



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:46 PM UTC

PDB ID : 5HN8 / pdb_00005hn8
Title : Crystal structure of Plasmodium vivax geranylgeranylpyrophosphate synthase complexed with BPH-1182
Authors : Liu, Y.-L.; Zhang, Y.; Oldfield, E.
Deposited on : 2016-01-18
Resolution : 2.70 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

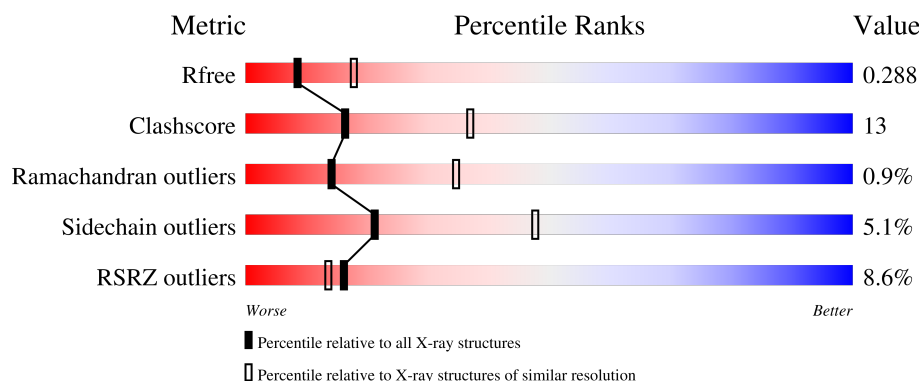
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	375	12% 65% 18% • 14%
1	B	375	4% 68% 17% • 13%
1	C	375	9% 64% 22% • 11%
1	D	375	5% 67% 20% • 11%

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	HXK	D	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10771 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.

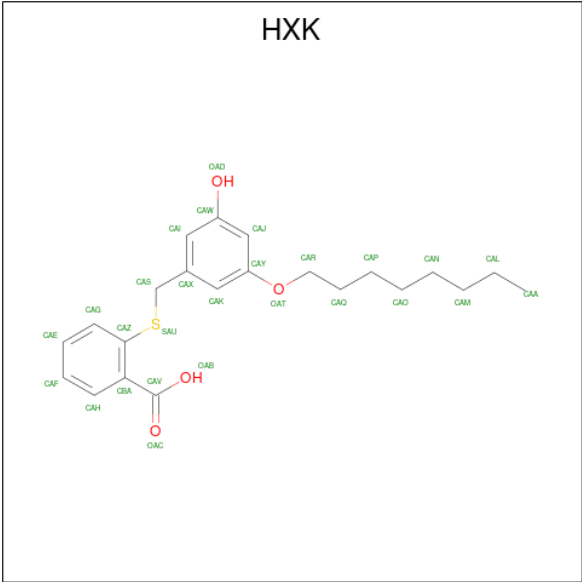
- Molecule 1 is a protein called Farnesyl pyrophosphate synthase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2580	1682	405	479	14			
1	B	326	Total	C	N	O	S	0	0	0
			2595	1684	414	483	14			
1	C	334	Total	C	N	O	S	0	0	0
			2662	1730	426	491	15			
1	D	334	Total	C	N	O	S	0	0	0
			2660	1731	424	490	15			

There are 8 discrepancies between the modelled and reference sequences:

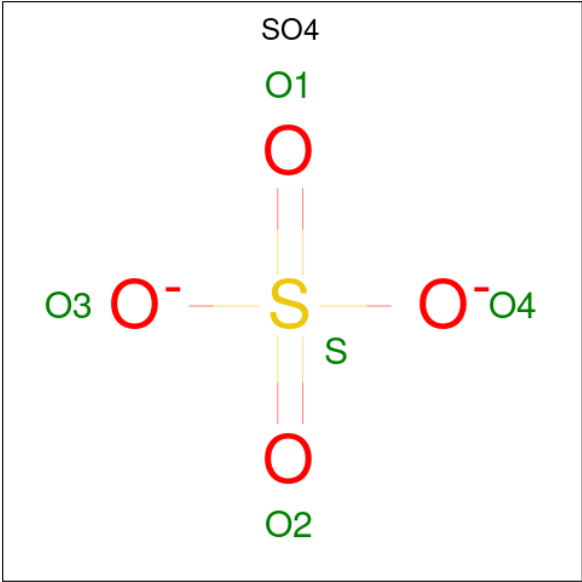
Chain	Residue	Modelled	Actual	Comment	Reference
A	134	MET	THR	SEE REMARK 999	UNP A5K4U6
A	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
B	134	MET	THR	SEE REMARK 999	UNP A5K4U6
B	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
C	134	MET	THR	SEE REMARK 999	UNP A5K4U6
C	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
D	134	MET	THR	SEE REMARK 999	UNP A5K4U6
D	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6

- Molecule 2 is 2-([3-hydroxy-5-(octyloxy)benzyl]sulfanyl)benzoic acid (CCD ID: HXK) (formula: C₂₂H₂₈O₄S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			27	22	4	1		
2	B	1	Total	C	O	S	0	0
			27	22	4	1		
2	C	1	Total	C	O	S	0	0
			27	22	4	1		
2	D	1	Total	C	O	S	0	0
			27	22	4	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

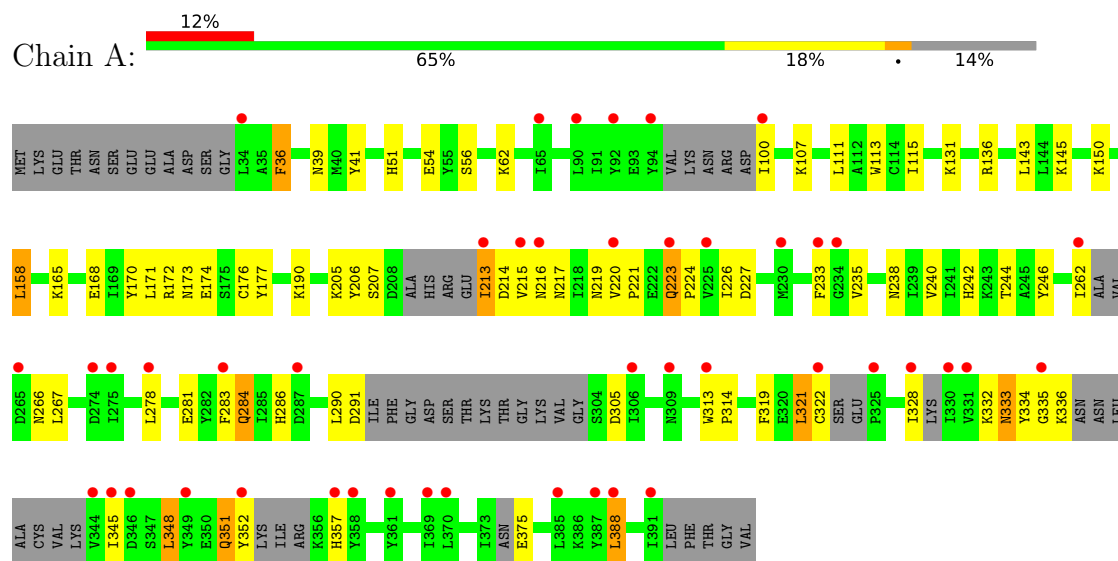
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	60	Total	O		0	0
			60	60			
4	B	19	Total	O		0	0
			19	19			
4	C	38	Total	O		0	0
			38	38			
4	D	44	Total	O		0	0
			44	44			

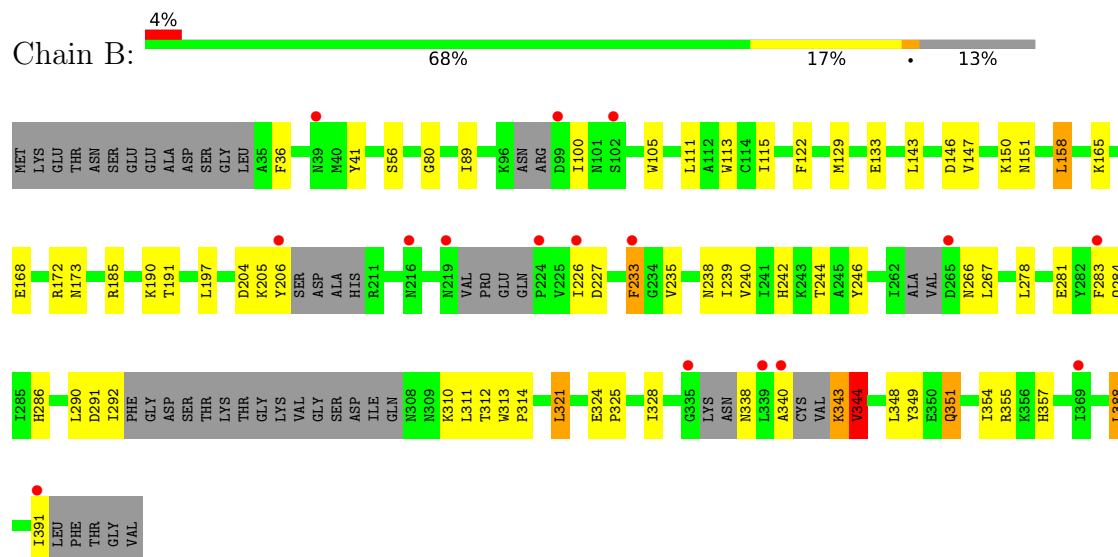
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

