



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:04 PM UTC

PDB ID : 9V61 / pdb_00009v61
Title : Human Serum Albumin in I 1 2 1 space group
Authors : Cetinok, H.; DeMirici, H.
Deposited on : 2025-05-26
Resolution : 2.50 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

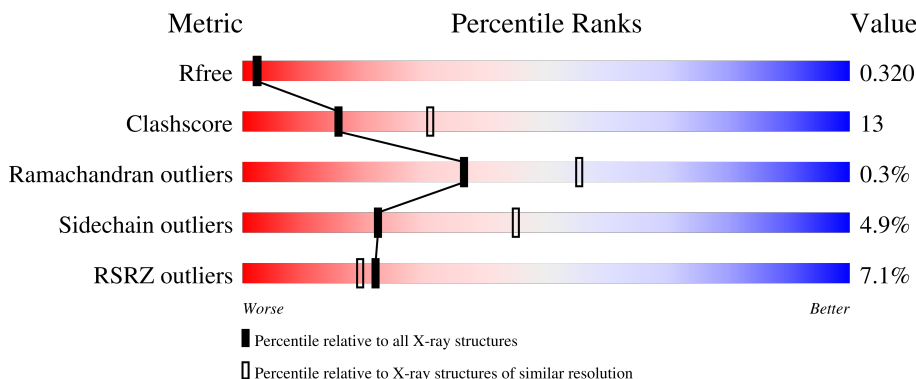
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	582	6% 71% 26% ..
1	B	582	9% 63% 32% ..
1	C	582	6% 67% 30% ..

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	PO4	A	601	-	-	X	-

2 Entry composition [i](#)

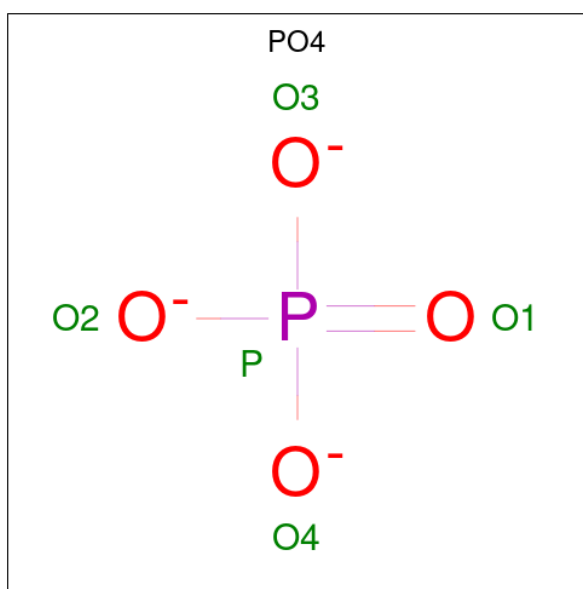
There are 3 unique types of molecules in this entry. The entry contains 13946 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	0	0
			4556	2876	771	869	40			
1	B	569	Total	C	N	O	S	0	0	0
			4533	2863	767	863	40			
1	C	569	Total	C	N	O	S	0	0	0
			4533	2863	767	863	40			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

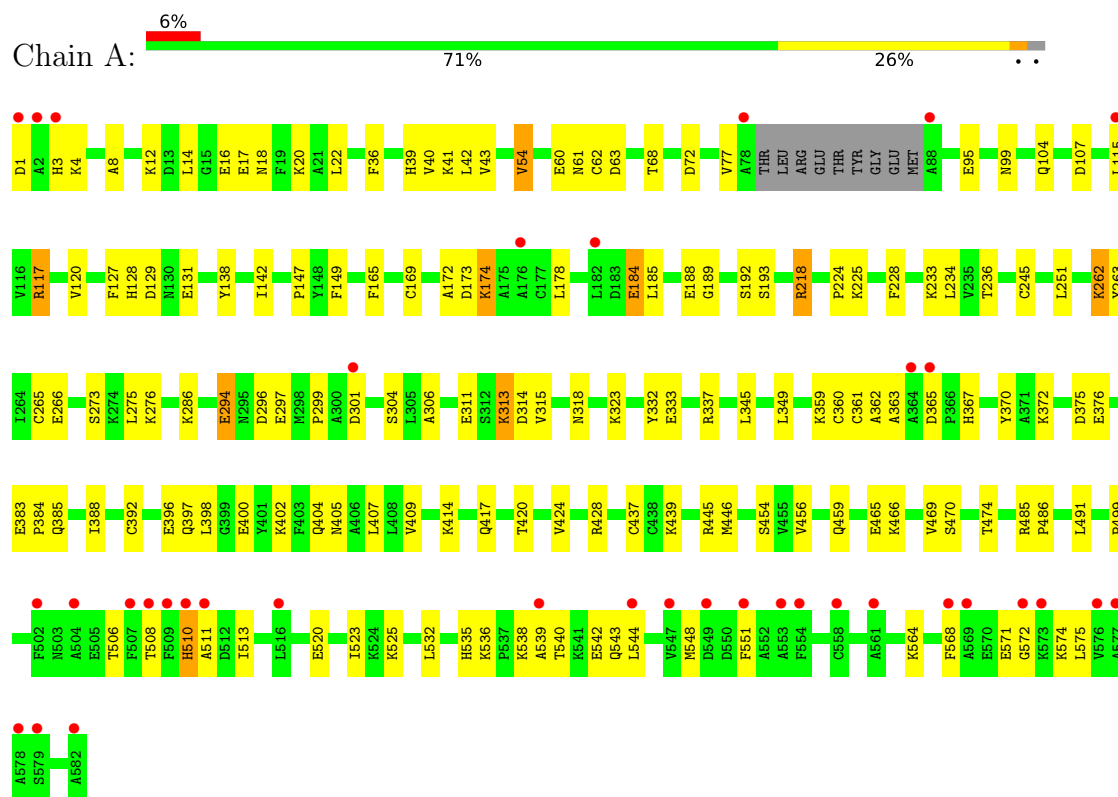
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total 102	O 102	0	0
3	B	120	Total 120	O 120	0	0
3	C	97	Total 97	O 97	0	0

