



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:44 AM UTC

PDB ID : 3ZLV / pdb_00003zlv
Title : Crystal structure of mouse acetylcholinesterase in complex with tabun and HI-6
Authors : Artursson, E.; Andersson, P.O.; Akfur, C.; Linusson, A.; Borjegen, S.; Ekstrom, F.
Deposited on : 2013-02-04
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

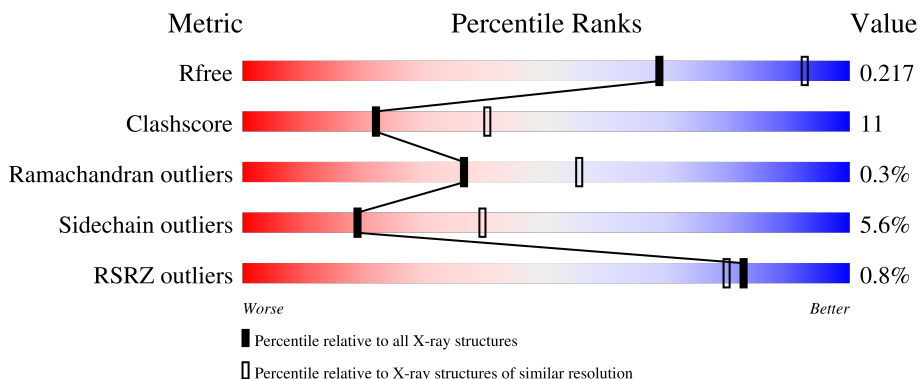
1 Overall quality at a glance

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	543	 78% 19% ..
1	B	543	 71% 25% ..

2 Entry composition [i](#)

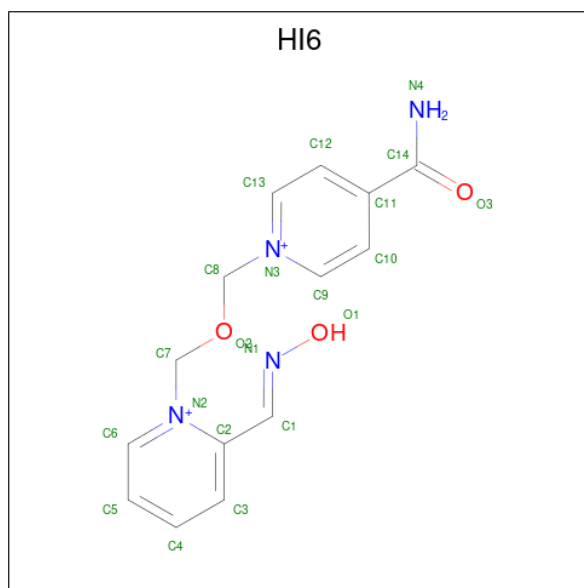
There are 6 unique types of molecules in this entry. The entry contains 9211 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

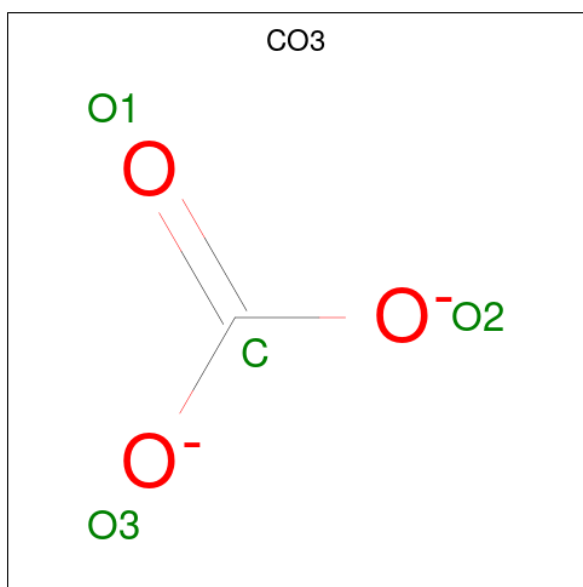
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	P	S	0	4	0
			4224	2708	734	767	1	14			
1	B	535	Total	C	N	O	P	S	0	4	0
			4225	2709	734	767	1	14			

- Molecule 2 is 4-(AMINOCARBONYL)-1-[(2-[(E)-(HYDROXYIMINO)METHYL]PYRIDINIUM-1-YL}METHOXY)METHYL]PYRIDINIUM (CCD ID: HI6) (formula: C₁₄H₁₆N₄O₃).



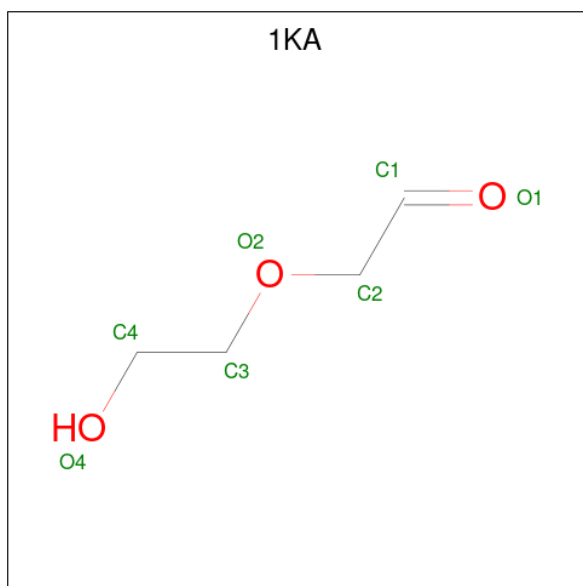
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	8	2	2		
2	B	1	Total	C	N	O	0	0
			12	8	2	2		

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is (2-hydroxyethoxy)acetaldehyde (CCD ID: 1KA) (formula: C₄H₈O₃).