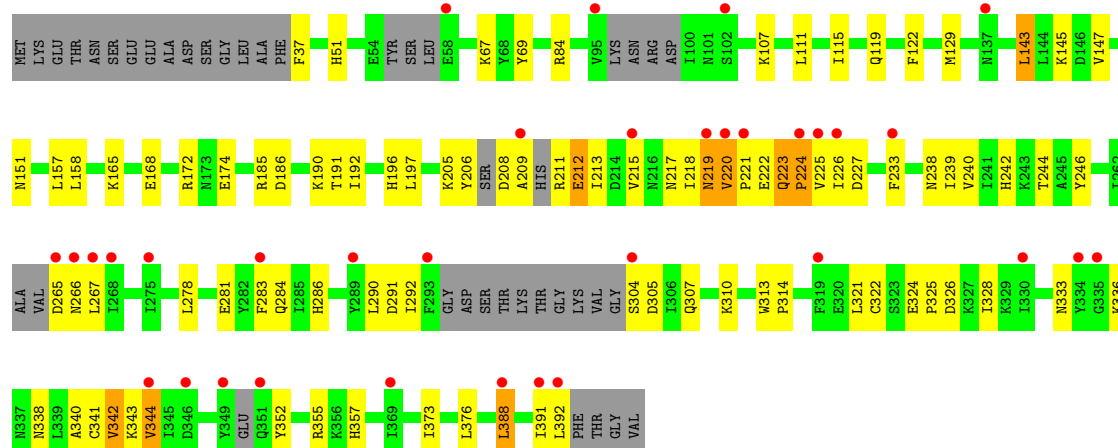
- Molecule 1: Farnesyl pyrophosphate synthase, putative



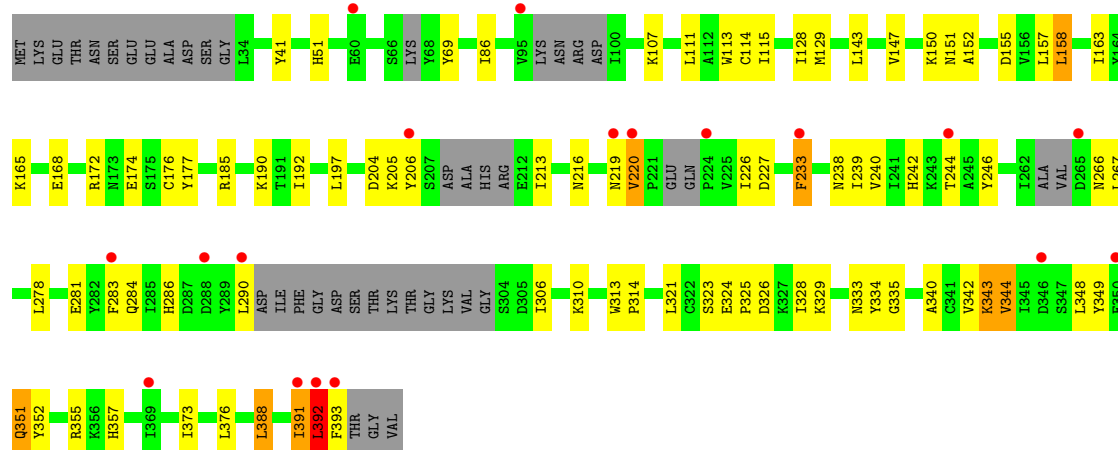
- Molecule 1: Farnesyl pyrophosphate synthase, putative



- Molecule 1: Farnesyl pyrophosphate synthase, putative



- Molecule 1: Farnesyl pyrophosphate synthase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.07Å 117.22Å 92.79Å 90.00° 116.20° 90.00°	Depositor
Resolution (Å)	31.10 – 2.70 31.10 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.0 (31.10-2.70) 91.9 (31.10-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.259 , 0.296 0.259 , 0.288	Depositor DCC
R_{free} test set	2075 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10771	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 4.87% 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: HXK, SO4

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	0/2631	0.98	7/3559 (0.2%)
1	B	0.74	0/2645	0.94	3/3582 (0.1%)
1	C	0.76	0/2712	0.91	1/3673 (0.0%)
1	D	0.74	0/2712	0.97	3/3675 (0.1%)
All	All	0.76	0/10700	0.95	14/14489 (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	B	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	391	ILE	N-CA-C	11.63	121.57	111.56
1	A	345	ILE	N-CA-C	-7.04	103.66	110.42
1	A	351	GLN	CB-CA-C	-6.89	100.01	110.90
1	B	344	VAL	N-CA-C	-6.71	95.38	109.34
1	A	36	PHE	N-CA-C	-6.30	104.34	111.14
1	C	305	ASP	N-CA-C	6.03	118.62	111.33
1	A	284	GLN	N-CA-C	-5.97	104.78	111.28
1	D	391	ILE	CB-CA-C	-5.57	106.15	111.44
1	D	155	ASP	N-CA-C	5.56	118.10	111.71
1	A	223	GLN	CA-C-N	5.55	125.72	119.90
1	A	223	GLN	C-N-CA	5.55	125.72	119.90
1	B	36	PHE	N-CA-C	-5.44	106.48	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ILE	N-CA-C	5.02	114.80	107.37
1	A	351	GLN	CA-CB-CG	5.02	124.13	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	343	LYS	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2580	0	2433	63	0
1	B	2595	0	2431	58	0
1	C	2662	0	2528	83	0
1	D	2660	0	2523	84	0
2	A	27	0	0	3	0
2	B	27	0	0	6	0
2	C	27	0	0	2	0
2	D	27	0	0	13	0
3	D	5	0	0	0	0
4	A	60	0	0	12	0
4	B	19	0	0	4	0
4	C	38	0	0	4	0
4	D	44	0	0	5	0
All	All	10771	0	9915	267	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 13.

