



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:18 PM EDT

PDB ID : 3F6X / pdb_00003f6x
Title : c-Src kinase domain in complex with small molecule inhibitor
Authors : Seeliger, M.A.; Statsuk, A.V.; Maly, D.J.; Patrick, P.Z.; Kuriyan, J.; Shokat, K.M.
Deposited on : 2008-11-06
Resolution : 2.35 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

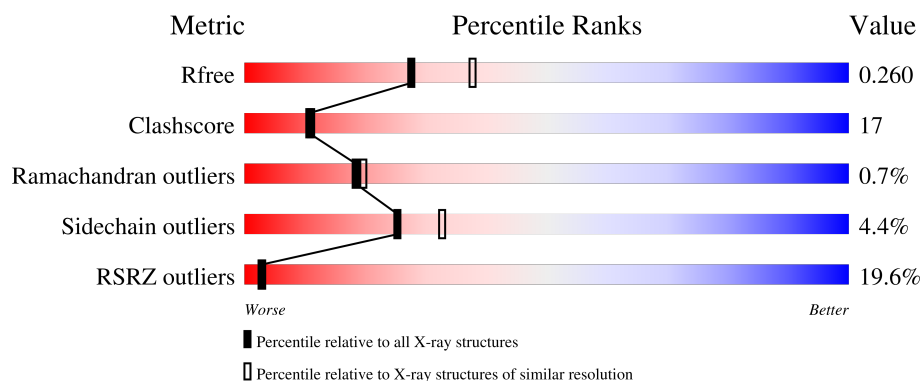
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	286	
1	B	286	
1	C	286	
1	D	286	

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	IHH	B	1	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8872 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.

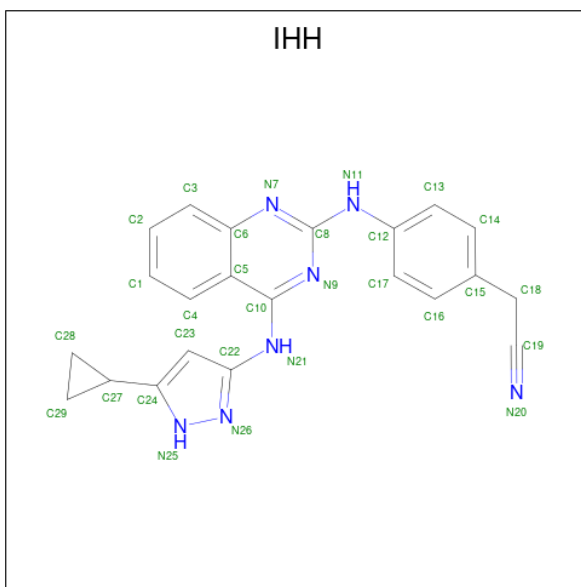
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2124	1364	355	389	16			
1	B	267	Total	C	N	O	S	0	0	0
			2137	1372	358	391	16			
1	C	265	Total	C	N	O	S	0	0	0
			2133	1373	357	387	16			
1	D	267	Total	C	N	O	S	0	0	0
			2142	1375	359	391	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP P00523
A	249	HIS	-	expression tag	UNP P00523
A	250	MET	-	expression tag	UNP P00523
B	248	GLY	-	expression tag	UNP P00523
B	249	HIS	-	expression tag	UNP P00523
B	250	MET	-	expression tag	UNP P00523
C	248	GLY	-	expression tag	UNP P00523
C	249	HIS	-	expression tag	UNP P00523
C	250	MET	-	expression tag	UNP P00523
D	248	GLY	-	expression tag	UNP P00523
D	249	HIS	-	expression tag	UNP P00523
D	250	MET	-	expression tag	UNP P00523

- Molecule 2 is [4-({4-[(5-cyclopropyl-1H-pyrazol-3-yl)amino]quinazolin-2-yl}amino)phenyl]acetonitrile (CCD ID: IHH) (formula: C₂₂H₁₉N₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			29	22	7		
2	B	1	Total	C	N	0	0
			29	22	7		
2	C	1	Total	C	N	0	0
			29	22	7		
2	D	1	Total	C	N	0	0
			29	22	7		

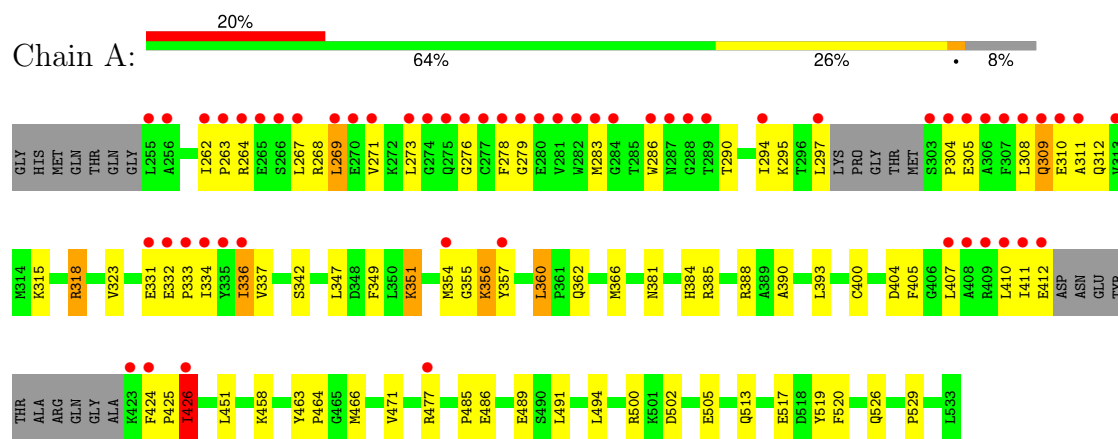
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		
3	B	57	Total	O	0	0
			57	57		
3	C	47	Total	O	0	0
			47	47		
3	D	65	Total	O	0	0
			65	65		

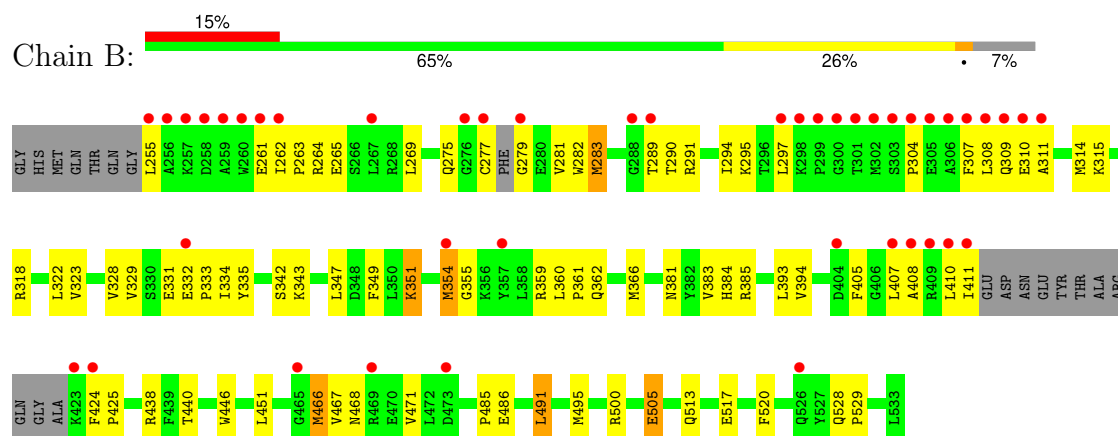
3 Residue-property plots [i](#)

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.

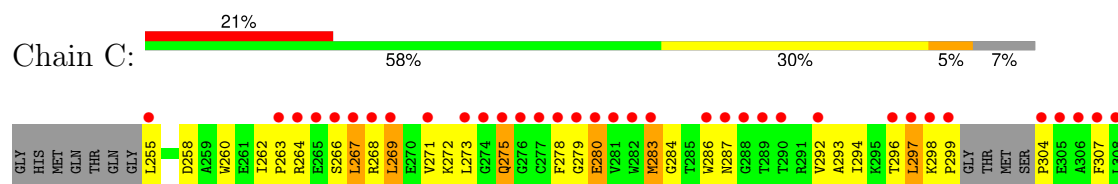
- Molecule 1: Proto-oncogene tyrosine-protein kinase Src

