



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:13 AM UTC

PDB ID : 1W22 / pdb_00001w22
Title : Crystal structure of inhibited human HDAC8
Authors : Vannini, A.; Volpari, C.; Caroli Casavola, E.; Di Marco, S.
Deposited on : 2004-06-25
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

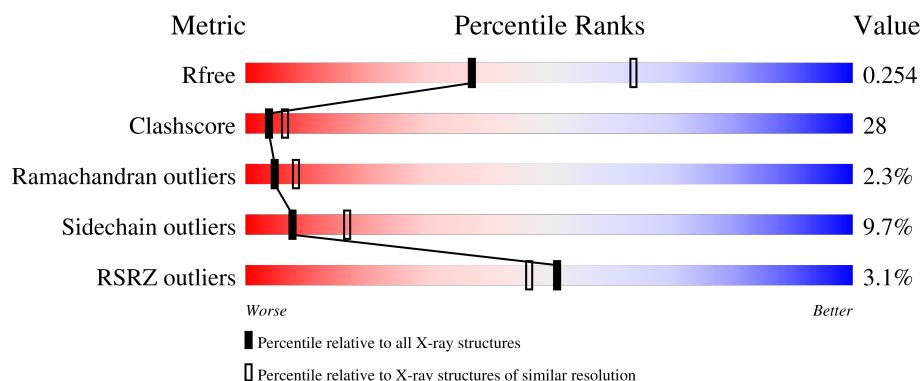
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

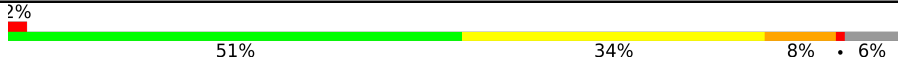
The reported resolution of this entry is 2.50 Å.

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	377	
1	B	377	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5815 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 HISTONE DEACETYLASE 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	1
			2745	1763	456	507	19			
1	B	351	Total	C	N	O	S	0	0	1
			2732	1754	455	504	19			

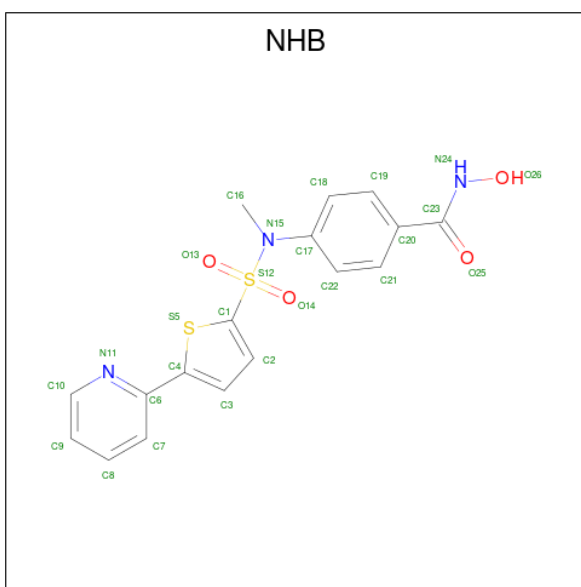
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	K	0	0
			2	2		
3	B	2	Total	K	0	0
			2	2		

- Molecule 4 is N-HYDROXY-4-(METHYL{[5-(2-PYRIDINYL)-2-THIENYL]SULFONYL} AMINO)BENZAMIDE (CCD ID: NHB) (formula: C₁₇H₁₅N₃O₄S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	17	3	4	2		
4	B	1	Total	C	N	O	S	0	0
			26	17	3	4	2		

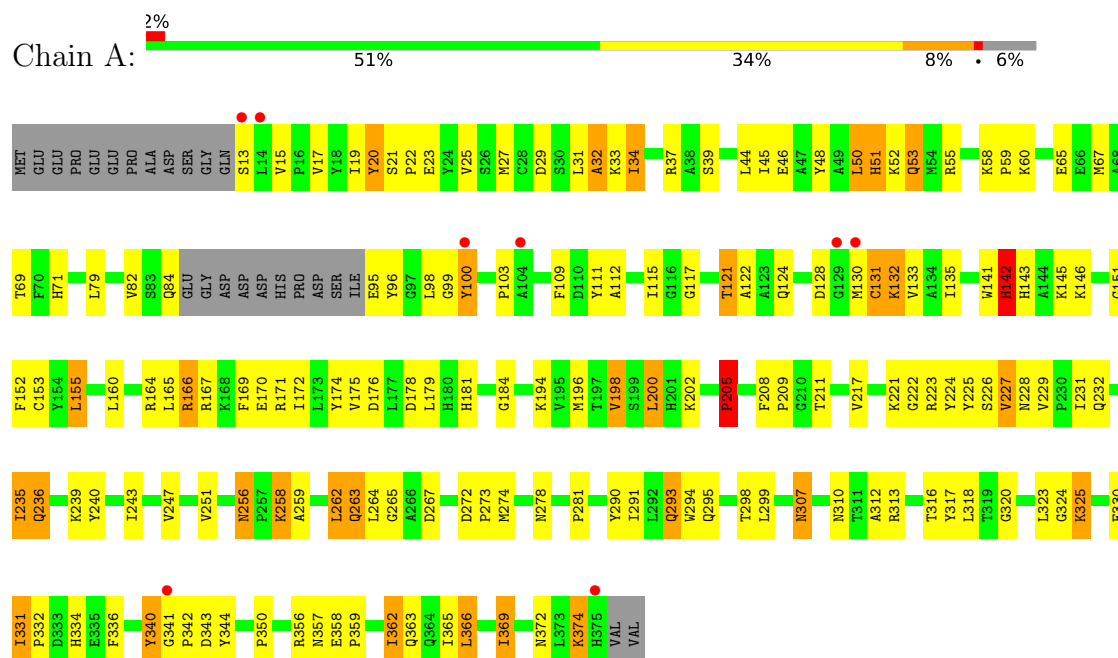
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	154	Total	O	0	0
			154	154		
5	B	126	Total	O	0	0
			126	126		