All (267) 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)
2:A:401:H XK:CAA	1:C:157:LEU:HD12	1.85	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:PHE:CE1	1:C:392:LEU:HG	1.90	1.05
1:D:283:PHE:CD2	2:D:401:H XK:CAH	2.41	1.02
1:A:335:GLY:HA3	4:A:501:HOH:O	1.61	1.01
1:A:291:ASP:OD2	1:A:305:ASP:HB2	1.67	0.95
1:D:283:PHE:CE2	2:D:401:H XK:CAH	2.49	0.95
1:B:150:LYS:O	1:D:129:MET:HE3	1.66	0.93
2:A:401:H XK:CAA	1:C:157:LEU:CD1	2.49	0.89
1:D:283:PHE:CE2	2:D:401:H XK:CAV	2.55	0.88
1:D:283:PHE:CE2	2:D:401:H XK:CBA	2.60	0.85
1:A:165:LYS:NZ	1:C:185:ARG:HH22	1.76	0.83
1:D:283:PHE:HD2	2:D:401:H XK:CAH	1.92	0.79
1:A:190:LYS:HD3	1:A:246:TYR:CD1	2.19	0.78
1:C:265:ASP:CB	4:C:537:HOH:O	2.30	0.78
1:C:208:ASP:CG	1:C:209:ALA:H	1.93	0.77
1:D:190:LYS:HD3	1:D:246:TYR:CD1	2.20	0.77
1:A:262:ILE:CB	4:A:551:HOH:O	2.32	0.77
2:B:401:H XK:CAA	1:D:157:LEU:HD12	2.16	0.76
1:B:129:MET:HE3	1:D:150:LYS:O	1.86	0.75
1:D:283:PHE:HD2	2:D:401:H XK:CAF	2.00	0.75
1:D:391:ILE:C	1:D:393:PHE:N	2.41	0.74
1:A:221:PRO:HA	1:C:145:LYS:HG3	1.69	0.74
1:A:51:HIS:O	1:A:54:GLU:HG2	1.88	0.73
4:A:545:HOH:O	1:C:242:HIS:HE1	1.69	0.73
1:A:165:LYS:HZ1	1:C:185:ARG:HH22	1.35	0.72
1:C:185:ARG:NH2	1:C:186:ASP:OD1	2.22	0.72
1:C:190:LYS:HD3	1:C:246:TYR:CD1	2.25	0.71
1:C:223:GLN:O	1:C:225:VAL:HG13	1.91	0.71
1:B:165:LYS:NZ	1:D:185:ARG:HH11	1.89	0.70
1:A:100:ILE:N	4:A:502:HOH:O	2.23	0.70
1:C:119:GLN:HE22	2:C:401:H XK:CAS	2.03	0.70
1:B:321:LEU:HD21	1:B:357:HIS:HE1	1.56	0.70
1:A:240:VAL:HG22	1:A:284:GLN:HG2	1.74	0.70
1:B:340:ALA:H	1:B:343:LYS:HB2	1.57	0.69
2:D:401:H XK:OAD	4:D:501:HOH:O	2.10	0.69
1:A:319:PHE:HD1	4:A:523:HOH:O	1.74	0.68
1:A:286:HIS:O	1:A:290:LEU:HD12	1.93	0.68
1:A:145:LYS:HG3	1:C:219:ASN:O	1.94	0.68
1:D:283:PHE:HE2	2:D:401:H XK:CAV	2.04	0.67
1:D:321:LEU:HD21	1:D:357:HIS:HE1	1.58	0.67
1:B:190:LYS:HD3	1:B:246:TYR:CD1	2.31	0.66
1:C:290:LEU:O	1:C:292:ILE:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASN:HD22	1:A:336:LYS:HD3	1.58	0.66
1:A:165:LYS:NZ	1:C:185:ARG:NH2	2.44	0.66
1:A:41:TYR:HB2	1:A:113:TRP:CZ2	2.31	0.65
1:A:150:LYS:O	1:C:129:MET:HE3	1.97	0.65
1:A:145:LYS:HG3	1:C:220:VAL:O	1.97	0.64
1:B:391:ILE:C	4:B:502:HOH:O	2.39	0.64
1:C:342:VAL:C	1:C:344:VAL:H	2.04	0.64
1:C:240:VAL:HG22	1:C:284:GLN:HG2	1.78	0.64
1:A:321:LEU:HD21	1:A:357:HIS:HE1	1.63	0.64
1:C:208:ASP:CG	1:C:209:ALA:N	2.56	0.63
1:D:391:ILE:O	1:D:392:LEU:C	2.40	0.63
1:A:334:TYR:O	4:A:501:HOH:O	2.15	0.63
1:C:313:TRP:HB3	1:C:314:PRO:HD3	1.80	0.63
1:B:266:ASN:OD1	1:B:267:LEU:N	2.32	0.63
1:C:338:ASN:HD21	1:C:340:ALA:HB3	1.64	0.63
1:D:306:ILE:HG23	1:D:334:TYR:CD1	2.34	0.62
1:A:321:LEU:HD21	1:A:357:HIS:CE1	2.34	0.62
1:B:286:HIS:O	1:B:290:LEU:HD12	2.00	0.62
1:B:321:LEU:HD21	1:B:357:HIS:CE1	2.34	0.62
1:A:219:ASN:O	1:A:220:VAL:C	2.41	0.62
2:B:401:H XK:CAS	2:B:401:H XK:CAV	2.78	0.62
1:B:173:ASN:HB2	4:B:506:HOH:O	2.00	0.62
1:D:286:HIS:O	1:D:290:LEU:HD12	1.99	0.62
1:B:165:LYS:HZ1	1:D:185:ARG:HH11	1.47	0.61
1:D:388:LEU:HD13	1:D:392:LEU:HD13	1.82	0.61
1:C:290:LEU:C	1:C:292:ILE:H	2.07	0.61
1:C:321:LEU:HD21	1:C:357:HIS:HE1	1.66	0.61
1:A:313:TRP:HB3	1:A:314:PRO:HD3	1.82	0.61
1:D:391:ILE:O	1:D:393:PHE:N	2.34	0.61
1:A:238:ASN:O	1:A:242:HIS:HD2	1.83	0.60
1:B:240:VAL:HG22	1:B:284:GLN:HG2	1.82	0.60
1:D:283:PHE:HE2	2:D:401:H XK:CAH	2.09	0.60
1:C:283:PHE:CD1	1:C:392:LEU:HG	2.36	0.60
1:D:321:LEU:HD21	1:D:357:HIS:CE1	2.36	0.60
1:C:37:PHE:N	4:C:501:HOH:O	2.34	0.60
2:B:401:H XK:CAA	1:D:157:LEU:CD1	2.79	0.60
1:C:321:LEU:HD21	1:C:357:HIS:CE1	2.36	0.60
1:A:266:ASN:OD1	1:A:267:LEU:N	2.33	0.60
1:C:266:ASN:OD1	1:C:267:LEU:N	2.35	0.60
1:D:313:TRP:HB3	1:D:314:PRO:HD3	1.84	0.60
1:A:51:HIS:CE1	1:A:165:LYS:HE3	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ASN:ND2	1:C:145:LYS:HD3	2.17	0.59
1:D:342:VAL:O	1:D:344:VAL:N	2.35	0.59
1:D:306:ILE:HG23	1:D:334:TYR:CE1	2.38	0.59
1:B:292:ILE:C	1:B:355:ARG:NH1	2.61	0.59
1:D:342:VAL:C	1:D:344:VAL:H	2.10	0.58
1:D:266:ASN:OD1	1:D:267:LEU:N	2.35	0.58
1:D:238:ASN:O	1:D:242:HIS:HD2	1.86	0.58
1:C:119:GLN:NE2	2:C:401:HXK:CAS	2.67	0.58
1:C:338:ASN:ND2	1:C:340:ALA:HB3	2.18	0.58
1:C:168:GLU:O	1:C:172:ARG:HB3	2.03	0.57
1:B:168:GLU:CD	1:D:185:ARG:HH12	2.12	0.57
1:A:322:CYS:HA	1:A:352:TYR:CE1	2.40	0.57
1:A:281:GLU:C	1:A:283:PHE:H	2.12	0.57
1:C:322:CYS:HA	1:C:352:TYR:CE1	2.40	0.57
1:D:283:PHE:CD2	2:D:401:HXK:CAF	2.82	0.56
1:B:238:ASN:O	1:B:242:HIS:HD2	1.89	0.56
1:B:313:TRP:HB3	1:B:314:PRO:HD3	1.88	0.56
1:A:168:GLU:O	1:A:172:ARG:HB3	2.06	0.55
1:C:209:ALA:N	1:C:211:ARG:N	2.55	0.55
1:D:240:VAL:O	1:D:244:THR:HG22	2.06	0.55
1:A:322:CYS:HA	1:A:352:TYR:CZ	2.41	0.55
1:D:51:HIS:CE1	1:D:165:LYS:HE3	2.42	0.54
1:C:238:ASN:O	1:C:242:HIS:HD2	1.89	0.54
1:B:185:ARG:HH11	1:D:165:LYS:HZ1	1.56	0.54
1:B:168:GLU:O	1:B:172:ARG:HB3	2.08	0.54
1:B:324:GLU:N	1:B:325:PRO:HD2	2.23	0.54
1:C:344:VAL:HG23	4:C:517:HOH:O	2.08	0.54
1:D:326:ASP:OD2	1:D:352:TYR:OH	2.27	0.53
1:C:304:SER:O	1:C:307:GLN:HG3	2.08	0.53
1:B:286:HIS:CE1	1:B:290:LEU:HD11	2.44	0.53
4:A:545:HOH:O	1:C:242:HIS:CE1	2.50	0.53
1:D:114:CYS:HB3	1:D:163:ILE:HG23	1.91	0.53
1:D:324:GLU:N	1:D:325:PRO:HD2	2.23	0.53
1:D:168:GLU:O	1:D:172:ARG:HB3	2.08	0.53
1:B:158:LEU:HB2	1:D:192:ILE:HG21	1.92	0.52
1:C:373:ILE:O	1:C:376:LEU:HB2	2.08	0.52
1:C:212:GLU:CG	1:C:213:ILE:N	2.72	0.52
1:B:111:LEU:O	1:B:115:ILE:HG12	2.09	0.52
1:A:62:LYS:NZ	4:A:504:HOH:O	2.42	0.52
1:C:222:GLU:O	1:C:224:PRO:N	2.43	0.51
1:A:375:GLU:N	4:A:506:HOH:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ILE:C	1:B:355:ARG:HH12	2.19	0.51
1:B:281:GLU:C	1:B:283:PHE:H	2.19	0.50
1:D:283:PHE:CD2	2:D:401:H XK:CBA	2.89	0.50
1:A:333:ASN:ND2	1:A:336:LYS:HD3	2.26	0.50
1:A:214:ASP:OD1	1:A:216:ASN:N	2.38	0.50
1:B:147:VAL:O	1:B:151:ASN:HB2	2.11	0.50
1:B:290:LEU:O	1:B:292:ILE:N	2.44	0.50
1:C:219:ASN:O	1:C:220:VAL:O	2.30	0.50
1:D:286:HIS:CE1	1:D:290:LEU:HD11	2.47	0.50
1:C:283:PHE:CZ	1:C:392:LEU:HG	2.45	0.49
1:B:240:VAL:O	1:B:244:THR:HG22	2.12	0.49