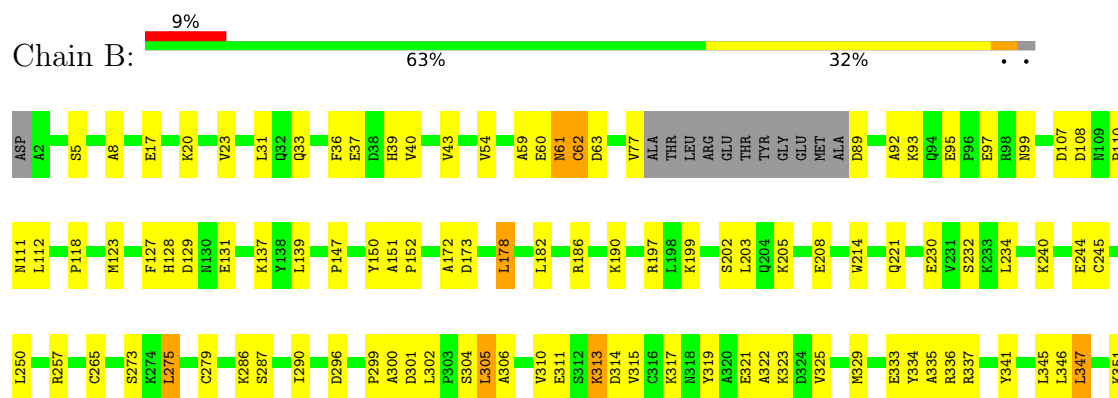
3 Residue-property plots

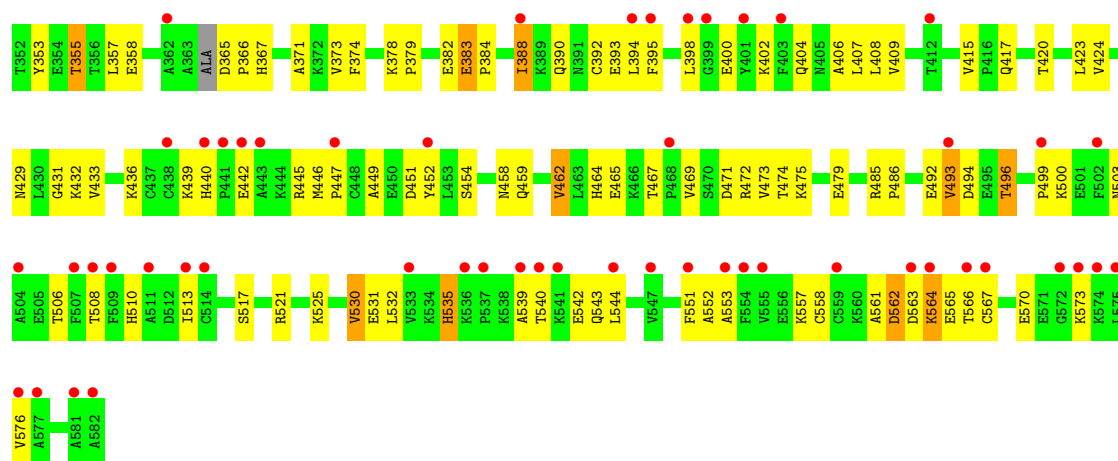
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

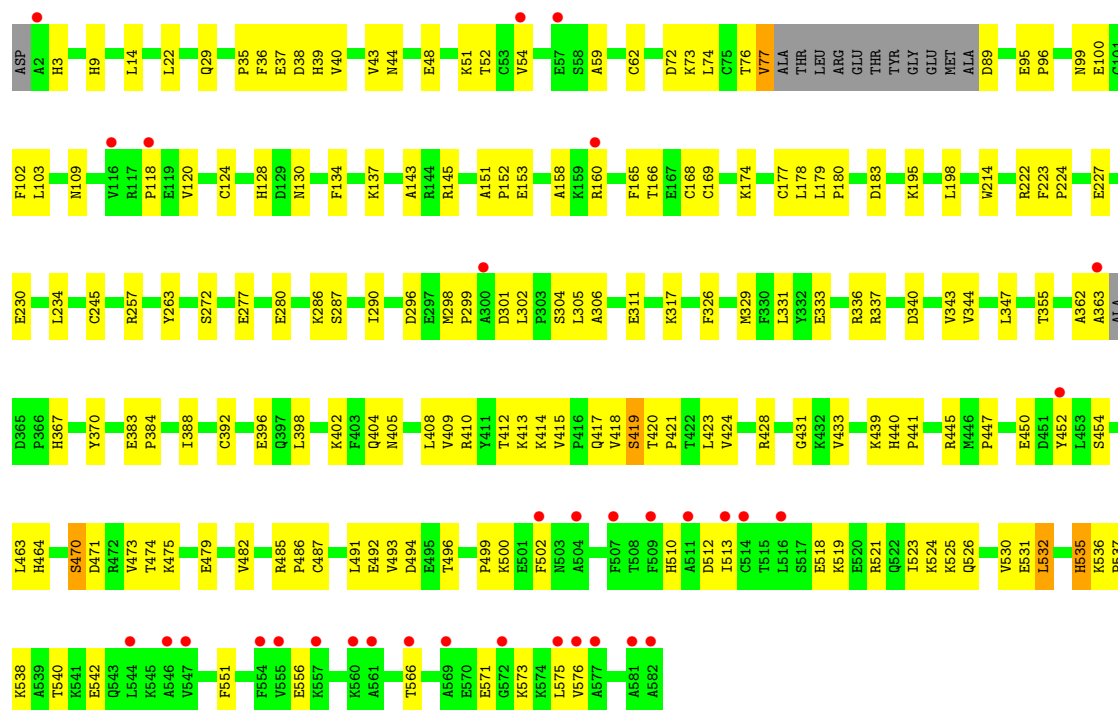


• Molecule 1: Albumin





• Molecule 1: Albumin



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.45Å 115.80Å 207.81Å 90.00° 99.71° 90.00°	Depositor
Resolution (Å)	29.41 – 2.50 29.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	86.7 (29.41-2.50) 86.6 (29.41-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.254 , 0.320 0.261 , 0.320	Depositor DCC
R_{free} test set	2000 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 80.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13946	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	1/4644 (0.0%)	0.84	1/6263 (0.0%)
1	B	0.50	0/4620	0.83	6/6228 (0.1%)
1	C	0.52	3/4620 (0.1%)	0.77	2/6228 (0.0%)
All	All	0.52	4/13884 (0.0%)	0.81	9/18719 (0.0%)

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	C	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	531	GLU	C-N	6.29	1.41	1.33
1	C	158	ALA	C-N	-5.81	1.25	1.33
1	C	532	LEU	C-N	-5.60	1.27	1.34
1	A	184	GLU	C-N	-5.34	1.26	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ASN	CB-CA-C	7.79	125.49	116.54
1	B	313	LYS	N-CA-C	-7.28	99.14	110.42
1	B	315	VAL	N-CA-C	-6.13	104.37	110.62
1	A	363	ALA	N-CA-C	5.60	115.67	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ASN	N-CA-C	-5.58	99.83	108.31
1	B	394	LEU	N-CA-C	-5.47	105.32	111.28
1	C	134	PHE	CA-CB-CG	5.37	119.17	113.80
1	B	60	GLU	N-CA-CB	-5.35	102.61	110.26
1	C	531	GLU	O-C-N	5.16	127.66	122.09

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain
1	A	218	ARG	Sidechain
1	C	160	ARG	Sidechain

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	4556	0	4478	104	7
1	B	4533	0	4455	145	5
1	C	4533	0	4455	112	1
2	A	5	0	0	2	0
3	A	102	0	0	17	0
3	B	120	0	0	13	0
3	C	97	0	0	8	0
All	All	13946	0	13388	358	12

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 13.