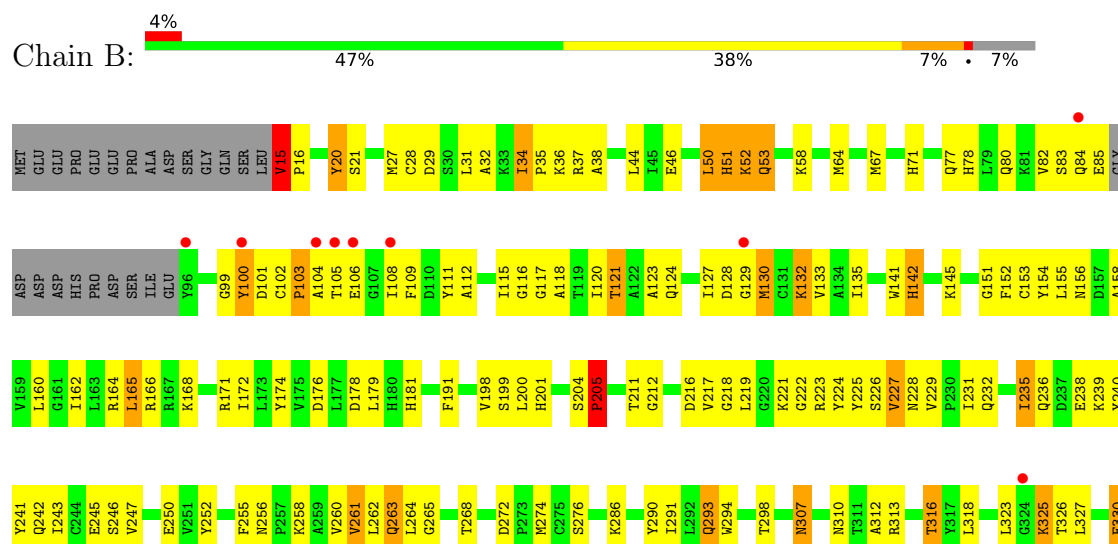
3 Residue-property plots

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: HISTONE DEACETYLASE 8



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.75Å 83.53Å 94.65Å 90.00° 97.48° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 97.7 (50.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.51Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.210 , 0.250 0.210 , 0.254	Depositor DCC
R_{free} test set	1322 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5815	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: K, NHB, ZN

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	0.48	1/2812 (0.0%)	1.02	15/3812 (0.4%)
1	B	0.45	1/2799 (0.0%)	1.02	15/3795 (0.4%)
All	All	0.47	2/5611 (0.0%)	1.02	30/7607 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	LYS	C-N	-5.71	1.25	1.33
1	B	374	LYS	C-N	-5.67	1.25	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	GLN	N-CA-C	-8.83	101.49	112.88
1	A	135	ILE	N-CA-C	7.38	118.50	108.17
1	A	331	ILE	CA-C-N	7.30	127.06	119.76
1	A	331	ILE	C-N-CA	7.30	127.06	119.76
1	A	69	THR	N-CA-C	-6.37	105.36	113.01
1	B	358	GLU	CA-C-N	6.28	127.69	119.84
1	B	358	GLU	C-N-CA	6.28	127.69	119.84
1	B	363	GLN	N-CA-C	-6.19	104.53	111.28
1	A	53	GLN	N-CA-C	-6.08	104.67	114.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	TYR	N-CA-C	6.03	117.68	108.52
1	B	142	HIS	N-CA-C	6.01	120.47	113.20
1	A	128	ASP	N-CA-C	-5.90	102.20	110.35
1	B	261	VAL	N-CA-C	-5.84	99.99	108.17
1	B	268	THR	N-CA-C	-5.77	106.22	113.72
1	A	294	TRP	N-CA-C	-5.74	105.53	112.54
1	B	15	VAL	CA-C-N	5.73	125.68	119.78
1	B	15	VAL	C-N-CA	5.73	125.68	119.78
1	A	122	ALA	N-CA-C	-5.59	105.26	111.36
1	A	48	TYR	N-CA-C	-5.52	106.40	113.02
1	A	142	HIS	N-CA-C	5.45	119.55	113.01
1	B	294	TRP	N-CA-C	-5.42	106.67	113.72
1	B	135	ILE	N-CA-C	5.39	115.66	108.11
1	A	298	THR	N-CA-C	5.39	117.18	108.34
1	B	358	GLU	N-CA-C	5.34	121.61	109.81
1	A	32	ALA	N-CA-C	5.28	117.44	111.11
1	B	327	LEU	N-CA-C	5.15	117.76	110.50
1	A	262	LEU	N-CA-C	5.07	116.68	108.41
1	B	258	LYS	N-CA-C	-5.07	107.64	113.88
1	A	20	TYR	N-CA-C	5.03	116.70	108.76
1	A	258	LYS	N-CA-C	-5.02	106.84	113.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	TYR	Sidechain

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	2745	0	2711	145	0
1	B	2732	0	2696	169	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
4	A	26	0	14	0	0
4	B	26	0	14	4	0
5	A	154	0	0	9	0
5	B	126	0	0	15	0
All	All	5815	0	5435	311	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 28.