1:B:290:LEU:C	1:B:292:ILE:N	2.69	0.49
1:D:388:LEU:C	1:D:388:LEU:HD12	2.37	0.49
1:D:205:LYS:N	4:D:504:HOH:O	2.38	0.49
1:D:240:VAL:HG22	1:D:284:GLN:HG2	1.95	0.49
1:C:51:HIS:CE1	1:C:165:LYS:HE3	2.48	0.49
1:D:41:TYR:HB2	1:D:113:TRP:CZ2	2.47	0.49
1:A:213:ILE:N	4:A:508:HOH:O	2.46	0.48
1:C:281:GLU:C	1:C:283:PHE:H	2.20	0.48
1:C:286:HIS:CE1	1:C:290:LEU:HD11	2.48	0.48
4:A:542:HOH:O	1:C:67:LYS:HD3	2.11	0.48
1:A:168:GLU:OE2	1:C:185:ARG:NH1	2.46	0.48
1:B:168:GLU:HG3	4:B:505:HOH:O	2.14	0.48
1:D:227:ASP:OD1	1:D:227:ASP:C	2.56	0.48
1:C:286:HIS:O	1:C:290:LEU:HD12	2.13	0.48
1:D:205:LYS:HG3	1:D:206:TYR:HD2	1.79	0.48
1:A:136:ARG:HE	2:A:401:H XK:CAF	2.27	0.48
1:D:233:PHE:HE1	1:D:313:TRP:CD1	2.31	0.48
1:C:222:GLU:O	1:C:223:GLN:C	2.56	0.48
1:A:281:GLU:C	1:A:283:PHE:N	2.70	0.48
1:C:147:VAL:O	1:C:151:ASN:HB2	2.14	0.48
1:C:391:ILE:O	1:C:392:LEU:C	2.57	0.48
1:D:128:ILE:HD11	1:D:152:ALA:HB1	1.95	0.48
1:D:348:LEU:O	1:D:352:TYR:HD2	1.97	0.48
1:B:205:LYS:HG3	1:B:206:TYR:HD2	1.78	0.47
1:B:80:GLY:CA	2:B:401:H XK:CAF	2.92	0.47
1:C:209:ALA:O	1:C:211:ARG:N	2.47	0.47
1:C:223:GLN:O	1:C:224:PRO:C	2.56	0.47
1:B:286:HIS:NE2	1:B:290:LEU:HD11	2.29	0.47
1:C:388:LEU:HD13	1:C:392:LEU:HD13	1.97	0.47
1:C:217:ASN:OD1	1:C:217:ASN:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:GLU:C	1:D:283:PHE:H	2.22	0.47
1:D:283:PHE:CZ	2:D:401:HXK:OAB	2.68	0.47
1:B:185:ARG:HH11	1:D:165:LYS:NZ	2.12	0.47
1:A:214:ASP:OD1	1:A:214:ASP:C	2.58	0.47
1:D:373:ILE:O	1:D:376:LEU:HB2	2.15	0.47
1:B:348:LEU:O	1:B:351:GLN:HB3	2.14	0.46
1:C:333:ASN:HB3	1:C:341:CYS:O	2.15	0.46
1:B:122:PHE:CE2	1:B:191:THR:HG21	2.50	0.46
1:B:388:LEU:HD12	1:B:388:LEU:C	2.40	0.46
1:A:217:ASN:ND2	1:C:145:LYS:CD	2.78	0.46
1:A:348:LEU:O	1:A:351:GLN:HB2	2.15	0.46
1:A:111:LEU:O	1:A:115:ILE:HG12	2.16	0.46
1:C:205:LYS:HG3	1:C:206:TYR:HD2	1.81	0.46
1:B:80:GLY:HA3	2:B:401:HXK:CAF	2.46	0.46
1:B:227:ASP:C	1:B:227:ASP:OD1	2.59	0.46
1:C:338:ASN:O	1:C:341:CYS:HB2	2.15	0.46
1:D:391:ILE:C	1:D:393:PHE:H	2.19	0.46
1:C:69:TYR:CE1	1:C:158:LEU:HD22	2.51	0.46
1:C:107:LYS:HE2	1:C:174:GLU:OE2	2.16	0.46
1:C:240:VAL:HG11	1:C:281:GLU:HA	1.98	0.46
1:B:41:TYR:HB2	1:B:113:TRP:CZ2	2.51	0.45
1:B:340:ALA:N	1:B:343:LYS:HB2	2.27	0.45
1:C:324:GLU:N	1:C:325:PRO:HD2	2.31	0.45
1:B:168:GLU:CD	1:D:185:ARG:NH1	2.75	0.45
1:B:349:TYR:C	1:B:351:GLN:H	2.23	0.45
1:A:322:CYS:HA	1:A:352:TYR:OH	2.16	0.45
1:A:170:TYR:C	1:A:171:LEU:HD12	2.41	0.45
1:B:89:ILE:HG23	1:B:105:TRP:HZ3	1.81	0.45
1:A:107:LYS:HE2	1:A:174:GLU:OE2	2.17	0.45
1:B:340:ALA:HA	1:B:343:LYS:N	2.32	0.45
1:A:158:LEU:O	1:A:158:LEU:HG	2.13	0.45
1:B:197:LEU:HB3	1:B:239:ILE:HG12	1.99	0.45
1:D:197:LEU:HB3	1:D:239:ILE:HG12	1.99	0.45
1:A:145:LYS:HE2	1:C:218:ILE:O	2.18	0.44
2:B:401:HXK:OAC	2:B:401:HXK:SAU	2.75	0.44
1:D:158:LEU:O	1:D:158:LEU:HG	2.09	0.44
1:A:145:LYS:HD3	1:A:145:LYS:HA	1.69	0.44
1:D:86:ILE:H	1:D:86:ILE:HG13	1.70	0.44
1:B:239:ILE:HD12	1:B:311:LEU:HD23	1.99	0.44
1:C:240:VAL:O	1:C:244:THR:HG22	2.18	0.44
1:D:69:TYR:CE1	1:D:158:LEU:HD22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:VAL:C	1:C:344:VAL:N	2.70	0.44
1:B:233:PHE:HE1	1:B:313:TRP:CD1	2.36	0.43
1:C:326:ASP:OD2	1:C:352:TYR:OH	2.36	0.43
1:D:107:LYS:HE2	1:D:174:GLU:OE2	2.18	0.43
1:D:128:ILE:HD11	1:D:152:ALA:CB	2.48	0.43
1:D:349:TYR:C	1:D:351:GLN:H	2.26	0.43
1:C:281:GLU:C	1:C:283:PHE:N	2.76	0.43
1:D:111:LEU:O	1:D:115:ILE:HG12	2.17	0.43
1:D:176:CYS:O	1:D:177:TYR:C	2.61	0.43
1:D:326:ASP:OD1	1:D:329:LYS:HE3	2.19	0.43
1:D:329:LYS:O	1:D:333:ASN:ND2	2.52	0.43
1:A:158:LEU:HB2	1:C:192:ILE:HG21	1.99	0.43
1:C:196:HIS:HE1	1:C:206:TYR:OH	2.01	0.43
1:A:165:LYS:HZ3	1:C:185:ARG:HH22	1.62	0.43
1:A:223:GLN:HA	1:A:224:PRO:HD3	1.76	0.43
1:C:122:PHE:CE2	1:C:191:THR:HG21	2.54	0.43
1:D:219:ASN:CA	4:D:539:HOH:O	2.67	0.43
1:D:340:ALA:HA	1:D:343:LYS:HB2	2.00	0.43
1:A:205:LYS:HG3	1:A:206:TYR:HD2	1.84	0.43
1:D:306:ILE:O	1:D:335:GLY:HA2	2.19	0.43
1:B:338:ASN:N	4:B:504:HOH:O	2.51	0.43
1:D:219:ASN:HB2	1:D:220:VAL:H	1.10	0.43
1:A:173:ASN:ND2	4:A:511:HOH:O	2.51	0.42
1:B:165:LYS:HZ3	1:D:185:ARG:HH11	1.67	0.42
1:D:283:PHE:CE2	2:D:401:H XK:OAB	2.72	0.42
1:C:111:LEU:O	1:C:115:ILE:HG12	2.19	0.42
1:D:323:SER:OG	1:D:325:PRO:HG2	2.19	0.42
1:A:281:GLU:O	1:A:283:PHE:N	2.52	0.42
1:D:205:LYS:HG3	1:D:206:TYR:CD2	2.55	0.42
1:B:340:ALA:H	1:B:343:LYS:CB	2.29	0.42
1:C:310:LYS:HA	1:C:310:LYS:HD2	1.92	0.42
1:A:36:PHE:O	1:A:39:ASN:HB2	2.19	0.42
1:C:84:ARG:HB3	1:C:115:ILE:HG21	2.01	0.42
1:D:147:VAL:O	1:D:151:ASN:HB2	2.20	0.42
1:D:310:LYS:HD2	1:D:310:LYS:HA	1.87	0.42
1:B:290:LEU:C	1:B:292:ILE:H	2.27	0.41
1:C:290:LEU:C	1:C:292:ILE:N	2.73	0.41
1:D:190:LYS:HE2	1:D:246:TYR:HE1	1.85	0.41
1:A:332:LYS:O	1:A:332:LYS:HG2	2.20	0.41
1:B:235:VAL:O	1:B:238:ASN:HB2	2.19	0.41
1:D:219:ASN:HA	4:D:539:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:O	1:A:238:ASN:HB2	2.19	0.41
1:C:197:LEU:HB3	1:C:239:ILE:HG12	2.01	0.41
1:B:146:ASP:HB2	1:D:213:ILE:HG23	2.02	0.41
1:B:281:GLU:C	1:B:283:PHE:N	2.77	0.41
1:A:240:VAL:O	1:A:244:THR:HG22	2.21	0.41
1:C:143:LEU:HD12	1:C:143:LEU:HA	1.93	0.41
1:C:205:LYS:HG3	1:C:206:TYR:CD2	2.55	0.41
1:A:219:ASN:O	1:A:220:VAL:O	2.37	0.41
1:D:190:LYS:HE2	1:D:246:TYR:CE1	2.56	0.41
1:D:216:ASN:OD1	4:D:502:HOH:O	2.22	0.41
1:A:388:LEU:C	1:A:388:LEU:HD12	2.45	0.41
1:B:310:LYS:HD2	1:B:310:LYS:HA	1.90	0.41
1:C:227:ASP:OD1	1:C:227:ASP:C	2.63	0.41
1:A:227:ASP:OD1	1:A:227:ASP:C	2.64	0.41
1:A:176:CYS:O	1:A:177:TYR:C	2.64	0.40
1:B:292:ILE:CB	1:B:355:ARG:HH12	2.34	0.40
1:B:312:THR:HB	1:B:314:PRO:HD2	2.02	0.40
1:D:190:LYS:CE	1:D:246:TYR:CE1	3.04	0.40
1:C:344:VAL:CG2	4:C:517:HOH:O	2.68	0.40
1:D:348:LEU:O	1:D:351:GLN:HB3	2.20	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	301/375 (80%)	286 (95%)	15 (5%)	0	100	100
1	B	310/375 (83%)	295 (95%)	13 (4%)	2 (1%)	21	44
1	C	318/375 (85%)	292 (92%)	20 (6%)	6 (2%)	6	17
1	D	320/375 (85%)	300 (94%)	17 (5%)	3 (1%)	14	35
All	All	1249/1500 (83%)	1173 (94%)	65 (5%)	11 (1%)	14	35