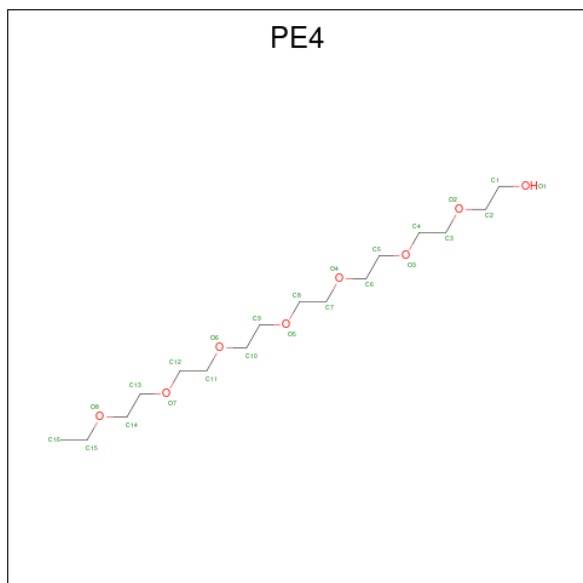
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			23	15	8		

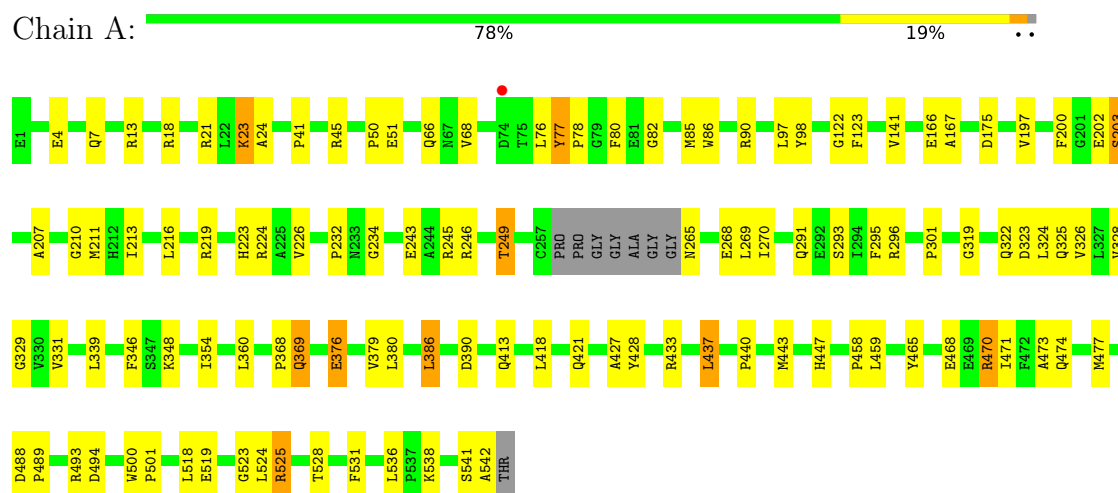
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	394	Total	O	0	0
			394	394		
6	B	282	Total	O	0	0
			282	282		

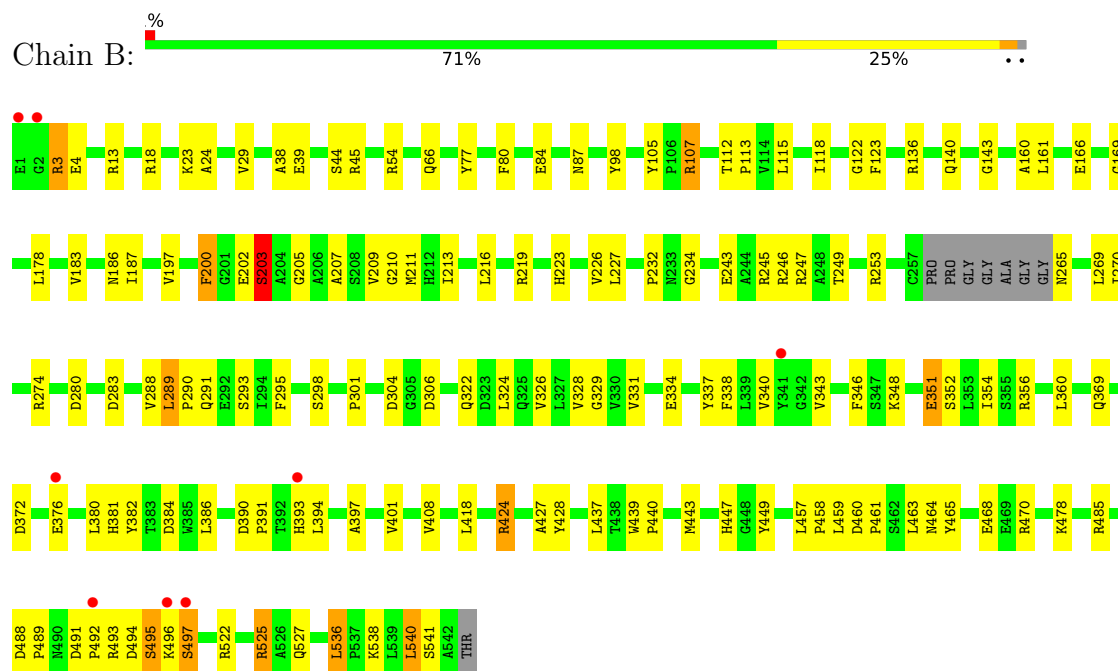
3 Residue-property plots

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: ACETYLCHOLINESTERASE



• Molecule 1: ACETYLCHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.57Å 112.38Å 226.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.19 – 2.50 29.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.19-2.50) 99.9 (29.19-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.176 , 0.226 0.170 , 0.217	Depositor DCC
R_{free} test set	1428 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9211	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: HI6, PE4, CO3, SUN, 1KA

