



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:37 AM UTC

PDB ID : 3KDS / pdb_00003kds
Title : apo-FtsH crystal structure
Authors : Bieniossek, C.; Niederhauser, B.; Baumann, U.
Deposited on : 2009-10-23
Resolution : 2.60 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

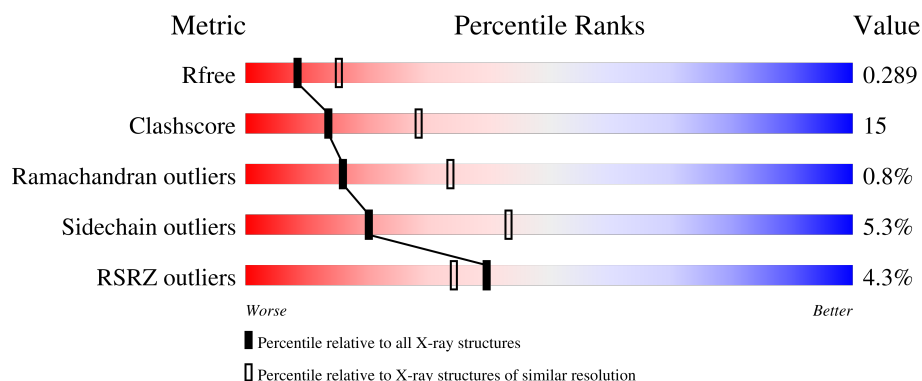
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	E	465	4% 66% 22% 8%
1	F	465	3% 61% 28% 8%
1	G	465	5% 58% 31% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9994 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 Cell division protein FtsH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	427	Total	C	N	O	S	0	0	0
			3301	2083	584	624	10			
1	F	426	Total	C	N	O	S	0	0	0
			3295	2080	583	622	10			
1	G	426	Total	C	N	O	S	0	0	0
			3296	2080	583	623	10			

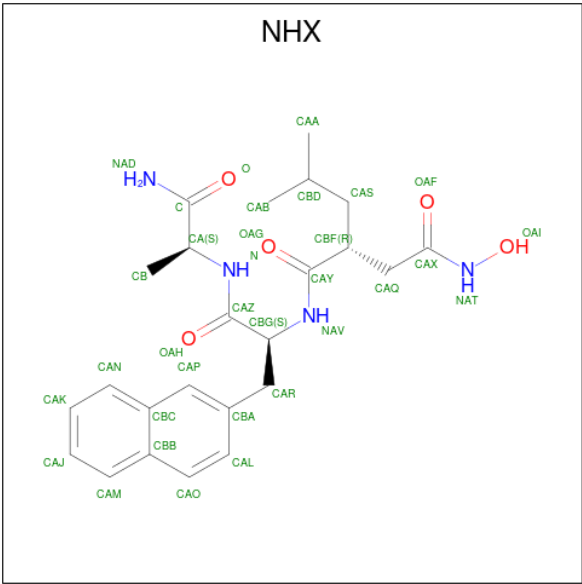
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	146	MET	-	expression tag	UNP Q9WZ49
E	207	ALA	LYS	engineered mutation	UNP Q9WZ49
E	410	LEU	LYS	engineered mutation	UNP Q9WZ49
E	415	ALA	LYS	engineered mutation	UNP Q9WZ49
F	146	MET	-	expression tag	UNP Q9WZ49
F	207	ALA	LYS	engineered mutation	UNP Q9WZ49
F	410	LEU	LYS	engineered mutation	UNP Q9WZ49
F	415	ALA	LYS	engineered mutation	UNP Q9WZ49
G	146	MET	-	expression tag	UNP Q9WZ49
G	207	ALA	LYS	engineered mutation	UNP Q9WZ49
G	410	LEU	LYS	engineered mutation	UNP Q9WZ49
G	415	ALA	LYS	engineered mutation	UNP Q9WZ49

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		
2	G	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-{(2R)-2-[2-(hydroxyamino)-2-oxoethyl]-4-methylpentanoyl}-3-naphthalen-2-yl-L-alanyl-L-alaninamide (CCD ID: NHX) (formula: C₂₄H₃₂N₄O₅).

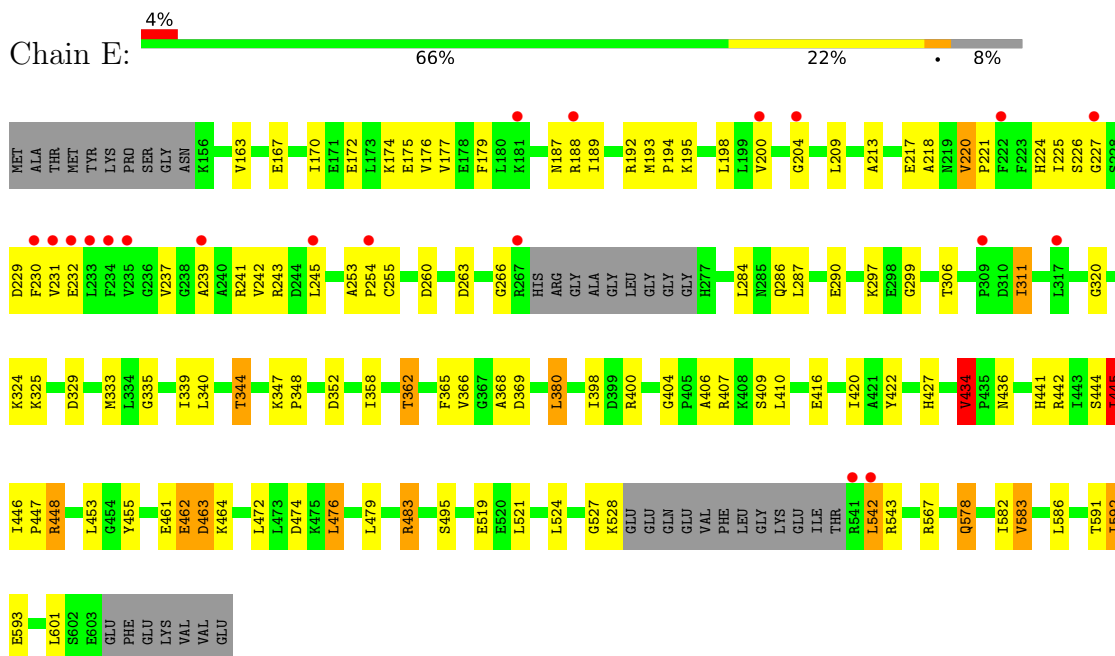


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			33	24	4	5		
3	F	1	Total	C	N	O	0	0
			33	24	4	5		
3	G	1	Total	C	N	O	0	0
			33	24	4	5		

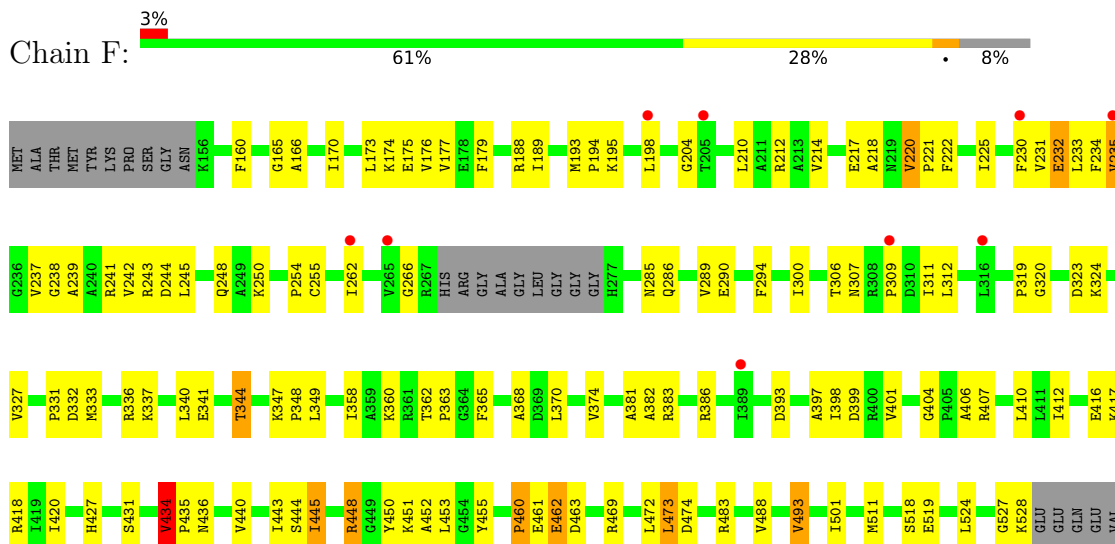
3 Residue-property plots [i](#)