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	344	VAL
1	C	291	ASP
1	D	343	LYS
1	D	392	LEU
1	B	291	ASP
1	C	221	PRO
1	D	220	VAL
1	C	343	LYS
1	C	220	VAL
1	C	223	GLN
1	C	224	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/339 (77%)	246 (94%)	15 (6%)	18	43
1	B	258/339 (76%)	244 (95%)	14 (5%)	20	45
1	C	268/339 (79%)	255 (95%)	13 (5%)	22	49
1	D	268/339 (79%)	256 (96%)	12 (4%)	24	52
All	All	1055/1356 (78%)	1001 (95%)	54 (5%)	21	48

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	131	LYS
1	A	143	LEU
1	A	158	LEU
1	A	207	SER
1	A	213	ILE
1	A	215	VAL
1	A	226	ILE
1	A	233	PHE

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Mol	Chain	Res	Type
1	A	278	LEU
1	A	321	LEU
1	A	328	ILE
1	A	333	ASN
1	A	348	LEU
1	A	388	LEU
1	B	56	SER
1	B	133	GLU
1	B	143	LEU
1	B	158	LEU
1	B	204	ASP
1	B	226	ILE
1	B	233	PHE
1	B	278	LEU
1	B	321	LEU
1	B	328	ILE
1	B	344	VAL
1	B	351	GLN
1	B	354	ILE
1	B	388	LEU
1	C	143	LEU
1	C	212	GLU
1	C	215	VAL
1	C	219	ASN
1	C	226	ILE
1	C	233	PHE
1	C	278	LEU
1	C	328	ILE
1	C	336	LYS
1	C	342	VAL
1	C	344	VAL
1	C	355	ARG
1	C	388	LEU
1	D	143	LEU
1	D	158	LEU
1	D	204	ASP
1	D	226	ILE
1	D	233	PHE
1	D	278	LEU
1	D	328	ILE
1	D	344	VAL
1	D	351	GLN

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Mol	Chain	Res	Type
1	D	355	ARG
1	D	388	LEU
1	D	392	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	173	ASN
1	A	196	HIS
1	A	238	ASN
1	A	242	HIS
1	A	333	ASN
1	A	357	HIS
1	B	82	ASN
1	B	196	HIS
1	B	242	HIS
1	B	338	ASN
1	B	357	HIS
1	B	374	ASN
1	C	173	ASN
1	C	196	HIS
1	C	242	HIS
1	C	333	ASN
1	C	338	ASN
1	C	357	HIS
1	D	51	HIS
1	D	53	ASN
1	D	173	ASN
1	D	196	HIS
1	D	216	ASN
1	D	242	HIS
1	D	284	GLN
1	D	338	ASN
1	D	357	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HXK	A	401	-	28,28,28	1.34	2 (7%)	35,35,35	1.09	3 (8%)
2	HXK	B	401	-	28,28,28	0.92	0	35,35,35	1.05	2 (5%)
2	HXK	C	401	-	28,28,28	1.13	2 (7%)	35,35,35	1.35	4 (11%)
3	SO4	D	402	-	4,4,4	0.33	0	6,6,6	0.41	0
2	HXK	D	401	-	28,28,28	1.00	1 (3%)	35,35,35	0.95	1 (2%)

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	HXK	D	401	-	-	12/18/18/18	0/2/2/2
2	HXK	A	401	-	-	7/18/18/18	0/2/2/2
2	HXK	B	401	-	-	13/18/18/18	0/2/2/2
2	HXK	C	401	-	-	13/18/18/18	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HXK	CBA-CAV	4.87	1.60	1.49
2	D	401	HXK	CAZ-SAU	-2.69	1.73	1.77
2	C	401	HXK	OAB-CAV	-2.03	1.24	1.30
2	C	401	HXK	CAZ-SAU	-2.03	1.74	1.77
2	A	401	HXK	CAH-CBA	-2.02	1.36	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	HXK	CAS-SAU-CAZ	-4.12	95.14	102.67
2	B	401	HXK	CAZ-CBA-CAV	-3.22	117.49	121.99
2	A	401	HXK	CAS-SAU-CAZ	-2.67	97.79	102.67
2	D	401	HXK	OAC-CAV-CBA	-2.40	116.24	121.97
2	C	401	HXK	CAG-CAZ-SAU	-2.25	116.04	121.48
2	C	401	HXK	CBA-CAZ-SAU	2.24	122.97	120.36
2	A	401	HXK	CAG-CAZ-SAU	-2.24	116.06	121.48
2	B	401	HXK	OAC-CAV-CBA	-2.14	116.85	121.97
2	A	401	HXK	CBA-CAZ-SAU	2.04	122.74	120.36
2	C	401	HXK	CAX-CAS-SAU	2.03	118.74	110.67

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	HXK	CAX-CAS-SAU-CAZ
2	B	401	HXK	CBA-CAZ-SAU-CAS
2	C	401	HXK	CAJ-CAY-OAT-CAR
2	C	401	HXK	CAK-CAY-OAT-CAR
2	B	401	HXK	CAK-CAY-OAT-CAR
2	B	401	HXK	CAJ-CAY-OAT-CAR
2	A	401	HXK	CAO-CAP-CAQ-CAR
2	B	401	HXK	CAO-CAP-CAQ-CAR
2	A	401	HXK	CAK-CAY-OAT-CAR
2	A	401	HXK	CAJ-CAY-OAT-CAR
2	D	401	HXK	CAN-CAO-CAP-CAQ
2	C	401	HXK	CAQ-CAR-OAT-CAY
2	D	401	HXK	CAK-CAY-OAT-CAR
2	B	401	HXK	CAG-CAZ-SAU-CAS
2	C	401	HXK	SAU-CAS-CAX-CAI
2	D	401	HXK	CAJ-CAY-OAT-CAR
2	B	401	HXK	CAQ-CAR-OAT-CAY
2	C	401	HXK	CAM-CAN-CAO-CAP