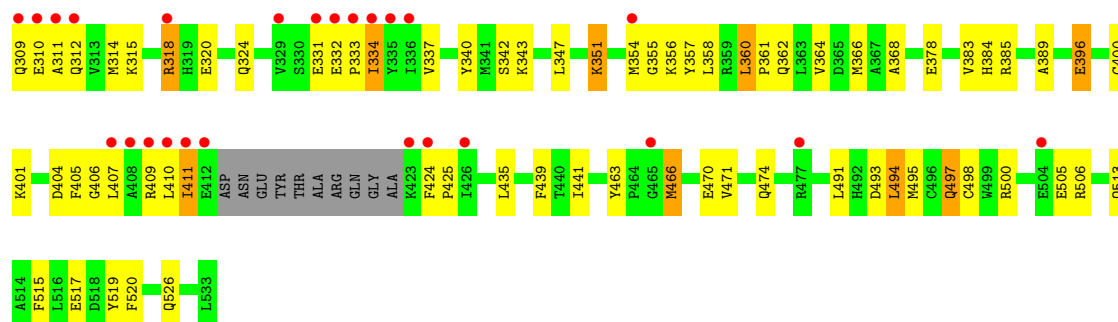


- Molecule 1: Proto-oncogene tyrosine-protein kinase Src

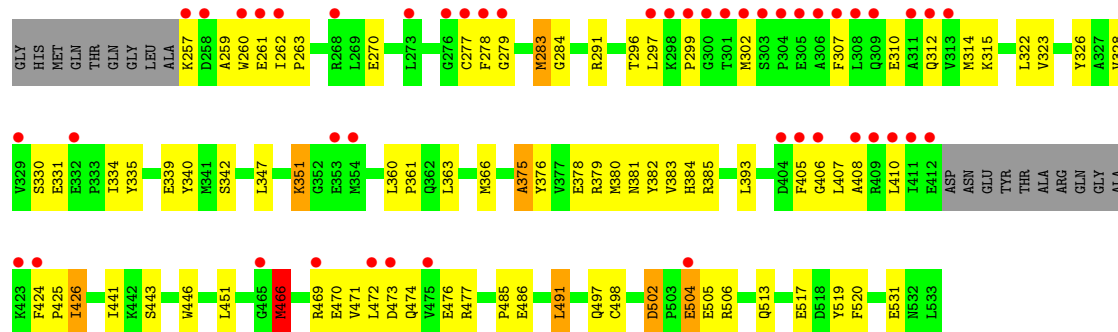


- Molecule 1: Proto-oncogene tyrosine-protein kinase Src





● Molecule 1: Proto-oncogene tyrosine-protein kinase Src



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.70Å 74.49Å 84.65Å 89.06° 89.97° 78.43°	Depositor
Resolution (Å)	34.99 – 2.35 34.99 – 2.35	Depositor EDS
% Data completeness (in resolution range)	79.8 (34.99-2.35) 79.8 (34.99-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.34Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.266 0.227 , 0.260	Depositor DCC
R_{free} test set	2984 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8872	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 91.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1880e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: IHH

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	0/2174	0.87	4/2942 (0.1%)
1	B	0.41	0/2187	0.93	5/2961 (0.2%)
1	C	0.43	0/2184	0.93	9/2955 (0.3%)
1	D	0.43	0/2194	0.96	9/2970 (0.3%)
All	All	0.42	0/8739	0.92	27/11828 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	SER	N-CA-C	7.48	121.50	112.38
1	D	259	ALA	N-CA-C	-7.44	104.18	113.18
1	B	466	MET	N-CA-C	7.12	120.00	109.24
1	B	468	ASN	N-CA-C	6.79	119.30	111.02
1	D	342	SER	N-CA-C	6.69	120.54	112.38
1	C	342	SER	N-CA-C	6.62	120.46	112.38
1	D	426	ILE	N-CA-C	6.38	117.89	110.62
1	D	466	MET	N-CA-C	6.26	118.58	109.07
1	D	330	SER	N-CA-C	6.00	120.46	113.20
1	D	519	TYR	N-CA-C	5.99	121.20	111.37
1	C	519	TYR	N-CA-C	5.90	121.05	111.37
1	B	355	GLY	N-CA-C	5.90	120.03	112.83
1	C	297	LEU	N-CA-C	-5.86	104.63	113.89
1	D	443	SER	N-CA-C	-5.74	105.17	111.82
1	C	466	MET	N-CA-C	5.62	118.97	109.76
1	C	389	ALA	N-CA-C	5.51	117.99	111.33
1	C	463	TYR	CA-C-N	5.41	126.61	119.84
1	C	463	TYR	C-N-CA	5.41	126.61	119.84
1	A	426	ILE	N-CA-C	5.41	116.78	110.62
1	A	494	LEU	N-CA-C	-5.34	105.35	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	SER	N-CA-C	5.23	118.92	112.54
1	A	519	TYR	N-CA-C	5.23	120.00	111.37
1	C	494	LEU	N-CA-C	-5.07	105.67	111.14
1	D	497	GLN	N-CA-C	-5.07	105.84	111.36
1	D	375	ALA	N-CA-C	-5.06	105.95	111.82
1	C	497	GLN	N-CA-C	-5.03	105.98	111.82
1	B	309	GLN	N-CA-C	-5.03	105.50	111.69

There are no chirality outliers.

There are no planarity outliers.

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	2124	0	2104	71	0
1	B	2137	0	2123	60	0
1	C	2133	0	2125	79	0
1	D	2142	0	2124	57	0
2	A	29	0	19	6	0
2	B	29	0	19	9	0
2	C	29	0	19	5	0
2	D	29	0	19	8	0
3	A	51	0	0	2	0
3	B	57	0	0	1	0
3	C	47	0	0	1	0
3	D	65	0	0	1	0
All	All	8872	0	8552	288	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 17.