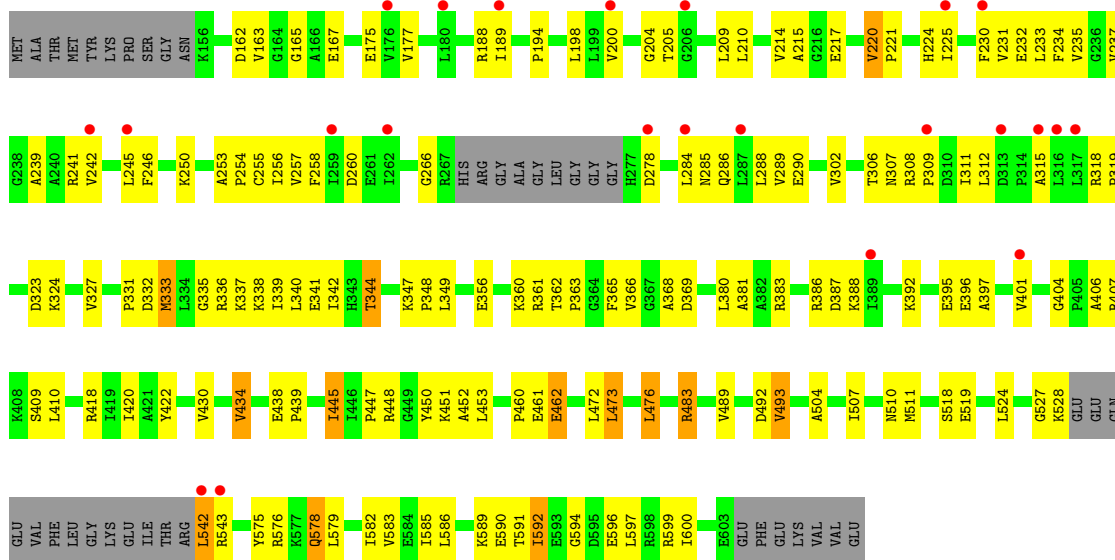
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Cell division protein FtsH





4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	190.50Å 190.50Å 152.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.76 – 2.60 45.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.76-2.60) 99.7 (45.76-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.223 , 0.287 0.224 , 0.289	Depositor DCC
R_{free} test set	1987 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 92.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9994	wwPDB-VP
Average B, all atoms (Å ²)	117.0	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 24.09 % 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 4.1018e-03. 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: NHX, 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	E	0.69	1/3348 (0.0%)	1.10	11/4519 (0.2%)
1	F	0.60	0/3342	1.01	11/4511 (0.2%)
1	G	0.54	0/3343	0.95	8/4512 (0.2%)
All	All	0.61	1/10033 (0.0%)	1.02	30/13542 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	427	HIS	CE1-NE2	5.17	1.37	1.32

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	436	ASN	N-CA-C	8.09	122.73	113.02
1	G	483	ARG	CG-CD-NE	-7.93	94.55	112.00
1	E	434	VAL	CA-C-N	7.64	129.40	119.84
1	E	434	VAL	C-N-CA	7.64	129.40	119.84
1	F	434	VAL	CA-C-N	7.42	126.96	119.24
1	F	434	VAL	C-N-CA	7.42	126.96	119.24
1	E	483	ARG	CG-CD-NE	-6.80	97.03	112.00
1	E	445	ILE	N-CA-C	-6.71	106.26	112.43
1	F	585	ILE	CB-CA-C	-6.59	103.25	112.14
1	F	404	GLY	CA-C-N	6.53	126.44	119.85
1	F	404	GLY	C-N-CA	6.53	126.44	119.85
1	F	327	VAL	CB-CA-C	-6.24	103.41	110.96
1	F	488	VAL	N-CA-C	6.12	116.86	110.62
1	G	404	GLY	CA-C-N	6.01	127.35	119.84
1	G	404	GLY	C-N-CA	6.01	127.35	119.84
1	E	329	ASP	CA-C-N	5.97	126.53	120.38
1	E	329	ASP	C-N-CA	5.97	126.53	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	434	VAL	CB-CA-C	5.93	116.46	110.94
1	G	492	ASP	CA-C-N	5.79	128.26	120.50
1	G	492	ASP	C-N-CA	5.79	128.26	120.50
1	E	441	HIS	N-CA-C	-5.62	106.47	113.55
1	E	446	ILE	N-CA-C	5.60	113.41	107.76
1	E	200	VAL	N-CA-C	5.44	115.78	108.17
1	E	362	THR	CB-CA-C	-5.36	104.25	111.11
1	G	308	ARG	CA-C-N	5.17	124.87	119.64
1	G	308	ARG	C-N-CA	5.17	124.87	119.64
1	F	436	ASN	N-CA-C	5.14	119.53	113.16
1	G	327	VAL	N-CA-C	5.11	114.97	108.12
1	F	501	ILE	N-CA-C	-5.04	105.50	111.00
1	F	469	ARG	CG-CD-NE	-5.00	100.99	112.00

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	E	3301	0	3364	86	0
1	F	3295	0	3362	98	0
1	G	3296	0	3362	103	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
3	E	33	0	31	7	0
3	F	33	0	31	5	0
3	G	33	0	31	4	0
All	All	9994	0	10181	295	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 15.