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	0.42	0/4335	0.80	8/5921 (0.1%)
1	B	0.40	0/4336	0.78	5/5922 (0.1%)
All	All	0.41	0/8671	0.79	13/11843 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	GLY	CA-C-N	6.54	126.12	119.19
1	A	234	GLY	C-N-CA	6.54	126.12	119.19
1	B	289	LEU	CA-C-N	6.36	126.57	119.32
1	B	289	LEU	C-N-CA	6.36	126.57	119.32
1	A	167	ALA	CA-C-N	5.44	124.95	119.19
1	A	167	ALA	C-N-CA	5.44	124.95	119.19
1	A	390	ASP	CA-C-N	5.42	125.06	119.05
1	A	390	ASP	C-N-CA	5.42	125.06	119.05
1	A	77	TYR	CA-C-N	5.41	125.67	119.83
1	A	77	TYR	C-N-CA	5.41	125.67	119.83
1	B	343	VAL	N-CA-C	5.17	113.13	107.60
1	B	234	GLY	CA-C-N	5.01	124.62	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	GLY	C-N-CA	5.01	124.62	119.56

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	GLU	Mainchain
1	B	202	GLU	Mainchain
1	B	203	SUN	Mainchain

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	4224	0	4097	78	0
1	B	4225	0	4099	103	0
2	A	12	0	8	0	0
2	B	12	0	8	0	0
3	A	4	0	0	0	0
4	A	21	0	24	1	0
4	B	14	0	16	2	0
5	B	23	0	29	5	0
6	A	394	0	0	8	0
6	B	282	0	0	2	0
All	All	9211	0	8281	180	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 11.