All (288) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ILE:HD13	1:C:334:ILE:H	1.29	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLU:HG2	1:B:314:MET:HE2	1.45	0.96
2:B:1:IHH:H17	2:B:1:IHH:H23	1.52	0.91
2:D:1:IHH:H17	2:D:1:IHH:H23	1.54	0.90
1:D:504:GLU:CD	1:D:504:GLU:H	1.85	0.84
1:C:262:ILE:HD13	1:C:286:TRP:HE1	1.44	0.83
2:B:1:IHH:H17	2:B:1:IHH:N9	1.93	0.82
1:B:289:THR:HG23	1:B:290:THR:HG23	1.61	0.80
1:C:310:GLU:HG3	1:C:405:PHE:C	2.08	0.79
1:C:513:GLN:O	1:C:517:GLU:HG3	1.84	0.77
2:C:1:IHH:H16	2:C:1:IHH:H28	1.66	0.77
2:A:1:IHH:H16	2:A:1:IHH:H28	1.64	0.76
2:D:1:IHH:H17	2:D:1:IHH:N9	1.99	0.75
2:A:1:IHH:N9	2:A:1:IHH:H17	2.02	0.75
1:C:334:ILE:H	1:C:334:ILE:CD1	1.99	0.75
1:B:269:LEU:HD23	1:B:294:ILE:HD12	1.68	0.74
1:C:262:ILE:CD1	1:C:286:TRP:HE1	2.02	0.73
1:D:283:MET:HG3	1:D:340:TYR:CE1	2.24	0.72
1:C:310:GLU:HG2	1:C:314:MET:HE2	1.71	0.72
1:D:363:LEU:HA	1:D:366:MET:HE3	1.71	0.72
1:C:309:GLN:NE2	1:C:312:GLN:HG3	2.05	0.72
1:B:347:LEU:O	1:B:351:LYS:HG2	1.88	0.71
1:C:410:LEU:H	1:C:410:LEU:HD23	1.55	0.71
1:C:297:LEU:O	1:C:297:LEU:HD23	1.90	0.71
1:A:310:GLU:HG3	1:A:405:PHE:C	2.16	0.70
1:C:298:LYS:HB3	1:C:299:PRO:HD3	1.73	0.70
1:B:297:LEU:HD22	1:B:307:PHE:HB2	1.73	0.70
1:C:334:ILE:HD13	1:C:334:ILE:N	2.07	0.69
1:D:297:LEU:HD11	1:D:302:MET:HB2	1.73	0.69
1:A:347:LEU:O	1:A:351:LYS:HG2	1.93	0.69
1:B:466:MET:CE	1:B:471:VAL:HA	2.23	0.69
1:C:356:LYS:HE3	1:C:357:TYR:CZ	2.27	0.69
1:D:473:ASP:HB2	1:D:477:ARG:NH2	2.07	0.69
1:B:311:ALA:O	1:B:315:LYS:HG3	1.93	0.68
1:B:393:LEU:HD11	2:B:1:IHH:H28	1.75	0.68
1:D:278:PHE:O	1:D:297:LEU:HD12	1.93	0.68
1:A:268:ARG:O	1:A:268:ARG:HG3	1.93	0.68
2:C:1:IHH:H17	2:C:1:IHH:N9	2.08	0.68
1:C:378:GLU:HG3	1:C:441:ILE:HG12	1.76	0.66
1:A:407:LEU:HD13	1:A:424:PHE:CE1	2.31	0.65
1:A:295:LYS:HB2	1:A:336:ILE:CG2	2.27	0.65
1:B:381:ASN:O	1:B:410:LEU:HD12	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:PHE:CZ	1:A:354:MET:HG2	2.32	0.64
2:A:1:IHH:H17	2:A:1:IHH:H23	1.79	0.64
1:A:513:GLN:O	1:A:517:GLU:HG3	1.98	0.64
1:A:334:ILE:HD12	1:A:334:ILE:H	1.62	0.63
2:C:1:IHH:H17	2:C:1:IHH:H23	1.80	0.63
1:D:257:LYS:HE3	1:D:261:GLU:HG2	1.80	0.63
1:A:407:LEU:HD13	1:A:424:PHE:HE1	1.63	0.63
1:C:366:MET:HE2	1:C:400:CYS:SG	2.39	0.63
1:C:262:ILE:CG1	1:C:263:PRO:HD2	2.29	0.62
1:C:280:GLU:HG3	1:C:299:PRO:HG2	1.79	0.62
1:A:331:GLU:O	1:A:334:ILE:HA	2.00	0.62
1:A:354:MET:HE1	1:C:435:LEU:HB3	1.81	0.62
1:B:297:LEU:HD22	1:B:307:PHE:CB	2.29	0.62
1:B:323:VAL:HG21	1:B:393:LEU:HD12	1.82	0.62
1:A:410:LEU:O	1:A:412:GLU:HG3	2.01	0.61
1:D:278:PHE:HA	1:D:302:MET:HG3	1.82	0.61
1:A:500:ARG:HD3	1:A:505:GLU:HG3	1.82	0.61
1:D:381:ASN:O	1:D:410:LEU:HD12	2.00	0.61
1:D:426:ILE:HD11	1:D:472:LEU:HB2	1.83	0.61
1:B:383:VAL:HG23	1:B:411:ILE:HB	1.84	0.60
1:C:356:LYS:HE3	1:C:357:TYR:OH	2.02	0.60
1:A:279:GLY:HA3	1:A:297:LEU:HA	1.84	0.59
1:C:262:ILE:HG13	1:C:263:PRO:HD2	1.84	0.59
1:C:267:LEU:N	1:C:267:LEU:HD23	2.16	0.59
1:D:312:GLN:HA	1:D:315:LYS:HD3	1.85	0.58
1:A:273:LEU:HD11	1:A:283:MET:HB2	1.85	0.58
1:D:466:MET:CE	1:D:471:VAL:HA	2.34	0.57
1:B:362:GLN:O	1:B:366:MET:HG3	2.03	0.57
1:D:376:TYR:CE1	1:D:380:MET:HE3	2.39	0.57
1:C:318:ARG:HD3	1:C:324:GLN:OE1	2.03	0.57
1:C:355:GLY:HA2	1:C:358:LEU:HD12	1.86	0.57
1:B:354:MET:HB2	3:B:72:HOH:O	2.04	0.57
1:B:513:GLN:O	1:B:517:GLU:HG3	2.04	0.57
1:D:513:GLN:O	1:D:517:GLU:HG3	2.05	0.56
2:B:1:IHH:N9	2:B:1:IHH:C17	2.63	0.56
1:D:283:MET:HE1	1:D:291:ARG:HH21	1.70	0.56
1:A:269:LEU:HD23	1:A:269:LEU:H	1.70	0.56
1:A:334:ILE:HD12	1:A:334:ILE:N	2.20	0.56
2:D:1:IHH:H16	2:D:1:IHH:C28	2.34	0.56
1:A:295:LYS:HB2	1:A:336:ILE:HG23	1.86	0.56
1:D:322:LEU:HG	1:D:405:PHE:HZ	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ALA:O	1:A:315:LYS:HG3	2.05	0.56
1:D:378:GLU:HG3	1:D:441:ILE:HG12	1.86	0.56
1:A:332:GLU:HA	1:A:333:PRO:C	2.29	0.55
1:B:467:VAL:O	1:B:471:VAL:HG23	2.06	0.55
1:B:466:MET:HE2	1:B:471:VAL:HG22	1.89	0.55
1:A:451:LEU:O	1:A:451:LEU:HD23	2.07	0.55
2:B:1:IHH:H16	2:B:1:IHH:C28	2.35	0.55
1:C:294:ILE:N	1:C:294:ILE:HD12	2.22	0.54
1:C:383:VAL:HG23	1:C:411:ILE:HG23	1.90	0.54
1:B:451:LEU:HD23	1:B:451:LEU:O	2.07	0.54
1:C:466:MET:CE	1:C:471:VAL:HA	2.38	0.54
1:B:261:GLU:HA	1:B:328:VAL:O	2.06	0.54
1:B:318:ARG:NH1	1:B:318:ARG:HB2	2.23	0.54
1:C:310:GLU:CG	1:C:314:MET:HE2	2.38	0.54
1:A:485:PRO:O	1:A:486:GLU:HB2	2.06	0.54
1:B:264:ARG:NH2	1:B:331:GLU:O	2.40	0.54
1:C:384:HIS:O	1:C:385:ARG:HB2	2.08	0.54
1:B:411:ILE:HD12	1:B:440:THR:HA	1.89	0.54
1:C:273:LEU:HD11	1:C:283:MET:HB2	1.88	0.54
1:D:283:MET:CE	1:D:291:ARG:HH21	2.21	0.54
1:D:375:ALA:O	1:D:379:ARG:HG3	2.08	0.53
2:A:1:IHH:N9	2:A:1:IHH:C17	2.70	0.53
1:A:331:GLU:OE2	1:A:331:GLU:HA	2.07	0.53
1:C:354:MET:HB2	3:C:129:HOH:O	2.09	0.53
2:A:1:IHH:H28	2:A:1:IHH:C16	2.34	0.53
1:A:502:ASP:HB3	1:A:505:GLU:HG2	1.90	0.52
1:C:258:ASP:OD1	1:C:260:TRP:HB2	2.09	0.52
1:C:383:VAL:CG2	1:C:411:ILE:HG23	2.39	0.52
2:D:1:IHH:H16	2:D:1:IHH:H28	1.91	0.52
1:A:297:LEU:HD23	1:A:297:LEU:C	2.35	0.52
1:D:393:LEU:HD11	2:D:1:IHH:H28	1.92	0.52
1:A:318:ARG:HG2	1:A:318:ARG:HH11	1.75	0.52
1:B:318:ARG:HB2	1:B:318:ARG:HH11	1.74	0.52
2:B:1:IHH:H28	2:B:1:IHH:H16	1.91	0.52
1:D:310:GLU:O	1:D:314:MET:HG3	2.09	0.52
1:B:283:MET:HE1	1:B:291:ARG:HD3	1.91	0.52
1:D:270:GLU:HG3	1:D:284:GLY:HA2	1.92	0.52
1:C:268:ARG:O	1:C:268:ARG:HG3	2.10	0.51
1:C:260:TRP:NE1	1:C:315:LYS:HB2	2.26	0.51
2:B:1:IHH:H23	2:B:1:IHH:C17	2.35	0.51
1:C:362:GLN:O	1:C:366:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:ARG:NH2	1:C:439:PHE:HB2	2.26	0.51
1:D:261:GLU:HA	1:D:328:VAL:O	2.09	0.51
1:C:292:VAL:HG23	1:C:294:ILE:HD11	1.93	0.51
1:C:283:MET:HG3	1:C:340:TYR:CE1	2.45	0.50
1:D:424:PHE:HB3	1:D:425:PRO:HD2	1.92	0.50
1:B:269:LEU:HD23	1:B:294:ILE:CD1	2.40	0.50
1:C:493:ASP:O	1:C:497:GLN:HG3	2.10	0.50
1:B:269:LEU:HD22	1:B:282:TRP:HB2	1.92	0.50
1:B:304:PRO:O	1:B:308:LEU:HG	2.11	0.50
1:A:269:LEU:HD23	1:A:269:LEU:N	2.26	0.50
1:C:385:ARG:HG2	1:C:439:PHE:CD2	2.47	0.50
1:A:323:VAL:HG21	1:A:393:LEU:HD12	1.94	0.50
1:C:293:ALA:C	1:C:294:ILE:HD12	2.37	0.50
1:B:261:GLU:OE2	1:B:329:VAL:HA	2.12	0.50
1:D:279:GLY:HA3	1:D:296:THR:O	2.12	0.50
2:D:1:IHH:N9	2:D:1:IHH:C17	2.68	0.50
1:A:308:LEU:O	1:A:312:GLN:HG2	2.12	0.50
1:B:310:GLU:CG	1:B:314:MET:HE2	2.32	0.49
1:B:485:PRO:O	1:B:486:GLU:HB2	2.13	0.49
1:B:383:VAL:CG2	1:B:411:ILE:HB	2.43	0.49
1:D:323:VAL:HG21	1:D:393:LEU:HD12	1.94	0.49
1:A:276:GLY:HA3	1:A:279:GLY:O	2.13	0.49
1:A:309:GLN:HA	1:A:312:GLN:HG2	1.95	0.49
1:A:354:MET:CE	1:C:435:LEU:HB3	2.41	0.49
1:C:500:ARG:HD3	1:C:505:GLU:HG3	1.95	0.49
1:A:354:MET:HE1	1:C:435:LEU:CB	2.42	0.48
1:D:382:TYR:CE1	1:D:410:LEU:HD13	2.48	0.48
1:D:485:PRO:O	1:D:486:GLU:HB2	2.13	0.48