All (295) 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:E:204:GLY:HA3	1:E:368:ALA:HB2	1.31	1.12
3:E:998:NHX:OAH	3:E:998:NHX:HAP	1.62	0.98
1:F:542:LEU:HD13	1:F:543:ARG:H	1.28	0.95
1:G:204:GLY:HA3	1:G:368:ALA:HB2	1.47	0.94
3:E:998:NHX:HAP	3:E:998:NHX:CAZ	2.01	0.88
1:F:340:LEU:O	1:F:344:THR:HB	1.75	0.87
1:G:410:LEU:HD11	1:G:447:PRO:HG2	1.57	0.85
1:F:204:GLY:HA3	1:F:368:ALA:HB2	1.60	0.84
1:E:462:GLU:O	1:E:463:ASP:HB2	1.79	0.81
1:F:461:GLU:HG3	1:F:461:GLU:O	1.81	0.79
1:G:542:LEU:HD13	1:G:543:ARG:H	1.47	0.77
1:F:233:LEU:HD13	1:F:237:VAL:HG12	1.65	0.75
1:E:410:LEU:HD11	1:E:447:PRO:HG2	1.68	0.75
3:F:998:NHX:CAZ	3:F:998:NHX:HAP	2.18	0.73
1:F:337:LYS:O	1:F:341:GLU:HG3	1.88	0.73
1:G:266:GLY:HA2	1:G:284:LEU:HD13	1.72	0.72
1:E:340:LEU:O	1:E:344:THR:HB	1.90	0.70
1:E:225:ILE:HG13	1:E:245:LEU:HD22	1.73	0.69
1:E:410:LEU:HD12	1:E:410:LEU:O	1.92	0.68
1:E:586:LEU:HD13	1:E:592:ILE:HG22	1.74	0.68
1:F:225:ILE:HG13	1:F:245:LEU:HD22	1.75	0.67
1:G:340:LEU:O	1:G:344:THR:HB	1.95	0.67
1:G:231:VAL:O	1:G:232:GLU:HB2	1.95	0.66
1:F:231:VAL:O	1:F:232:GLU:HB2	1.93	0.66
1:F:460:PRO:O	1:F:461:GLU:HG2	1.96	0.66
1:G:333:MET:HE1	1:G:356:GLU:HG3	1.78	0.65
1:F:225:ILE:HG13	1:F:245:LEU:CD2	2.26	0.65
1:G:410:LEU:O	1:G:410:LEU:HD12	1.96	0.65
1:F:358:ILE:HG23	1:F:398:ILE:HD11	1.78	0.65
1:F:344:THR:OG1	1:F:349:LEU:HD11	1.97	0.65
1:F:382:ALA:HB2	1:G:189:ILE:HD11	1.79	0.65
3:E:998:NHX:CAZ	3:E:998:NHX:CAP	2.76	0.65
1:E:542:LEU:HD13	1:E:543:ARG:H	1.61	0.64
1:E:231:VAL:O	1:E:232:GLU:HB2	1.96	0.64
1:F:453:LEU:HB2	3:F:998:NHX:HAB	1.78	0.64
1:F:383:ARG:HE	1:G:175:GLU:HB3	1.62	0.64
1:G:188:ARG:HG3	1:G:189:ILE:HG23	1.80	0.64
1:E:578:GLN:CD	1:E:578:GLN:H	2.05	0.64
1:G:542:LEU:HD13	1:G:543:ARG:N	2.13	0.64
1:F:586:LEU:O	1:F:590:GLU:HA	1.97	0.63
1:E:188:ARG:HG3	1:E:189:ILE:HG23	1.81	0.63
1:G:361:ARG:NH1	1:G:395:GLU:HG2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:VAL:HG13	1:G:255:CYS:HA	1.81	0.62
1:G:461:GLU:O	1:G:462:GLU:HB2	2.00	0.62
1:G:483:ARG:HD2	1:G:493:VAL:HG22	1.82	0.61
1:G:473:LEU:HD13	1:G:511:MET:HE1	1.82	0.61
1:E:434:VAL:HG22	1:E:567:ARG:NH2	2.15	0.61
1:E:578:GLN:HG3	1:E:601:LEU:HD23	1.82	0.61
1:E:179:PHE:CG	1:E:193:MET:HG3	2.36	0.60
1:F:462:GLU:CD	1:F:463:ASP:H	2.09	0.60
1:G:366:VAL:HG22	1:G:369:ASP:OD2	2.00	0.60
1:F:578:GLN:CD	1:F:578:GLN:H	2.08	0.60
1:G:586:LEU:HD13	1:G:592:ILE:HG22	1.84	0.60
1:E:220:VAL:HG13	1:E:255:CYS:HA	1.83	0.60
1:E:266:GLY:HA2	1:E:284:LEU:HD13	1.82	0.59
1:G:344:THR:OG1	1:G:349:LEU:HD11	2.02	0.59
1:F:483:ARG:HD2	1:F:493:VAL:HG22	1.83	0.59
1:G:397:ALA:O	1:G:401:VAL:HG23	2.03	0.58
1:F:460:PRO:HB3	1:F:462:GLU:HG3	1.86	0.58
1:E:442:ARG:HD3	1:E:593:GLU:OE2	2.03	0.58
1:E:461:GLU:H	1:E:462:GLU:HG3	1.69	0.57
1:E:462:GLU:CD	1:E:463:ASP:H	2.12	0.57
1:F:230:PHE:CE2	1:F:241:ARG:HB2	2.40	0.57
1:F:596:GLU:O	1:F:600:ILE:HG13	2.05	0.57
1:G:579:LEU:O	1:G:583:VAL:HG23	2.04	0.57
1:F:170:ILE:O	1:F:174:LYS:HG3	2.05	0.56
1:E:224:HIS:O	1:E:225:ILE:HD13	2.04	0.56
1:G:507:ILE:O	1:G:511:MET:HG3	2.05	0.56
1:F:407:ARG:HB3	1:F:410:LEU:HD13	1.87	0.56
1:F:307:ASN:C	1:F:309:PRO:HD3	2.30	0.56
1:F:445:ILE:HG23	1:F:445:ILE:O	2.06	0.56
1:G:220:VAL:HG22	1:G:221:PRO:HD2	1.86	0.56
1:E:194:PRO:HG3	1:E:324:LYS:HD3	1.87	0.55
1:G:258:PHE:CE2	1:G:260:ASP:HB2	2.42	0.55
1:E:362:THR:HG22	1:E:365:PHE:CE2	2.42	0.55
1:F:188:ARG:HG3	1:F:189:ILE:HG23	1.87	0.55
1:F:362:THR:N	1:F:363:PRO:HD3	2.22	0.55
1:G:257:VAL:HB	1:G:302:VAL:HG22	1.89	0.55
1:E:225:ILE:HG13	1:E:245:LEU:CD2	2.36	0.55
1:F:160:PHE:CE1	1:F:217:GLU:HG2	2.41	0.55
1:F:445:ILE:O	1:F:445:ILE:CG2	2.54	0.55
1:F:462:GLU:O	1:F:463:ASP:HB2	2.06	0.55
1:G:163:VAL:HG22	1:G:209:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:462:GLU:HB3	1:E:464:LYS:HE3	1.88	0.54
1:F:434:VAL:CG1	1:F:474:ASP:HB3	2.38	0.54
1:G:165:GLY:HA3	1:G:331:PRO:HB3	1.90	0.54
1:F:360:LYS:O	1:F:460:PRO:HG2	2.07	0.54
3:F:998:NHX:HABB	3:F:998:NHX:CAY	2.37	0.54
1:F:234:PHE:CD2	1:F:235:VAL:N	2.76	0.53
1:F:370:LEU:O	1:F:374:VAL:HG23	2.08	0.53
1:G:306:THR:HG21	1:G:312:LEU:HD11	1.90	0.53
3:E:998:NHX:HAA	3:E:998:NHX:CAY	2.39	0.53
1:E:195:LYS:HD3	1:E:320:GLY:O	2.08	0.53
1:E:434:VAL:CG1	1:E:474:ASP:HB3	2.39	0.53
1:F:230:PHE:HE2	1:F:241:ARG:HB2	1.74	0.52
1:G:582:ILE:O	1:G:586:LEU:HB2	2.10	0.52
1:E:192:ARG:O	1:E:192:ARG:HG3	2.08	0.52
1:G:362:THR:O	1:G:365:PHE:HB2	2.09	0.52
1:E:462:GLU:HB2	1:E:464:LYS:HG3	1.91	0.52
1:G:596:GLU:O	1:G:600:ILE:HG13	2.10	0.52
1:G:225:ILE:HG13	1:G:245:LEU:HD22	1.91	0.52
1:G:406:ALA:HB2	1:G:448:ARG:NH1	2.24	0.52
1:E:172:GLU:O	1:E:175:GLU:HG2	2.09	0.52
1:F:527:GLY:O	1:F:528:LYS:HB2	2.10	0.52
1:F:381:ALA:HA	1:F:386:ARG:NH2	2.25	0.51
1:G:242:VAL:HG12	1:G:290:GLU:HG3	1.93	0.51
1:E:253:ALA:HA	1:E:254:PRO:C	2.36	0.51
1:F:220:VAL:HG13	1:F:255:CYS:HA	1.90	0.51
1:G:285:ASN:HD22	1:G:288:LEU:HD12	1.76	0.51
1:E:177:VAL:HG13	1:E:218:ALA:HB2	1.92	0.51
1:G:198:LEU:HD11	1:G:306:THR:HG22	1.92	0.51
1:G:163:VAL:HG11	1:G:210:LEU:HD21	1.93	0.51
1:E:187:ASN:ND2	1:E:297:LYS:HB3	2.26	0.51
3:F:998:NHX:CAZ	3:F:998:NHX:CAP	2.87	0.50
1:E:527:GLY:O	1:E:528:LYS:HB2	2.12	0.50
1:F:427:HIS:O	1:F:431:SER:HB2	2.12	0.50
1:G:585:ILE:HG23	1:G:589:LYS:HD3	1.93	0.50
1:G:200:VAL:HG13	1:G:309:PRO:HG3	1.93	0.50
1:F:473:LEU:HD13	1:F:511:MET:HE1	1.92	0.50
1:F:397:ALA:O	1:F:401:VAL:HG23	2.12	0.50
1:G:233:LEU:HD13	1:G:237:VAL:HG12	1.94	0.50
1:E:306:THR:HG23	1:E:306:THR:O	2.10	0.49
1:E:410:LEU:HD12	1:E:410:LEU:C	2.37	0.49
1:G:307:ASN:C	1:G:309:PRO:HD3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:PHE:HE2	1:E:241:ARG:HB2	1.77	0.49
1:E:445:ILE:O	1:E:445:ILE:CG2	2.61	0.49
1:G:387:ASP:OD2	1:G:388:LYS:HG3	2.12	0.49
1:F:416:GLU:O	1:F:420:ILE:HG13	2.13	0.49
1:G:246:PHE:O	1:G:250:LYS:HG3	2.12	0.49
1:E:400:ARG:HA	1:E:404:GLY:O	2.13	0.49
1:G:380:LEU:HA	1:G:383:ARG:NH1	2.28	0.49
1:F:250:LYS:HA	1:F:300:ILE:HD11	1.94	0.48
1:E:242:VAL:HG12	1:E:290:GLU:HG3	1.95	0.48
1:E:170:ILE:O	1:E:174:LYS:HG3	2.12	0.48
1:E:445:ILE:O	1:E:445:ILE:HG23	2.14	0.48
1:G:360:LYS:HD3	1:G:460:PRO:O	2.13	0.48
1:F:175:GLU:HG3	1:F:176:VAL:N	2.28	0.48
1:F:524:LEU:N	1:F:524:LEU:HD12	2.28	0.48
1:G:594:GLY:O	1:G:597:LEU:HB3	2.13	0.48
1:F:234:PHE:HB3	1:F:237:VAL:CG2	2.43	0.48
1:G:220:VAL:CG1	1:G:255:CYS:HA	2.43	0.48
1:F:195:LYS:HD3	1:F:320:GLY:O	2.12	0.48
1:F:412:ILE:O	1:F:417:LYS:HE3	2.14	0.48
1:G:286:GLN:O	1:G:290:GLU:HG2	2.13	0.48
1:F:434:VAL:HG13	1:F:474:ASP:HB3	1.96	0.48
1:F:542:LEU:CD1	1:F:543:ARG:H	2.13	0.48
1:E:239:ALA:O	1:E:286:GLN:HG2	2.14	0.47
1:E:472:LEU:O	1:E:476:LEU:HB2	2.14	0.47
1:G:162:ASP:O	1:G:209:LEU:HD21	2.15	0.47
1:F:285:ASN:O	1:F:289:VAL:HG23	2.15	0.47
1:G:451:LYS:O	3:G:998:NHX:HAP	2.15	0.47
1:E:358:ILE:HG23	1:E:398:ILE:HD11	1.97	0.47
1:E:407:ARG:C	1:E:409:SER:H	2.23	0.47
1:G:230:PHE:CE2	1:G:241:ARG:HB2	2.50	0.47