All (311) 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:263:GLN:NE2	1:B:265:GLY:H	1.49	1.11
1:A:263:GLN:NE2	1:A:265:GLY:H	1.52	1.06
1:A:181:HIS:HD1	1:A:211:THR:HG23	1.25	1.00
1:B:117:GLY:O	1:B:121:THR:HG22	1.65	0.97
1:A:374:LYS:HB3	5:A:2151:HOH:O	1.63	0.97
1:B:124:GLN:HE21	1:B:164:ARG:HE	0.97	0.93
1:B:263:GLN:HE22	1:B:265:GLY:H	1.14	0.91
1:A:34:ILE:HD11	1:A:37:ARG:NE	1.89	0.88
1:B:232:GLN:H	1:B:357:ASN:HD21	1.22	0.88
1:A:205:PRO:HB2	1:B:353:ARG:HG3	1.58	0.86
1:B:364:GLN:C	1:B:364:GLN:HE21	1.86	0.83
1:B:124:GLN:NE2	1:B:164:ARG:HE	1.75	0.82
1:B:312:ALA:O	1:B:316:THR:HG23	1.78	0.81
1:B:15:VAL:HG12	1:B:130:MET:HE2	1.62	0.79
1:B:123:ALA:HB1	1:B:165:LEU:HD13	1.65	0.78
1:B:358:GLU:O	1:B:358:GLU:CD	2.27	0.78
1:B:357:ASN:O	1:B:358:GLU:HG3	1.83	0.78
1:A:181:HIS:ND1	1:A:211:THR:HG23	1.99	0.77
1:A:312:ALA:O	1:A:316:THR:HG23	1.83	0.77
1:B:51:HIS:O	1:B:52:LYS:HG2	1.83	0.77
1:A:169:PHE:HB2	1:A:172:ILE:HD11	1.67	0.77
1:A:166:ARG:HG2	1:A:166:ARG:HH11	1.51	0.76
1:A:34:ILE:HD11	1:A:37:ARG:CZ	2.16	0.76
1:A:263:GLN:HE21	1:A:265:GLY:H	1.34	0.75
1:A:307:ASN:HD22	1:A:310:ASN:H	1.35	0.74
1:A:141:TRP:HB3	1:A:153:CYS:SG	2.28	0.74
1:A:290:TYR:O	1:A:293:GLN:HG3	1.89	0.73
1:A:51:HIS:O	1:A:52:LYS:HG2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:TYR:HD2	1:B:261:VAL:HG13	1.54	0.73
1:B:171:ARG:HH21	1:B:256:ASN:HB3	1.55	0.72
1:A:235:ILE:HD12	1:A:240:TYR:HB2	1.72	0.72
1:A:209:PRO:HG2	1:A:211:THR:HG22	1.71	0.72
1:B:307:ASN:C	1:B:307:ASN:HD22	1.97	0.71
1:A:95:GLU:HG3	5:B:2102:HOH:O	1.91	0.70
1:B:124:GLN:HE21	1:B:164:ARG:NE	1.81	0.70
1:A:60:LYS:H	1:A:121:THR:HG21	1.54	0.70
1:A:205:PRO:CB	1:B:353:ARG:HG3	2.22	0.70
1:B:263:GLN:HE22	1:B:265:GLY:N	1.90	0.69
1:A:179:LEU:HD23	1:A:274:MET:HG2	1.73	0.69
1:A:263:GLN:NE2	1:A:265:GLY:N	2.36	0.69
1:B:179:LEU:HD23	1:B:274:MET:HG2	1.74	0.69
1:B:264:LEU:HD13	1:B:318:LEU:HD13	1.73	0.69
1:B:361:ARG:O	1:B:365:ILE:HG12	1.93	0.69
1:B:34:ILE:HD11	1:B:37:ARG:NE	2.09	0.68
1:B:53:GLN:HE22	1:B:325:LYS:NZ	1.91	0.68
1:B:132:LYS:HD3	1:B:133:VAL:HG23	1.75	0.68
1:B:99:GLY:O	1:B:103:PRO:HA	1.92	0.68
1:A:178:ASP:HB2	1:A:263:GLN:NE2	2.08	0.68
1:B:16:PRO:HG3	1:B:132:LYS:HE3	1.76	0.67
1:A:217:VAL:HA	1:A:226:SER:O	1.93	0.67
1:B:307:ASN:ND2	1:B:310:ASN:H	1.92	0.67
1:A:325:LYS:HZ3	1:A:325:LYS:HB3	1.60	0.67
1:A:164:ARG:HD2	1:A:167:ARG:HD2	1.77	0.67
1:A:132:LYS:HD2	1:A:133:VAL:HG23	1.77	0.66
1:B:238:GLU:O	1:B:242:GLN:HG3	1.97	0.65
1:A:46:GLU:HG3	1:A:51:HIS:CE1	2.32	0.65
1:B:28:CYS:SG	1:B:115:ILE:HD11	2.37	0.64
1:B:44:LEU:HB3	1:B:316:THR:HG21	1.78	0.64
1:B:51:HIS:C	1:B:53:GLN:H	2.04	0.64
1:A:31:LEU:HD23	1:A:34:ILE:CG2	2.27	0.63
1:A:31:LEU:HD23	1:A:34:ILE:HG21	1.81	0.63
1:B:27:MET:HE2	1:B:111:TYR:HB2	1.78	0.63
1:B:100:TYR:O	1:B:103:PRO:HD3	1.98	0.63
1:A:100:TYR:O	1:A:103:PRO:HD3	1.97	0.63
1:A:307:ASN:ND2	1:A:310:ASN:H	1.97	0.63
1:B:34:ILE:HG12	1:B:34:ILE:O	1.99	0.62
1:A:53:GLN:HE22	1:A:325:LYS:NZ	1.98	0.62
1:A:258:LYS:HA	1:A:258:LYS:HE2	1.82	0.61
1:A:363:GLN:HG3	5:A:2143:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:HD13	1:B:156:ASN:N	2.15	0.61
1:A:117:GLY:O	1:A:121:THR:HG23	2.01	0.60
1:A:365:ILE:O	1:A:369:ILE:HG22	2.00	0.60
1:B:174:TYR:CD2	1:B:261:VAL:HG13	2.37	0.60
1:A:205:PRO:HB2	1:B:353:ARG:CG	2.30	0.60
1:A:235:ILE:HD13	1:A:236:GLN:N	2.16	0.60
1:A:263:GLN:HE22	1:A:265:GLY:H	1.42	0.60
1:A:235:ILE:HD13	1:A:236:GLN:H	1.67	0.59
1:A:71:HIS:HA	1:A:146:LYS:O	2.03	0.59
1:B:343:ASP:HB2	1:B:345:VAL:HG22	1.85	0.59
1:B:101:ASP:HB3	4:B:1378:NHB:C16	2.33	0.58
1:B:191:PHE:O	1:B:221:LYS:HB2	2.04	0.58
1:B:179:LEU:CD2	1:B:274:MET:HG2	2.33	0.58
1:A:31:LEU:HD22	1:A:111:TYR:OH	2.03	0.58
1:A:130:MET:HE3	1:A:130:MET:H	1.69	0.58
1:B:366:LEU:O	1:B:369:ILE:HG22	2.04	0.58
1:A:19:ILE:HG22	1:A:59:PRO:HG3	1.86	0.57
1:A:295:GLN:HB2	5:A:2118:HOH:O	2.03	0.57
1:B:53:GLN:HG2	5:B:2017:HOH:O	2.03	0.57
1:B:145:LYS:HE3	5:B:2044:HOH:O	2.05	0.57
1:B:263:GLN:NE2	1:B:265:GLY:N	2.35	0.57
1:A:179:LEU:CD2	1:A:274:MET:HG2	2.33	0.57
1:B:51:HIS:O	1:B:53:GLN:N	2.38	0.57
1:B:217:VAL:HA	1:B:226:SER:O	2.04	0.57
1:B:231:ILE:HG22	1:B:232:GLN:N	2.20	0.57
1:A:172:ILE:HD12	1:A:259:ALA:HB3	1.87	0.57
1:B:371:GLY:O	1:B:373:LEU:N	2.38	0.57
1:B:178:ASP:HB2	1:B:263:GLN:NE2	2.19	0.56
1:B:330:GLU:HB3	5:B:2100:HOH:O	2.06	0.56
1:A:53:GLN:CD	1:A:325:LYS:HZ1	2.12	0.56
1:B:373:LEU:C	1:B:374:LYS:HG3	2.30	0.56
1:A:32:ALA:HB1	5:A:2010:HOH:O	2.06	0.56
1:A:239:LYS:O	1:A:243:ILE:HG13	2.06	0.56
1:A:372:ASN:O	1:A:374:LYS:HG2	2.06	0.56
1:A:175:VAL:HA	1:A:198:VAL:HG13	1.86	0.56
