE1	2.41	0.56
1:C:177:THR:OG1	1:C:179:LYS:NZ	2.34	0.56
1:C:199:SER:C	1:C:201:ASP:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HG3	1:A:255:GLU:OE2	2.06	0.56
1:B:336:GLY:HA2	1:B:339:ILE:HD12	1.88	0.56
1:B:338:ASP:O	1:B:342:VAL:HG23	2.06	0.56
1:C:222:ARG:HG2	1:C:266:ASP:OD2	2.06	0.56
1:C:168:GLY:HA3	1:C:290:PHE:HA	1.87	0.55
1:B:237:LEU:O	1:B:253:LYS:HD3	2.06	0.55
1:B:208:GLY:C	1:B:210:SER:H	2.13	0.55
1:B:284:SER:HB2	1:B:288:ARG:NH1	2.21	0.55
1:C:179:LYS:HB3	4:C:501:EDO:H22	1.89	0.55
1:C:204:SER:O	1:C:205:LYS:HG3	2.07	0.55
1:C:263:VAL:CB	1:C:289:ARG:NH2	2.61	0.55
1:C:293:ARG:O	1:C:434:GLN:NE2	2.40	0.55
1:B:374:THR:CG2	1:B:375:PRO:HD3	2.14	0.55
1:A:316:PRO:HG3	1:A:398:GLU:OE2	2.07	0.54
1:B:256:LEU:O	1:B:260:MET:HG3	2.07	0.54
1:C:195:PHE:CZ	1:C:220:MET:HB3	2.42	0.54
1:C:278:ILE:HG22	1:C:278:ILE:O	2.05	0.54
1:C:349:GLN:N	1:C:350:PRO:HD2	2.23	0.54
1:A:429:THR:O	1:A:433:GLY:CA	2.56	0.54
1:B:204:SER:HA	1:B:207:MET:CE	2.37	0.54
1:A:166:THR:HG23	1:A:291:GLU:OE1	2.07	0.54
1:A:384:ILE:CD1	1:A:386:MET:CE	2.82	0.54
1:B:203:VAL:O	1:B:203:VAL:HG12	2.06	0.54
1:C:246:SER:O	1:C:247:GLU:HG2	2.08	0.54
1:C:134:ASP:N	1:C:134:ASP:OD1	2.41	0.53
1:C:301:LEU:N	1:C:304:ARG:HH21	2.06	0.53
1:A:137:GLY:O	1:A:142:LYS:HE3	2.08	0.53
1:C:156:PRO:C	1:C:158:LEU:N	2.62	0.53
1:C:176:GLY:N	4:C:501:EDO:H21	2.21	0.53
1:A:174:PRO:HD2	1:A:177:THR:HG21	1.91	0.53
1:A:348:MET:HB2	1:A:352:ARG:CZ	2.39	0.53
1:B:386:MET:CE	1:B:391:ILE:HG12	2.34	0.53
1:C:265:ASN:ND2	1:C:268:GLN:HB2	2.23	0.53
1:C:195:PHE:HE2	1:C:220:MET:C	2.16	0.53
1:A:331:THR:O	1:A:334:TYR:HB2	2.08	0.53
1:B:263:VAL:HG22	1:B:270:VAL:HG22	1.90	0.53
1:A:151:LEU:HD12	1:A:155:PHE:HD1	1.74	0.53
1:B:131:LYS:HA	1:B:189:GLU:OE2	2.09	0.53
2:B:501:AGS:O1A	2:B:501:AGS:H3'	2.10	0.52
1:C:139:GLU:HA	1:C:142:LYS:HE3	1.91	0.52
1:A:360:PHE:HB2	1:A:386:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:THR:C	1:A:367:ASP:H	2.17	0.52
1:B:392:GLU:O	1:B:395:GLU:HG2	2.10	0.52
1:C:218:PHE:HB3	1:C:259:GLN:OE1	2.08	0.52
1:C:278:ILE:HG21	1:C:281:GLN:OE1	2.09	0.52
1:B:179:LYS:HE2	1:B:277:ASN:OD1	2.10	0.52
1:B:240:THR:HA	1:B:250:ARG:HH22	1.74	0.52
1:C:434:GLN:O	1:C:435:GLU:HB2	2.10	0.52
1:B:358:THR:HG23	1:B:359:HIS:N	2.24	0.52
1:B:377:SER:OG	1:B:380:ASP:HB2	2.09	0.52
1:C:323:ASP:HB3	1:C:403:ILE:HG12	1.92	0.51
1:C:154:LYS:HE2	1:C:155:PHE:CZ	2.42	0.51
1:C:278:ILE:HG22	1:C:281:GLN:HB2	1.91	0.51
1:A:368:ASP:OD2	1:A:372:LYS:CD	2.55	0.51
1:A:265:ASN:O	1:A:267:SER:N	2.44	0.51
1:A:283:ASP:OD2	1:A:285:ALA:HB3	2.11	0.51
1:A:432:PHE:O	1:A:433:GLY:C	2.54	0.51
1:B:250:ARG:HH11	1:B:253:LYS:NZ	2.08	0.51
1:B:250:ARG:HA	1:B:253:LYS:HG3	1.93	0.51
1:C:225:LYS:NZ	1:C:267:SER:HB2	2.25	0.51
1:C:298:LEU:HD23	1:C:422:LEU:CD1	2.40	0.51
1:B:374:THR:HG22	1:B:375:PRO:O	2.11	0.50
1:B:130:VAL:O	1:B:185:ALA:HA	2.10	0.50
1:B:365:THR:O	1:B:367:ASP:N	2.45	0.50
1:B:420:ASP:C	1:B:422:LEU:H	2.18	0.50
1:C:166:THR:HG22	1:C:167:SER:N	2.27	0.50
1:C:180:SER:N	4:C:501:EDO:H12	2.25	0.50
1:A:143:GLU:OE2	1:B:355:GLN:NE2	2.45	0.50
1:A:321:LYS:O	1:A:325:ARG:HG3	2.11	0.50