1:A:304:PRO:HG2	1:A:305:GLU:H	1.77	0.48
1:C:360:LEU:HD22	1:C:364:VAL:HG23	1.96	0.48
1:C:470:GLU:O	1:C:474:GLN:HG2	2.14	0.48
1:A:384:HIS:O	1:A:385:ARG:HB2	2.13	0.48
1:C:310:GLU:O	1:C:314:MET:HG3	2.13	0.48
1:A:267:LEU:HD21	1:A:337:VAL:HG21	1.95	0.48
1:D:361:PRO:HA	1:D:520:PHE:CE2	2.48	0.48
1:C:271:VAL:HG12	1:C:272:LYS:N	2.29	0.47
1:D:310:GLU:HB3	1:D:406:GLY:HA2	1.95	0.47
1:A:362:GLN:O	1:A:366:MET:HG3	2.14	0.47
1:B:329:VAL:HB	1:B:335:TYR:HB2	1.96	0.47
1:D:470:GLU:O	1:D:474:GLN:HB2	2.14	0.47
1:B:500:ARG:HD3	1:B:505:GLU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:MET:HE2	1:C:284:GLY:CA	2.44	0.47
1:C:310:GLU:HG3	1:C:406:GLY:N	2.30	0.47
1:D:473:ASP:O	1:D:477:ARG:HG3	2.14	0.47
1:C:304:PRO:O	1:C:307:PHE:HB3	2.15	0.47
1:C:407:LEU:HD13	1:C:424:PHE:CE2	2.50	0.47
1:A:269:LEU:HD22	1:A:294:ILE:HD12	1.97	0.46
1:B:405:PHE:HB3	1:B:408:ALA:HB3	1.97	0.46
1:B:446:TRP:CD1	1:B:446:TRP:C	2.94	0.46
1:C:278:PHE:O	1:C:297:LEU:HG	2.16	0.46
1:C:495:MET:O	1:C:498:CYS:HB2	2.16	0.46
1:C:269:LEU:N	1:C:269:LEU:HD23	2.29	0.46
1:C:272:LYS:O	1:C:273:LEU:HD23	2.15	0.46
1:C:424:PHE:HD1	1:C:424:PHE:H	1.61	0.46
1:A:463:TYR:N	1:A:464:PRO:HD3	2.30	0.45
1:B:407:LEU:HD13	1:B:424:PHE:CE1	2.51	0.45
1:B:491:LEU:O	1:B:495:MET:HG3	2.16	0.45
1:C:283:MET:HE2	1:C:284:GLY:N	2.32	0.45
1:C:309:GLN:HA	1:C:312:GLN:HG2	1.98	0.45
1:A:336:ILE:HG23	1:A:336:ILE:O	2.15	0.45
1:C:320:GLU:O	1:C:401:LYS:HE2	2.16	0.45
1:A:489:GLU:HG2	3:A:181:HOH:O	2.16	0.45
1:A:356:LYS:HE3	1:A:357:TYR:CZ	2.52	0.45
1:D:451:LEU:O	1:D:451:LEU:HD23	2.17	0.45
1:A:424:PHE:O	1:A:426:ILE:N	2.49	0.45
1:C:361:PRO:HA	1:C:520:PHE:CE2	2.52	0.45
1:A:388:ARG:NH1	1:A:390:ALA:HB3	2.32	0.45
1:B:359:ARG:HA	1:B:359:ARG:HD3	1.82	0.45
1:D:283:MET:HG3	1:D:340:TYR:CZ	2.52	0.45
1:A:381:ASN:O	1:A:411:ILE:HG22	2.17	0.45
1:B:329:VAL:O	1:B:334:ILE:HG23	2.17	0.45
1:C:494:LEU:HD22	1:C:515:PHE:CE1	2.52	0.44
1:A:262:ILE:HB	1:A:263:PRO:HD2	1.99	0.44
1:C:262:ILE:HG12	1:C:263:PRO:HD2	1.98	0.44
1:B:393:LEU:HD11	2:B:1:IHH:C28	2.45	0.44
1:B:466:MET:HE2	1:B:471:VAL:HA	1.97	0.44
1:C:267:LEU:HD13	1:C:337:VAL:HG21	1.98	0.44
1:C:383:VAL:HG12	1:C:385:ARG:HG3	1.98	0.44
1:D:297:LEU:O	1:D:299:PRO:HD3	2.18	0.44
1:A:286:TRP:HB3	1:A:290:THR:OG1	2.18	0.44
1:D:446:TRP:CD1	1:D:446:TRP:C	2.96	0.44
2:B:1:IHH:H16	2:B:1:IHH:C29	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:MET:HE2	1:D:471:VAL:HG22	1.99	0.44
2:C:1:IHH:N9	2:C:1:IHH:H23	2.33	0.44
1:D:297:LEU:HD22	1:D:307:PHE:CB	2.48	0.44
1:D:476:GLU:OE2	1:D:476:GLU:HA	2.16	0.44
1:A:278:PHE:CD1	1:A:278:PHE:N	2.86	0.44
1:A:310:GLU:HG3	1:A:405:PHE:CA	2.47	0.44
1:B:262:ILE:HB	1:B:263:PRO:HD2	2.00	0.43
1:B:297:LEU:HD22	1:B:307:PHE:CG	2.53	0.43
1:C:332:GLU:OE1	1:C:334:ILE:HD12	2.17	0.43
1:C:347:LEU:O	1:C:351:LYS:HG2	2.17	0.43
1:D:331:GLU:C	1:D:334:ILE:HD13	2.43	0.43
1:A:477:ARG:HG3	1:A:477:ARG:HH11	1.83	0.43
1:A:529:PRO:HB3	3:A:82:HOH:O	2.19	0.43
1:B:264:ARG:HH12	1:B:333:PRO:HG2	1.83	0.43
1:C:498:CYS:O	1:C:506:ARG:HG2	2.18	0.43
1:A:500:ARG:HB3	1:A:505:GLU:HG3	2.00	0.43
1:D:262:ILE:HB	1:D:263:PRO:HD2	2.00	0.43
1:A:311:ALA:HB2	1:A:336:ILE:HD12	2.01	0.43
1:C:311:ALA:O	1:C:315:LYS:HG2	2.18	0.43
1:C:466:MET:CE	1:C:474:GLN:HG3	2.49	0.43
1:D:326:TYR:CE2	1:D:339:GLU:HA	2.54	0.43
2:D:1:IHH:H23	2:D:1:IHH:N9	2.34	0.43
1:A:426:ILE:HD13	1:A:426:ILE:C	2.44	0.43
1:A:502:ASP:O	1:A:505:GLU:HG2	2.19	0.43
1:A:360:LEU:HD13	1:A:520:PHE:HZ	1.84	0.43
1:C:264:ARG:HH11	1:C:333:PRO:HD2	1.84	0.42
1:D:407:LEU:HD13	1:D:424:PHE:CE2	2.54	0.42
1:D:347:LEU:O	1:D:351:LYS:HG2	2.19	0.42
2:D:1:IHH:H16	2:D:1:IHH:C29	2.50	0.42
1:A:354:MET:HE1	1:C:435:LEU:HD22	2.01	0.42
1:B:277:CYS:O	1:B:279:GLY:N	2.52	0.42
1:B:322:LEU:HG	1:B:405:PHE:HZ	1.85	0.42
1:D:283:MET:HE1	1:D:291:ARG:NH2	2.34	0.42
1:B:384:HIS:O	1:B:385:ARG:HB2	2.19	0.42
1:A:310:GLU:HG3	1:A:405:PHE:HB2	2.01	0.42
1:A:332:GLU:HA	1:A:334:ILE:N	2.35	0.42
1:A:500:ARG:CB	1:A:505:GLU:HG3	2.50	0.42
1:D:502:ASP:HB3	1:D:505:GLU:HG2	2.02	0.42
1:A:477:ARG:O	1:A:477:ARG:HG2	2.20	0.42
1:A:309:GLN:NE2	1:A:312:GLN:HG3	2.35	0.42
1:B:265:GLU:CD	1:B:265:GLU:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:ILE:HG22	1:D:335:TYR:N	2.35	0.42
1:D:466:MET:HE3	1:D:471:VAL:HA	2.02	0.42
1:D:498:CYS:O	1:D:506:ARG:HG2	2.20	0.42
1:A:273:LEU:CD1	1:A:283:MET:HB2	2.49	0.42
1:B:361:PRO:HA	1:B:520:PHE:CE2	2.55	0.42
1:C:279:GLY:HA3	1:C:296:THR:O	2.19	0.42
1:D:383:VAL:O	1:D:408:ALA:HA	2.20	0.42
1:A:308:LEU:HD21	1:A:334:ILE:CG2	2.50	0.41
2:A:1:IHH:N9	2:A:1:IHH:H23	2.34	0.41
1:B:275:GLN:NE2	1:B:275:GLN:HA	2.35	0.41
1:B:407:LEU:HD13	1:B:424:PHE:HE1	1.85	0.41
1:B:343:LYS:HB2	1:B:394:VAL:HB	2.03	0.41
1:B:349:PHE:CZ	1:B:354:MET:HG3	2.56	0.41
1:C:266:SER:HB2	1:C:287:ASN:OD1	2.21	0.41
2:C:1:IHH:N9	2:C:1:IHH:C23	2.83	0.41
1:A:318:ARG:HH11	1:A:318:ARG:CG	2.33	0.41
1:B:281:VAL:HG22	1:B:295:LYS:HG2	2.02	0.41
1:D:260:TRP:NE1	1:D:315:LYS:HG2	2.35	0.41
1:A:466:MET:HE2	1:A:471:VAL:HA	2.02	0.41
1:B:411:ILE:HD11	1:B:440:THR:HG22	2.01	0.41
1:D:260:TRP:CD1	1:D:315:LYS:HE3	2.55	0.41
1:D:384:HIS:O	1:D:385:ARG:HB2	2.20	0.41
1:D:491:LEU:HD23	1:D:491:LEU:HA	1.94	0.41
1:B:331:GLU:O	1:B:332:GLU:C	2.63	0.41
1:A:332:GLU:HA	1:A:334:ILE:HD12	2.03	0.41
1:A:411:ILE:HG23	1:A:411:ILE:O	2.21	0.41
1:C:255:LEU:HD11	1:C:331:GLU:OE2	2.20	0.41
1:A:355:GLY:O	1:A:458:LYS:HE2	2.20	0.41
1:A:366:MET:HE2	1:A:400:CYS:SG	2.61	0.41
1:C:272:LYS:HE2	1:C:275:GLN:OE1	2.20	0.41
1:C:343:LYS:HE3	1:C:396:GLU:OE1	2.21	0.41
1:D:351:LYS:HE3	3:D:176:HOH:O	2.20	0.41
1:C:309:GLN:HA	1:C:312:GLN:CG	2.51	0.40
1:D:531:GLU:HA	1:D:531:GLU:OE2	2.22	0.40
1:B:275:GLN:CA	1:B:275:GLN:HE21	2.35	0.40
1:B:283:MET:HE1	1:B:291:ARG:CD	2.50	0.40
1:C:368:ALA:HB1	1:C:517:GLU:HG2	2.03	0.40
1:D:363:LEU:HD23	1:D:366:MET:CE	2.51	0.40
1:A:334:ILE:H	1:A:334:ILE:CD1	2.32	0.40
1:B:528:GLN:HA	1:B:529:PRO:HD3	1.98	0.40
1:B:269:LEU:CD2	1:B:294:ILE:HD12	2.45	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	258/286 (90%)	240 (93%)	15 (6%)	3 (1%)	10	9
1	B	261/286 (91%)	246 (94%)	14 (5%)	1 (0%)	30	34
1	C	259/286 (91%)	245 (95%)	11 (4%)	3 (1%)	10	9
1	D	263/286 (92%)	254 (97%)	9 (3%)	0	100	100
All	All	1041/1144 (91%)	985 (95%)	49 (5%)	7 (1%)	18	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	404	ASP
1	A	336	ILE
1	A	425	PRO
1	A	404	ASP
1	C	411	ILE
1	C	425	PRO
1	B	425	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	227/245 (93%)	216 (95%)	11 (5%)	23	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	228/245 (93%)	220 (96%)	8 (4%)	32	42
1	C	228/245 (93%)	216 (95%)	12 (5%)	20	25
1	D	229/245 (94%)	220 (96%)	9 (4%)	28	39
All	All	912/980 (93%)	872 (96%)	40 (4%)	25	33