All (358) 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:465:GLU:HB3	3:A:705:HOH:O	1.48	1.11
1:C:518:GLU:HA	1:C:521:ARG:HE	1.34	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:PRO:HB2	1:A:446:MET:HE2	1.61	0.82
1:A:525:LYS:HD3	1:A:551:PHE:HE2	1.46	0.81
1:C:412:THR:HG22	1:C:423:LEU:HD13	1.64	0.79
1:B:110:PRO:HB2	1:B:112:LEU:HD13	1.62	0.79
1:B:500:LYS:HE3	1:B:531:GLU:OE2	1.84	0.78
1:B:398:LEU:HA	1:B:402:LYS:HZ3	1.53	0.74
1:A:323:LYS:HE3	1:B:205:LYS:HE3	1.70	0.72
1:B:398:LEU:HD13	1:B:402:LYS:HE2	1.70	0.72
1:C:433:VAL:HG22	1:C:452:TYR:CD2	2.25	0.72
1:A:417:GLN:HB2	1:A:470:SER:HB2	1.71	0.72
1:C:317:LYS:NZ	3:C:601:HOH:O	2.23	0.71
1:B:333:GLU:HB3	1:B:337:ARG:HH21	1.56	0.71
1:B:61:ASN:O	1:B:63:ASP:N	2.23	0.70
1:C:174:LYS:HA	3:C:604:HOH:O	1.91	0.69
1:C:419:SER:HB2	1:C:421:PRO:HD2	1.74	0.69
1:A:414:LYS:HD3	1:A:491:LEU:HB2	1.74	0.68
1:A:95:GLU:OE1	1:A:99:ASN:HB2	1.93	0.68
1:B:296:ASP:HB3	3:B:640:HOH:O	1.93	0.68
1:B:95:GLU:OE1	1:B:99:ASN:HB2	1.94	0.68
1:B:475:LYS:O	1:B:479:GLU:HB2	1.94	0.67
1:A:396:GLU:OE2	3:A:701:HOH:O	2.11	0.67
1:A:225:LYS:HG2	1:A:299:PRO:HG3	1.77	0.67
1:C:224:PRO:HD2	1:C:296:ASP:HB3	1.75	0.66
1:B:465:GLU:CD	3:B:601:HOH:O	2.38	0.66
1:B:525:LYS:HG2	1:B:551:PHE:HE2	1.61	0.65
1:A:61:ASN:O	1:A:63:ASP:N	2.28	0.65
1:C:153:GLU:HG2	1:C:257:ARG:HH12	1.62	0.65
1:C:95:GLU:OE2	1:C:99:ASN:HB2	1.97	0.64
1:C:415:VAL:HG12	1:C:418:VAL:HG12	1.78	0.64
1:C:433:VAL:HG22	1:C:452:TYR:HD2	1.63	0.64
1:C:89:ASP:N	3:C:602:HOH:O	2.31	0.64
1:C:485:ARG:HB3	1:C:486:PRO:HD3	1.80	0.64
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.78	0.63
1:A:306:ALA:O	1:A:311:GLU:HG2	1.98	0.63
1:B:465:GLU:OE1	3:B:601:HOH:O	2.15	0.63
1:C:59:ALA:HB3	1:C:62:CYS:SG	2.38	0.63
1:A:439:LYS:NZ	3:A:704:HOH:O	2.20	0.63
1:B:429:ASN:O	1:B:433:VAL:HG23	1.98	0.63
1:B:178:LEU:HG	1:B:182:LEU:HD13	1.81	0.62
1:B:445:ARG:NH1	1:B:446:MET:HA	2.13	0.62
1:A:360:CYS:C	1:A:362:ALA:H	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:GLU:HA	1:A:574:LYS:HD2	1.82	0.62
1:B:89:ASP:O	3:B:602:HOH:O	2.16	0.61
1:B:127:PHE:O	1:B:131:GLU:HG2	1.99	0.61
1:C:230:GLU:O	1:C:234:LEU:HD23	2.00	0.61
1:A:61:ASN:C	1:A:63:ASP:H	2.07	0.61
1:C:439:LYS:HE3	1:C:440:HIS:HE1	1.65	0.60
1:B:172:ALA:O	1:B:173:ASP:C	2.43	0.60
1:B:445:ARG:NH1	1:B:449:ALA:HB3	2.17	0.60
1:A:12:LYS:NZ	1:A:54:VAL:HG23	2.16	0.60
1:A:273:SER:O	1:A:276:LYS:HE3	2.02	0.60
1:B:471:ASP:HA	1:B:474:THR:HG22	1.84	0.59
1:A:456:VAL:O	1:A:459:GLN:HB2	2.02	0.59
1:B:492:GLU:HG2	1:B:493:VAL:HG12	1.84	0.59
1:B:404:GLN:HG2	1:B:431:GLY:HA3	1.85	0.59
1:B:517:SER:O	1:B:521:ARG:HG3	2.03	0.59
1:C:100:GLU:HG2	1:C:103:LEU:HD12	1.85	0.59
1:C:408:LEU:HD11	1:C:530:VAL:HG22	1.83	0.59
1:C:392:CYS:O	1:C:396:GLU:HG2	2.03	0.58
1:B:186:ARG:O	1:B:190:LYS:HG2	2.02	0.58
1:B:302:LEU:HB3	1:B:337:ARG:NH1	2.18	0.58
1:C:306:ALA:O	1:C:311:GLU:HG2	2.03	0.58
1:B:494:ASP:OD1	1:B:496:THR:HG22	2.04	0.58
1:A:539:ALA:HB1	1:A:543:GLN:HB2	1.86	0.58
1:B:500:LYS:HE3	1:B:531:GLU:CD	2.28	0.57
1:C:475:LYS:O	1:C:479:GLU:HB2	2.03	0.57
1:A:392:CYS:O	1:A:396:GLU:HG2	2.05	0.57
1:A:499:PRO:HB3	1:A:535:HIS:O	2.04	0.57
1:B:539:ALA:HB1	1:B:543:GLN:HB2	1.87	0.57
1:C:499:PRO:HB3	1:C:535:HIS:O	2.05	0.57
1:B:265:CYS:SG	1:B:286:LYS:HD3	2.45	0.56
1:A:385:GLN:HG3	1:A:446:MET:HE3	1.87	0.56
1:A:189:GLY:C	3:A:710:HOH:O	2.49	0.56
1:B:573:LYS:HA	1:B:576:VAL:HG12	1.88	0.56
1:C:3:HIS:CD2	1:C:9:HIS:CE1	2.93	0.56
1:C:388:ILE:HD11	1:C:445:ARG:HG2	1.87	0.56
1:B:388:ILE:HG21	1:B:445:ARG:NH2	2.19	0.56
1:C:513:ILE:HG12	1:C:524:LYS:HD3	1.87	0.56
1:B:395:PHE:HA	1:B:398:LEU:HB2	1.88	0.55
1:B:447:PRO:O	1:B:451:ASP:HB2	2.06	0.55
1:B:525:LYS:HG2	1:B:551:PHE:CE2	2.41	0.55
1:B:275:LEU:HD11	1:B:290:ILE:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:HE2	1:A:297:GLU:O	2.06	0.55
1:B:240:LYS:HG2	1:B:244:GLU:OE2	2.06	0.55
1:A:192:SER:N	3:A:710:HOH:O	2.40	0.55
1:B:302:LEU:HB3	1:B:337:ARG:HH12	1.71	0.55
1:B:351:LYS:O	1:B:355:THR:HG22	2.06	0.54
1:B:406:ALA:O	1:B:409:VAL:HG12	2.06	0.54
1:B:500:LYS:HB3	1:B:535:HIS:HA	1.88	0.54
1:C:439:LYS:HE3	1:C:440:HIS:CE1	2.43	0.54
1:A:420:THR:O	1:A:424:VAL:HG23	2.07	0.54
1:B:279:CYS:HA	1:B:286:LYS:HE2	1.89	0.54
1:C:35:PRO:HD2	1:C:38:ASP:OD2	2.06	0.54
1:C:305:LEU:HD11	1:C:333:GLU:HB2	1.88	0.54
1:C:573:LYS:O	1:C:576:VAL:HG12	2.08	0.54
1:B:111:ASN:HA	3:B:645:HOH:O	2.07	0.54
1:C:333:GLU:O	1:C:336:ARG:HG2	2.07	0.54
1:B:305:LEU:HD21	1:B:333:GLU:HB3	1.89	0.54
1:B:400:GLU:OE2	1:B:432:LYS:HA	2.08	0.54
1:B:446:MET:N	1:B:447:PRO:HD2	2.22	0.54
1:C:471:ASP:HA	1:C:474:THR:HB	1.89	0.53
1:B:150:TYR:CD1	1:B:152:PRO:HD2	2.43	0.53
1:A:511:ALA:HA	1:A:568:PHE:HE2	1.74	0.53
1:B:59:ALA:O	1:B:62:CYS:HB2	2.09	0.53
1:C:72:ASP:O	1:C:76:THR:HG23	2.09	0.53
1:C:573:LYS:O	1:C:573:LYS:HD3	2.08	0.53
1:B:61:ASN:C	1:B:63:ASP:H	2.15	0.53
1:A:61:ASN:C	1:A:63:ASP:N	2.67	0.52
1:B:492:GLU:CG	1:B:493:VAL:H	2.21	0.52
1:A:372:LYS:O	1:A:375:ASP:HB2	2.09	0.52
1:B:433:VAL:HG22	1:B:452:TYR:CD2	2.44	0.52
1:B:458:ASN:O	1:B:462:VAL:HG13	2.09	0.52
1:A:525:LYS:HD3	1:A:551:PHE:CE2	2.37	0.52
1:B:398:LEU:HA	1:B:402:LYS:NZ	2.24	0.52
1:C:214:TRP:CD1	1:C:343:VAL:HG11	2.44	0.52
1:B:374:PHE:C	3:B:603:HOH:O	2.52	0.52