1:C:359:HIS:CE1	1:C:378:PRO:HG3	2.46	0.50
1:A:151:LEU:HD12	1:A:155:PHE:CD1	2.47	0.50
1:B:246:SER:HA	1:B:250:ARG:HG3	1.94	0.50
1:C:264:GLY:HA2	1:C:265:ASN:CB	2.27	0.50
1:C:311:ASN:HB3	1:C:343:VAL:HG11	1.94	0.50
1:C:154:LYS:C	1:C:156:PRO:HD3	2.35	0.50
1:B:220:MET:O	1:B:224:ASN:ND2	2.29	0.49
1:C:429:THR:O	1:C:433:GLY:N	2.45	0.49
1:A:354:ILE:HD11	1:A:398:GLU:HA	1.94	0.49
1:C:138:LEU:O	1:C:142:LYS:HE2	2.12	0.49
1:B:386:MET:HE3	1:B:390:ASP:HB3	1.94	0.49
1:A:279:PRO:HB2	1:A:428:PHE:CD2	2.47	0.49
1:A:364:SER:OG	1:A:371:ARG:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:LEU:CG	1:C:296:ILE:HD11	2.43	0.49
1:B:284:SER:HB2	1:B:288:ARG:HH11	1.76	0.49
1:A:260:MET:C	1:A:289:ARG:HH22	2.21	0.49
1:C:360:PHE:CE2	1:C:387:SER:HA	2.41	0.49
1:A:165:PRO:HG2	1:A:268:GLN:OE1	2.12	0.49
1:C:202:LEU:HB3	1:C:207:MET:HG3	1.95	0.49
1:A:307:MET:HE2	1:A:339:ILE:HD12	1.94	0.49
1:B:143:GLU:O	1:B:144:ALA:C	2.56	0.49
1:B:203:VAL:O	1:B:203:VAL:CG1	2.60	0.49
1:C:374:THR:OG1	1:C:397:LYS:O	2.21	0.49
1:A:131:LYS:HA	1:A:189:GLU:OE2	2.12	0.48
1:C:167:SER:HB2	1:C:263:VAL:CG1	2.43	0.48
1:C:260:MET:O	1:C:289:ARG:NH2	2.36	0.48
1:C:326:THR:HG22	1:C:330:MET:CE	2.42	0.48
1:C:138:LEU:HD23	1:C:297:PRO:HD2	1.95	0.48
1:C:319:LEU:CD2	1:C:403:ILE:HG13	2.43	0.48
1:A:349:GLN:NE2	1:A:408:LYS:HD3	2.28	0.48
1:C:165:PRO:HD2	1:C:268:GLN:HG2	1.94	0.48
1:C:358:THR:HB	1:C:359:HIS:CE1	2.48	0.48
1:C:277:ASN:C	1:C:278:ILE:HG13	2.38	0.48
1:A:319:LEU:HD21	1:A:403:ILE:HD13	1.92	0.48
1:B:131:LYS:HE3	1:B:133:GLU:HB2	1.94	0.48
1:B:204:SER:HA	1:B:207:MET:HE2	1.95	0.48
1:C:222:ARG:HA	1:C:225:LYS:HE3	1.95	0.48
1:B:403:ILE:CG1	1:B:404:LYS:N	2.77	0.48
1:A:209:GLU:HB3	1:A:212:LYS:HD3	1.95	0.48
1:C:124:LEU:HB2	1:C:196:SER:HB3	1.96	0.48
1:B:402:THR:O	1:B:403:ILE:C	2.56	0.48
1:B:135:VAL:HG22	1:B:181:TYR:CD2	2.48	0.48
1:B:307:MET:O	1:B:308:PHE:C	2.57	0.48
1:C:228:ILE:O	1:C:228:ILE:CG2	2.61	0.47
1:C:374:THR:CG2	1:C:375:PRO:HD2	2.44	0.47
1:B:347:LEU:HA	1:B:401:LEU:HD21	1.95	0.47
1:C:179:LYS:N	4:C:501:EDO:H11	2.28	0.47
1:C:287:ARG:CG	1:C:293:ARG:NH2	2.53	0.47
1:C:360:PHE:HD2	1:C:386:MET:HG3	1.78	0.47
1:B:231:ILE:CG2	1:B:234:VAL:HG12	2.44	0.47
1:C:260:MET:HE2	1:C:289:ARG:CZ	2.45	0.47
1:B:155:PHE:N	1:B:156:PRO:HD3	2.30	0.47
1:C:436:GLY:HA3	1:C:437:ASN:HA	1.50	0.47
1:B:241:ARG:HB3	1:B:245:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:VAL:H	1:C:188:THR:HG21	1.78	0.47
1:C:301:LEU:HD12	1:C:304:ARG:NH2	2.29	0.47
1:C:171:LEU:CD2	1:C:296:ILE:HD11	2.45	0.47
1:B:173:GLY:O	1:B:277:ASN:HA	2.14	0.47
1:A:135:VAL:HG22	1:A:181:TYR:HD2	1.80	0.47
1:C:385:GLU:O	1:C:386:MET:CB	2.63	0.47
1:A:335:SER:O	1:A:338:ASP:HB2	2.15	0.47
1:B:323:ASP:CG	1:B:403:ILE:CG2	2.88	0.47
1:A:190:ALA:O	1:A:191:ASN:C	2.58	0.46
1:A:384:ILE:HD12	1:A:386:MET:HE1	1.94	0.46
1:B:231:ILE:HG22	1:B:234:VAL:HG12	1.97	0.46
1:A:276:THR:O	1:A:276:THR:HG23	2.13	0.46
1:C:125:SER:O	1:C:126:GLU:HB2	2.16	0.46
1:A:167:SER:O	1:A:271:LEU:HD12	2.15	0.46
1:A:384:ILE:CD1	1:A:386:MET:HE1	2.46	0.46
1:B:210:SER:HB2	1:B:252:ILE:HG12	1.98	0.46
1:C:199:SER:C	1:C:201:ASP:N	2.74	0.46