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	ARG
1	A	269	LEU
1	A	271	VAL
1	A	309	GLN
1	A	318	ARG
1	A	351	LYS
1	A	356	LYS
1	A	360	LEU
1	A	426	ILE
1	A	491	LEU
1	A	526	GLN
1	B	255	LEU
1	B	283	MET
1	B	351	LYS
1	B	354	MET
1	B	360	LEU
1	B	438	ARG
1	B	491	LEU
1	B	505	GLU
1	C	267	LEU
1	C	269	LEU
1	C	275	GLN
1	C	280	GLU
1	C	283	MET
1	C	318	ARG
1	C	334	ILE
1	C	351	LYS
1	C	360	LEU
1	C	396	GLU
1	C	491	LEU
1	C	526	GLN
1	D	277	CYS
1	D	283	MET

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Mol	Chain	Res	Type
1	D	351	LYS
1	D	360	LEU
1	D	466	MET
1	D	469	ARG
1	D	491	LEU
1	D	502	ASP
1	D	504	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	309	GLN
1	C	309	GLN
1	C	381	ASN
1	C	468	ASN

5.3.3 RNA [i](#)

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IHH	B	1	-	32,33,33	1.98	8 (25%)	42,46,46	2.28	13 (30%)
2	IHH	A	1	-	32,33,33	1.95	7 (21%)	42,46,46	2.31	12 (28%)
2	IHH	C	1	-	32,33,33	1.95	7 (21%)	42,46,46	2.30	14 (33%)
2	IHH	D	1	-	32,33,33	1.98	8 (25%)	42,46,46	2.26	13 (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
2	IHH	B	1	-	-	0/14/17/17	0/5/5/5
2	IHH	A	1	-	-	0/14/17/17	0/5/5/5
2	IHH	C	1	-	-	0/14/17/17	0/5/5/5
2	IHH	D	1	-	-	0/14/17/17	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	IHH	N25-N26	-6.31	1.23	1.36
2	D	1	IHH	N25-N26	-6.30	1.23	1.36
2	A	1	IHH	N25-N26	-6.24	1.23	1.36
2	C	1	IHH	N25-N26	-6.18	1.23	1.36
2	B	1	IHH	C10-C5	-4.51	1.39	1.44
2	D	1	IHH	C10-C5	-4.49	1.39	1.44
2	C	1	IHH	C10-C5	-4.25	1.39	1.44
2	A	1	IHH	C10-C5	-4.24	1.39	1.44
2	B	1	IHH	C23-C22	-3.95	1.33	1.40
2	C	1	IHH	C23-C22	-3.95	1.33	1.40
2	A	1	IHH	C23-C22	-3.94	1.33	1.40
2	D	1	IHH	C23-C22	-3.93	1.33	1.40
2	B	1	IHH	C12-N11	-3.40	1.33	1.40
2	C	1	IHH	C12-N11	-3.40	1.33	1.40
2	A	1	IHH	C12-N11	-3.38	1.33	1.40
2	D	1	IHH	C12-N11	-3.31	1.33	1.40
2	D	1	IHH	C22-N21	-2.50	1.33	1.37
2	D	1	IHH	C23-C24	-2.46	1.33	1.37
2	A	1	IHH	C23-C24	-2.45	1.33	1.37
2	C	1	IHH	C23-C24	-2.44	1.33	1.37
2	B	1	IHH	C23-C24	-2.44	1.33	1.37
2	B	1	IHH	C22-N21	-2.39	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	IHH	C6-N7	-2.35	1.33	1.37
2	A	1	IHH	C22-N21	-2.24	1.33	1.37
2	D	1	IHH	C6-N7	-2.23	1.34	1.37
2	C	1	IHH	C22-N21	-2.23	1.33	1.37
2	A	1	IHH	C6-N7	-2.23	1.34	1.37
2	B	1	IHH	C6-N7	-2.17	1.34	1.37
2	B	1	IHH	C5-C6	-2.02	1.39	1.42
2	D	1	IHH	C5-C6	-2.00	1.39	1.42

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	IHH	C22-N26-N25	7.54	109.19	103.71
2	B	1	IHH	C22-N26-N25	7.50	109.17	103.71
2	C	1	IHH	C22-N26-N25	7.40	109.09	103.71
2	D	1	IHH	C22-N26-N25	7.27	109.00	103.71
2	A	1	IHH	C10-C5-C6	6.21	119.53	115.86
2	B	1	IHH	C10-C5-C6	6.19	119.52	115.86
2	C	1	IHH	C10-C5-C6	6.00	119.40	115.86
2	D	1	IHH	C10-C5-C6	5.86	119.32	115.86
2	C	1	IHH	C23-C24-N25	4.60	110.02	106.19
2	B	1	IHH	C23-C24-N25	4.45	109.90	106.19
2	D	1	IHH	C23-C24-N25	4.43	109.88	106.19
2	A	1	IHH	C23-C24-N25	4.31	109.78	106.19
2	A	1	IHH	C23-C22-N26	-4.09	109.21	112.14
2	B	1	IHH	C23-C22-N26	-3.91	109.34	112.14
2	D	1	IHH	C23-C22-N26	-3.79	109.43	112.14
2	C	1	IHH	C23-C22-N26	-3.72	109.48	112.14
2	B	1	IHH	C5-C6-N7	-3.70	118.88	122.80
2	C	1	IHH	C5-C6-N7	-3.61	118.98	122.80
2	D	1	IHH	C5-C6-N7	-3.56	119.03	122.80
2	A	1	IHH	C5-C6-N7	-3.50	119.10	122.80
2	D	1	IHH	C8-N7-C6	3.49	121.07	115.54
2	C	1	IHH	C8-N7-C6	3.48	121.07	115.54
2	B	1	IHH	C8-N7-C6	3.40	120.93	115.54
2	C	1	IHH	C27-C24-C23	-3.35	125.69	131.09
2	A	1	IHH	C8-N7-C6	3.35	120.85	115.54
2	D	1	IHH	N7-C8-N9	-3.33	120.81	126.25
2	A	1	IHH	C27-C24-C23	-3.31	125.75	131.09
2	A	1	IHH	N7-C8-N9	-3.19	121.02	126.25
2	C	1	IHH	N7-C8-N9	-3.17	121.06	126.25
2	B	1	IHH	N7-C8-N9	-3.11	121.17	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	IHH	C27-C24-C23	-2.97	126.30	131.09
2	D	1	IHH	C5-C10-N21	-2.79	116.99	119.78
2	B	1	IHH	C27-C24-C23	-2.71	126.73	131.09
2	B	1	IHH	C5-C10-N21	-2.50	117.28	119.78
2	C	1	IHH	N11-C8-N9	2.41	125.17	116.90
2	A	1	IHH	C5-C10-N9	-2.34	118.57	122.07
2	C	1	IHH	C24-C23-C22	-2.32	103.16	104.78
2	A	1	IHH	N21-C22-N26	2.30	123.05	117.81
2	D	1	IHH	N21-C22-N26	2.26	122.96	117.81
2	A	1	IHH	N11-C8-N9	2.25	124.62	116.90
2	D	1	IHH	C24-C23-C22	-2.21	103.23	104.78
2	C	1	IHH	C3-C6-C5	2.19	121.49	119.13
2	B	1	IHH	C24-C23-C22	-2.17	103.26	104.78
2	D	1	IHH	C4-C5-C10	-2.16	121.04	124.16
2	C	1	IHH	N21-C22-N26	2.14	122.71	117.81
2	C	1	IHH	C5-C10-N9	-2.14	118.86	122.07
2	B	1	IHH	N21-C22-N26	2.12	122.66	117.81
2	A	1	IHH	C3-C6-C5	2.12	121.42	119.13
2	B	1	IHH	C4-C5-C10	-2.08	121.17	124.16
2	B	1	IHH	C5-C10-N9	-2.07	118.97	122.07
2	D	1	IHH	C5-C10-N9	-2.05	119.00	122.07
2	C	1	IHH	C5-C10-N21	-2.03	117.75	119.78

There are no chirality outliers.

There are no torsion outliers.