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Mol	Chain	Res	Type	Atoms
2	C	401	HXK	CAP-CAQ-CAR-OAT
2	C	401	HXK	SAU-CAS-CAX-CAK
2	A	401	HXK	CAA-CAL-CAM-CAN
2	C	401	HXK	CAA-CAL-CAM-CAN
2	D	401	HXK	CAA-CAL-CAM-CAN
2	A	401	HXK	CAQ-CAR-OAT-CAY
2	B	401	HXK	CAA-CAL-CAM-CAN
2	D	401	HXK	CAL-CAM-CAN-CAO
2	B	401	HXK	CAL-CAM-CAN-CAO
2	D	401	HXK	OAC-CAV-CBA-CAZ
2	D	401	HXK	CAM-CAN-CAO-CAP
2	B	401	HXK	SAU-CAS-CAX-CAK
2	A	401	HXK	CAX-CAS-SAU-CAZ
2	B	401	HXK	SAU-CAS-CAX-CAI
2	D	401	HXK	OAB-CAV-CBA-CAZ
2	C	401	HXK	OAC-CAV-CBA-CAH
2	C	401	HXK	OAB-CAV-CBA-CAH
2	A	401	HXK	CAL-CAM-CAN-CAO
2	C	401	HXK	CAN-CAO-CAP-CAQ
2	B	401	HXK	CAM-CAN-CAO-CAP
2	D	401	HXK	OAC-CAV-CBA-CAH
2	D	401	HXK	OAB-CAV-CBA-CAH
2	B	401	HXK	CAX-CAS-SAU-CAZ
2	C	401	HXK	CBA-CAZ-SAU-CAS
2	D	401	HXK	SAU-CAS-CAX-CAK
2	B	401	HXK	OAB-CAV-CBA-CAH
2	D	401	HXK	SAU-CAS-CAX-CAI

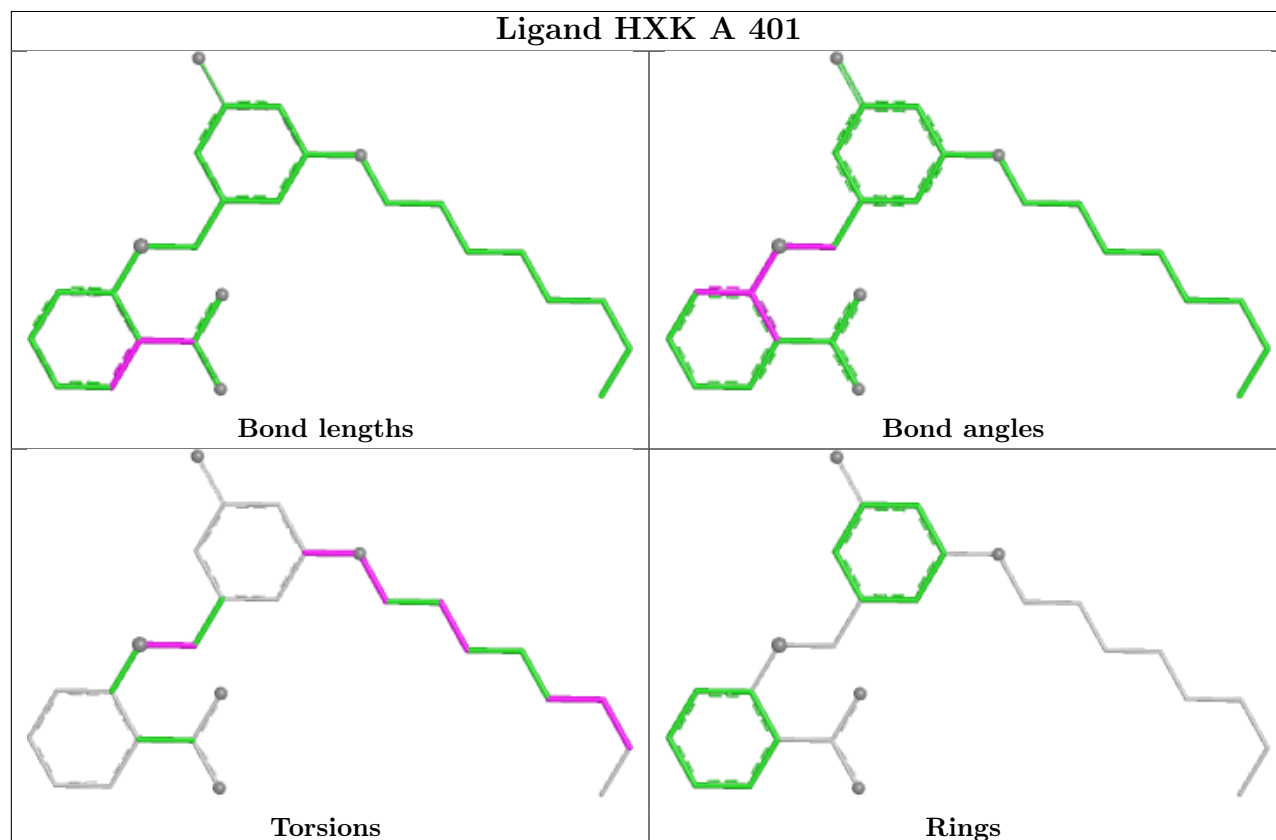
There are no ring outliers.