1:B:232:GLN:H	1:B:357:ASN:ND2	1.98	0.56
1:B:67:MET:HE1	1:B:109:PHE:CZ	2.41	0.55
1:A:272:ASP:OD2	1:A:274:MET:HB2	2.07	0.55
1:A:247:VAL:HG22	1:A:369:ILE:HD13	1.87	0.55
1:B:118:ALA:O	1:B:121:THR:HG23	2.06	0.55
1:B:112:ALA:HB1	1:B:155:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HB3	1:A:316:THR:HG21	1.89	0.54
1:B:241:TYR:CD2	1:B:286:LYS:HE2	2.42	0.54
1:B:358:GLU:O	1:B:360:HIS:N	2.40	0.54
1:A:34:ILE:HD11	1:A:37:ARG:CD	2.37	0.54
1:B:276:SER:O	1:B:353:ARG:NH2	2.39	0.54
1:A:67:MET:HE1	1:A:109:PHE:CZ	2.43	0.54
1:A:132:LYS:CD	1:A:133:VAL:HG23	2.37	0.54
1:A:27:MET:HE2	1:A:111:TYR:HB2	1.90	0.54
1:A:325:LYS:NZ	1:A:325:LYS:CB	2.71	0.54
1:B:199:SER:OG	1:B:201:HIS:HD2	1.90	0.54
1:A:13:SER:OG	1:A:15:VAL:HG22	2.08	0.53
1:A:34:ILE:CD1	1:A:37:ARG:CZ	2.86	0.53
1:B:250:GLU:HG3	1:B:373:LEU:HD21	1.91	0.53
1:B:313:ARG:NH2	5:B:2103:HOH:O	2.42	0.53
1:A:71:HIS:CD2	1:A:155:LEU:HD22	2.43	0.53
1:B:372:ASN:O	1:B:373:LEU:HD12	2.09	0.52
1:B:46:GLU:HG3	1:B:51:HIS:CE1	2.45	0.52
1:A:208:PHE:CE1	1:A:209:PRO:HB3	2.45	0.52
1:A:171:ARG:HH21	1:A:256:ASN:HB3	1.75	0.52
1:B:174:TYR:HD2	1:B:261:VAL:CG1	2.21	0.52
1:B:15:VAL:HG12	1:B:130:MET:CE	2.37	0.52
1:A:45:ILE:HG13	1:A:316:THR:HG22	1.91	0.51
1:B:341:GLY:N	5:B:2103:HOH:O	2.27	0.51
1:A:53:GLN:NE2	1:A:325:LYS:HZ1	2.08	0.51
1:A:142:HIS:CD2	1:A:142:HIS:H	2.26	0.51
1:B:171:ARG:HD2	1:B:255:PHE:CE1	2.45	0.51
1:B:252:TYR:O	1:B:255:PHE:O	2.29	0.51
1:A:130:MET:HE3	5:A:2051:HOH:O	2.11	0.51
1:A:130:MET:O	1:A:131:CYS:HB2	2.10	0.51
1:B:366:LEU:O	1:B:366:LEU:HD23	2.11	0.51
1:B:32:ALA:O	1:B:35:PRO:HD3	2.11	0.51
1:A:334:HIS:CD2	1:A:336:PHE:H	2.29	0.51
1:B:178:ASP:HB2	1:B:263:GLN:CD	2.36	0.51
1:A:366:LEU:O	1:A:369:ILE:HG23	2.11	0.50
1:B:20:TYR:CG	1:B:21:SER:N	2.78	0.50
1:A:174:TYR:O	1:A:198:VAL:HG12	2.11	0.50
1:A:117:GLY:O	1:A:121:THR:CG2	2.59	0.50
1:B:243:ILE:O	1:B:247:VAL:HG23	2.11	0.49
1:B:218:GLY:HA3	5:B:2063:HOH:O	2.12	0.49
1:B:357:ASN:O	1:B:358:GLU:CG	2.58	0.49
1:B:34:ILE:HD11	1:B:37:ARG:CZ	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:PRO:HA	5:B:2049:HOH:O	2.12	0.49
1:A:34:ILE:O	1:A:34:ILE:HG12	2.10	0.49
1:B:217:VAL:C	1:B:226:SER:HB2	2.37	0.49
1:A:55:ARG:NH2	5:A:2022:HOH:O	2.46	0.49
1:B:116:GLY:O	1:B:120:ILE:HG13	2.13	0.49
1:A:51:HIS:C	1:A:53:GLN:N	2.68	0.49
1:B:235:ILE:HD12	1:B:240:TYR:HB2	1.93	0.49
1:A:247:VAL:HG13	1:A:369:ILE:HD11	1.95	0.49
1:A:374:LYS:HG3	1:A:374:LYS:O	2.12	0.49
1:A:170:GLU:HG3	1:A:194:LYS:HE3	1.95	0.49
1:B:104:ALA:HB3	5:B:2035:HOH:O	2.12	0.49
1:B:340:TYR:O	1:B:341:GLY:O	2.31	0.48
1:A:236:GLN:HG3	5:A:2101:HOH:O	2.13	0.48
1:A:60:LYS:O	1:A:117:GLY:HA3	2.13	0.48
1:A:196:MET:SD	1:A:251:VAL:HG13	2.53	0.48
1:B:84:GLN:O	1:B:85:GLU:HB2	2.13	0.48
1:A:166:ARG:CZ	1:A:194:LYS:HG2	2.43	0.48
1:A:176:ASP:CG	1:A:263:GLN:HG2	2.39	0.48
1:A:273:PRO:HB3	4:B:1378:NHB:C1	2.43	0.48
1:B:307:ASN:C	1:B:307:ASN:ND2	2.68	0.48
1:A:178:ASP:HB2	1:A:263:GLN:CD	2.38	0.48
1:A:325:LYS:HZ3	1:A:325:LYS:CB	2.24	0.48
1:A:124:GLN:OE1	1:A:164:ARG:NE	2.46	0.48
1:B:99:GLY:O	1:B:103:PRO:CA	2.59	0.48
1:A:178:ASP:OD1	1:A:265:GLY:HA3	2.14	0.48
1:B:155:LEU:HD11	1:B:160:LEU:CD1	2.44	0.48
1:A:217:VAL:C	1:A:226:SER:HB2	2.40	0.47
1:B:31:LEU:HD23	1:B:34:ILE:CG2	2.44	0.47
1:B:369:ILE:HG23	1:B:370:LYS:N	2.30	0.47
1:A:263:GLN:HE22	1:A:265:GLY:N	2.07	0.47
1:B:108:ILE:HD11	1:B:154:TYR:CD1	2.49	0.47
1:B:246:SER:OG	1:B:366:LEU:HD11	2.15	0.47
1:A:50:LEU:C	1:A:51:HIS:O	2.56	0.47
1:A:166:ARG:HG2	1:A:166:ARG:NH1	2.26	0.47
1:B:245:GLU:O	1:B:246:SER:C	2.56	0.47
1:A:235:ILE:HD11	1:A:240:TYR:N	2.29	0.47
1:A:278:ASN:ND2	1:A:350:PRO:HB2	2.29	0.47
1:A:175:VAL:HG22	1:A:198:VAL:CG1	2.45	0.47
1:B:50:LEU:C	1:B:51:HIS:O	2.54	0.47
1:A:51:HIS:C	1:A:53:GLN:H	2.23	0.46
1:B:53:GLN:NE2	1:B:325:LYS:NZ	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:HIS:CD2	1:B:155:LEU:HD22	2.49	0.46
1:B:201:HIS:HE1	1:B:212:GLY:O	1.98	0.46
1:B:44:LEU:HD12	1:B:44:LEU:HA	1.75	0.46
1:B:67:MET:HE1	1:B:109:PHE:CE1	2.50	0.46
1:B:239:LYS:O	1:B:243:ILE:HG13	2.14	0.46
1:A:273:PRO:HB3	4:B:1378:NHB:C2	2.45	0.46
1:A:22:PRO:HG2	1:A:23:GLU:OE1	2.15	0.46
1:B:375:HIS:N	5:B:2124:HOH:O	2.48	0.46
1:B:166:ARG:HG2	1:B:166:ARG:HH11	1.80	0.46
1:B:325:LYS:NZ	1:B:325:LYS:CB	2.79	0.46
1:A:34:ILE:O	1:A:34:ILE:HG23	2.15	0.46
1:B:21:SER:HB3	1:B:58:LYS:HG3	1.98	0.46
1:A:320:GLY:O	1:A:324:GLY:N	2.49	0.46
1:B:358:GLU:O	1:B:358:GLU:OE2	2.34	0.46
1:B:83:SER:HB2	1:B:109:PHE:HB2	1.97	0.46
1:B:343:ASP:HB3	5:B:2105:HOH:O	2.16	0.46
1:A:223:ARG:O	1:A:224:TYR:HB2	2.17	0.45
1:B:142:HIS:H	1:B:142:HIS:CD2	2.34	0.45