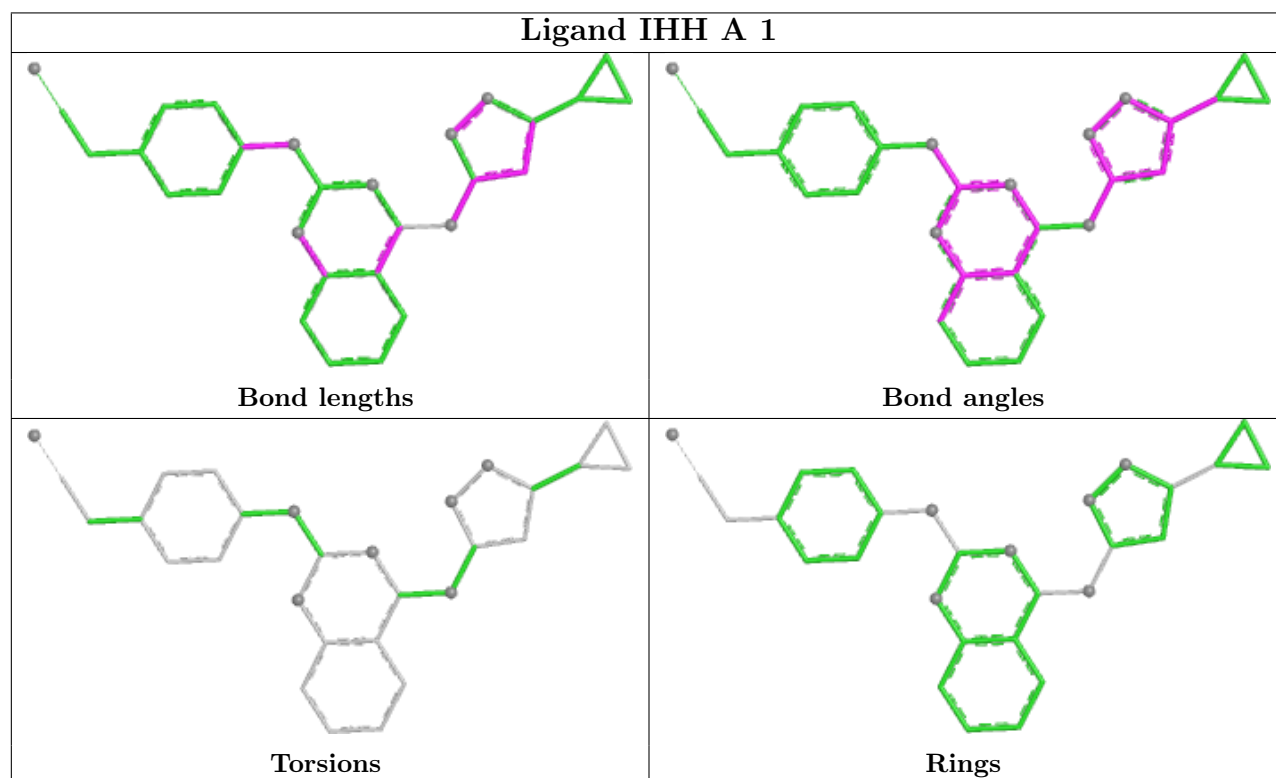
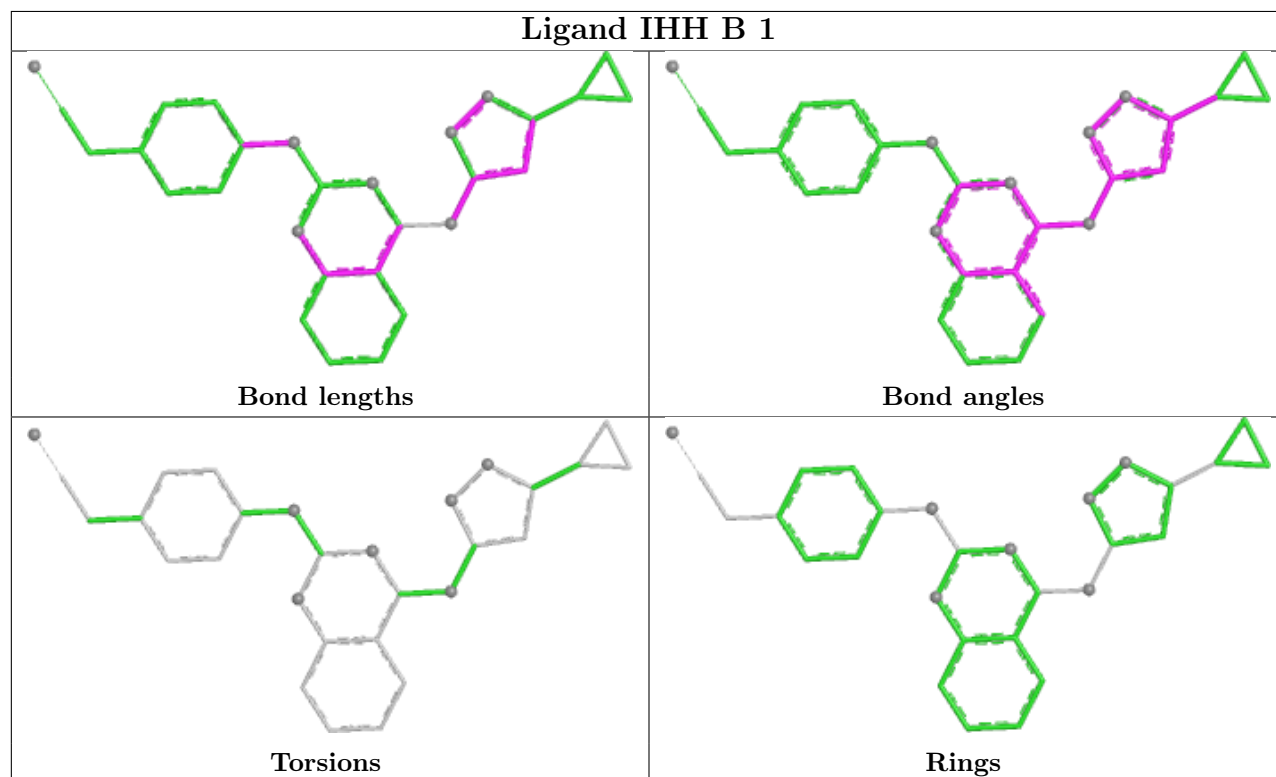
There are no ring outliers.

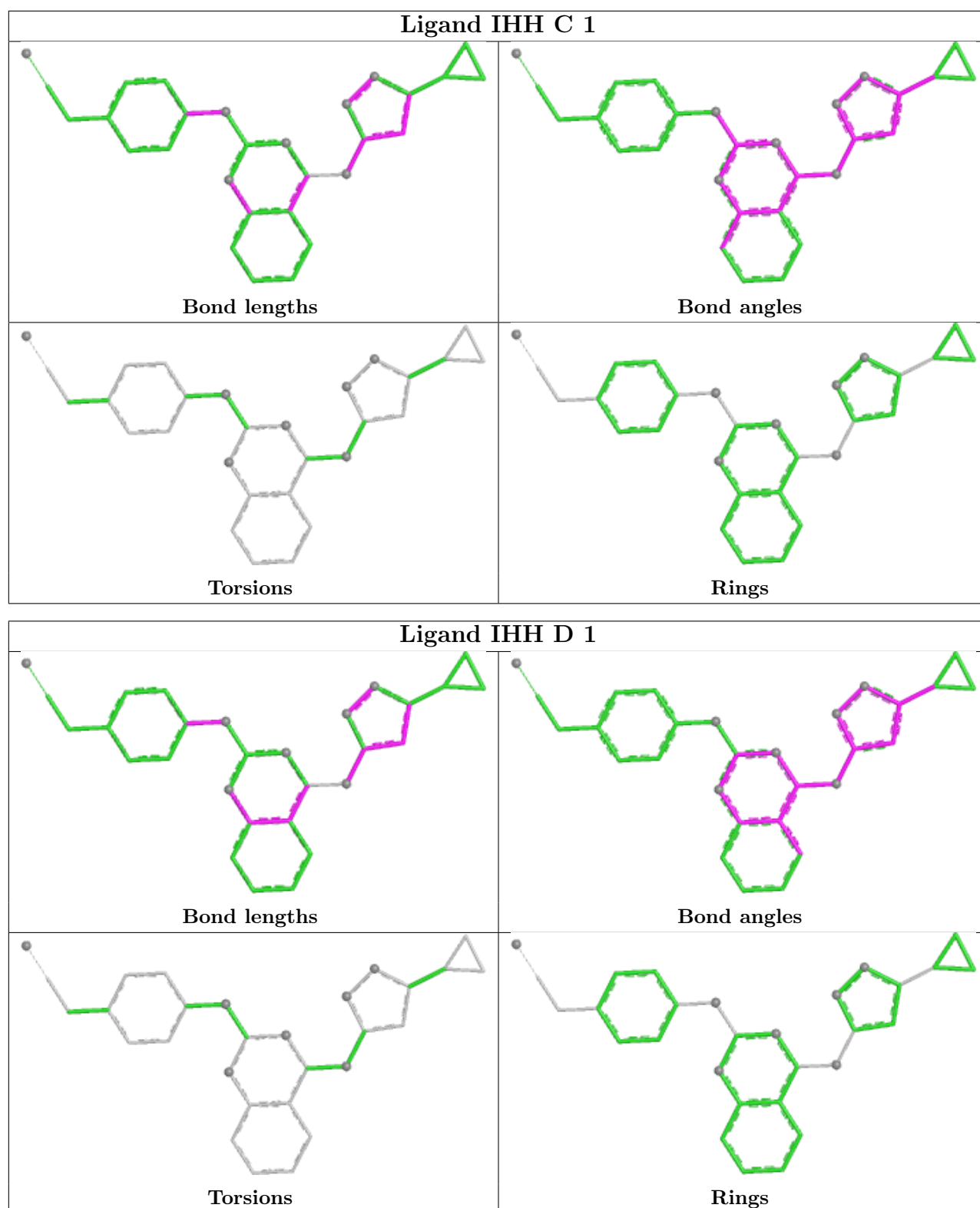
4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	IHH	9	0
2	A	1	IHH	6	0
2	C	1	IHH	5	0
2	D	1	IHH	8	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 ⓘ