All (180) 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:B:107:ARG:HH11	1:B:107:ARG:HG3	1.06	1.07
1:B:424:ARG:HG2	1:B:424:ARG:HH11	1.28	0.95
1:B:210:GLY:HA3	1:B:232:PRO:HG3	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:H	1:A:223:HIS:HD2	1.08	0.92
1:A:376:GLU:HG3	6:A:2310:HOH:O	1.72	0.89
1:B:197:VAL:H	1:B:223:HIS:HD2	1.17	0.88
1:A:369:GLN:HE21	1:A:369:GLN:H	1.17	0.87
1:A:210:GLY:HA3	1:A:232:PRO:HG3	1.57	0.84
1:B:107:ARG:HG3	1:B:107:ARG:NH1	1.83	0.82
1:B:197:VAL:H	1:B:223:HIS:CD2	1.97	0.82
1:A:197:VAL:H	1:A:223:HIS:CD2	1.98	0.80
1:B:166:GLU:HB2	1:B:270:ILE:HD13	1.68	0.75
1:A:369:GLN:H	1:A:369:GLN:NE2	1.85	0.75
1:B:493:ARG:HG3	1:B:494:ASP:H	1.52	0.73
1:A:50:PRO:HG3	1:A:175:ASP:OD1	1.88	0.73
1:A:525:ARG:HH11	1:A:525:ARG:CG	2.02	0.73
1:A:376:GLU:O	1:A:380:LEU:HG	1.93	0.69
1:B:424:ARG:HG2	1:B:424:ARG:NH1	2.04	0.68
1:A:376:GLU:OE2	1:B:538:LYS:HE3	1.93	0.68
1:B:527:GLN:HE21	5:B:1545:PE4:H12	1.56	0.68
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.29	0.68
1:A:519:GLU:HB2	6:A:2360:HOH:O	1.93	0.67
1:B:210:GLY:CA	1:B:232:PRO:HG3	2.23	0.67
1:B:112:THR:HG21	1:B:143:GLY:O	1.95	0.67
1:A:369:GLN:HE21	1:A:369:GLN:N	1.92	0.66
1:A:525:ARG:HH11	1:A:525:ARG:HG2	1.62	0.65
5:B:1545:PE4:H132	4:B:1546:1KA:H7	1.80	0.64
1:B:245:ARG:O	1:B:249:THR:HG23	1.97	0.64
1:B:372:ASP:O	1:B:376[B]:GLU:HG3	1.98	0.63
1:B:243:GLU:O	1:B:247:ARG:HG3	1.99	0.63
1:A:265:ASN:OD1	1:A:268:GLU:HG3	1.99	0.61
1:B:536:LEU:HD13	1:B:540:LEU:HD13	1.81	0.61
1:A:7:GLN:HG3	6:A:2012:HOH:O	1.99	0.61
1:A:360:LEU:HD22	1:A:379:VAL:HG21	1.83	0.61
1:B:107:ARG:HH11	1:B:107:ARG:CG	1.96	0.61
1:A:213:ILE:O	1:A:219:ARG:HD3	2.02	0.60
1:B:207:ALA:O	1:B:211:MET:HG2	2.01	0.60
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.82	0.60
1:B:351:GLU:OE1	1:B:351:GLU:HA	2.01	0.60
1:B:424:ARG:NH1	1:B:424:ARG:CG	2.64	0.59
4:B:1546:1KA:H5	6:B:2208:HOH:O	2.00	0.59
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.37	0.59
1:A:348:LYS:O	1:A:440:PRO:HG3	2.02	0.59
1:B:382:TYR:O	1:B:393[A]:HIS:HE1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.84	0.59
1:A:433:ARG:HG3	1:A:437:LEU:HD23	1.86	0.58
1:A:245:ARG:O	1:A:249:THR:CG2	2.52	0.57
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.85	0.57
1:B:213:ILE:O	1:B:219:ARG:HD3	2.05	0.57
1:A:7:GLN:CG	6:A:2012:HOH:O	2.52	0.57
1:B:337:TYR:HA	1:B:443:MET:CE	2.35	0.56
1:A:538:LYS:HD3	1:B:376[B]:GLU:OE1	2.05	0.56
1:B:424:ARG:HH11	1:B:424:ARG:CG	2.04	0.56
1:A:296:ARG:HH21	1:A:369:GLN:NE2	2.04	0.55
1:B:203:SUN:HBC2	1:B:447[A]:HIS:NE2	2.21	0.55
1:B:326:VAL:HG12	1:B:328:VAL:HG13	1.89	0.55
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.89	0.54
1:A:293:SER:HB3	1:A:368:PRO:HG3	1.88	0.54
1:A:525:ARG:CG	1:A:525:ARG:NH1	2.64	0.54
1:B:328:VAL:O	1:B:427:ALA:HA	2.08	0.54
1:A:296:ARG:HH21	1:A:369:GLN:HE22	1.54	0.54
1:B:3:ARG:HB2	1:B:3:ARG:HH11	1.73	0.54
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.89	0.53
1:B:122:GLY:O	1:B:123:PHE:HB2	2.08	0.53
1:A:328:VAL:O	1:A:427:ALA:HA	2.07	0.53
1:B:288:VAL:CG2	1:B:298:SER:HB3	2.38	0.53
1:B:3:ARG:HB2	1:B:3:ARG:NH1	2.24	0.52
1:B:540:LEU:HD23	1:B:541:SER:N	2.24	0.52
1:B:45:ARG:HG2	6:B:2037:HOH:O	2.09	0.52
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.91	0.52
1:B:84:GLU:HA	1:B:87:ASN:HD22	1.74	0.51
1:A:380:LEU:HB2	5:B:1545:PE4:H41	1.92	0.51
1:A:41:PRO:HG3	1:A:97:LEU:CD1	2.41	0.51
1:B:39:GLU:OE1	1:B:54:ARG:HD3	2.11	0.51
1:A:245:ARG:O	1:A:249:THR:HG23	2.10	0.51
1:A:368:PRO:HD2	1:A:369:GLN:NE2	2.26	0.51
1:B:13:ARG:HG3	1:B:186:ASN:OD1	2.11	0.51
1:B:390:ASP:OD2	1:B:393[B]:HIS:ND1	2.42	0.51
1:B:203:SUN:H4C2	1:B:338[B]:PHE:HZ	1.76	0.51
4:A:1547:1KA:H3	6:A:2226:HOH:O	2.11	0.50
1:A:210:GLY:CA	1:A:232:PRO:HG3	2.37	0.50
1:A:470:ARG:HB3	1:A:470:ARG:CZ	2.42	0.49
1:A:77:TYR:O	1:A:80:PHE:HB3	2.13	0.49
1:A:440:PRO:HD2	1:A:443:MET:SD	2.52	0.49
1:B:346:PHE:HA	1:B:352:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:GLN:NE2	6:A:2215:HOH:O	2.45	0.49
1:B:66:GLN:HG3	1:B:98:TYR:CD2	2.48	0.48
1:A:523:GLY:HA3	1:B:386:LEU:HD21	1.95	0.48
1:A:319:GLY:O	1:A:421:GLN:NE2	2.47	0.48
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.49	0.48
1:A:368:PRO:HD2	1:A:369:GLN:HE22	1.79	0.48
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.49	0.48
1:A:493:ARG:HB2	1:A:493:ARG:NH1	2.29	0.48
1:A:80:PHE:CE2	1:A:82:GLY:HA3	2.49	0.47
1:B:334:GLU:O	1:B:338[A]:PHE:HE1	1.96	0.47
1:B:463:LEU:O	1:B:464:ASN:HB2	2.14	0.47
1:B:66:GLN:HG3	1:B:98:TYR:CG	2.49	0.47
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.97	0.47
1:B:211:MET:HE3	1:B:301:PRO:HG2	1.97	0.47
1:B:381:HIS:HA	5:B:1545:PE4:H112	1.96	0.47
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.97	0.46
1:A:51:GLU:HG2	6:A:2058:HOH:O	2.14	0.46
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.95	0.46
1:B:38:ALA:HB2	1:B:178:LEU:HD23	1.96	0.46
1:B:160:ALA:HB2	1:B:169:GLY:HA2	1.96	0.46
1:A:245:ARG:O	1:A:249:THR:HG22	2.16	0.46
1:B:331:VAL:HG22	1:B:334:GLU:OE2	2.16	0.46
1:B:356:ARG:O	1:B:360:LEU:HG	2.16	0.46
1:B:44:SER:HA	1:B:274:ARG:HD2	1.97	0.46
1:A:528:THR:O	1:A:531:PHE:HB3	2.17	0.45
1:B:329:GLY:HA3	1:B:428:TYR:CE1	2.51	0.45
1:A:76:LEU:C	1:A:78:PRO:HD3	2.42	0.45
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.52	0.45
1:A:331:VAL:HG21	1:A:447[B]:HIS:HA	1.98	0.45
1:A:211:MET:HE3	1:A:301:PRO:HG2	1.98	0.45
1:B:460:ASP:O	1:B:463:LEU:HB2	2.16	0.44
1:B:493:ARG:HG3	1:B:494:ASP:N	2.26	0.44
1:B:457:LEU:N	1:B:458:PRO:CD	2.80	0.44
1:B:488:ASP:OD1	1:B:489:PRO:HD2	2.18	0.44
1:A:324:LEU:HG	1:A:326:VAL:HG23	2.00	0.44
1:B:105:TYR:C	1:B:105:TYR:CD1	2.96	0.44
1:A:207:ALA:O	1:A:211:MET:HG2	2.17	0.44
1:B:29:VAL:HG21	1:B:136:ARG:HB2	1.99	0.44
1:B:118:ILE:O	1:B:205:GLY:HA3	2.18	0.44
1:B:337:TYR:HA	1:B:443:MET:HE1	2.00	0.44
1:B:107:ARG:NH1	1:B:107:ARG:CG	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:TRP:HB3	1:B:440:PRO:HD2	1.99	0.43
1:B:495:SER:O	1:B:497:SER:N	2.52	0.43
1:A:243:GLU:OE2	1:A:246:ARG:NH1	2.51	0.43
1:A:339:LEU:HD13	1:A:346:PHE:CE2	2.53	0.43
1:B:354:ILE:O	1:B:391:PRO:HB3	2.18	0.43
1:B:540:LEU:HD23	1:B:540:LEU:C	2.43	0.43
1:A:265:ASN:HA	6:A:2242:HOH:O	2.17	0.43
1:A:122:GLY:O	1:A:123:PHE:HB2	2.18	0.43
1:A:524:LEU:O	1:A:525:ARG:C	2.62	0.43
1:B:536:LEU:O	1:B:540:LEU:HD22	2.18	0.43
1:B:380:LEU:HB2	5:B:1545:PE4:H82	2.01	0.43
1:B:183:VAL:HG13	1:B:187:ILE:HB	2.01	0.43
1:A:203:SUN:HBC2	1:A:447[A]:HIS:NE2	2.33	0.43
1:B:80:PHE:O	1:B:84:GLU:HG2	2.19	0.43
1:B:200:PHE:CB	1:B:226:VAL:HB	2.49	0.43
1:B:205:GLY:O	1:B:209:VAL:HG23	2.19	0.43
1:B:331:VAL:HG21	1:B:447[B]:HIS:HA	2.01	0.43
1:A:85:MET:HE2	1:A:86:TRP:CZ2	2.53	0.42
1:A:473:ALA:O	1:A:477:MET:HG3	2.19	0.42
1:A:524:LEU:HD12	1:A:524:LEU:HA	1.74	0.42
1:A:4:GLU:OE1	1:A:18:ARG:HD3	2.18	0.42
1:B:203:SUN:H4C2	1:B:203:SUN:H1C2	2.01	0.42
1:A:541:SER:O	1:A:542:ALA:HB2	2.17	0.42
1:B:324:LEU:HG	1:B:326:VAL:HG23	2.02	0.42
1:B:491:ASP:HA	1:B:492:PRO:HD3	1.81	0.42
1:A:141:VAL:HG21	1:A:459:LEU:CD2	2.50	0.42
1:A:525:ARG:NH1	1:A:525:ARG:HG3	2.33	0.42
1:B:463:LEU:HD23	1:B:463:LEU:HA	1.86	0.42
1:A:68:VAL:HG23	1:A:90:ARG:HB2	2.02	0.41
1:B:384:ASP:OD1	1:B:384:ASP:C	2.63	0.41
1:A:200:PHE:CB	1:A:226:VAL:HB	2.50	0.41
1:B:280:ASP:O	1:B:283:ASP:HB2	2.19	0.41
1:A:386:LEU:HD21	1:B:522:ARG:HB3	2.01	0.41
1:B:437:LEU:HD11	1:B:449:TYR:CD2	2.55	0.41
1:B:390:ASP:HA	1:B:391:PRO:HD3	1.83	0.41
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.56	0.41
1:A:470:ARG:NH1	1:A:474:GLN:OE1	2.53	0.41
1:B:77:TYR:CD1	1:B:348:LYS:HE3	2.55	0.41
1:B:304:ASP:OD2	1:B:306:ASP:HB3	2.21	0.41
1:A:23:LYS:HE2	1:A:24:ALA:O	2.21	0.41
1:A:293:SER:HB3	1:A:368:PRO:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:TYR:CD1	1:A:428:TYR:C	2.98	0.41
1:A:488:ASP:HA	1:A:489:PRO:HD3	1.92	0.41
1:B:394:LEU:HD23	1:B:394:LEU:HA	1.95	0.41
1:A:500:TRP:HA	1:A:501:PRO:HD3	1.90	0.40
1:B:459:LEU:O	1:B:461:PRO:HD3	2.21	0.40
1:B:337:TYR:CD2	1:B:447[B]:HIS:CE1	3.09	0.40
1:B:351:GLU:OE1	1:B:351:GLU:CA	2.68	0.40
1:A:269:LEU:C	1:A:269:LEU:HD23	2.46	0.40
1:B:337:TYR:HB3	1:B:447[B]:HIS:NE2	2.36	0.40
1:B:352:SER:O	1:B:354:ILE:HG23	2.22	0.40
1:B:397:ALA:O	1:B:401:VAL:HG23	2.21	0.40
1:A:166:GLU:HB2	1:A:270:ILE:HD13	2.03	0.40
1:B:289:LEU:HA	1:B:290:PRO:HD2	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	534/543 (98%)	517 (97%)	16 (3%)	1 (0%)	43	63
1	B	534/543 (98%)	510 (96%)	22 (4%)	2 (0%)	30	49
All	All	1068/1086 (98%)	1027 (96%)	38 (4%)	3 (0%)	36	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	495	SER
1	B	496	LYS
1	A	494	ASP