1:G:578:GLN:H	1:G:578:GLN:CD	2.22	0.47
1:F:210:LEU:O	1:F:214:VAL:HG23	2.14	0.47
1:F:440:VAL:HG11	1:F:443:ILE:HD11	1.97	0.47
1:F:445:ILE:HD12	1:F:445:ILE:HA	1.67	0.47
1:G:476:LEU:CD2	1:G:504:ALA:HB1	2.45	0.46
1:F:434:VAL:HA	1:F:435:PRO:HD3	1.77	0.46
1:G:230:PHE:HE2	1:G:241:ARG:HB2	1.80	0.46
1:F:166:ALA:O	1:F:170:ILE:HG13	2.15	0.46
1:F:165:GLY:HA3	1:F:331:PRO:HB3	1.97	0.46
1:F:306:THR:HG21	1:F:312:LEU:HD11	1.96	0.46
1:F:231:VAL:O	1:F:232:GLU:CB	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:243:ARG:HG3	1:F:286:GLN:NE2	2.30	0.46
1:F:173:LEU:O	1:F:177:VAL:HG23	2.15	0.46
1:G:188:ARG:HG3	1:G:189:ILE:N	2.29	0.46
1:G:337:LYS:O	1:G:341:GLU:HG3	2.15	0.46
1:F:233:LEU:HD12	1:F:238:GLY:HA2	1.97	0.46
1:G:225:ILE:HG13	1:G:245:LEU:CD2	2.46	0.46
1:G:344:THR:HG1	1:G:349:LEU:HD11	1.79	0.46
1:G:461:GLU:O	1:G:462:GLU:CB	2.61	0.46
1:E:167:GLU:H	1:E:167:GLU:CD	2.24	0.46
1:E:362:THR:HB	1:E:365:PHE:CG	2.51	0.46
1:F:237:VAL:O	1:F:241:ARG:HG2	2.15	0.46
1:F:244:ASP:O	1:F:248:GLN:HG2	2.15	0.46
1:E:220:VAL:HG22	1:E:221:PRO:HD2	1.96	0.46
1:F:575:TYR:HA	1:F:578:GLN:OE1	2.15	0.46
1:F:362:THR:O	1:F:365:PHE:HB2	2.16	0.45
1:G:231:VAL:O	1:G:232:GLU:CB	2.64	0.45
1:E:362:THR:HB	1:E:365:PHE:CD2	2.51	0.45
1:E:444:SER:HB3	1:E:455:TYR:CE2	2.51	0.45
1:F:266:GLY:O	1:F:312:LEU:HA	2.15	0.45
1:E:453:LEU:HD21	3:E:998:NHX:HB	1.98	0.45
1:E:495:SER:HB2	3:E:998:NHX:HAK	1.97	0.45
1:F:332:ASP:O	1:F:336:ARG:HG3	2.16	0.45
1:E:445:ILE:HA	1:E:445:ILE:HD12	1.57	0.45
1:G:430:VAL:O	1:G:434:VAL:HB	2.17	0.45
1:G:575:TYR:O	1:G:578:GLN:HG2	2.16	0.45
1:G:445:ILE:HG23	1:G:445:ILE:O	2.17	0.45
1:F:195:LYS:HB3	1:F:294:PHE:CZ	2.51	0.45
1:G:234:PHE:CG	1:G:235:VAL:N	2.85	0.45
1:E:227:GLY:N	1:E:260:ASP:O	2.41	0.45
1:E:362:THR:O	1:E:365:PHE:HB2	2.17	0.45
1:E:420:ILE:HD13	1:E:453:LEU:HB3	1.99	0.45
3:E:998:NHX:NAT	3:E:998:NHX:HAS	2.32	0.45
1:G:335:GLY:O	1:G:339:ILE:HG13	2.16	0.45
1:E:175:GLU:HG3	1:E:176:VAL:N	2.31	0.45
1:E:230:PHE:CE2	1:E:241:ARG:HB2	2.52	0.44
1:G:472:LEU:O	1:G:476:LEU:HB2	2.16	0.44
1:G:401:VAL:O	1:G:401:VAL:HG12	2.18	0.44
1:E:231:VAL:O	1:E:232:GLU:CB	2.63	0.44
1:G:266:GLY:O	1:G:312:LEU:HA	2.17	0.44
1:E:462:GLU:CB	1:E:464:LYS:HE3	2.48	0.44
3:G:998:NHX:HAB	3:G:998:NHX:HBF	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:445:ILE:HA	1:G:445:ILE:HD12	1.49	0.44
1:G:422:TYR:CD2	1:G:583:VAL:HG21	2.53	0.44
1:F:399:ASP:CB	1:F:448:ARG:HH21	2.30	0.43
1:E:243:ARG:HG3	1:E:286:GLN:NE2	2.33	0.43
1:F:381:ALA:HB2	1:F:393:ASP:OD2	2.18	0.43
1:G:332:ASP:O	1:G:336:ARG:HG3	2.18	0.43
1:G:422:TYR:CE2	1:G:583:VAL:HG21	2.52	0.43
1:G:527:GLY:O	1:G:528:LYS:HB2	2.18	0.43
1:E:189:ILE:O	1:E:189:ILE:HG13	2.19	0.43
1:G:381:ALA:HA	1:G:386:ARG:NH2	2.32	0.43
1:E:521:LEU:HD23	1:E:521:LEU:HA	1.79	0.43
1:F:239:ALA:O	1:F:286:GLN:HG2	2.17	0.43
1:E:163:VAL:HG22	1:E:209:LEU:HG	1.99	0.43
1:F:220:VAL:HG22	1:F:221:PRO:HD2	2.00	0.43
1:E:352:ASP:C	1:E:352:ASP:OD1	2.61	0.43
1:F:242:VAL:HG12	1:F:290:GLU:HG3	2.00	0.43
1:G:285:ASN:O	1:G:289:VAL:HG23	2.19	0.43
1:E:366:VAL:HG22	1:E:369:ASP:OD2	2.19	0.43
1:E:226:SER:HB3	1:E:229:ASP:OD1	2.19	0.43
1:E:422:TYR:CD2	1:E:583:VAL:HG11	2.53	0.43
1:F:286:GLN:O	1:F:290:GLU:HG2	2.19	0.43
1:G:253:ALA:HA	1:G:254:PRO:C	2.44	0.43
1:G:448:ARG:O	1:G:452:ALA:HB3	2.17	0.43
1:G:319:PRO:HA	1:G:323:ASP:HB3	2.00	0.43
1:F:188:ARG:HG3	1:F:189:ILE:N	2.32	0.43
1:G:239:ALA:O	1:G:286:GLN:HG2	2.19	0.43
1:F:177:VAL:HG13	1:F:218:ALA:HB2	2.00	0.42
3:F:998:NHX:HAP	3:F:998:NHX:OAH	2.19	0.42
1:G:194:PRO:HG3	1:G:324:LYS:HD3	1.99	0.42
1:G:347:LYS:HA	1:G:348:PRO:HD3	1.86	0.42
1:G:362:THR:N	1:G:363:PRO:CD	2.82	0.42
1:E:380:LEU:HA	1:E:380:LEU:HD12	1.61	0.42
1:F:179:PHE:CG	1:F:193:MET:HG3	2.54	0.42
1:F:234:PHE:HB3	1:F:237:VAL:HG23	2.01	0.42
1:F:347:LYS:HA	1:F:348:PRO:HD3	1.75	0.42
1:G:215:ALA:HB2	1:G:256:ILE:HD12	2.00	0.42
1:E:434:VAL:HG13	1:E:474:ASP:HB3	2.01	0.42
1:G:392:LYS:O	1:G:396:GLU:HB2	2.19	0.42
1:G:407:ARG:C	1:G:409:SER:H	2.27	0.42
1:E:213:ALA:O	1:E:217:GLU:HB2	2.19	0.42
1:F:262:ILE:HG23	1:F:312:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:GLU:H	1:G:167:GLU:CD	2.26	0.42
1:E:347:LYS:HA	1:E:348:PRO:HD3	1.77	0.42
1:F:362:THR:HB	1:F:365:PHE:CG	2.54	0.42
1:F:160:PHE:HB3	1:F:170:ILE:HD13	2.02	0.42
1:F:406:ALA:HB2	1:F:448:ARG:NH1	2.34	0.42
1:F:448:ARG:O	1:F:452:ALA:HB3	2.19	0.42
1:G:489:VAL:HG22	1:G:576:ARG:CZ	2.50	0.42
1:F:460:PRO:O	1:F:461:GLU:CG	2.65	0.42
1:G:242:VAL:O	1:G:246:PHE:HD1	2.02	0.42
1:E:263:ASP:HB2	1:E:311:ILE:CG2	2.50	0.42
1:G:224:HIS:O	1:G:225:ILE:HD13	2.20	0.42
1:F:220:VAL:HG22	1:F:254:PRO:O	2.20	0.41
1:E:237:VAL:O	1:E:241:ARG:HG2	2.19	0.41
1:F:212:ARG:HG2	1:F:222:PHE:CE2	2.55	0.41
1:G:524:LEU:HD12	1:G:524:LEU:N	2.35	0.41
1:G:246:PHE:CG	1:G:290:GLU:HB3	2.55	0.41
1:E:335:GLY:O	1:E:339:ILE:HG13	2.20	0.41
1:F:472:LEU:HD23	1:F:472:LEU:HA	1.86	0.41
1:E:416:GLU:O	1:E:420:ILE:HG13	2.20	0.41
1:E:578:GLN:CD	1:E:578:GLN:N	2.77	0.41
1:F:194:PRO:HG2	1:F:324:LYS:HD3	2.02	0.41
1:F:586:LEU:HD13	1:F:592:ILE:HG22	2.03	0.41
1:G:177:VAL:HG11	1:G:217:GLU:HG3	2.03	0.41
1:G:420:ILE:HG23	3:G:998:NHX:HAA	2.02	0.41
1:G:586:LEU:O	1:G:590:GLU:HA	2.21	0.41
1:E:406:ALA:HA	1:E:448:ARG:HD2	2.01	0.41
1:F:319:PRO:HA	1:F:323:ASP:HB3	2.03	0.41
1:G:205:THR:HG22	1:G:366:VAL:HB	2.02	0.41
1:G:315:ALA:HA	1:G:318:ARG:NE	2.36	0.41
1:G:420:ILE:HG12	3:G:998:NHX:HAAB	2.02	0.41
1:G:338:LYS:O	1:G:342:ILE:HG13	2.21	0.41
1:G:476:LEU:HD21	1:G:504:ALA:HB1	2.01	0.41
1:E:444:SER:HB3	1:E:455:TYR:CZ	2.55	0.41
1:E:582:ILE:O	1:E:586:LEU:HB2	2.21	0.41
1:F:198:LEU:HD11	1:F:306:THR:HG22	2.01	0.41
1:F:575:TYR:O	1:F:578:GLN:HG2	2.20	0.41
1:G:420:ILE:HD13	1:G:453:LEU:HB3	2.03	0.41
1:F:444:SER:HB3	1:F:455:TYR:CZ	2.56	0.41
1:G:210:LEU:O	1:G:214:VAL:HG23	2.21	0.41
1:E:194:PRO:HG3	1:E:324:LYS:CD	2.51	0.40
1:E:542:LEU:HD13	1:E:543:ARG:N	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:THR:HG23	1:F:306:THR:O	2.19	0.40
1:E:198:LEU:O	1:E:325:LYS:HA	2.22	0.40
1:E:297:LYS:C	1:E:299:GLY:H	2.27	0.40
1:F:460:PRO:HB3	1:F:462:GLU:CG	2.50	0.40
1:E:179:PHE:CD1	1:E:193:MET:HG3	2.56	0.40
1:E:179:PHE:CD2	1:E:193:MET:HG3	2.56	0.40
1:G:438:GLU:HA	1:G:439:PRO:HD3	1.96	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	E	355/465 (76%)	329 (93%)	25 (7%)	1 (0%)	36	58
1	F	420/465 (90%)	390 (93%)	25 (6%)	5 (1%)	10	23
1	G	375/465 (81%)	347 (92%)	25 (7%)	3 (1%)	16	34
All	All	1150/1395 (82%)	1066 (93%)	75 (6%)	9 (1%)	16	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	463	ASP
1	G	462	GLU
1	F	235	VAL
1	F	450	TYR
1	G	450	TYR
1	F	451	LYS
1	F	232	GLU
1	F	460	PRO
1	G	278	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	348/381 (91%)	328 (94%)	20 (6%)	18	40
1	F	348/381 (91%)	331 (95%)	17 (5%)	22	47
1	G	348/381 (91%)	330 (95%)	18 (5%)	21	44
All	All	1044/1143 (91%)	989 (95%)	55 (5%)	20	43