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	264/286 (92%)	0.90	57 (21%) 2 2	12, 30, 76, 98	0
1	B	267/286 (93%)	0.81	44 (16%) 4 5	11, 31, 75, 86	0
1	C	265/286 (92%)	0.96	60 (22%) 2 1	12, 31, 78, 90	0
1	D	267/286 (93%)	0.92	47 (17%) 4 4	12, 32, 75, 84	0
All	All	1063/1144 (92%)	0.90	208 (19%) 3 3	11, 31, 77, 98	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	277	CYS	8.3
1	D	278	PHE	7.7
1	B	277	CYS	7.5
1	B	255	LEU	7.2
1	D	412	GLU	7.0
1	B	301	THR	6.9
1	C	267	LEU	6.5
1	C	273	LEU	6.0
1	D	354	MET	6.0
1	C	308	LEU	5.9
1	D	411	ILE	5.7
1	C	412	GLU	5.6
1	C	297	LEU	5.5
1	B	300	GLY	5.3
1	D	408	ALA	5.2
1	A	267	LEU	5.1
1	C	333	PRO	5.0
1	D	299	PRO	5.0
1	B	299	PRO	4.9
1	D	300	GLY	4.8
1	B	411	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	411	ILE	4.7
1	C	269	LEU	4.6
1	A	304	PRO	4.6
1	A	303	SER	4.6
1	C	408	ALA	4.6
1	A	255	LEU	4.6
1	C	304	PRO	4.5
1	A	308	LEU	4.5
1	A	288	GLY	4.5
1	A	269	LEU	4.5
1	D	301	THR	4.4
1	C	411	ILE	4.4
1	A	289	THR	4.3
1	D	257	LYS	4.3
1	C	306	ALA	4.3
1	B	409	ARG	4.2
1	B	408	ALA	4.2
1	C	288	GLY	4.2
1	A	333	PRO	4.2
1	D	258	ASP	4.1
1	C	299	PRO	4.1
1	A	306	ALA	4.1
1	D	279	GLY	4.1
1	C	274	GLY	4.0
1	C	265	GLU	4.0
1	C	307	PHE	4.0
1	C	334	ILE	4.0
1	B	469	ARG	3.9
1	D	309	GLN	3.9
1	B	256	ALA	3.9
1	B	423	LYS	3.9
1	D	465	GLY	3.9
1	A	273	LEU	3.8
1	D	424	PHE	3.8
1	D	268	ARG	3.7
1	A	297	LEU	3.6
1	D	308	LEU	3.6
1	A	408	ALA	3.6
1	B	304	PRO	3.6
1	B	298	LYS	3.6
1	A	305	GLU	3.6
1	A	277	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	309	GLN	3.5
1	A	276	GLY	3.5
1	C	298	LYS	3.5
1	A	334	ILE	3.5
1	C	255	LEU	3.5
1	B	276	GLY	3.5
1	A	278	PHE	3.5
1	A	407	LEU	3.5
1	B	424	PHE	3.5
1	A	287	ASN	3.5
1	A	307	PHE	3.5
1	D	306	ALA	3.4
1	C	278	PHE	3.4
1	A	310	GLU	3.4
1	D	409	ARG	3.4
1	B	259	ALA	3.4
1	C	409	ARG	3.4
1	D	472	LEU	3.4
1	A	331	GLU	3.4
1	D	304	PRO	3.3
1	C	424	PHE	3.3
1	D	311	ALA	3.3
1	B	465	GLY	3.3
1	A	335	TYR	3.3
1	C	282	TRP	3.3
1	C	271	VAL	3.3
1	C	332	GLU	3.2
1	A	286	TRP	3.2
1	A	423	LYS	3.2
1	C	276	GLY	3.2
1	A	309	GLN	3.2
1	A	311	ALA	3.1
1	C	287	ASN	3.1
1	D	423	LYS	3.1
1	D	473	ASP	3.1
1	A	271	VAL	3.1
1	D	307	PHE	3.1
1	B	308	LEU	3.1
1	B	306	ALA	3.1
1	B	257	LYS	3.1
1	D	303	SER	3.0
1	D	298	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	280	GLU	3.0
1	C	268	ARG	3.0
1	A	424	PHE	3.0
1	D	313	VAL	2.9
1	B	289	THR	2.9
1	C	335	TYR	2.9
1	A	332	GLU	2.9
1	B	297	LEU	2.9
1	C	277	CYS	2.9
1	C	264	ARG	2.9
1	C	407	LEU	2.9
1	C	281	VAL	2.9
1	C	266	SER	2.8
1	D	276	GLY	2.8
1	D	302	MET	2.8
1	B	258	ASP	2.8
1	A	263	PRO	2.8
1	C	410	LEU	2.8
1	D	297	LEU	2.8
1	B	310	GLU	2.8
1	C	504	GLU	2.8
1	A	283	MET	2.8
1	A	282	TRP	2.8
1	B	357	TYR	2.8
1	B	302	MET	2.8
1	C	275	GLN	2.7
1	C	279	GLY	2.7
1	A	265	GLU	2.7
1	D	353	GLU	2.7
1	D	405	PHE	2.7
1	B	260	TRP	2.7
1	D	260	TRP	2.7
1	A	313	VAL	2.7
1	A	426	ILE	2.7
1	B	279	GLY	2.7
1	C	354	MET	2.7
1	D	404	ASP	2.7
1	A	410	LEU	2.7
1	D	305	GLU	2.6
1	C	296	THR	2.6
1	C	283	MET	2.6
1	C	465	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	266	SER	2.6
1	B	407	LEU	2.6
1	D	410	LEU	2.6
1	C	311	ALA	2.6
1	A	412	GLU	2.6
1	B	305	GLU	2.6
1	C	305	GLU	2.6
1	B	404	ASP	2.6
1	A	274	GLY	2.6
1	C	309	GLN	2.5
1	A	270	GLU	2.5
1	B	354	MET	2.5
1	C	280	GLU	2.5
1	C	310	GLU	2.5
1	C	286	TRP	2.4
1	C	312	GLN	2.4
1	A	409	ARG	2.4
1	D	406	GLY	2.4
1	D	469	ARG	2.4
1	A	294	ILE	2.4
1	A	357	TYR	2.4
1	B	307	PHE	2.4
1	D	262	ILE	2.4
1	B	261	GLU	2.4
1	D	332	GLU	2.4
1	C	426	ILE	2.4
1	A	275	GLN	2.3
1	D	261	GLU	2.3
1	B	473	ASP	2.3
1	A	354	MET	2.3
1	A	336	ILE	2.3
1	A	281	VAL	2.3
1	C	331	GLU	2.3
1	D	475	VAL	2.3
1	C	423	LYS	2.3
1	C	329	VAL	2.3
1	A	477	ARG	2.2
1	C	289	THR	2.2
1	A	264	ARG	2.2
1	C	263	PRO	2.2
1	A	284	GLY	2.2
1	B	410	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	504	GLU	2.2
1	A	256	ALA	2.2
1	B	332	GLU	2.1
1	B	303	SER	2.1
1	A	279	GLY	2.1
1	B	288	GLY	2.1
1	C	318	ARG	2.1
1	C	477	ARG	2.1
1	B	311	ALA	2.1
1	A	262	ILE	2.1
1	B	262	ILE	2.1
1	B	526	GLN	2.1
1	D	312	GLN	2.1
1	D	329	VAL	2.1
1	C	336	ILE	2.1
1	C	292	VAL	2.1
1	B	267	LEU	2.0
1	D	273	LEU	2.0
1	C	290	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](#)