1:A:379:GLY:O	1:A:380:ASP:HB2	2.16	0.46
1:B:234:VAL:HG22	1:B:275:ALA:O	2.16	0.45
1:B:392:GLU:HB2	1:B:395:GLU:OE2	2.16	0.45
1:C:298:LEU:HD22	1:C:422:LEU:CD1	2.44	0.45
1:B:306:THR:HG22	1:B:310:ILE:CD1	2.46	0.45
1:A:135:VAL:HG11	1:A:182:LEU:HD13	1.97	0.45
1:A:260:MET:C	1:A:289:ARG:NH2	2.74	0.45
1:B:306:THR:HG22	1:B:310:ILE:HD12	1.99	0.45
1:C:130:VAL:N	1:C:188:THR:HG21	2.31	0.45
1:C:225:LYS:HZ2	1:C:267:SER:HB2	1.81	0.45
1:C:403:ILE:H	1:C:403:ILE:HD12	1.81	0.45
1:A:348:MET:HB2	1:A:352:ARG:NH1	2.32	0.45
1:B:301:LEU:O	1:B:302:ALA:C	2.60	0.45
1:C:265:ASN:HD22	1:C:268:GLN:H	1.61	0.45
1:A:357:ALA:HB1	1:A:359:HIS:N	2.28	0.45
1:C:287:ARG:O	1:C:293:ARG:NH2	2.50	0.45
1:C:210:SER:O	1:C:252:ILE:HG13	2.17	0.45
1:C:403:ILE:HD12	1:C:403:ILE:N	2.32	0.45
1:B:178:GLY:HA2	2:B:501:AGS:O1A	2.16	0.45
1:C:293:ARG:HD2	1:C:432:PHE:O	2.17	0.45
1:C:331:THR:O	1:C:332:GLU:C	2.59	0.44
1:C:360:PHE:CD1	1:C:375:PRO:HA	2.52	0.44
1:C:427:GLN:HE21	1:C:431:ASP:CG	2.24	0.44
1:A:120:SER:HB3	1:A:121:SER:H	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LYS:HG2	1:C:193:THR:CA	2.36	0.44
1:A:135:VAL:HG22	1:A:181:TYR:CD2	2.51	0.44
1:C:298:LEU:HD23	1:C:422:LEU:HD12	2.00	0.44
1:C:323:ASP:HB3	1:C:403:ILE:CG1	2.47	0.44
1:C:402:THR:C	1:C:404:LYS:N	2.75	0.44
1:A:358:THR:O	1:A:385:GLU:HA	2.18	0.44
1:B:359:HIS:HA	1:B:384:ILE:O	2.18	0.44
1:C:235:ASP:OD2	1:C:276:THR:CG2	2.63	0.44
1:B:197:VAL:HG21	1:B:202:LEU:HD12	1.98	0.44
1:C:280:TRP:HZ3	1:C:425:GLN:CD	2.24	0.44
1:A:235:ASP:C	1:A:237:LEU:H	2.26	0.44
1:B:166:THR:HG23	1:B:291:GLU:OE1	2.17	0.44
1:C:182:LEU:O	1:C:182:LEU:HG	2.18	0.44
1:C:235:ASP:HB3	1:C:276:THR:CG2	2.48	0.44
1:C:385:GLU:O	1:C:386:MET:HB3	2.17	0.44
1:A:174:PRO:HB3	1:A:421:ASP:OD2	2.18	0.44
1:A:330:MET:O	1:A:330:MET:HG2	2.18	0.44
1:B:307:MET:SD	1:B:336:GLY:HA2	2.58	0.44
1:B:334:TYR:CD2	1:B:338:ASP:HB3	2.53	0.44
1:B:348:MET:O	1:B:352:ARG:HG3	2.17	0.44
1:B:374:THR:HG22	1:B:375:PRO:CD	2.36	0.44
1:B:204:SER:HA	1:B:207:MET:HE3	2.00	0.43
1:C:327:LEU:HA	1:C:330:MET:HG2	2.00	0.43
1:C:179:LYS:HE2	4:C:501:EDO:H22	1.99	0.43
1:C:195:PHE:CZ	1:C:220:MET:HE2	2.53	0.43
1:C:238:THR:OG1	1:C:283:ASP:HB2	2.19	0.43
1:C:320:THR:O	1:C:323:ASP:N	2.47	0.43
1:A:278:ILE:O	1:A:278:ILE:HG22	2.18	0.43
1:B:123:ILE:HD13	1:B:217:LEU:HB2	2.00	0.43
1:B:299:PRO:HB2	1:B:304:ARG:HG3	2.00	0.43
1:C:174:PRO:HB3	1:C:417:VAL:HG21	2.00	0.43
1:C:222:ARG:HE	1:C:266:ASP:HB3	1.84	0.43
1:B:429:THR:O	1:B:430:ARG:C	2.61	0.43
1:B:435:GLU:O	1:B:435:GLU:CD	2.61	0.43
1:A:138:LEU:HD21	1:A:296:ILE:HG23	2.00	0.43
1:A:199:SER:HB2	1:A:233:GLN:HB2	2.00	0.43
1:A:295:TYR:CE2	1:A:297:PRO:HB3	2.54	0.43
1:C:299:PRO:HB2	1:C:304:ARG:HG3	2.00	0.43
1:C:188:THR:C	1:C:190:ALA:H	2.27	0.43
1:A:349:GLN:HG3	1:A:405:ASP:OD1	2.19	0.43
1:B:131:LYS:HE3	1:B:133:GLU:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ILE:HD12	1:B:351:ILE:H	1.82	0.43
1:A:143:GLU:OE1	1:A:143:GLU:HA	2.19	0.42
1:B:431:ASP:O	1:B:432:PHE:CD2	2.71	0.42
1:B:283:ASP:OD1	1:B:283:ASP:C	2.62	0.42
1:C:252:ILE:H	1:C:252:ILE:HD12	1.84	0.42
1:B:351:ILE:N	1:B:351:ILE:CD1	2.81	0.42