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	220	VAL
1	E	287	LEU
1	E	311	ILE
1	E	333	MET
1	E	344	THR
1	E	380	LEU
1	E	434	VAL
1	E	445	ILE
1	E	448	ARG
1	E	462	GLU
1	E	476	LEU
1	E	479	LEU
1	E	483	ARG
1	E	519	GLU
1	E	524	LEU
1	E	542	LEU
1	E	578	GLN
1	E	583	VAL
1	E	591	THR
1	E	592	ILE
1	F	220	VAL
1	F	311	ILE
1	F	333	MET
1	F	344	THR
1	F	418	ARG
1	F	434	VAL

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Mol	Chain	Res	Type
1	F	445	ILE
1	F	448	ARG
1	F	462	GLU
1	F	473	LEU
1	F	493	VAL
1	F	518	SER
1	F	519	GLU
1	F	542	LEU
1	F	578	GLN
1	F	591	THR
1	F	592	ILE
1	G	220	VAL
1	G	311	ILE
1	G	333	MET
1	G	344	THR
1	G	418	ARG
1	G	434	VAL
1	G	445	ILE
1	G	473	LEU
1	G	476	LEU
1	G	493	VAL
1	G	510	ASN
1	G	518	SER
1	G	519	GLU
1	G	542	LEU
1	G	578	GLN
1	G	591	THR
1	G	592	ILE
1	G	599	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	187	ASN
1	E	277	HIS
1	E	343	HIS
1	F	277	HIS
1	F	286	GLN
1	F	514	GLN
1	G	277	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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$
3	NHX	E	998	2	34,34,34	0.89	0	44,46,46	1.45	4 (9%)
3	NHX	F	998	2	34,34,34	0.94	0	44,46,46	1.43	4 (9%)
3	NHX	G	998	2	34,34,34	1.25	1 (2%)	44,46,46	1.27	4 (9%)