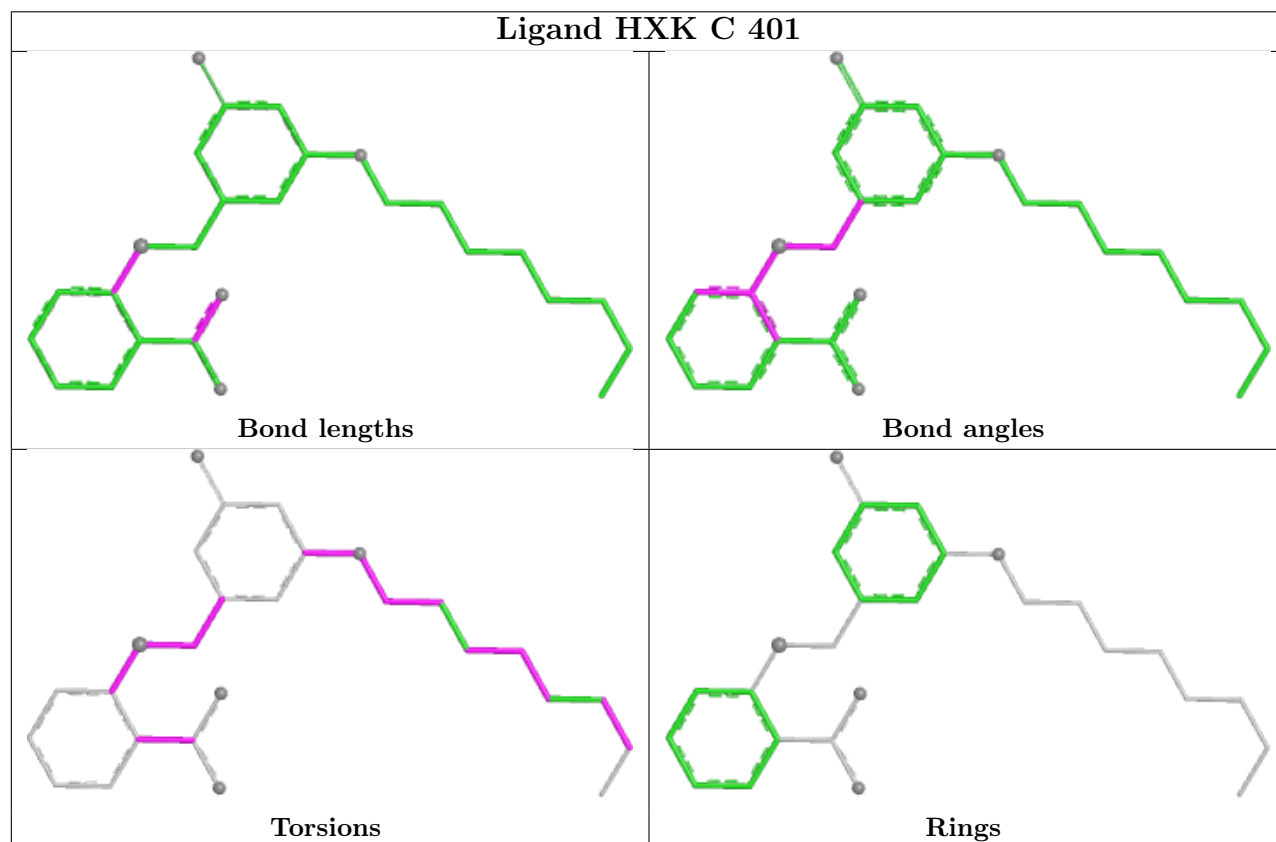
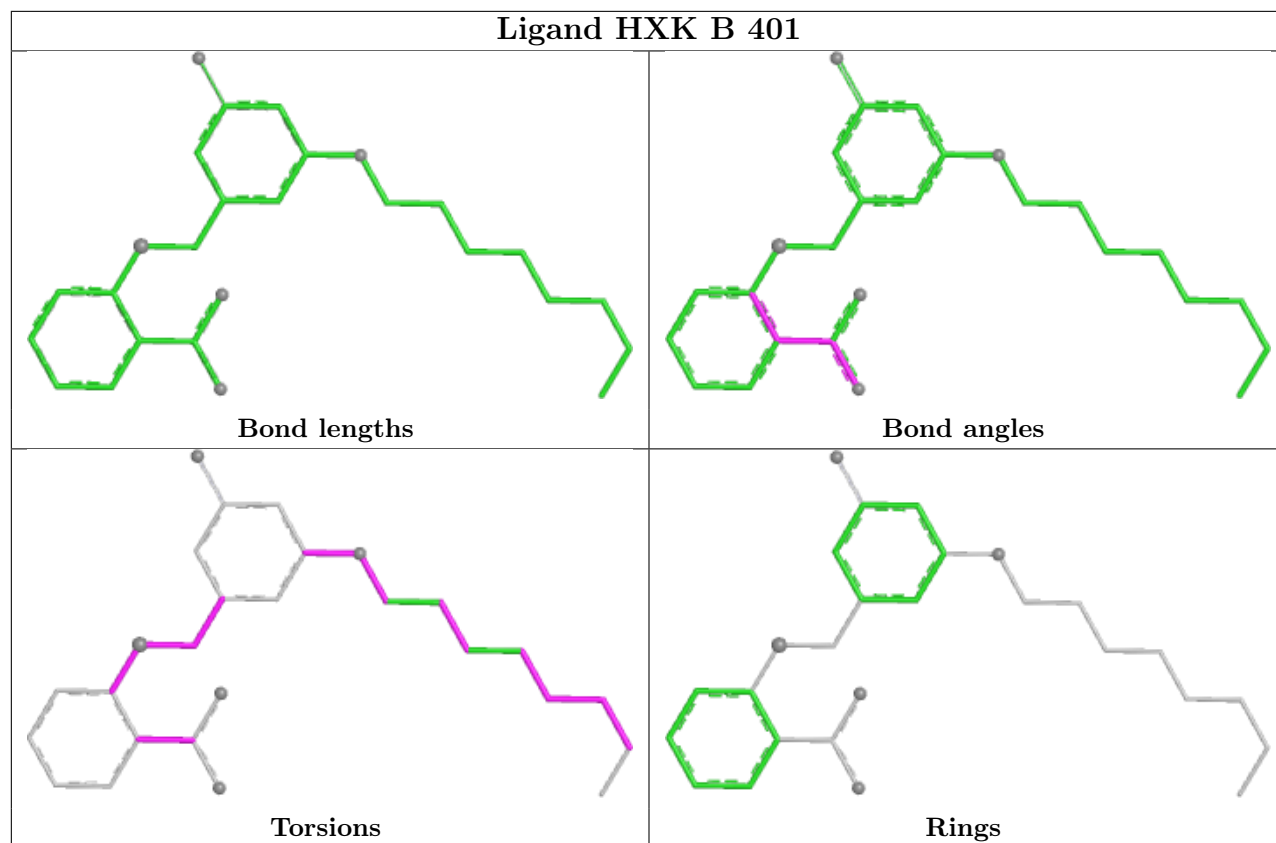
4 monomers are involved in 24 short contacts:

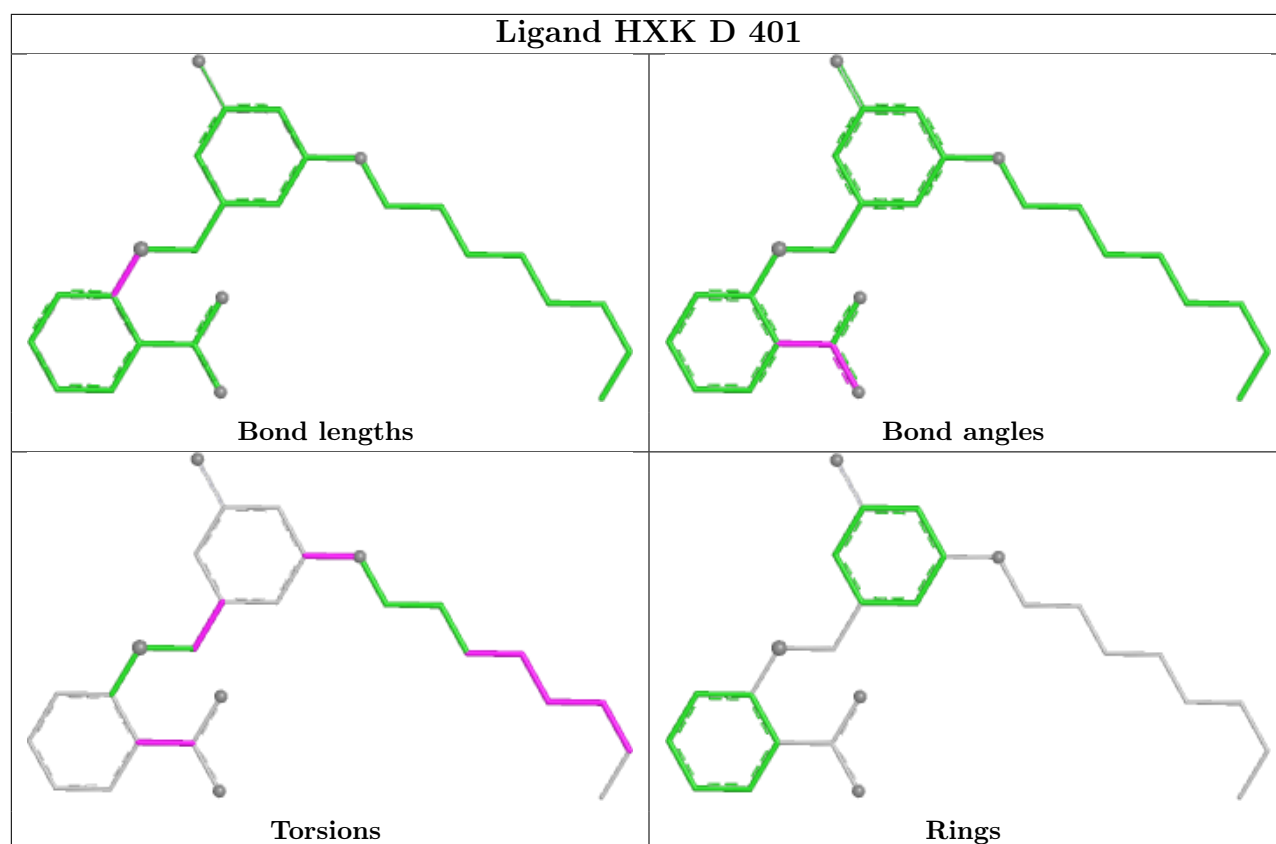
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HXK	3	0
2	B	401	HXK	6	0
2	C	401	HXK	2	0
2	D	401	HXK	13	0