1:B:277:ASN:C	1:B:279:PRO:HD3	2.45	0.42
1:C:265:ASN:HD22	1:C:268:GLN:CB	2.33	0.42
1:C:350:PRO:HG3	1:C:401:LEU:HD21	2.00	0.42
1:A:402:THR:O	1:A:405:ASP:HB2	2.19	0.42
1:C:167:SER:HB3	1:C:268:GLN:NE2	2.34	0.42
1:A:189:GLU:HA	1:A:189:GLU:OE1	2.20	0.42
1:B:170:LEU:HD12	1:B:274:GLY:O	2.20	0.42
1:C:131:LYS:C	1:C:133:GLU:H	2.28	0.42
1:C:195:PHE:CE2	1:C:220:MET:CB	2.91	0.42
1:C:279:PRO:HD2	1:C:425:GLN:HE22	1.85	0.42
1:C:287:ARG:HG3	1:C:293:ARG:HE	1.83	0.42
1:A:197:VAL:HG21	1:A:202:LEU:HD22	2.02	0.42
1:B:121:SER:C	1:B:123:ILE:N	2.77	0.42
1:B:306:THR:O	1:B:307:MET:C	2.63	0.42
1:B:402:THR:C	1:B:404:LYS:N	2.75	0.42
1:C:320:THR:O	1:C:321:LYS:C	2.62	0.42
1:C:410:ILE:O	1:C:413:THR:O	2.37	0.42
1:A:125:SER:O	1:A:126:GLU:CB	2.64	0.42
1:B:131:LYS:HG3	1:B:133:GLU:HB2	2.02	0.42
1:C:182:LEU:O	1:C:186:VAL:HG23	2.20	0.42
1:C:215:LYS:HA	1:C:259:GLN:NE2	2.35	0.42
1:C:292:ARG:HE	1:C:292:ARG:HB2	1.61	0.41
1:B:263:VAL:CG2	1:B:270:VAL:CG2	2.98	0.41
1:C:309:GLU:O	1:C:310:ILE:C	2.63	0.41
1:A:298:LEU:HD21	1:A:417:VAL:HG21	2.03	0.41
1:B:214:VAL:HG11	1:B:255:GLU:HG3	2.02	0.41
2:B:501:AGS:N3	2:B:501:AGS:H2'	2.36	0.41
1:A:147:GLU:HB2	1:B:355:GLN:CD	2.36	0.41
1:A:278:ILE:HG21	1:A:281:GLN:CD	2.45	0.41
1:B:278:ILE:N	1:B:278:ILE:HD12	2.35	0.41
1:B:402:THR:HB	1:B:404:LYS:HB2	2.02	0.41
1:B:133:GLU:CD	1:B:133:GLU:H	2.29	0.41
1:B:190:ALA:O	1:B:192:SER:N	2.54	0.41
1:C:375:PRO:O	1:C:376:CYS:CB	2.65	0.41
1:C:138:LEU:CD2	1:C:297:PRO:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:SER:HG	1:C:226:PRO:HB2	1.81	0.41
1:A:163:ARG:HH11	1:B:351:ILE:HD11	1.81	0.41
1:B:263:VAL:HA	1:B:268:GLN:HB3	2.03	0.41
1:C:127:LYS:HA	1:C:128:PRO:HD3	1.80	0.41
1:C:132:TRP:HB3	1:C:142:LYS:HD2	2.02	0.41
1:C:232:ASP:OD1	1:C:275:ALA:HB3	2.21	0.41
1:C:417:VAL:HG13	1:C:421:ASP:HB3	2.03	0.41
1:A:169:ILE:HB	1:A:273:LEU:HD23	2.02	0.41
1:A:198:SER:O	1:A:199:SER:C	2.64	0.41
1:A:319:LEU:CD2	1:A:403:ILE:CD1	2.80	0.41
1:A:143:GLU:O	1:A:144:ALA:C	2.63	0.41
1:B:203:VAL:HG21	1:B:237:LEU:HD23	2.02	0.41
1:A:349:GLN:HE22	1:A:408:LYS:HE2	1.85	0.40
1:B:418:ASN:OD1	1:B:418:ASN:C	2.64	0.40
1:B:260:MET:HE2	1:B:289:ARG:HG2	2.02	0.40
1:B:263:VAL:O	1:B:268:GLN:HG2	2.20	0.40
1:B:265:ASN:O	1:B:268:GLN:NE2	2.54	0.40
1:C:184:LYS:O	1:C:186:VAL:N	2.50	0.40
1:C:214:VAL:HG11	1:C:255:GLU:O	2.21	0.40
1:C:360:PHE:CE2	1:C:386:MET:O	2.74	0.40
1:A:224:ASN:O	1:A:225:LYS:C	2.64	0.40
2:A:501:AGS:O2A	2:A:501:AGS:O2G	2.40	0.40
1:B:249:SER:O	1:B:253:LYS:HG3	2.21	0.40
1:B:413:THR:CG2	1:B:414:ARG:O	2.68	0.40
1:C:177:THR:H	4:C:501:EDO:H21	1.86	0.40
1:B:386:MET:HE1	1:B:391:ILE:HG12	1.96	0.40
1:C:246:SER:O	1:C:247:GLU:CB	2.68	0.40
1:C:360:PHE:CD2	1:C:386:MET:O	2.75	0.40
1:B:353:LYS:O	1:B:357:ALA:HB2	2.21	0.40
1:B:387:SER:O	1:B:390:ASP:HB2	2.21	0.40
1:C:148:ALA:HB2	1:C:292:ARG:NH1	2.36	0.40
1:C:185:ALA:O	1:C:189:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/340 (93%)	267 (84%)	40 (13%)	10 (3%)	3	18
1	B	314/340 (92%)	252 (80%)	47 (15%)	15 (5%)	2	11
1	C	306/340 (90%)	227 (74%)	59 (19%)	20 (6%)	1	7
All	All	937/1020 (92%)	746 (80%)	146 (16%)	45 (5%)	2	11