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
3	NHX	E	998	2	-	5/34/34/34	0/2/2/2
3	NHX	F	998	2	-	9/34/34/34	0/2/2/2
3	NHX	G	998	2	-	0/34/34/34	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	998	NHX	CAX-NAT	-4.33	1.27	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	998	NHX	OAI-NAT-CAX	-5.05	112.33	119.79
3	F	998	NHX	CBF-CAQ-CAX	-4.84	102.83	112.33
3	F	998	NHX	OAI-NAT-CAX	-4.14	113.68	119.79
3	E	998	NHX	CBF-CAQ-CAX	-4.11	104.26	112.33
3	F	998	NHX	CBG-NAV-CAY	-3.96	113.14	121.65
3	G	998	NHX	OAI-NAT-CAX	-3.96	113.94	119.79
3	E	998	NHX	CBG-NAV-CAY	-3.47	114.19	121.65
3	G	998	NHX	CBF-CAS-CBD	-3.31	108.72	115.60
3	G	998	NHX	CBF-CAQ-CAX	-3.24	105.97	112.33
3	G	998	NHX	CAQ-CBF-CAY	-2.27	106.49	109.71
3	F	998	NHX	CAQ-CBF-CAY	-2.21	106.57	109.71
3	E	998	NHX	CAQ-CBF-CAY	-2.03	106.82	109.71

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	998	NHX	OAH-CAZ-CBG-CAR
3	F	998	NHX	N-CAZ-CBG-CAR
3	F	998	NHX	CBG-CAR-CBA-CAP
3	F	998	NHX	CBG-CAR-CBA-CAL
3	E	998	NHX	CBG-CAR-CBA-CAL
3	E	998	NHX	CBG-CAR-CBA-CAP
3	F	998	NHX	OAH-CAZ-CBG-NAV
3	E	998	NHX	NAD-C-CA-N
3	F	998	NHX	N-CAZ-CBG-NAV
3	E	998	NHX	CBF-CAQ-CAX-OAF
3	E	998	NHX	O-C-CA-N
3	F	998	NHX	O-C-CA-CB
3	F	998	NHX	NAD-C-CA-N
3	F	998	NHX	NAD-C-CA-CB

There are no ring outliers.

3 monomers are involved in 16 short contacts:

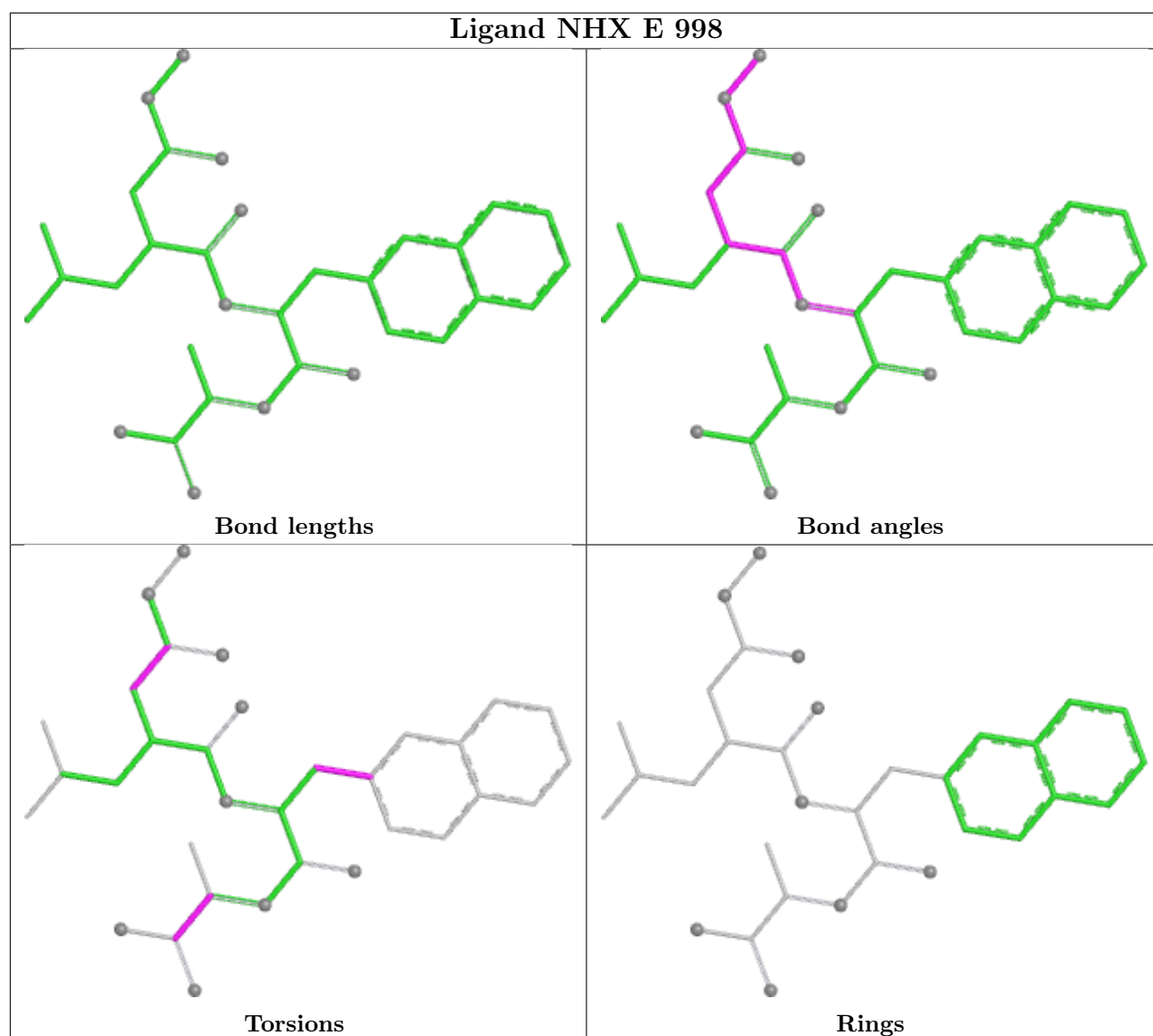
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	998	NHX	7	0