1:A:142:HIS:O	1:A:184:GLY:HA3	2.16	0.45
1:B:132:LYS:HD2	1:B:133:VAL:N	2.30	0.45
1:B:50:LEU:HD11	1:B:325:LYS:HE2	1.98	0.45
1:B:80:GLN:O	1:B:83:SER:HB3	2.16	0.45
1:B:102:CYS:HB3	1:B:154:TYR:CE1	2.52	0.45
1:A:151:GLY:O	1:A:152:PHE:HB2	2.16	0.45
1:B:141:TRP:HB3	1:B:153:CYS:SG	2.56	0.45
1:B:181:HIS:CD2	1:B:228:ASN:ND2	2.85	0.45
1:B:200:LEU:HD13	1:B:229:VAL:HB	1.99	0.45
1:B:325:LYS:NZ	1:B:325:LYS:HB3	2.31	0.45
1:A:221:LYS:HE3	1:A:221:LYS:HB3	1.78	0.45
1:B:340:TYR:C	1:B:341:GLY:O	2.59	0.45
1:A:143:HIS:O	1:A:145:LYS:HD2	2.17	0.45
1:A:313:ARG:NH2	5:A:2125:HOH:O	2.49	0.45
1:B:29:ASP:OD2	1:B:38:ALA:HB3	2.17	0.45
1:B:222:GLY:O	1:B:225:TYR:HB2	2.17	0.45
1:B:223:ARG:HG3	1:B:223:ARG:HH11	1.81	0.45
1:A:205:PRO:CG	1:B:353:ARG:HG3	2.48	0.45
1:B:127:ILE:HG23	1:B:168:LYS:CD	2.47	0.45
1:A:281:PRO:HB2	1:A:317:TYR:CD2	2.52	0.44
1:B:216:ASP:C	1:B:216:ASP:OD2	2.59	0.44
1:B:290:TYR:O	1:B:293:GLN:HG3	2.17	0.44
1:A:343:ASP:O	1:A:344:TYR:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PRO:O	1:B:36:LYS:HB2	2.18	0.44
1:A:20:TYR:CG	1:A:21:SER:N	2.85	0.44
1:A:99:GLY:O	1:A:103:PRO:CA	2.66	0.44
1:A:247:VAL:HG13	1:A:369:ILE:CD1	2.47	0.44
1:B:375:HIS:N	5:B:2125:HOH:O	2.51	0.44
1:B:129:GLY:O	1:B:130:MET:C	2.60	0.44
1:B:171:ARG:HB3	1:B:255:PHE:CZ	2.53	0.44
1:A:65:GLU:CD	1:A:65:GLU:H	2.26	0.43
1:B:224:TYR:CD2	1:B:374:LYS:HD2	2.52	0.43
1:B:247:VAL:HG13	1:B:369:ILE:HD13	1.99	0.43
1:A:227:VAL:HG21	1:A:369:ILE:HD12	1.99	0.43
1:B:123:ALA:CB	1:B:165:LEU:HD13	2.40	0.43
1:B:198:VAL:O	1:B:198:VAL:HG23	2.16	0.43
1:B:272:ASP:OD2	1:B:274:MET:HB2	2.18	0.43
1:A:112:ALA:HB1	1:A:155:LEU:HB2	2.00	0.43
1:B:50:LEU:HA	1:B:50:LEU:HD12	1.79	0.43
1:B:357:ASN:C	1:B:358:GLU:HG3	2.40	0.43
1:A:231:ILE:HG22	1:A:232:GLN:N	2.34	0.43
1:B:218:GLY:C	1:B:219:LEU:HG	2.43	0.43
1:A:171:ARG:HA	1:A:194:LYS:O	2.19	0.43
1:B:78:HIS:O	1:B:82:VAL:HG13	2.18	0.43
1:B:77:GLN:NE2	5:B:2026:HOH:O	2.52	0.43
1:B:132:LYS:HD2	1:B:132:LYS:H	1.84	0.43
1:B:198:VAL:HA	1:B:227:VAL:HG22	2.01	0.43
1:B:223:ARG:HG3	1:B:223:ARG:NH1	2.32	0.43
1:B:231:ILE:CG2	1:B:232:GLN:N	2.81	0.43
1:A:20:TYR:HE1	1:A:25:VAL:HG21	1.83	0.43
1:A:331:ILE:HA	1:A:332:PRO:HD3	1.76	0.43
1:B:174:TYR:HA	1:B:261:VAL:HG13	2.00	0.43
1:A:172:ILE:CD1	1:A:259:ALA:HB3	2.49	0.43
1:B:127:ILE:HG23	1:B:168:LYS:HD2	2.01	0.43
1:A:202:LYS:HA	1:A:231:ILE:O	2.19	0.43
1:B:21:SER:CB	1:B:58:LYS:HG3	2.49	0.43
1:B:83:SER:HA	1:B:108:ILE:HG22	2.00	0.42
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.84	0.42
1:B:293:GLN:HE21	1:B:293:GLN:HB2	1.51	0.42
1:A:82:VAL:C	1:A:84:GLN:H	2.26	0.42
1:A:111:TYR:O	1:A:115:ILE:HG12	2.19	0.42
1:A:51:HIS:O	1:A:53:GLN:N	2.52	0.42
1:A:155:LEU:HD11	1:A:160:LEU:CD1	2.49	0.42
1:B:151:GLY:O	1:B:152:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LEU:O	1:B:374:LYS:HG3	2.18	0.42
1:B:358:GLU:HB3	5:B:2116:HOH:O	2.18	0.42
1:A:340:TYR:N	1:A:340:TYR:CD1	2.87	0.42
1:B:235:ILE:HD13	1:B:236:GLN:N	2.35	0.42
1:A:29:ASP:OD1	1:A:39:SER:OG	2.34	0.42
1:A:243:ILE:HG12	1:A:362:ILE:HD11	2.02	0.42
1:B:158:ALA:O	1:B:162:ILE:HG13	2.20	0.42
1:A:142:HIS:CD2	1:A:142:HIS:N	2.83	0.42
1:B:199:SER:OG	1:B:201:HIS:CD2	2.72	0.41
1:A:262:LEU:HD22	1:A:291:ILE:HD12	2.01	0.41
1:B:262:LEU:HD22	1:B:291:ILE:HD12	2.03	0.41
1:A:181:HIS:NE2	1:A:228:ASN:ND2	2.67	0.41
1:A:200:LEU:HD22	1:A:229:VAL:HG21	2.02	0.41
1:A:358:GLU:HA	1:A:359:PRO:HD3	1.93	0.41
1:B:204:SER:O	1:B:205:PRO:C	2.63	0.41
1:A:17:VAL:HG23	1:A:131:CYS:SG	2.61	0.41
1:A:82:VAL:C	1:A:84:GLN:N	2.78	0.41
1:B:34:ILE:CD1	1:B:37:ARG:CZ	2.98	0.41
1:B:176:ASP:CG	1:B:263:GLN:HG2	2.45	0.41
1:B:325:LYS:HB3	1:B:325:LYS:HZ3	1.85	0.41
1:A:222:GLY:O	1:A:225:TYR:HB2	2.21	0.41
1:B:162:ILE:HG23	1:B:172:ILE:HG21	2.03	0.41
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.59	0.41
1:A:155:LEU:HD11	1:A:160:LEU:HD11	2.03	0.41
1:A:264:LEU:HD13	1:A:318:LEU:HD13	2.02	0.41
1:B:223:ARG:O	1:B:224:TYR:HB2	2.21	0.41
1:B:331:ILE:HA	1:B:332:PRO:HD3	1.94	0.41
1:B:85:GLU:HA	1:B:85:GLU:OE1	2.21	0.41
1:B:235:ILE:HD11	1:B:239:LYS:HG2	2.02	0.41
1:B:263:GLN:O	1:B:263:GLN:HG3	2.21	0.41
4:B:1378:NHB:H3	5:B:2126:HOH:O	2.20	0.41
1:A:96:TYR:HB2	1:A:98:LEU:HD23	2.02	0.40
1:A:211:THR:HG21	5:A:2072:HOH:O	2.19	0.40
1:B:198:VAL:O	1:B:198:VAL:CG2	2.69	0.40
1:B:260:VAL:O	1:B:298:THR:HA	2.21	0.40
1:B:263:GLN:HE21	1:B:265:GLY:H	1.51	0.40
1:A:232:GLN:HB2	1:A:357:ASN:OD1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/377 (93%)	316 (90%)	27 (8%)	6 (2%)	7	13
1	B	347/377 (92%)	309 (89%)	28 (8%)	10 (3%)	3	5
All	All	696/754 (92%)	625 (90%)	55 (8%)	16 (2%)	5	8