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ASP
1	B	191	ASN
1	B	210	SER
1	B	291	GLU
1	B	366	GLU
1	B	390	ASP
1	B	432	PHE
1	C	138	LEU
1	C	157	HIS
1	C	197	VAL
1	C	386	MET
1	C	403	ILE
1	A	366	GLU
1	A	380	ASP
1	A	433	GLY
1	A	435	GLU
1	B	161	GLY
1	B	238	THR
1	B	268	GLN
1	C	185	ALA
1	C	247	GLU
1	B	133	GLU
1	B	139	GLU
1	C	154	LYS
1	C	156	PRO
1	C	301	LEU
1	C	321	LYS
1	C	332	GLU
1	A	126	GLU
1	A	238	THR

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Mol	Chain	Res	Type
1	A	358	THR
1	B	143	GLU
1	B	427	GLN
1	C	237	LEU
1	C	246	SER
1	A	121	SER
1	C	189	GLU
1	C	200	SER
1	C	297	PRO
1	C	383	ALA
1	A	318	VAL
1	B	265	ASN
1	B	239	GLY
1	C	310	ILE
1	C	354	ILE

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	272/287 (95%)	253 (93%)	19 (7%)	14	40
1	B	270/287 (94%)	257 (95%)	13 (5%)	23	50
1	C	266/287 (93%)	238 (90%)	28 (10%)	6	24
All	All	808/861 (94%)	748 (93%)	60 (7%)	13	38