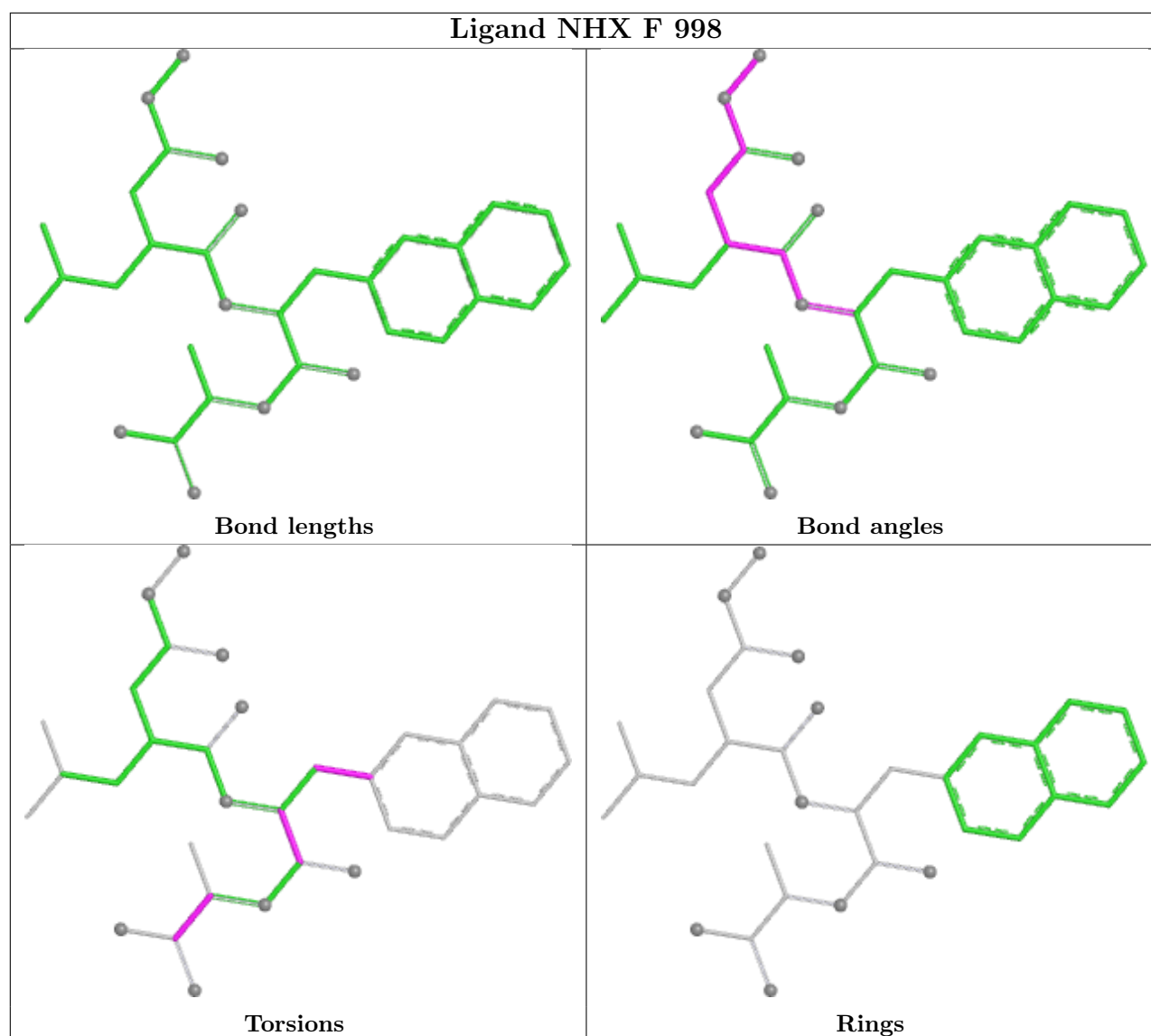
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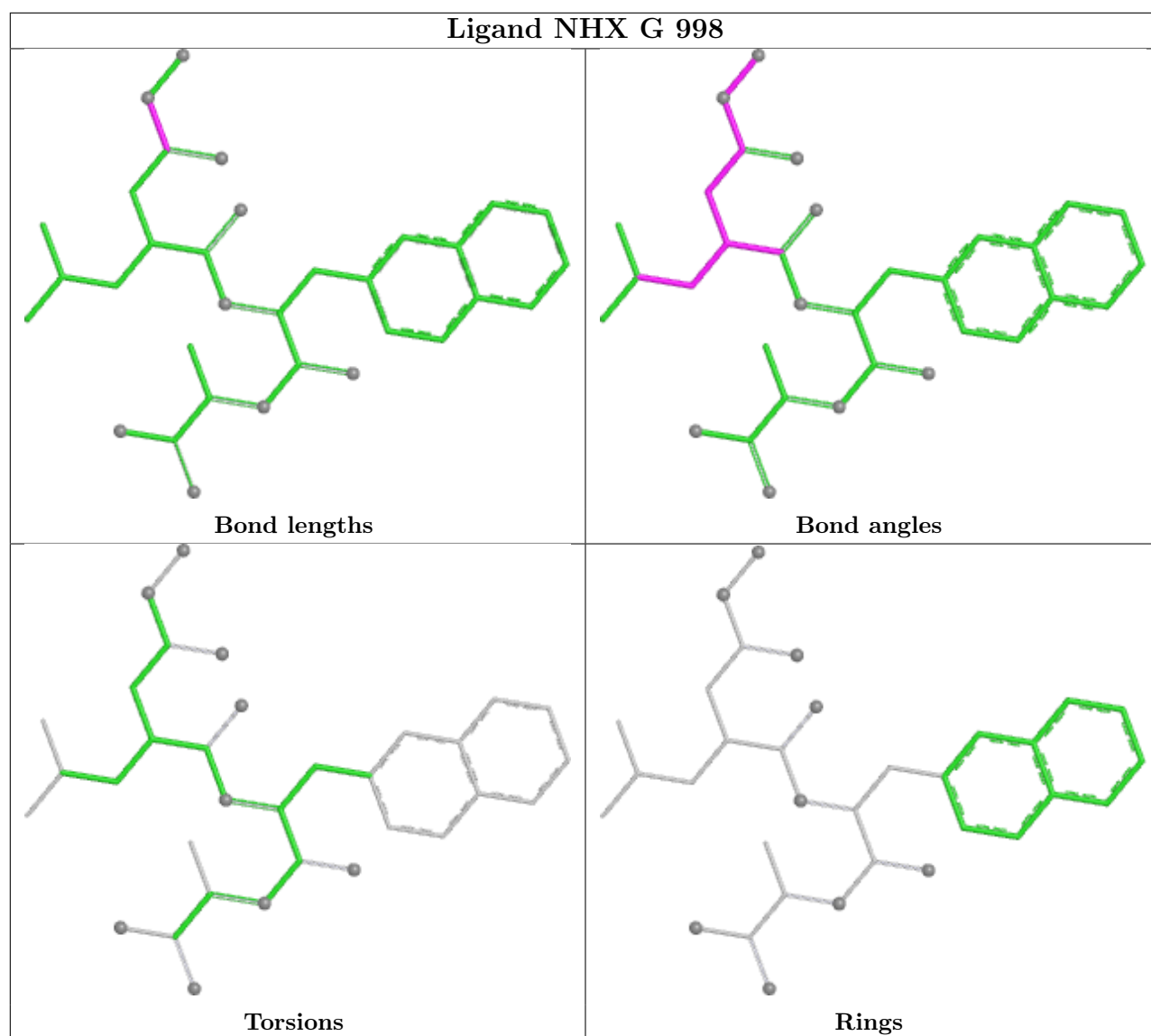
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	998	NHX	5	0
3	G	998	NHX	4	0

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	E	427/465 (91%)	0.14	20 (4%) 36 30	35, 78, 200, 347	0
1	F	426/465 (91%)	0.20	12 (2%) 55 49	46, 105, 229, 324	0
1	G	426/465 (91%)	0.35	23 (5%) 31 26	46, 124, 289, 360	0
All	All	1279/1395 (91%)	0.23	55 (4%) 40 34	35, 99, 258, 360	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	230	PHE	5.1
1	G	284	LEU	3.9
1	G	287	LEU	3.6
1	F	230	PHE	3.2
1	E	204	GLY	3.2
1	G	189	ILE	3.0
1	G	389	ILE	3.0
1	G	317	LEU	2.9
1	G	309	PRO	2.9
1	E	309	PRO	2.8
1	F	389	ILE	2.8
1	F	265	VAL	2.8
1	G	230	PHE	2.8
1	G	313	ASP	2.7
1	E	231	VAL	2.7
1	G	316	LEU	2.6
1	G	176	VAL	2.6
1	G	543	ARG	2.6
1	G	315	ALA	2.6
1	G	401	VAL	2.6
1	G	245	LEU	2.6
1	E	234	PHE	2.5
1	E	267	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	262	ILE	2.4
1	F	309	PRO	2.4
1	G	180	LEU	2.4
1	F	198	LEU	2.4
1	F	542	LEU	2.4
1	F	316	LEU	2.4
1	G	259	ILE	2.4
1	E	317	LEU	2.3
1	G	542	LEU	2.3
1	G	206	GLY	2.3
1	F	235	VAL	2.3
1	E	232	GLU	2.3
1	G	278	ASP	2.3
1	E	541	ARG	2.3
1	F	262	ILE	2.2
1	E	239	ALA	2.2
1	G	225	ILE	2.2
1	F	205	THR	2.2
1	E	235	VAL	2.2
1	E	233	LEU	2.2
1	E	188	ARG	2.1
1	F	552	LYS	2.1
1	E	222	PHE	2.1
1	E	181	LYS	2.1
1	E	200	VAL	2.1
1	E	254	PRO	2.1
1	E	542	LEU	2.1
1	G	200	VAL	2.1
1	E	245	LEU	2.1
1	F	543	ARG	2.0
1	E	227	GLY	2.0
1	G	242	VAL	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](#)