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	128	ASP
1	B	130	MET
1	B	359	PRO
1	B	372	ASN
1	A	51	HIS
1	A	205	PRO
1	A	341	GLY
1	B	103	PRO
1	B	341	GLY
1	A	131	CYS
1	B	51	HIS
1	B	52	LYS
1	A	356	ARG
1	B	205	PRO
1	A	342	PRO
1	B	358	GLU

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	293/316 (93%)	263 (90%)	30 (10%)	7	15
1	B	292/316 (92%)	265 (91%)	27 (9%)	8	19
All	All	585/632 (93%)	528 (90%)	57 (10%)	8	17

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	34	ILE
1	A	50	LEU
1	A	58	LYS
1	A	79	LEU
1	A	100	TYR
1	A	121	THR
1	A	132	LYS
1	A	142	HIS
1	A	155	LEU
1	A	165	LEU
1	A	166	ARG
1	A	198	VAL
1	A	200	LEU
1	A	205	PRO
1	A	227	VAL
1	A	235	ILE
1	A	236	GLN
1	A	256	ASN
1	A	263	GLN
1	A	267	ASP
1	A	293	GLN
1	A	299	LEU
1	A	307	ASN
1	A	323	LEU
1	A	325	LYS
1	A	330	GLU
1	A	362	ILE
1	A	366	LEU
1	A	369	ILE
1	B	15	VAL
1	B	34	ILE
1	B	50	LEU
1	B	64	MET
1	B	100	TYR