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	321/375 (85%)	0.84	45 (14%) 6 5	21, 49, 70, 80	0
1	B	326/375 (86%)	0.47	16 (4%) 35 31	21, 49, 72, 99	0
1	C	334/375 (89%)	0.72	34 (10%) 12 10	21, 51, 71, 80	0
1	D	334/375 (89%)	0.58	18 (5%) 31 27	21, 50, 71, 80	0
All	All	1315/1500 (87%)	0.65	113 (8%) 16 13	21, 50, 71, 99	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	283	PHE	6.4
1	D	265	ASP	5.1
1	A	265	ASP	4.5
1	C	220	VAL	4.4
1	C	265	ASP	4.4
1	B	340	ALA	4.3
1	C	283	PHE	4.1
1	B	265	ASP	4.0
1	A	283	PHE	3.8
1	A	388	LEU	3.7
1	B	339	LEU	3.7
1	A	361	TYR	3.6
1	D	206	TYR	3.6
1	B	283	PHE	3.6
1	A	213	ILE	3.5
1	A	387	TYR	3.3
1	C	224	PRO	3.3
1	C	349	TYR	3.3
1	A	287	ASP	3.2
1	B	219	ASN	3.1
1	A	262	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	95	VAL	3.0
1	A	34	LEU	3.0
1	C	392	LEU	3.0
1	C	268	ILE	3.0
1	A	215	VAL	2.9
1	A	225	VAL	2.9
1	D	233	PHE	2.9
1	B	369	ILE	2.8
1	A	325	PRO	2.8
1	C	219	ASN	2.8
1	C	351	GLN	2.8
1	C	267	LEU	2.8
1	A	322	CYS	2.7
1	C	388	LEU	2.7
1	C	335	GLY	2.7
1	A	331	VAL	2.7
1	A	100	ILE	2.7
1	A	275	ILE	2.7
1	D	392	LEU	2.7
1	A	358	TYR	2.6
1	C	226	ILE	2.6
1	C	319	PHE	2.6
1	A	385	LEU	2.6
1	C	102	SER	2.6
1	C	330	ILE	2.6
1	A	344	VAL	2.6
1	A	233	PHE	2.6
1	C	233	PHE	2.6
1	D	346	ASP	2.5
1	A	369	ILE	2.5
1	A	370	LEU	2.5
1	D	219	ASN	2.5
1	B	206	TYR	2.5
1	A	92	TYR	2.5
1	A	335	GLY	2.5
1	C	266	ASN	2.5
1	D	393	PHE	2.5
1	A	90	LEU	2.4
1	C	209	ALA	2.4
1	A	223	GLN	2.4
1	A	349	TYR	2.4
1	B	226	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	230	MET	2.4
1	B	224	PRO	2.4
1	B	335	GLY	2.4
1	A	391	ILE	2.4
1	D	290	LEU	2.3
1	D	350	GLU	2.3
1	B	102	SER	2.3
1	C	221	PRO	2.3
1	C	344	VAL	2.3
1	B	99	ASP	2.3
1	A	309	ASN	2.3
1	B	233	PHE	2.3
1	C	275	ILE	2.3
1	C	369	ILE	2.3
1	D	391	ILE	2.3
1	A	94	TYR	2.3
1	D	220	VAL	2.3
1	D	60	GLU	2.2
1	C	334	TYR	2.2
1	C	289	TYR	2.2
1	A	216	ASN	2.2
1	C	137	ASN	2.2
1	C	304	SER	2.2
1	D	369	ILE	2.2
1	C	58	GLU	2.2
1	A	65	ILE	2.2
1	D	224	PRO	2.2
1	A	346	ASP	2.2
1	A	306	ILE	2.2
1	C	391	ILE	2.2
1	D	244	THR	2.1
1	A	220	VAL	2.1
1	A	274	ASP	2.1
1	C	225	VAL	2.1
1	A	278	LEU	2.1
1	A	234	GLY	2.1
1	A	352	TYR	2.1
1	C	215	VAL	2.1
1	C	293	PHE	2.1
1	C	346	ASP	2.1
1	A	313	TRP	2.1
1	B	216	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	357	HIS	2.1
1	A	345	ILE	2.1
1	B	391	ILE	2.1
1	D	95	VAL	2.1
1	D	288	ASP	2.0
1	B	39	ASN	2.0
1	A	328	ILE	2.0
1	A	330	ILE	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](#)

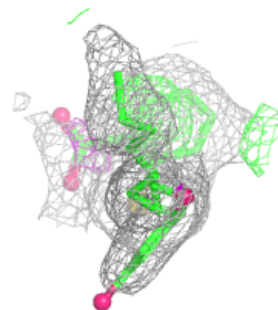
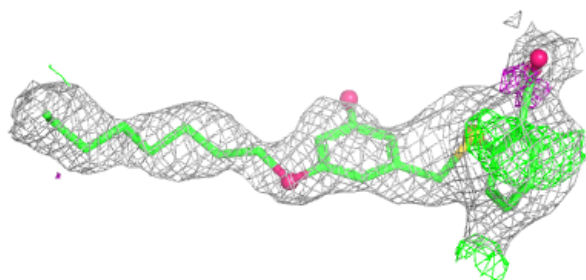
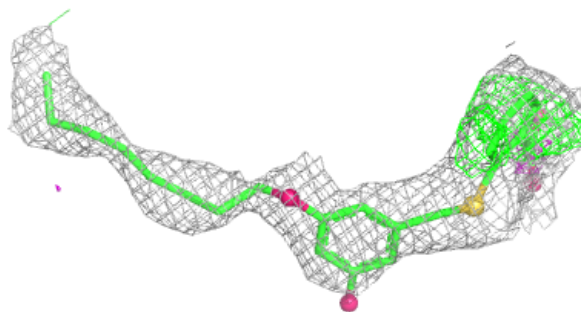
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	HXK	A	401	27/27	0.79	0.18	34,52,57,59	0
2	HXK	B	401	27/27	0.79	0.18	31,56,62,63	0
2	HXK	C	401	27/27	0.83	0.18	47,63,72,72	0
2	HXK	D	401	27/27	0.84	0.14	38,49,53,54	0
3	SO4	D	402	5/5	0.96	0.07	43,43,45,46	0

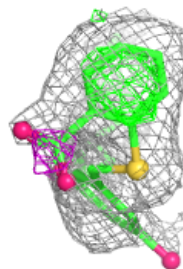
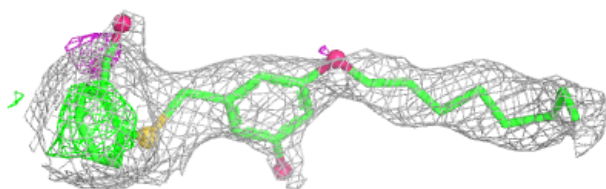
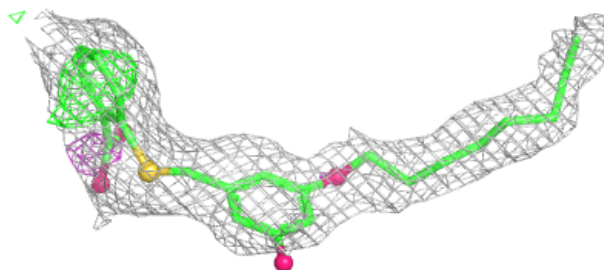
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HXK A 401:

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

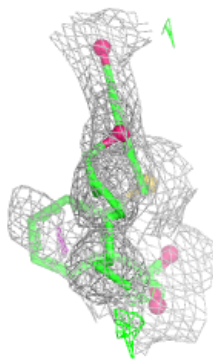
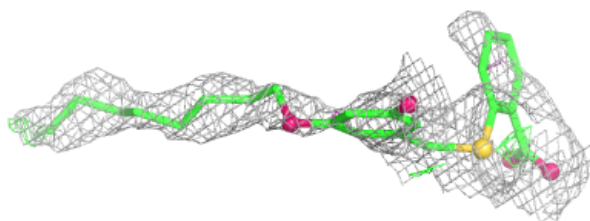
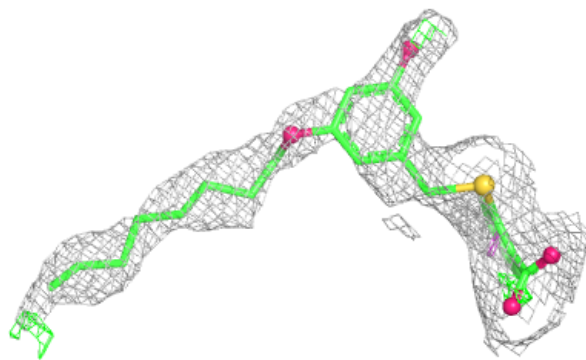
**Electron density around HXK B 401:**

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

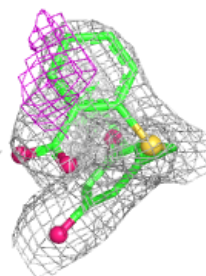
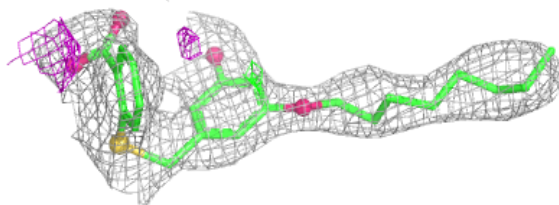
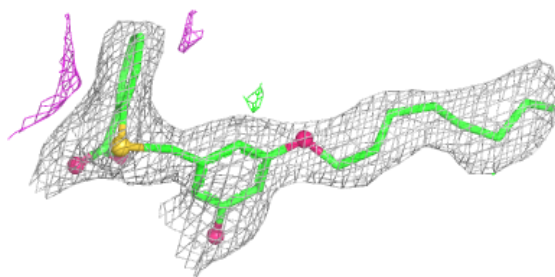


Electron density around HXK C 401:

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

**Electron density around HXK D 401:**

$2mF_o-DF_c$ (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.