1:C:518:GLU:HB2	1:C:521:ARG:HH21	1.75	0.52
1:B:20:LYS:HD2	3:B:628:HOH:O	2.10	0.51
1:C:433:VAL:HG22	1:C:452:TYR:CE2	2.44	0.51
1:B:107:ASP:O	1:B:147:PRO:HG3	2.10	0.51
1:C:526:GLN:O	1:C:530:VAL:HG23	2.10	0.51
1:C:177:CYS:HB3	3:C:604:HOH:O	2.10	0.51
1:B:420:THR:HG23	1:B:530:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:556:GLU:OE1	1:C:556:GLU:HA	2.10	0.51
1:C:14:LEU:HD13	1:C:22:LEU:HD12	1.93	0.51
1:C:305:LEU:HD21	1:C:337:ARG:NH1	2.26	0.51
1:B:230:GLU:O	1:B:234:LEU:HD23	2.11	0.50
1:B:417:GLN:HB3	1:B:469:VAL:HG12	1.92	0.50
1:A:149:PHE:CD2	1:A:193:SER:HB2	2.46	0.50
1:A:172:ALA:O	1:A:173:ASP:HB3	2.12	0.50
1:C:48:GLU:O	1:C:52:THR:HG23	2.11	0.50
1:A:192:SER:HB3	3:A:710:HOH:O	2.10	0.50
1:B:566:THR:O	1:B:570:GLU:HG2	2.10	0.50
1:A:16:GLU:O	1:A:20:LYS:HG2	2.11	0.50
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.93	0.50
1:A:17:GLU:HG3	3:A:782:HOH:O	2.12	0.50
1:C:571:GLU:O	1:C:575:LEU:HD23	2.12	0.50
1:B:532:LEU:O	1:B:535:HIS:HB3	2.12	0.50
1:C:326:PHE:HA	1:C:329:MET:HE2	1.94	0.49
1:B:353:TYR:CZ	1:B:357:LEU:HD11	2.47	0.49
1:C:73:LYS:O	1:C:77:VAL:HG23	2.13	0.49
1:A:12:LYS:HZ3	1:A:54:VAL:HG23	1.77	0.49
1:B:341:TYR:HD2	1:B:346:LEU:HD21	1.76	0.49
1:B:447:PRO:HD3	3:B:621:HOH:O	2.12	0.49
1:C:405:ASN:O	1:C:409:VAL:HG23	2.12	0.49
1:C:518:GLU:CA	1:C:521:ARG:HE	2.16	0.49
1:A:294:GLU:O	3:A:703:HOH:O	2.20	0.49
1:A:540:THR:HG23	1:A:542:GLU:H	1.77	0.49
1:B:365:ASP:N	1:B:366:PRO:HD3	2.28	0.49
1:C:464:HIS:HE1	1:C:470:SER:H	1.61	0.49
1:C:492:GLU:HG2	1:C:493:VAL:HG12	1.95	0.49
1:C:367:HIS:HA	1:C:370:TYR:CE2	2.47	0.49
1:A:286:LYS:NZ	1:A:286:LYS:HB3	2.27	0.49
1:C:424:VAL:O	1:C:428:ARG:HG3	2.13	0.49
1:C:525:LYS:HG2	1:C:551:PHE:CE2	2.48	0.49
1:B:445:ARG:CZ	1:B:446:MET:HA	2.43	0.48
1:B:553:ALA:O	1:B:557:LYS:HD3	2.12	0.48
1:A:14:LEU:HD13	1:A:22:LEU:HD12	1.95	0.48
1:A:532:LEU:O	1:A:535:HIS:HB3	2.13	0.48
1:B:383:GLU:CD	1:B:485:ARG:HH22	2.21	0.48
1:A:14:LEU:O	1:A:18:ASN:HB2	2.14	0.48
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.95	0.48
1:A:439:LYS:NZ	3:A:711:HOH:O	2.44	0.48
1:A:384:PRO:O	1:A:388:ILE:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLU:HB3	3:A:725:HOH:O	2.14	0.48
1:A:439:LYS:CE	3:A:704:HOH:O	2.61	0.48
1:B:186:ARG:O	1:B:190:LYS:HE3	2.14	0.48
1:B:499:PRO:HB3	1:B:535:HIS:O	2.14	0.48
1:C:151:ALA:HB3	1:C:152:PRO:HD3	1.96	0.48
1:B:61:ASN:C	1:B:63:ASP:N	2.72	0.47
1:A:4:LYS:HA	1:A:4:LYS:HD3	1.62	0.47
1:C:51:LYS:HA	1:C:54:VAL:HG12	1.96	0.47
1:B:31:LEU:HD11	1:B:77:VAL:HG21	1.96	0.47
1:B:36:PHE:O	1:B:40:VAL:HG23	2.15	0.47
1:A:510:HIS:O	1:A:513:ILE:HD12	2.15	0.47
1:C:540:THR:HG23	1:C:542:GLU:H	1.79	0.47
1:A:572:GLY:HA2	1:A:575:LEU:HB2	1.97	0.47
1:C:180:PRO:HA	1:C:183:ASP:HB3	1.96	0.47
1:C:367:HIS:HA	1:C:370:TYR:CZ	2.50	0.47
1:B:23:VAL:HG12	1:B:43:VAL:HG22	1.98	0.46
1:A:120:VAL:HG13	1:A:178:LEU:HD23	1.97	0.46
1:B:510:HIS:O	1:B:513:ILE:HD12	2.15	0.46
1:A:571:GLU:O	1:A:575:LEU:HD23	2.15	0.46
1:A:417:GLN:HB3	1:A:469:VAL:HG12	1.96	0.46
1:C:109:ASN:HB2	1:C:463:LEU:HD21	1.98	0.46
1:A:251:LEU:HD13	2:A:601:PO4:O4	2.15	0.46
1:B:37:GLU:CD	1:B:37:GLU:H	2.23	0.46
1:B:306:ALA:O	1:B:311:GLU:HG2	2.15	0.46
1:A:165:PHE:O	1:A:169:CYS:HB2	2.15	0.46
1:C:222:ARG:HG2	1:C:223:PHE:CE1	2.51	0.46
1:C:417:GLN:HB2	1:C:470:SER:OG	2.15	0.46
1:A:397:GLN:C	1:A:398:LEU:HD22	2.41	0.46
1:C:120:VAL:HG13	1:C:178:LEU:HD23	1.98	0.46
1:C:168:CYS:HB3	3:C:604:HOH:O	2.15	0.46
1:C:257:ARG:NH2	1:C:287:SER:HB3	2.31	0.45
1:A:424:VAL:O	1:A:428:ARG:HG3	2.16	0.45
1:A:520:GLU:HA	1:A:523:ILE:HG22	1.98	0.45
1:C:340:ASP:O	1:C:447:PRO:HD3	2.16	0.45
1:C:299:PRO:HG2	1:C:302:LEU:HD11	1.99	0.45
1:B:273:SER:HA	3:B:637:HOH:O	2.15	0.45
1:B:313:LYS:O	1:B:314:ASP:HB2	2.16	0.45
1:B:472:ARG:HG3	3:B:634:HOH:O	2.15	0.45
1:C:234:LEU:HD21	1:C:263:TYR:HE2	1.81	0.45
1:C:487:CYS:O	1:C:491:LEU:HG	2.16	0.45
1:B:128:HIS:O	1:B:129:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:VAL:HG13	1:B:373:VAL:HG12	1.98	0.45
1:B:345:LEU:C	1:B:345:LEU:HD23	2.42	0.45
1:C:299:PRO:HG3	1:C:336:ARG:HH21	1.81	0.45
1:B:382:GLU:OE2	1:B:382:GLU:HA	2.17	0.45
1:B:436:LYS:N	1:B:436:LYS:HD2	2.31	0.45
1:C:413:LYS:HE3	1:C:537:PRO:O	2.16	0.45
1:B:433:VAL:HG22	1:B:452:TYR:CE2	2.52	0.45
1:B:558:CYS:HA	1:B:561:ALA:HB3	1.98	0.45
1:C:299:PRO:HG3	1:C:336:ARG:NH2	2.32	0.45
1:C:383:GLU:HB3	1:C:384:PRO:HD3	1.99	0.45
1:A:39:HIS:O	1:A:43:VAL:HG12	2.17	0.45
1:B:544:LEU:HD13	1:B:544:LEU:HA	1.80	0.45
1:A:8:ALA:O	1:A:12:LYS:HG3	2.17	0.45
1:A:548:MET:HA	1:A:551:PHE:HB3	1.98	0.45
1:B:304:SER:HB2	3:B:673:HOH:O	2.16	0.45
1:B:525:LYS:NZ	1:B:552:ALA:HB2	2.32	0.45
1:A:424:VAL:HB	3:A:707:HOH:O	2.17	0.45
1:B:563:ASP:O	1:B:567:CYS:HB2	2.18	0.44
1:A:345:LEU:HD23	1:A:349:LEU:HG	1.99	0.44
1:A:360:CYS:C	1:A:362:ALA:N	2.73	0.44
1:B:299:PRO:HG2	1:B:302:LEU:HD21	1.98	0.44
1:B:378:LYS:HB3	1:B:379:PRO:HD3	1.99	0.44
1:A:41:LYS:HB3	1:A:41:LYS:HE2	1.76	0.44
1:B:314:ASP:HA	1:B:317:LYS:CG	2.47	0.44
1:B:384:PRO:O	1:B:388:ILE:HG22	2.17	0.44
1:A:400:GLU:HB2	3:A:721:HOH:O	2.17	0.44
1:B:420:THR:HG23	1:B:530:VAL:CG1	2.47	0.44
1:B:432:LYS:O	1:B:436:LYS:HD3	2.18	0.44
1:B:459:GLN:OE1	1:B:459:GLN:HA	2.17	0.44
1:B:473:VAL:HG23	1:B:474:THR:N	2.32	0.44
1:C:441:PRO:O	1:C:445:ARG:HB2	2.18	0.44