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Mol	Chain	Res	Type
1	B	105	THR
1	B	106	GLU
1	B	121	THR
1	B	132	LYS
1	B	165	LEU
1	B	205	PRO
1	B	211	THR
1	B	227	VAL
1	B	235	ILE
1	B	263	GLN
1	B	293	GLN
1	B	307	ASN
1	B	316	THR
1	B	323	LEU
1	B	325	LYS
1	B	326	THR
1	B	330	GLU
1	B	358	GLU
1	B	359	PRO
1	B	362	ILE
1	B	364	GLN
1	B	366	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	77	GLN
1	A	80	GLN
1	A	136	ASN
1	A	228	ASN
1	A	242	GLN
1	A	263	GLN
1	A	293	GLN
1	A	307	ASN
1	A	363	GLN
1	A	372	ASN
1	B	51	HIS
1	B	77	GLN
1	B	80	GLN
1	B	124	GLN
1	B	136	ASN

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Mol	Chain	Res	Type
1	B	201	HIS
1	B	228	ASN
1	B	236	GLN
1	B	242	GLN
1	B	253	GLN
1	B	263	GLN
1	B	293	GLN
1	B	295	GLN
1	B	307	ASN
1	B	357	ASN
1	B	363	GLN
1	B	364	GLN
1	B	372	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](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NHB	B	1378	2	25,28,28	2.71	5 (20%)	37,40,40	2.43	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NHB	A	1378	2	25,28,28	2.46	5 (20%)	37,40,40	2.46	11 (29%)

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	NHB	B	1378	2	-	4/26/26/26	0/3/3/3
4	NHB	A	1378	2	-	5/26/26/26	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1378	NHB	O14-S12	8.31	1.51	1.43
4	B	1378	NHB	O14-S12	8.22	1.51	1.43
4	B	1378	NHB	O13-S12	6.89	1.50	1.43
4	A	1378	NHB	O13-S12	6.18	1.49	1.43
4	B	1378	NHB	C6-C4	-5.41	1.39	1.46
4	A	1378	NHB	C6-C4	-4.63	1.40	1.46
4	B	1378	NHB	C1-S5	-4.55	1.63	1.71
4	A	1378	NHB	C20-C23	2.45	1.55	1.50
4	B	1378	NHB	C20-C23	2.33	1.55	1.50
4	A	1378	NHB	C1-S5	-2.23	1.67	1.71

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1378	NHB	O14-S12-N15	7.89	115.24	106.83
4	A	1378	NHB	O14-S12-O13	-7.35	109.15	119.69
4	A	1378	NHB	O14-S12-N15	6.52	113.78	106.83
4	B	1378	NHB	C1-S5-C4	6.35	96.05	90.41
4	A	1378	NHB	O13-S12-N15	5.37	112.55	106.83
4	A	1378	NHB	C1-S5-C4	5.14	94.97	90.41
4	B	1378	NHB	C2-C1-S5	-4.44	108.13	112.55
4	B	1378	NHB	O14-S12-O13	-4.37	113.42	119.69
4	A	1378	NHB	C2-C1-S5	-3.40	109.17	112.55
4	B	1378	NHB	C10-N11-C6	3.06	120.87	116.93
4	A	1378	NHB	C4-C6-N11	3.06	120.43	116.44
4	B	1378	NHB	C4-C6-N11	3.00	120.35	116.44
4	B	1378	NHB	C17-N15-S12	2.88	122.65	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1378	NHB	C3-C4-S5	-2.72	107.19	110.10
4	B	1378	NHB	C7-C6-C4	-2.60	118.35	121.92
4	B	1378	NHB	C3-C4-S5	-2.55	107.38	110.10
4	A	1378	NHB	C10-N11-C6	2.55	120.22	116.93
4	B	1378	NHB	C9-C8-C7	-2.20	117.52	120.24
4	A	1378	NHB	O14-S12-C1	2.07	110.88	107.30
4	A	1378	NHB	C17-N15-S12	2.06	121.25	117.75
4	A	1378	NHB	C9-C8-C7	-2.04	117.72	120.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