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	442/442 (100%)	420 (95%)	22 (5%)	22	44
1	B	442/442 (100%)	415 (94%)	27 (6%)	17	35
All	All	884/884 (100%)	835 (94%)	49 (6%)	19	40

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	21	ARG
1	A	23	LYS
1	A	45	ARG
1	A	216	LEU
1	A	249	THR
1	A	291	GLN
1	A	295	PHE
1	A	322	GLN
1	A	323	ASP
1	A	354	ILE
1	A	369	GLN
1	A	376	GLU
1	A	386	LEU
1	A	418	LEU
1	A	437	LEU
1	A	468	GLU
1	A	470	ARG
1	A	471	ILE
1	A	518	LEU
1	A	525	ARG
1	A	536	LEU
1	B	3	ARG
1	B	4	GLU
1	B	18	ARG
1	B	23	LYS
1	B	107	ARG

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Mol	Chain	Res	Type
1	B	115	LEU
1	B	200	PHE
1	B	216	LEU
1	B	246	ARG
1	B	253	ARG
1	B	265	ASN
1	B	291	GLN
1	B	293	SER
1	B	295	PHE
1	B	322	GLN
1	B	340	VAL
1	B	351	GLU
1	B	369	GLN
1	B	418	LEU
1	B	424	ARG
1	B	468	GLU
1	B	470	ARG
1	B	478	LYS
1	B	497	SER
1	B	525	ARG
1	B	536	LEU
1	B	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	284	HIS
1	A	291	GLN
1	A	369	GLN
1	A	421	GLN
1	A	509	GLN
1	B	87	ASN
1	B	223	HIS
1	B	291	GLN
1	B	322	GLN
1	B	387	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	SUN	A	203	1	12,13,14	2.08	2 (16%)	10,17,19	2.10	3 (30%)
1	SUN	B	203	1	12,13,14	2.05	3 (25%)	10,17,19	1.98	3 (30%)