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	SER
1	A	121	SER
1	A	124	LEU
1	A	157	HIS
1	A	180	SER
1	A	193	THR
1	A	257	LEU

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Mol	Chain	Res	Type
1	A	263	VAL
1	A	267	SER
1	A	271	LEU
1	A	307	MET
1	A	331	THR
1	A	358	THR
1	A	384	ILE
1	A	385	GLU
1	A	391	ILE
1	A	403	ILE
1	A	416	THR
1	A	434	GLN
1	B	138	LEU
1	B	150	ILE
1	B	164	LYS
1	B	206	TRP
1	B	209	GLU
1	B	227	SER
1	B	268	GLN
1	B	270	VAL
1	B	315	THR
1	B	347	LEU
1	B	351	ILE
1	B	374	THR
1	B	402	THR
1	C	130	VAL
1	C	134	ASP
1	C	138	LEU
1	C	151	LEU
1	C	158	LEU
1	C	193	THR
1	C	197	VAL
1	C	228	ILE
1	C	234	VAL
1	C	238	THR
1	C	254	THR
1	C	270	VAL
1	C	276	THR
1	C	319	LEU
1	C	320	THR
1	C	323	ASP
1	C	326	THR

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Mol	Chain	Res	Type
1	C	331	THR
1	C	358	THR
1	C	363	VAL
1	C	364	SER
1	C	365	THR
1	C	377	SER
1	C	384	ILE
1	C	403	ILE
1	C	412	SER
1	C	417	VAL
1	C	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	B	259	GLN
1	B	261	ASN
1	C	261	ASN
1	C	265	ASN
1	C	268	GLN
1	C	359	HIS
1	C	425	GLN
1	C	427	GLN
1	C	437	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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
2	AGS	A	501	-	32,33,33	1.97	7 (21%)	45,52,52	1.92	11 (24%)
2	AGS	B	501	-	32,33,33	2.23	6 (18%)	45,52,52	2.07	11 (24%)
4	EDO	C	501	-	3,3,3	0.45	0	2,2,2	0.21	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	A	501	-	-	4/21/38/38	0/3/3/3
2	AGS	B	501	-	-	9/21/38/38	0/3/3/3
4	EDO	C	501	-	-	1/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	AGS	PG-S1G	8.19	2.08	1.90
2	A	501	AGS	PG-S1G	7.48	2.06	1.90
2	B	501	AGS	C5-C4	5.09	1.48	1.39
2	A	501	AGS	C5-C4	4.88	1.47	1.39
2	B	501	AGS	PA-O3A	4.59	1.64	1.59
2	B	501	AGS	PB-O3A	3.37	1.63	1.59
2	B	501	AGS	C5-C6	2.96	1.49	1.41
2	A	501	AGS	C5-N7	-2.75	1.34	1.39
2	B	501	AGS	C8-N7	2.49	1.36	1.31
2	A	501	AGS	PA-O3A	2.45	1.62	1.59
2	A	501	AGS	C5-C6	2.40	1.47	1.41
2	A	501	AGS	C8-N7	2.28	1.36	1.31
2	A	501	AGS	PB-O3A	2.06	1.61	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	AGS	C5-C4-N3	-6.05	118.39	126.72
2	B	501	AGS	C5-C4-N3	-5.46	119.20	126.72
2	A	501	AGS	N3-C4-N9	4.96	135.61	127.17
2	B	501	AGS	N3-C4-N9	4.80	135.32	127.17
2	A	501	AGS	PB-O3B-PG	-4.45	116.89	133.17
2	B	501	AGS	PB-O3B-PG	-4.26	117.57	133.17
2	B	501	AGS	C2-N3-C4	3.88	121.30	111.83
2	B	501	AGS	N3-C2-N1	-3.85	122.75	128.58
2	B	501	AGS	C2'-C1'-N9	-3.76	103.95	113.30
2	A	501	AGS	C2-N3-C4	3.62	120.67	111.83
2	B	501	AGS	C4-N9-C8	3.52	109.44	105.74
2	B	501	AGS	C4-C5-N7	-3.33	106.78	110.58
2	A	501	AGS	N3-C2-N1	-3.07	123.93	128.58
2	A	501	AGS	C4-C5-N7	-2.89	107.27	110.58
2	B	501	AGS	C5-N7-C8	2.85	107.93	103.45
2	B	501	AGS	C6-C5-N7	2.55	137.01	132.09
2	B	501	AGS	N9-C8-N7	-2.51	110.38	113.94
2	A	501	AGS	O3A-PA-O1A	-2.40	103.48	110.70
2	A	501	AGS	O3G-PG-O3B	2.29	112.29	104.64
2	A	501	AGS	C5-N7-C8	2.25	106.98	103.45
2	A	501	AGS	O2A-PA-O1A	2.07	122.08	112.44
2	A	501	AGS	O3'-C3'-C4'	2.03	116.91	111.08

There are no chirality outliers.

All (14) torsion outliers are listed below:

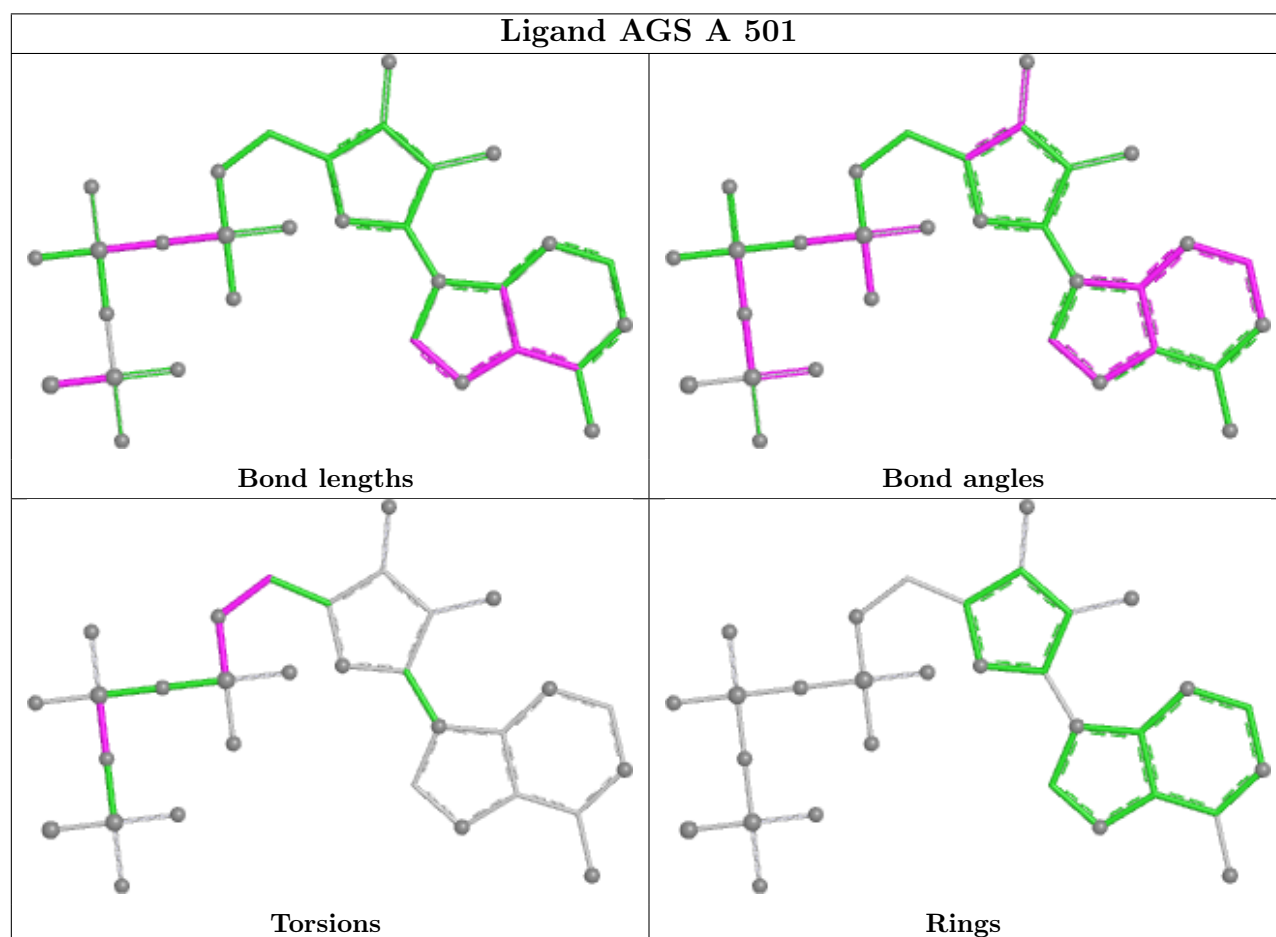
Mol	Chain	Res	Type	Atoms
2	A	501	AGS	C5'-O5'-PA-O3A
2	B	501	AGS	C5'-O5'-PA-O3A
2	B	501	AGS	PG-O3B-PB-O1B
2	B	501	AGS	PA-O3A-PB-O3B
2	B	501	AGS	PB-O3A-PA-O5'
2	B	501	AGS	C4'-C5'-O5'-PA
2	A	501	AGS	C5'-O5'-PA-O1A
2	B	501	AGS	C5'-O5'-PA-O1A
2	A	501	AGS	C4'-C5'-O5'-PA
4	C	501	EDO	O1-C1-C2-O2
2	A	501	AGS	PG-O3B-PB-O2B
2	B	501	AGS	PG-O3B-PB-O2B
2	B	501	AGS	PA-O3A-PB-O1B
2	B	501	AGS	PA-O3A-PB-O2B