1:B:93:LYS:HD3	1:B:97:GLU:HB3	1.99	0.44
1:B:319:TYR:HE2	1:B:358:GLU:OE1	2.00	0.44
1:C:492:GLU:HG2	1:C:493:VAL:H	1.83	0.44
1:C:492:GLU:CG	1:C:493:VAL:H	2.31	0.44
1:A:313:LYS:HB3	1:A:313:LYS:HE2	1.75	0.43
1:B:322:ALA:HB1	1:B:325:VAL:CG2	2.49	0.43
1:B:221:GLN:HG2	1:B:335:ALA:O	2.18	0.43
1:B:334:TYR:OH	1:B:341:TYR:HE2	2.02	0.43
1:C:420:THR:HG23	1:C:530:VAL:HB	2.00	0.43
1:C:532:LEU:O	1:C:535:HIS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:LYS:HE3	1:C:538:LYS:C	2.43	0.43
1:A:225:LYS:HD2	3:A:723:HOH:O	2.18	0.43
1:A:511:ALA:HA	1:A:568:PHE:CE2	2.54	0.43
1:B:325:VAL:O	1:B:329:MET:HG3	2.18	0.43
1:A:540:THR:O	1:A:544:LEU:HD23	2.18	0.43
1:C:463:LEU:HD23	1:C:463:LEU:HA	1.83	0.43
1:B:378:LYS:O	1:B:382:GLU:HG2	2.18	0.43
1:B:566:THR:HG22	1:B:570:GLU:HG2	2.01	0.43
1:A:233:LYS:HD3	1:A:234:LEU:HD23	2.01	0.43
3:A:735:HOH:O	1:B:208:GLU:HG2	2.18	0.43
1:C:223:PHE:CD1	1:C:272:SER:HB2	2.54	0.43
1:A:174:LYS:H	1:A:174:LYS:HG2	1.54	0.43
1:B:347:LEU:O	1:B:351:LYS:HG2	2.19	0.43
1:C:44:ASN:O	1:C:48:GLU:HG2	2.19	0.43
1:C:415:VAL:HG11	1:C:473:VAL:CG2	2.49	0.43
1:C:510:HIS:O	1:C:513:ILE:HD12	2.19	0.43
1:A:68:THR:HG22	1:A:72:ASP:OD2	2.18	0.43
1:B:367:HIS:O	1:B:371:ALA:HB2	2.19	0.43
1:B:205:LYS:HE2	1:B:205:LYS:HB3	1.93	0.43
1:B:503:ASN:OD1	1:B:506:THR:HG23	2.19	0.43
1:C:36:PHE:O	1:C:40:VAL:HG23	2.19	0.43
1:C:195:LYS:HE3	1:C:195:LYS:HB2	1.57	0.43
1:A:388:ILE:HD13	1:A:388:ILE:HG21	1.79	0.42
1:B:420:THR:O	1:B:424:VAL:HG23	2.18	0.42
1:B:540:THR:N	1:B:543:GLN:OE1	2.49	0.42
1:C:305:LEU:HD11	1:C:333:GLU:CB	2.48	0.42
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.99	0.42
1:C:95:GLU:O	1:C:96:PRO:C	2.60	0.42
1:C:362:ALA:O	1:C:363:ALA:C	2.62	0.42
1:B:402:LYS:HE2	1:B:402:LYS:HB2	1.70	0.42
1:B:492:GLU:HG2	1:B:493:VAL:H	1.83	0.42
1:A:172:ALA:O	1:A:173:ASP:CB	2.67	0.42
1:B:92:ALA:HB3	3:B:602:HOH:O	2.20	0.42
1:C:502:PHE:HD1	1:C:502:PHE:HA	1.72	0.42
1:C:502:PHE:HZ	1:C:532:LEU:HD12	1.85	0.42
1:A:138:TYR:O	1:A:142:ILE:HG12	2.18	0.42
1:A:333:GLU:HB3	1:A:337:ARG:NH1	2.34	0.42
1:B:439:LYS:HE3	1:B:440:HIS:CE1	2.55	0.42
1:C:29:GLN:HG3	1:C:143:ALA:HB1	2.00	0.42
1:A:127:PHE:CE1	1:A:131:GLU:HG3	2.55	0.42
1:A:184:GLU:HG2	1:A:188:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:GLN:O	1:A:398:LEU:HD22	2.19	0.42
1:B:108:ASP:CG	1:B:197:ARG:HE	2.27	0.42
1:C:145:ARG:NH1	3:C:609:HOH:O	2.53	0.42
1:A:173:ASP:O	1:A:174:LYS:C	2.62	0.42
1:A:265:CYS:SG	1:A:286:LYS:NZ	2.92	0.42
1:A:437:CYS:O	1:A:445:ARG:HG3	2.20	0.42
1:C:519:LYS:O	1:C:523:ILE:HD12	2.19	0.42
1:A:262:LYS:O	1:A:266:GLU:HG2	2.20	0.41
1:A:367:HIS:HA	1:A:370:TYR:CZ	2.54	0.41
1:B:275:LEU:HD13	1:B:275:LEU:HA	1.88	0.41
1:B:423:LEU:HA	1:B:423:LEU:HD23	1.83	0.41
1:C:37:GLU:H	1:C:37:GLU:CD	2.27	0.41
1:C:331:LEU:HD12	1:C:331:LEU:HA	1.75	0.41
1:A:36:PHE:O	1:A:40:VAL:HG23	2.20	0.41
1:A:318:ASN:ND2	3:A:702:HOH:O	2.16	0.41
1:A:323:LYS:CE	1:B:205:LYS:HE3	2.43	0.41
1:A:407:LEU:HD23	1:A:407:LEU:HA	1.63	0.41
1:B:346:LEU:HA	1:B:346:LEU:HD23	1.86	0.41
1:B:408:LEU:HD21	1:B:530:VAL:HG23	2.01	0.41
1:B:464:HIS:CD2	1:B:473:VAL:HG21	2.55	0.41
1:C:404:GLN:HG2	1:C:431:GLY:HA3	2.02	0.41
1:A:251:LEU:CD1	2:A:601:PO4:O4	2.67	0.41
1:B:374:PHE:HA	3:B:603:HOH:O	2.19	0.41
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.75	0.41
1:B:442:GLU:HA	1:B:445:ARG:HB2	2.00	0.41
1:A:128:HIS:O	1:A:129:ASP:C	2.63	0.41
1:A:263:TYR:CD2	1:A:263:TYR:C	2.98	0.41
1:B:333:GLU:O	1:B:336:ARG:HG2	2.20	0.41
1:B:345:LEU:HD12	1:B:446:MET:HE1	2.02	0.41
1:C:464:HIS:CE1	1:C:470:SER:H	2.39	0.41
1:A:400:GLU:O	1:A:404:GLN:HG3	2.21	0.41
1:C:214:TRP:HA	1:C:347:LEU:HD11	2.02	0.41
1:B:151:ALA:HB2	1:B:250:LEU:HD13	2.03	0.41
1:B:286:LYS:O	1:B:290:ILE:HG13	2.21	0.41
1:C:89:ASP:C	3:C:602:HOH:O	2.64	0.41
1:C:286:LYS:O	1:C:290:ILE:HG13	2.20	0.41
1:A:104:GLN:HB3	1:B:321:GLU:HG3	2.03	0.41
1:A:466:LYS:NZ	3:A:714:HOH:O	2.49	0.41
1:B:39:HIS:O	1:B:43:VAL:HG23	2.20	0.41
1:C:305:LEU:HD21	1:C:337:ARG:CZ	2.51	0.41
1:A:228:PHE:HB2	1:A:332:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:PRO:O	1:B:123:MET:HE2	2.20	0.41
1:B:367:HIS:CD2	1:B:367:HIS:C	2.99	0.41
1:B:510:HIS:H	1:B:513:ILE:HD12	1.86	0.41
1:C:410:ARG:HG2	1:C:414:LYS:HE2	2.02	0.41
1:A:107:ASP:O	1:A:147:PRO:HG3	2.21	0.41
1:A:398:LEU:HD12	1:A:402:LYS:CB	2.51	0.41
1:B:150:TYR:CE1	1:B:152:PRO:HD2	2.57	0.41
1:C:73:LYS:HD3	1:C:73:LYS:HA	1.71	0.41
1:C:124:CYS:HB3	1:C:169:CYS:HB3	1.88	0.41
1:C:344:VAL:HG21	1:C:450:GLU:HG3	2.02	0.41
1:C:494:ASP:OD1	1:C:496:THR:HG22	2.21	0.41
1:A:315:VAL:HB	1:A:370:TYR:CZ	2.56	0.40
1:B:17:GLU:H	1:B:17:GLU:CD	2.29	0.40
1:A:314:ASP:O	1:A:315:VAL:C	2.62	0.40
1:B:5:SER:HB3	1:B:8:ALA:HB3	2.02	0.40
1:B:199:LYS:HG2	1:B:214:TRP:CZ3	2.57	0.40
1:A:405:ASN:O	1:A:409:VAL:HG23	2.21	0.40
1:A:536:LYS:HG2	1:A:538:LYS:H	1.86	0.40
1:C:165:PHE:O	1:C:166:THR:C	2.64	0.40
1:C:179:LEU:HD23	1:C:179:LEU:HA	1.92	0.40
1:B:347:LEU:HD12	1:B:347:LEU:HA	1.86	0.40
1:B:564:LYS:HE3	1:B:564:LYS:HB3	1.69	0.40
1:C:74:LEU:HD12	1:C:102:PHE:CE2	2.57	0.40
1:C:227:GLU:CD	3:C:624:HOH:O	2.63	0.40
1:B:257:ARG:HH21	1:B:287:SER:HB3	1.87	0.40
1:C:39:HIS:O	1:C:43:VAL:HG13	2.21	0.40
1:C:40:VAL:O	1:C:43:VAL:HG22	2.22	0.40
1:C:398:LEU:O	1:C:402:LYS:HB2	2.21	0.40