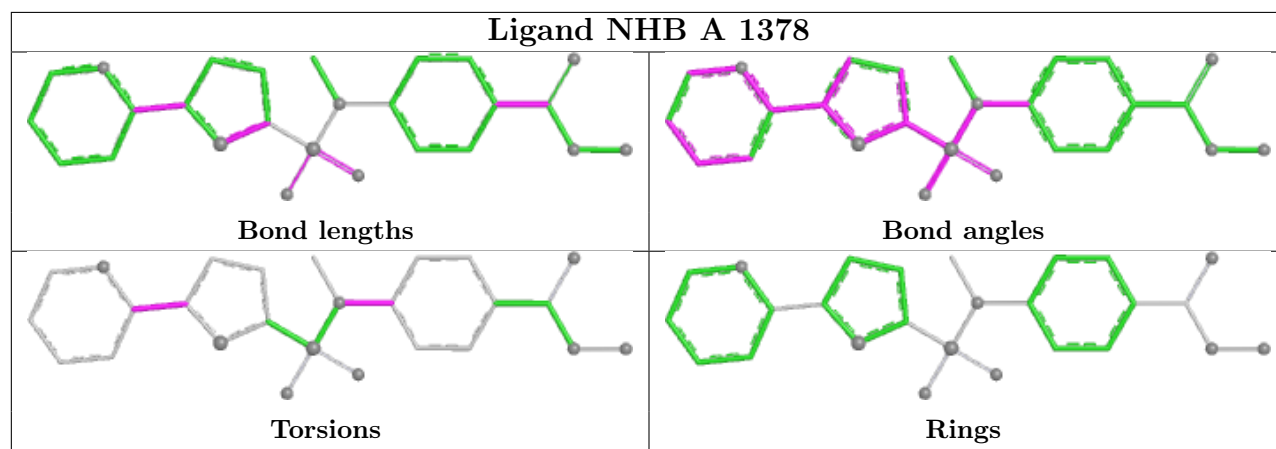
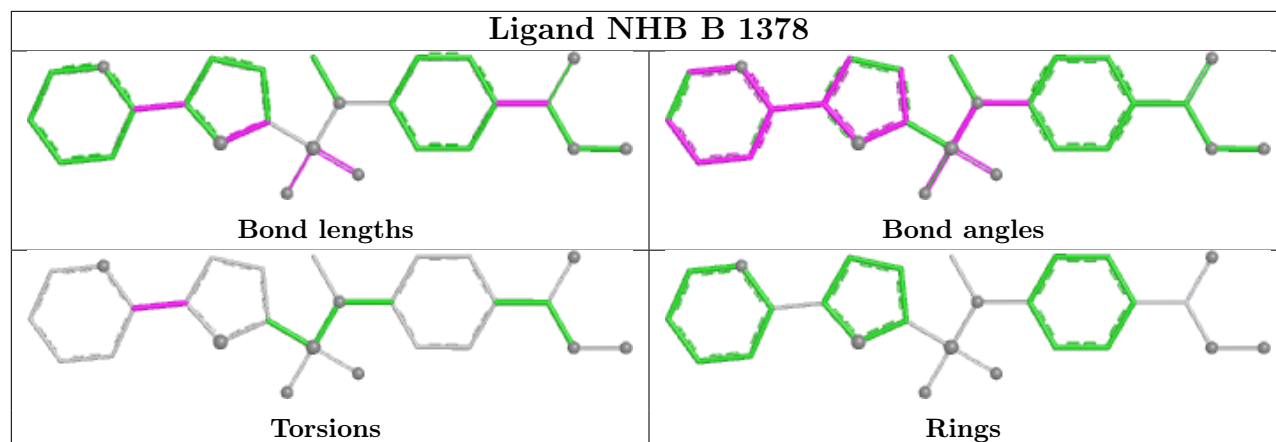
Mol	Chain	Res	Type	Atoms
4	A	1378	NHB	S5-C4-C6-N11
4	B	1378	NHB	S5-C4-C6-N11
4	A	1378	NHB	C3-C4-C6-N11
4	B	1378	NHB	C3-C4-C6-N11
4	A	1378	NHB	S5-C4-C6-C7
4	B	1378	NHB	S5-C4-C6-C7
4	A	1378	NHB	C3-C4-C6-C7
4	B	1378	NHB	C3-C4-C6-C7
4	A	1378	NHB	C18-C17-N15-C16

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1378	NHB	4	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	353/377 (93%)	-0.01	8 (2%) 61 57	19, 37, 61, 82	0
1	B	351/377 (93%)	0.23	14 (3%) 42 38	20, 41, 77, 96	0
All	All	704/754 (93%)	0.11	22 (3%) 51 47	19, 39, 68, 96	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	ALA	3.7
1	B	129	GLY	3.5
1	A	341	GLY	3.4
1	B	100	TYR	3.2
1	B	106	GLU	3.1
1	B	105	THR	3.0
1	A	375	HIS	3.0
1	A	100	TYR	2.9
1	A	104	ALA	2.9
1	A	129	GLY	2.5
1	B	324	GLY	2.5
1	A	130	MET	2.4
1	B	375	HIS	2.4
1	A	13	SER	2.3
1	B	369	ILE	2.3
1	B	373	LEU	2.2
1	A	14	LEU	2.2
1	B	96	TYR	2.2
1	B	84	GLN	2.1
1	B	368	TYR	2.1
1	B	108	ILE	2.1
1	B	341	GLY	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](#)

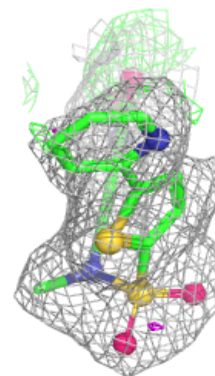
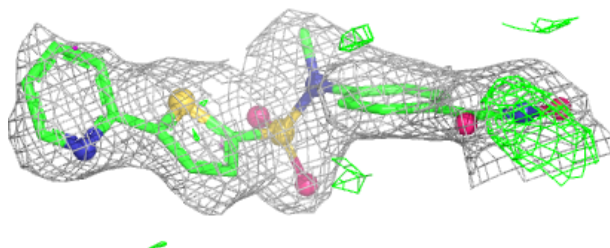
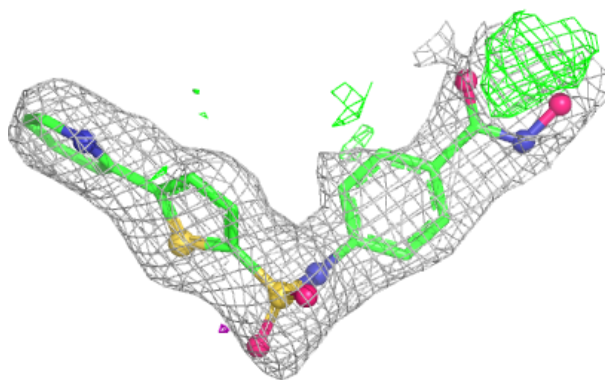
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	NHB	B	1378	26/26	0.90	0.13	40,49,55,56	0
4	NHB	A	1378	26/26	0.91	0.12	40,48,53,54	0
3	K	B	1377	1/1	0.94	0.07	40,40,40,40	0
2	ZN	A	1375	1/1	0.95	0.05	25,25,25,25	0
2	ZN	B	1375	1/1	0.95	0.05	27,27,27,27	0
3	K	A	1377	1/1	0.95	0.07	42,42,42,42	0
3	K	B	1376	1/1	0.96	0.04	31,31,31,31	0
3	K	A	1376	1/1	0.99	0.06	21,21,21,21	0

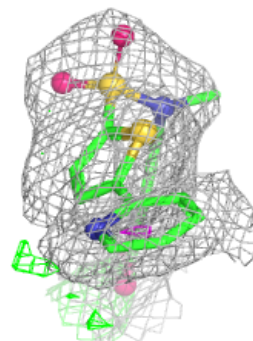
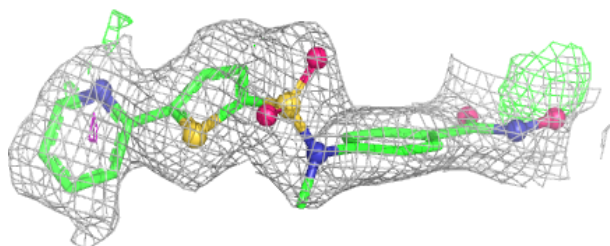
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NHB B 1378:

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

**Electron density around NHB A 1378:**

$2mF_o-DF_c$ (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.