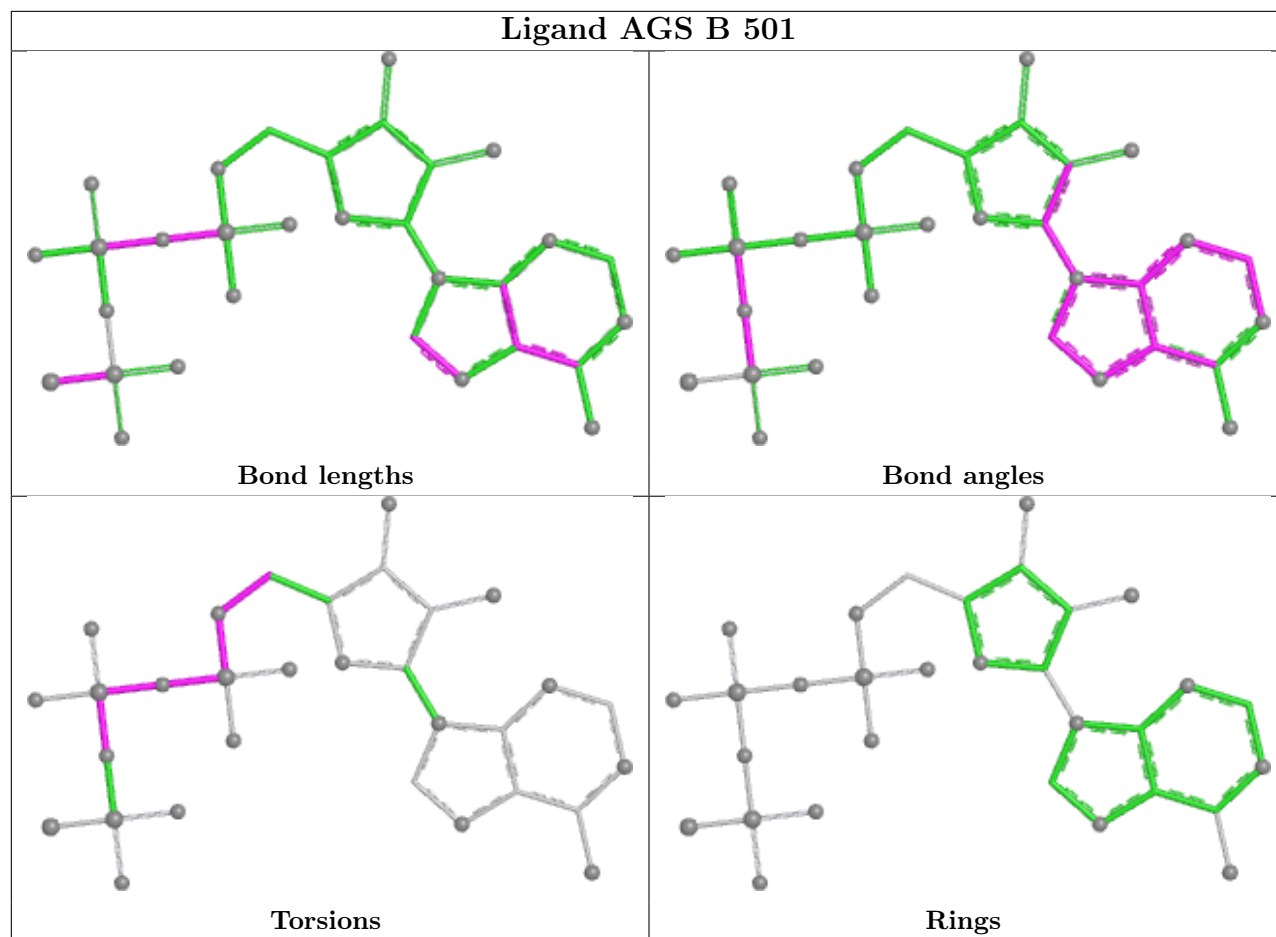
There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AGS	1	0
2	B	501	AGS	4	0
4	C	501	EDO	10	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.