All (12) 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:60:GLU:CD	1:A:301:ASP:OD1[4_444]	0.62	1.58
1:B:492:GLU:OE1	1:B:540:THR:OG1[2_455]	1.42	0.78
1:A:60:GLU:CG	1:A:301:ASP:OD1[4_444]	1.44	0.76
1:A:60:GLU:OE2	1:A:301:ASP:OD1[4_444]	1.47	0.73
1:A:60:GLU:OE1	1:A:301:ASP:OD1[4_444]	1.48	0.72
1:A:60:GLU:OE1	1:A:301:ASP:OD2[4_444]	1.60	0.60
1:A:60:GLU:OE1	1:A:301:ASP:CG[4_444]	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:CD	1:A:301:ASP:CG[4_444]	1.71	0.49
1:B:313:LYS:NZ	1:B:562:ASP:OD2[1_655]	1.80	0.40
1:B:313:LYS:CE	1:B:562:ASP:OD2[1_655]	1.89	0.31
1:B:390:GLN:NE2	1:B:542:GLU:OE2[2_455]	1.96	0.24
1:B:300:ALA:O	1:C:280:GLU:OE2[4_444]	2.01	0.19

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	569/582 (98%)	540 (95%)	27 (5%)	2 (0%)	30	49
1	B	563/582 (97%)	535 (95%)	27 (5%)	1 (0%)	43	63
1	C	563/582 (97%)	531 (94%)	30 (5%)	2 (0%)	30	49
All	All	1695/1746 (97%)	1606 (95%)	84 (5%)	5 (0%)	36	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	301	ASP
1	B	62	CYS
1	A	62	CYS
1	A	361	CYS
1	C	118	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	501/509 (98%)	476 (95%)	25 (5%)	22	44
1	B	500/509 (98%)	469 (94%)	31 (6%)	16	34
1	C	500/509 (98%)	482 (96%)	18 (4%)	31	58
All	All	1501/1527 (98%)	1427 (95%)	74 (5%)	22	45