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
1	SUN	A	203	1	-	5/16/18/20	-
1	SUN	B	203	1	-	4/16/18/20	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	SUN	O-C	5.25	1.39	1.20
1	B	203	SUN	O-C	5.20	1.39	1.20
1	A	203	SUN	P1-N1	3.54	1.70	1.62
1	B	203	SUN	P1-N1	3.41	1.70	1.62
1	B	203	SUN	P1-O2	2.09	1.65	1.57

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	SUN	OG-CB-CA	4.68	112.70	108.14
1	B	203	SUN	OG-CB-CA	4.49	112.52	108.14
1	A	203	SUN	O2-P1-OG	2.56	108.67	100.62
1	B	203	SUN	O2-P1-OG	2.53	108.57	100.62
1	A	203	SUN	OG-P1-O1	-2.32	108.30	115.71
1	B	203	SUN	OG-P1-O1	-2.17	108.78	115.71

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	203	SUN	C2-N1-P1-OG
1	A	203	SUN	C1-N1-P1-O2
1	B	203	SUN	C1-N1-P1-OG
1	B	203	SUN	C1-N1-P1-O2
1	B	203	SUN	C4-C3-O2-P1
1	A	203	SUN	C4-C3-O2-P1
1	A	203	SUN	C2-N1-P1-O1
1	A	203	SUN	N-CA-CB-OG
1	B	203	SUN	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	203	SUN	1	0
1	B	203	SUN	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
4	1KA	B	1546	-	6,6,6	1.58	1 (16%)	5,5,5	1.74	2 (40%)
2	HI6	A	1543	-	12,12,22	0.55	0	12,15,28	0.54	0
3	CO3	A	1544	-	3,3,3	0.95	0	2,3,3	0.17	0
4	1KA	A	1545	-	6,6,6	1.59	1 (16%)	5,5,5	1.93	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HI6	B	1543	-	12,12,22	0.55	0	12,15,28	0.51	0
4	1KA	B	1544	-	6,6,6	1.58	1 (16%)	5,5,5	1.83	1 (20%)
4	1KA	A	1547	-	6,6,6	1.60	1 (16%)	5,5,5	1.68	1 (20%)
4	1KA	A	1546	-	6,6,6	1.60	1 (16%)	5,5,5	1.74	1 (20%)
5	PE4	B	1545	-	22,22,23	0.55	0	21,21,22	1.58	1 (4%)

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
4	1KA	B	1546	-	-	2/3/4/4	-
2	HI6	A	1543	-	-	2/7/7/13	0/1/1/2
4	1KA	A	1545	-	-	3/3/4/4	-
2	HI6	B	1543	-	-	1/7/7/13	0/1/1/2
4	1KA	B	1544	-	-	1/3/4/4	-
4	1KA	A	1547	-	-	1/3/4/4	-
4	1KA	A	1546	-	-	1/3/4/4	-
5	PE4	B	1545	-	-	9/20/20/21	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1545	1KA	O1-C1	3.66	1.40	1.20
4	A	1547	1KA	O1-C1	3.66	1.40	1.20
4	A	1546	1KA	O1-C1	3.65	1.40	1.20
4	B	1544	1KA	O1-C1	3.62	1.40	1.20
4	B	1546	1KA	O1-C1	3.61	1.40	1.20

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1545	1KA	O1-C1-C2	-3.07	117.03	126.10
4	B	1544	1KA	O1-C1-C2	-2.91	117.51	126.10
4	A	1546	1KA	O1-C1-C2	-2.59	118.44	126.10
4	B	1546	1KA	O1-C1-C2	-2.56	118.52	126.10
4	A	1547	1KA	O1-C1-C2	-2.42	118.93	126.10
4	B	1546	1KA	O2-C3-C4	2.07	119.25	110.11
5	B	1545	PE4	O3-C5-C6	2.04	119.66	110.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1543	HI6	O2-C8-N3-C9
2	A	1543	HI6	O2-C8-N3-C13
2	B	1543	HI6	N3-C8-O2-C7
4	B	1544	1KA	C4-C3-O2-C2
4	A	1545	1KA	O2-C3-C4-O4
5	B	1545	PE4	O7-C13-C14-O8
4	A	1546	1KA	O2-C3-C4-O4
5	B	1545	PE4	O2-C3-C4-O3
5	B	1545	PE4	O4-C7-C8-O5
4	A	1545	1KA	C1-C2-O2-C3
4	B	1546	1KA	C4-C3-O2-C2
5	B	1545	PE4	C8-C7-O4-C6
5	B	1545	PE4	O6-C10-C9-O5
5	B	1545	PE4	C13-C14-O8-C15
5	B	1545	PE4	C5-C6-O4-C7
4	A	1547	1KA	O2-C3-C4-O4
5	B	1545	PE4	C3-C4-O3-C5
4	A	1545	1KA	C4-C3-O2-C2
4	B	1546	1KA	C1-C2-O2-C3
5	B	1545	PE4	O6-C11-C12-O7