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	319/340 (93%)	-0.01	9 (2%) 55 36	42, 68, 108, 124	0
1	B	316/340 (92%)	0.10	1 (0%) 90 82	51, 82, 122, 138	0
1	C	310/340 (91%)	0.56	13 (4%) 40 26	74, 105, 130, 136	0
All	All	945/1020 (92%)	0.21	23 (2%) 59 40	42, 84, 126, 138	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	LEU	5.4
1	C	231	ILE	4.2
1	C	199	SER	3.7
1	C	311	ASN	3.4
1	C	417	VAL	3.2
1	A	259	GLN	3.1
1	A	237	LEU	2.7
1	C	229	ILE	2.6
1	C	385	GLU	2.6
1	C	176	GLY	2.6
1	B	220	MET	2.5
1	A	239	GLY	2.5
1	C	419	GLU	2.4
1	A	238	THR	2.4
1	C	400	ASP	2.4
1	C	248	ALA	2.4
1	A	257	LEU	2.3
1	A	240	THR	2.3
1	C	123	ILE	2.3
1	A	236	ALA	2.3
1	C	197	VAL	2.1
1	A	268	GLN	2.1
1	C	401	LEU	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](#)

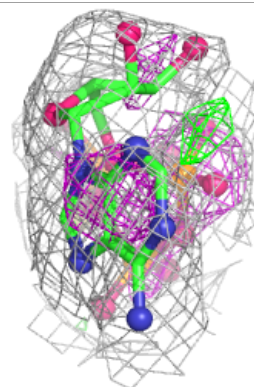
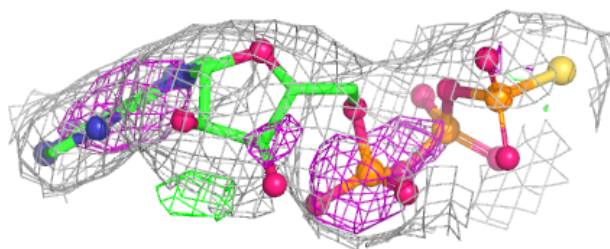
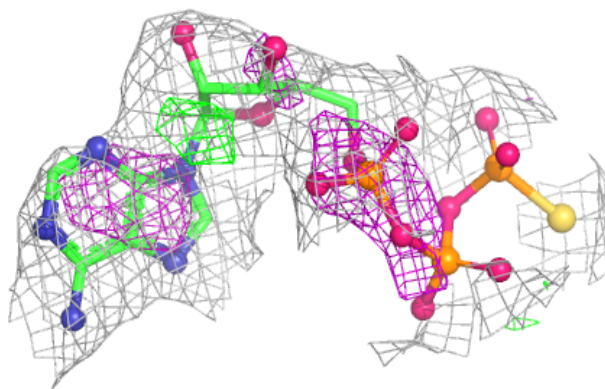
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	501	31/31	0.87	0.13	103,107,113,114	0
2	AGS	A	501	31/31	0.91	0.12	64,67,81,82	0
3	MG	C	502	1/1	0.91	0.12	100,100,100,100	0
4	EDO	C	501	4/4	0.92	0.09	54,56,58,61	0
3	MG	A	502	1/1	0.93	0.07	51,51,51,51	0
3	MG	B	502	1/1	0.98	0.05	59,59,59,59	0

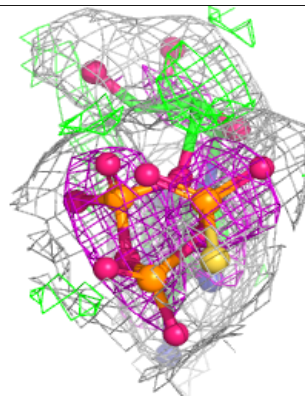
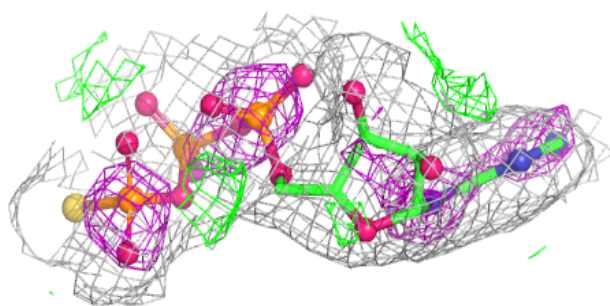
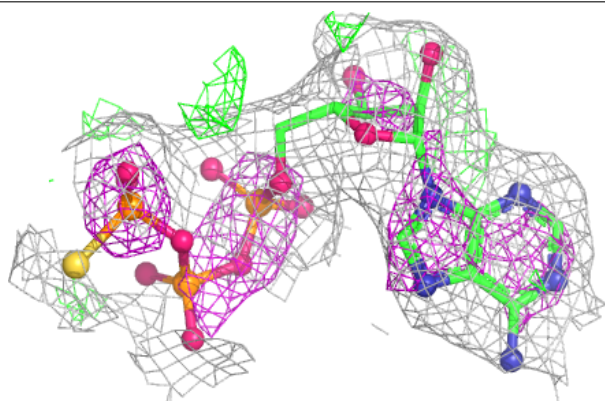
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS B 501:

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

**Electron density around AGS A 501:**

$2mF_o-DF_c$ (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.