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	3	HIS
1	A	42	LEU
1	A	54	VAL
1	A	77	VAL
1	A	115	LEU
1	A	117	ARG
1	A	174	LYS
1	A	185	LEU
1	A	218	ARG
1	A	236	THR
1	A	245	CYS
1	A	262	LYS
1	A	275	LEU
1	A	294	GLU
1	A	304	SER
1	A	313	LYS
1	A	359	LYS
1	A	365	ASP
1	A	454	SER
1	A	474	THR
1	A	506	THR
1	A	508	THR
1	A	510	HIS
1	A	564	LYS
1	B	33	GLN
1	B	54	VAL
1	B	137	LYS
1	B	139	LEU
1	B	178	LEU
1	B	202	SER
1	B	203	LEU
1	B	232	SER
1	B	245	CYS

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Mol	Chain	Res	Type
1	B	275	LEU
1	B	301	ASP
1	B	305	LEU
1	B	323	LYS
1	B	347	LEU
1	B	355	THR
1	B	383	GLU
1	B	388	ILE
1	B	392	CYS
1	B	393	GLU
1	B	415	VAL
1	B	454	SER
1	B	462	VAL
1	B	467	THR
1	B	493	VAL
1	B	496	THR
1	B	508	THR
1	B	530	VAL
1	B	535	HIS
1	B	562	ASP
1	B	564	LYS
1	B	565	GLU
1	C	77	VAL
1	C	128	HIS
1	C	130	ASN
1	C	137	LYS
1	C	198	LEU
1	C	245	CYS
1	C	277	GLU
1	C	298	MET
1	C	304	SER
1	C	355	THR
1	C	419	SER
1	C	454	SER
1	C	470	SER
1	C	482	VAL
1	C	500	LYS
1	C	512	ASP
1	C	535	HIS
1	C	566	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	61	ASN
1	A	94	GLN
1	A	221	GLN
1	A	247	HIS
1	A	288	HIS
1	A	390	GLN
1	A	405	ASN
1	A	522	GLN
1	A	526	GLN
1	B	9	HIS
1	B	44	ASN
1	B	67	HIS
1	B	94	GLN
1	B	99	ASN
1	B	105	HIS
1	B	221	GLN
1	B	367	HIS
1	B	440	HIS
1	C	109	ASN
1	C	221	GLN
1	C	367	HIS
1	C	459	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 ⓘ

1 ligand is 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	PO4	A	601	-	4,4,4	0.81	0	6,6,6	0.45	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

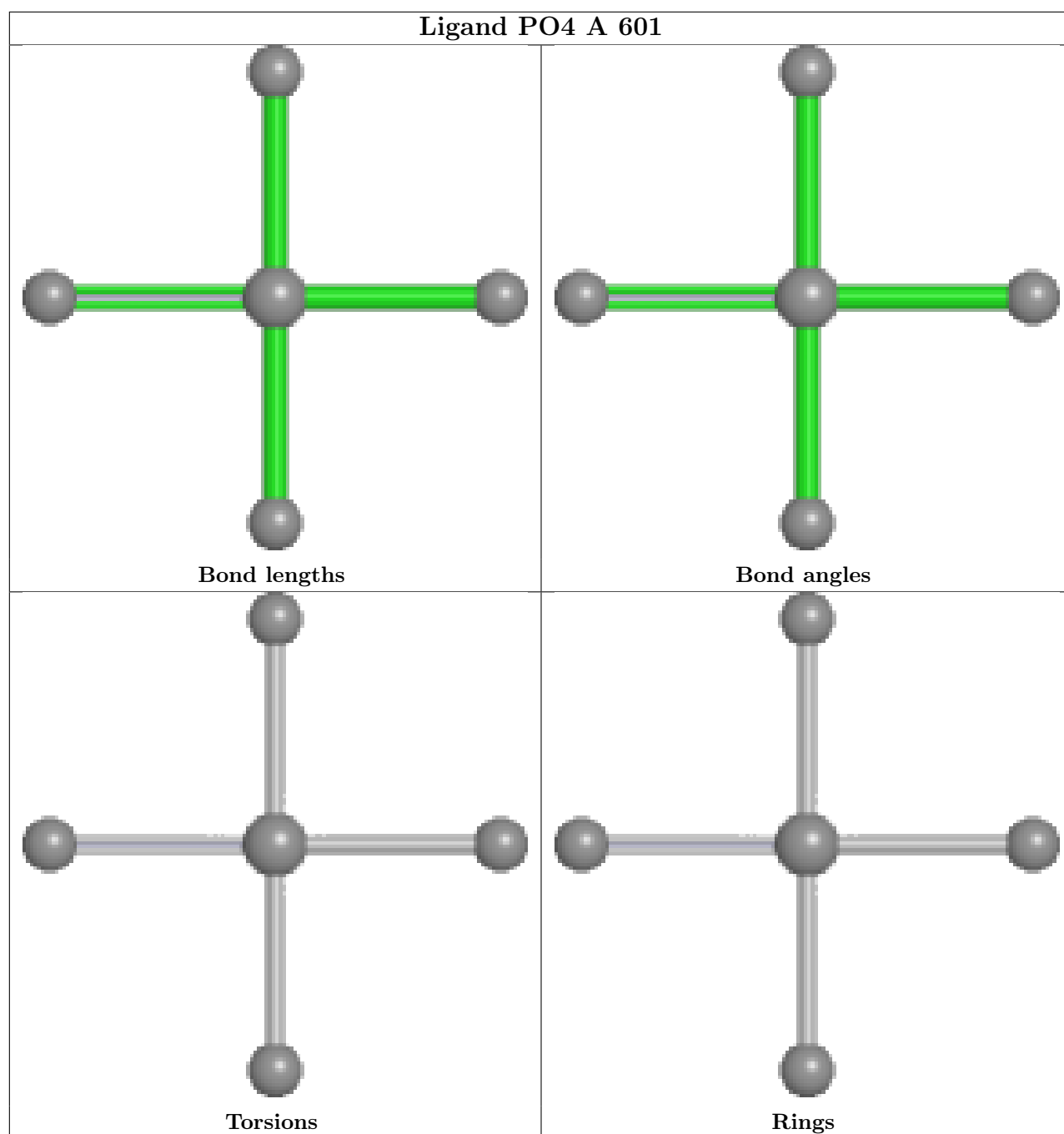
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PO4	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	573/582 (98%)	0.31	37 (6%)	25 22	30, 52, 119, 134	0
1	B	569/582 (97%)	0.51	52 (9%)	15 13	29, 57, 137, 153	0
1	C	569/582 (97%)	0.42	33 (5%)	29 25	33, 60, 118, 138	0
All	All	1711/1746 (97%)	0.41	122 (7%)	22 19	29, 56, 125, 153	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	363	ALA	5.3
1	B	539	ALA	4.5
1	B	443	ALA	4.4
1	C	576	VAL	4.2
1	A	78	ALA	4.1
1	B	504	ALA	4.0
1	A	507	PHE	3.8
1	C	547	VAL	3.7
1	A	539	ALA	3.7
1	C	507	PHE	3.7
1	B	576	VAL	3.7
1	A	582	ALA	3.7
1	B	447	PRO	3.6
1	A	572	GLY	3.6
1	A	554	PHE	3.6
1	A	553	ALA	3.5
1	A	561	ALA	3.5
1	B	582	ALA	3.5
1	B	575	LEU	3.5
1	B	362	ALA	3.5
1	C	502	PHE	3.4
1	C	557	LYS	3.4
1	B	581	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	573	LYS	3.3
1	A	509	PHE	3.2
1	B	513	ILE	3.2
1	A	301	ASP	3.2
1	B	493	VAL	3.1
1	B	559	CYS	3.1
1	A	568	PHE	3.1
1	A	365	ASP	3.0
1	B	403	PHE	3.0
1	C	555	VAL	3.0
1	B	537	PRO	3.0
1	B	509	PHE	3.0
1	B	441	PRO	3.0
1	B	399	GLY	3.0
1	B	507	PHE	2.9
1	A	508	THR	2.9
1	A	1	ASP	2.9
1	B	553	ALA	2.9
1	B	551	PHE	2.9
1	C	546	ALA	2.8
1	C	514	CYS	2.8
1	A	364	ALA	2.8
1	A	544	LEU	2.8
1	C	300	ALA	2.8
1	B	564	LYS	2.8
1	A	549	ASP	2.8
1	B	398	LEU	2.7
1	B	533	VAL	2.7
1	B	536	LYS	2.7
1	A	176	ALA	2.7
1	A	578	ALA	2.7
1	C	504	ALA	2.7
1	B	563	ASP	2.7
1	A	547	VAL	2.7
1	B	511	ALA	2.7
1	C	2	ALA	2.7
1	A	579	SER	2.6
1	A	576	VAL	2.6
1	A	2	ALA	2.6
1	B	541	LYS	2.6
1	C	118	PRO	2.6
1	A	577	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	573	LYS	2.5
1	C	582	ALA	2.5
1	B	554	PHE	2.5
1	C	509	PHE	2.5
1	B	540	THR	2.5
1	B	452	TYR	2.5
1	A	502	PHE	2.5
1	B	440	HIS	2.5
1	B	577	ALA	2.5
1	C	569	ALA	2.5
1	B	442	GLU	2.4
1	B	401	TYR	2.4
1	C	554	PHE	2.4
1	A	504	ALA	2.4
1	A	569	ALA	2.4
1	C	577	ALA	2.4
1	B	574	LYS	2.4
1	B	395	PHE	2.4
1	B	514	CYS	2.4
1	B	438	CYS	2.3
1	C	560	LYS	2.3
1	B	394	LEU	2.3
1	B	502	PHE	2.3
1	C	566	THR	2.3
1	B	544	LEU	2.3
1	B	567	CYS	2.3
1	A	511	ALA	2.3
1	C	544	LEU	2.3
1	C	57	GLU	2.3
1	A	3	HIS	2.2
1	C	452	TYR	2.2
1	B	572	GLY	2.2
1	A	182	LEU	2.2
1	C	513	ILE	2.2
1	C	511	ALA	2.2
1	C	575	LEU	2.2
1	B	547	VAL	2.2
1	C	116	VAL	2.2
1	C	516	LEU	2.2
1	C	561	ALA	2.1
1	C	54	VAL	2.1
1	A	510	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	2.1
1	A	516	LEU	2.1
1	B	468	PRO	2.1
1	A	88	ALA	2.1
1	B	566	THR	2.1
1	A	551	PHE	2.0
1	B	388	ILE	2.0
1	B	499	PRO	2.0
1	A	558	CYS	2.0
1	B	555	VAL	2.0
1	C	160	ARG	2.0
1	C	581	ALA	2.0
1	C	572	GLY	2.0
1	B	412	THR	2.0
1	B	508	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](#)