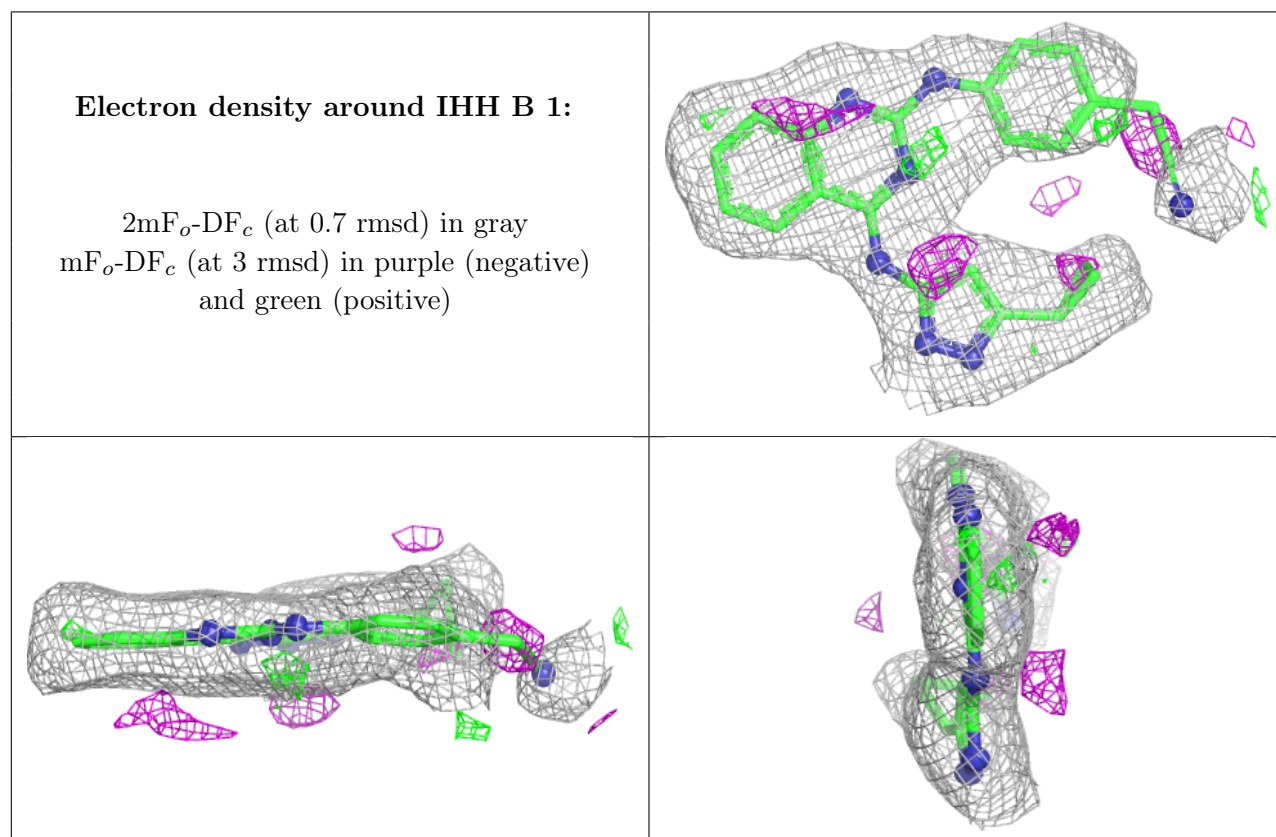
There are no oligosaccharides in this entry.

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.

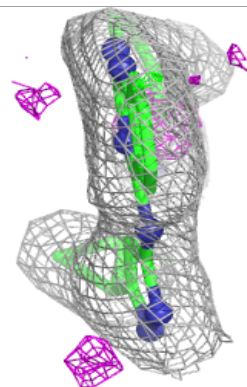
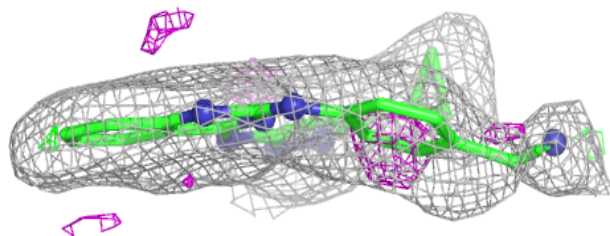
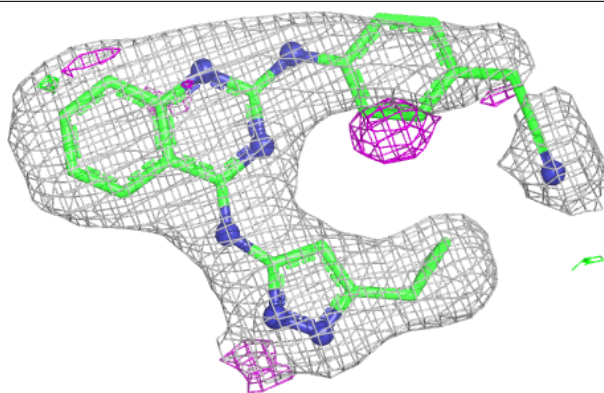
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IHH	B	1	29/29	0.87	0.14	31,34,59,61	0
2	IHH	A	1	29/29	0.88	0.13	30,33,54,55	0
2	IHH	C	1	29/29	0.89	0.13	32,34,54,56	0
2	IHH	D	1	29/29	0.89	0.13	28,30,51,53	0

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.

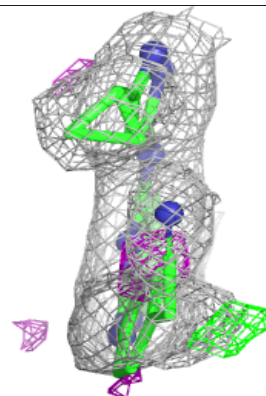
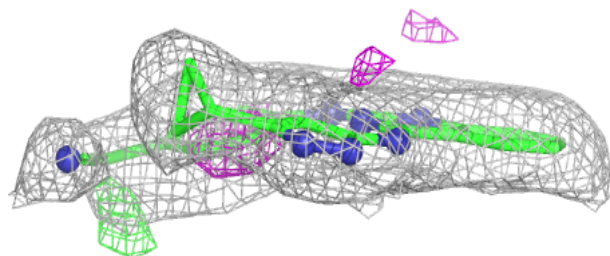
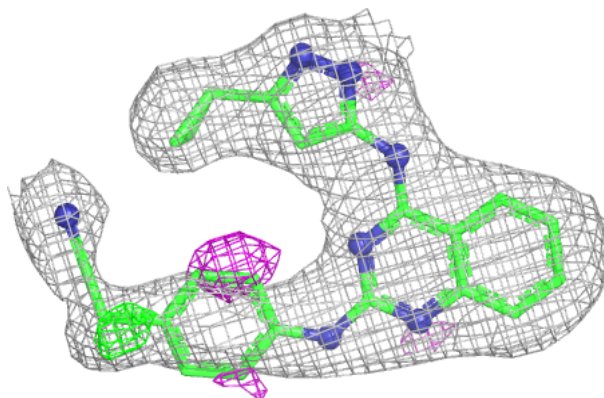


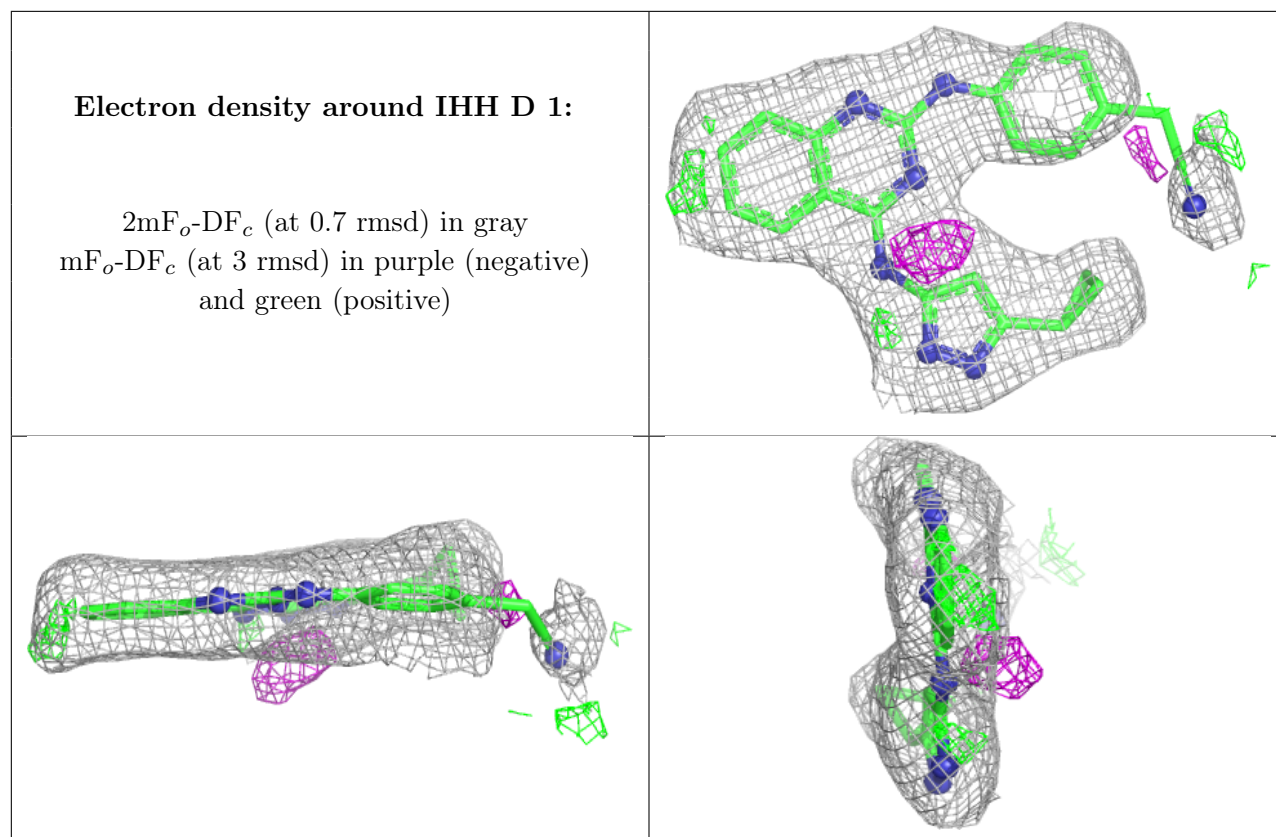
Electron density around IHH A 1:

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

**Electron density around IHH C 1:**

$2mF_o-DF_c$ (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.