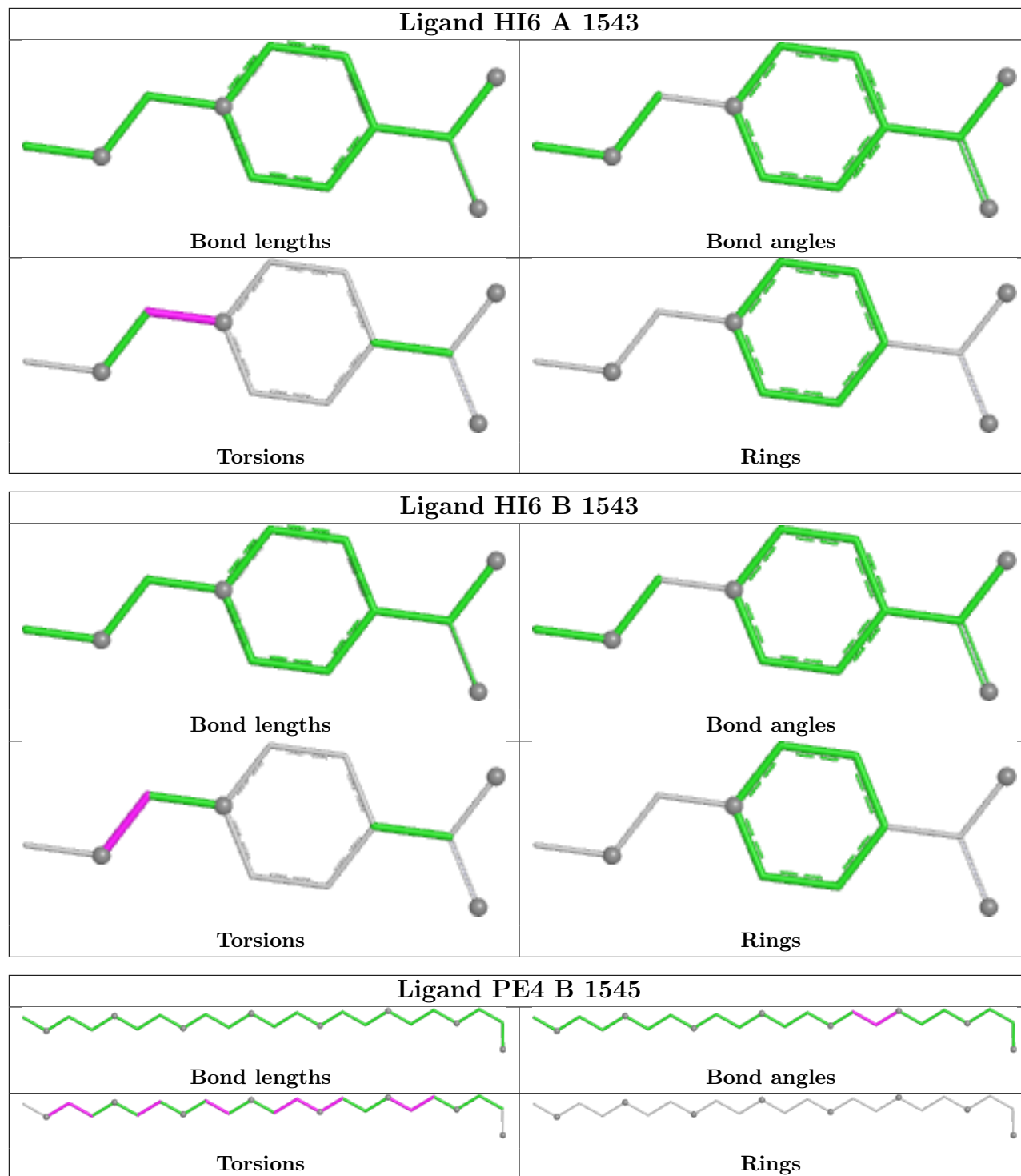
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1546	1KA	2	0
4	A	1547	1KA	1	0
5	B	1545	PE4	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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	534/543 (98%)	-0.50	1 (0%)	91 89	21, 43, 68, 119	4 (0%)
1	B	534/543 (98%)	-0.32	8 (1%)	72 68	23, 48, 73, 166	4 (0%)
All	All	1068/1086 (98%)	-0.41	9 (0%)	82 80	21, 45, 72, 166	8 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	393[A]	HIS	4.2
1	B	496	LYS	3.4
1	B	497	SER	3.2
1	B	1	GLU	3.2
1	B	376[A]	GLU	2.9
1	A	74[A]	ASP	2.8
1	B	2	GLY	2.2
1	B	492	PRO	2.0
1	B	341	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q < 0.9
1	SUN	A	203	14/15	0.98	0.07	32,36,48,54	0
1	SUN	B	203	14/15	0.98	0.06	32,41,52,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

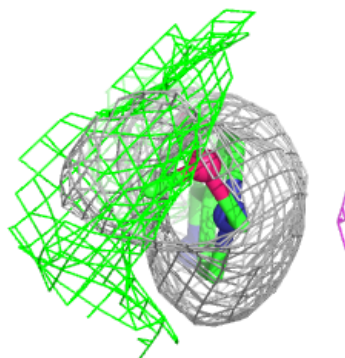
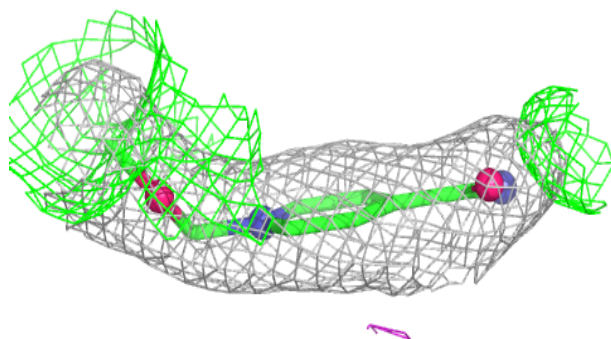
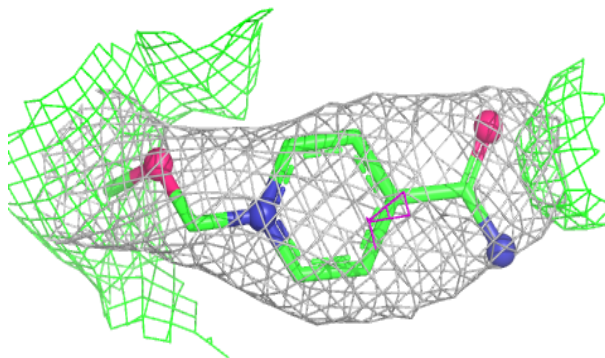
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	1KA	A	1547	7/7	0.75	0.19	55,70,80,83	0
2	HI6	B	1543	12/21	0.81	0.16	56,61,68,81	2
3	CO3	A	1544	4/4	0.81	0.14	67,77,77,79	0
2	HI6	A	1543	12/21	0.81	0.16	47,52,69,72	2
4	1KA	B	1544	7/7	0.82	0.15	65,68,75,79	0
4	1KA	A	1545	7/7	0.85	0.14	51,56,70,70	0
4	1KA	A	1546	7/7	0.88	0.14	55,65,82,86	0
4	1KA	B	1546	7/7	0.88	0.13	59,71,73,73	0
5	PE4	B	1545	23/24	0.88	0.15	45,57,80,83	0