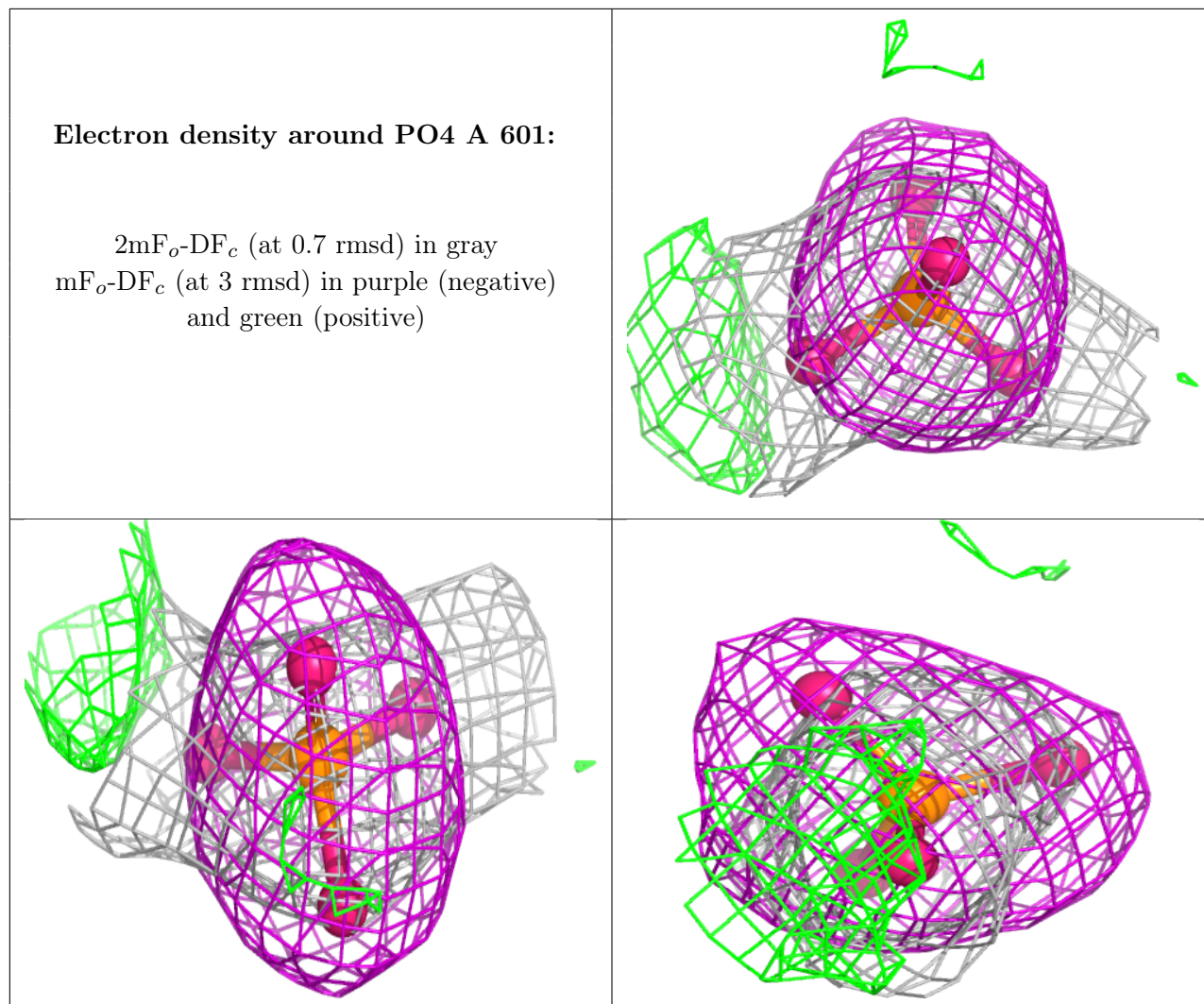
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PO4	A	601	5/5	0.75	0.38	20,20,20,20	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 PO4 A 601:

$2mF_o-DF_c$ (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.