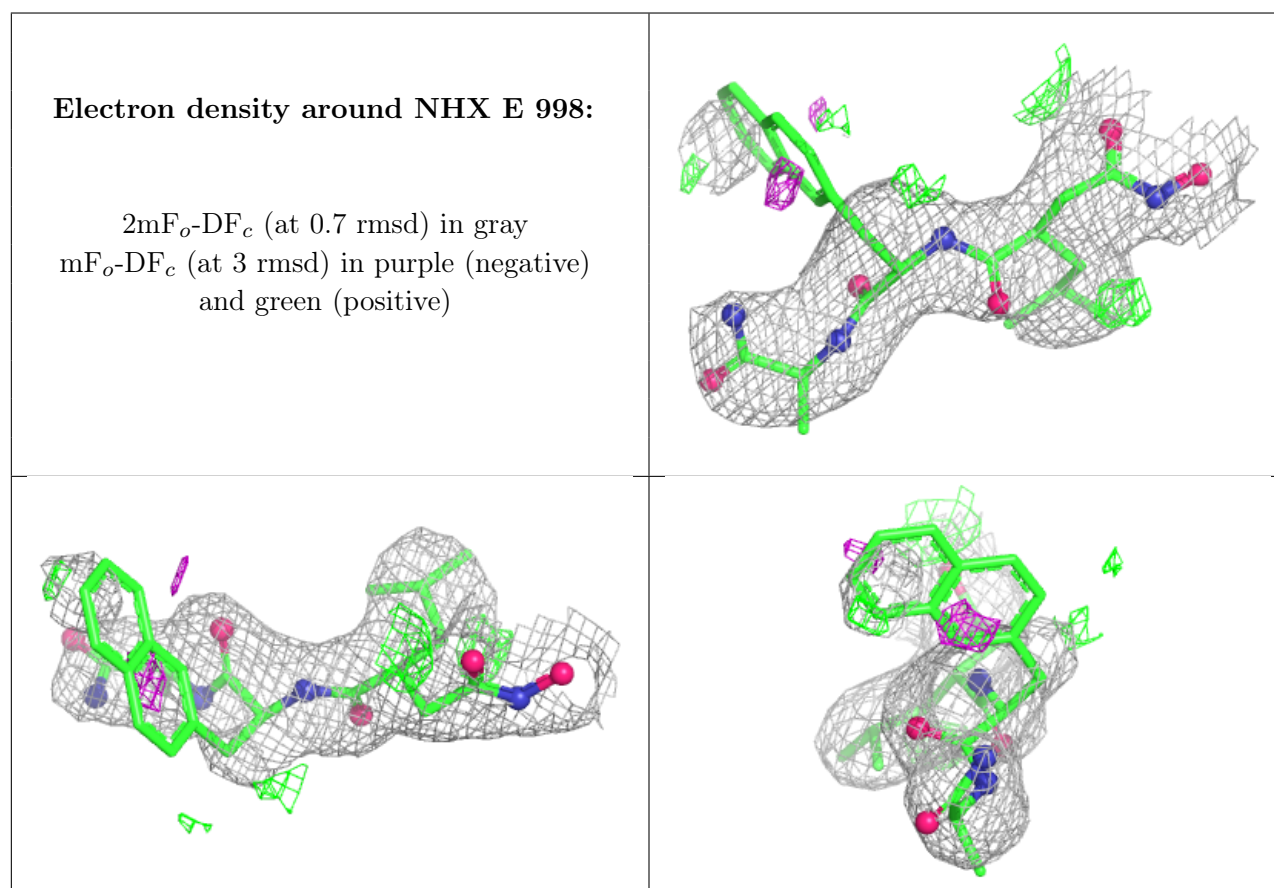
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

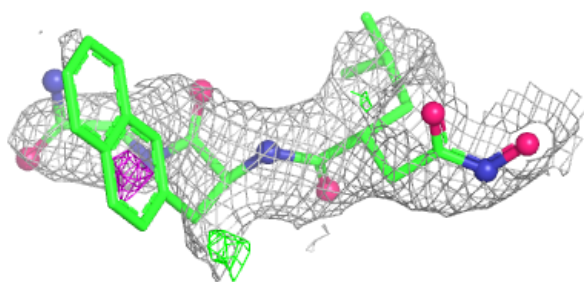
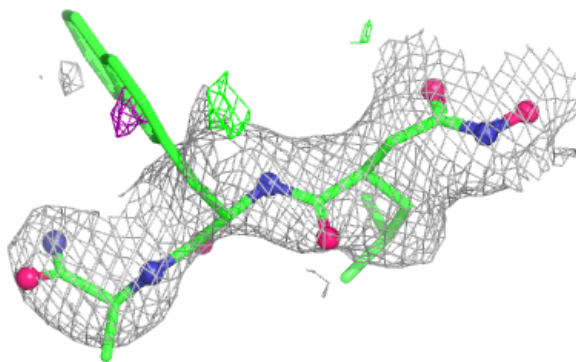
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NHX	E	998	33/33	0.89	0.15	43,90,166,169	0
3	NHX	F	998	33/33	0.89	0.15	65,138,183,184	0
3	NHX	G	998	33/33	0.91	0.11	53,87,112,115	0
2	ZN	E	996	1/1	0.99	0.03	55,55,55,55	0
2	ZN	F	996	1/1	0.99	0.03	70,70,70,70	0
2	ZN	G	996	1/1	0.99	0.04	65,65,65,65	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.



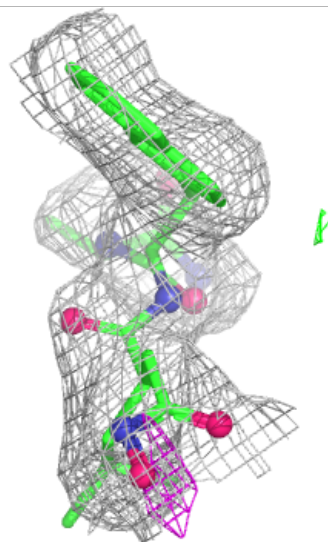
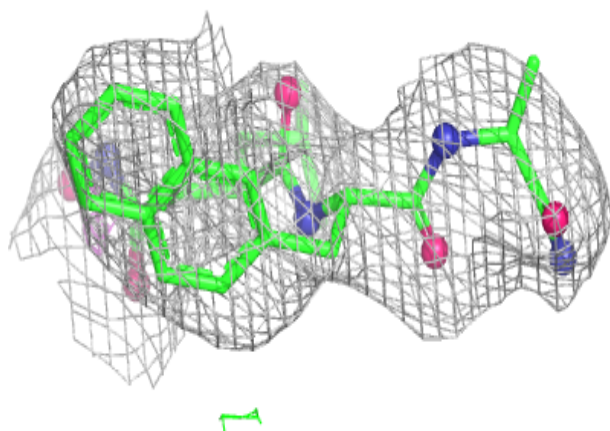
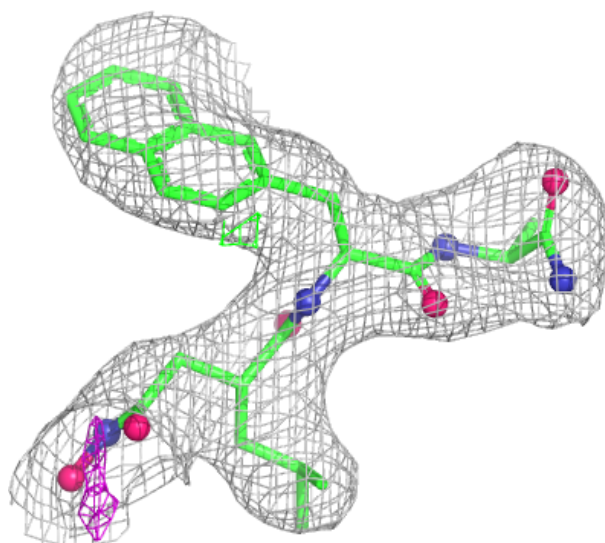
Electron density around NHX F 998:

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



Electron density around NHX G 998:

$2mF_o-DF_c$ (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.