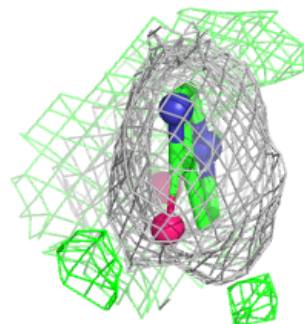
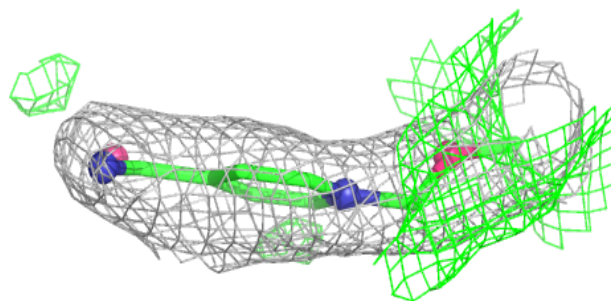
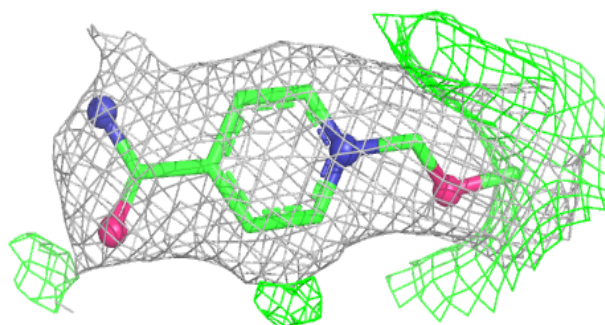
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

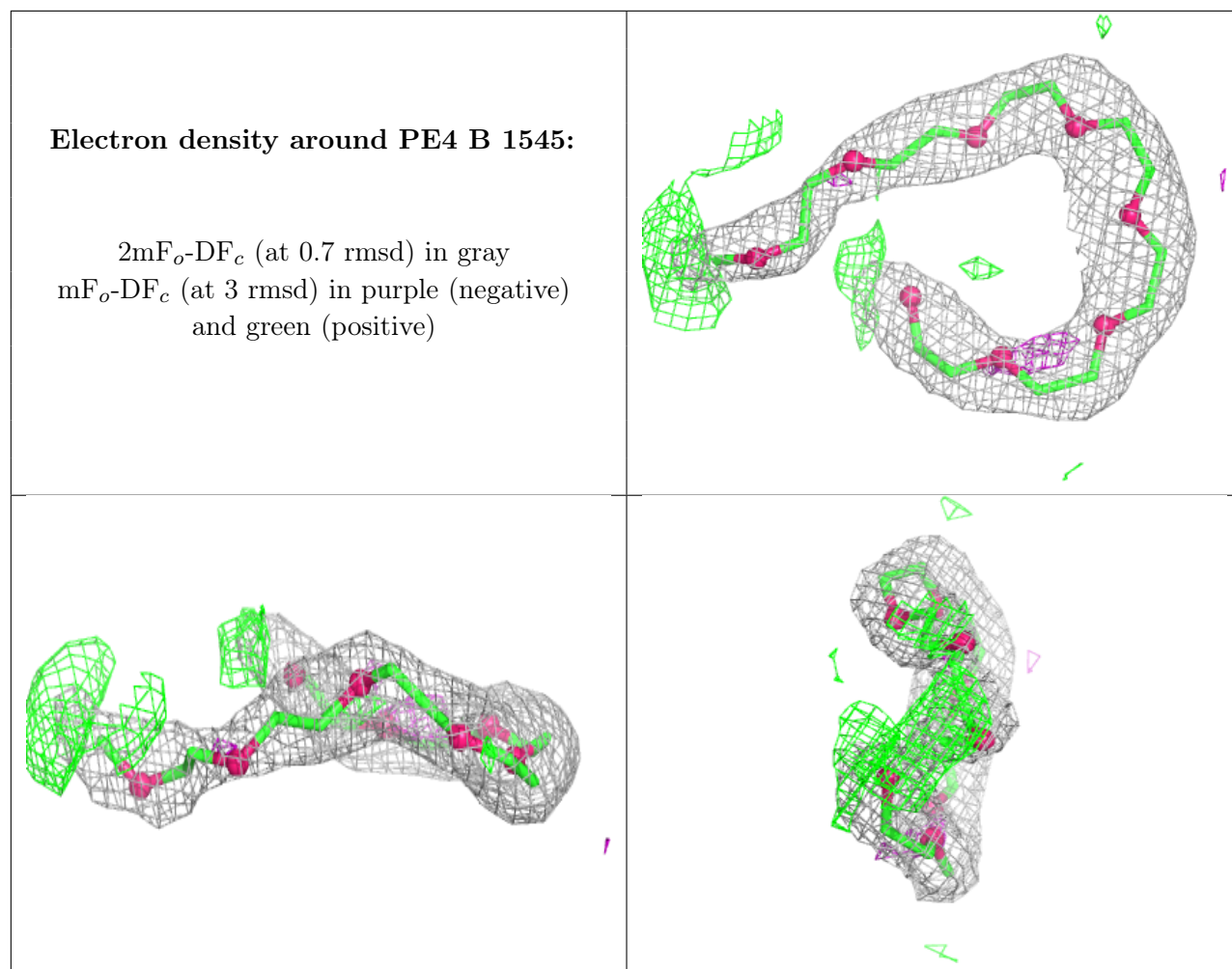
Electron density around HI6 B 1543:

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

**Electron density around HI6 A 1543:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.