



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2026 – 04:43 PM JST

PDB ID : 27XP / pdb_000027xp
Title : Crystal structure of monoalkyl phthalate hydrolase from *Rhodococcus* sp. EG-5 n complex with Paranitrophenyl butyrate (PNPB)
Authors : Aggarwal, S.; Jangid, K.; Singh, S.; Sharma, A.K.; Kumar, P.
Deposited on : 2026-06-16
Resolution : 2.80 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	:	1.8.5 (274361), CSD as541be (2020)
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

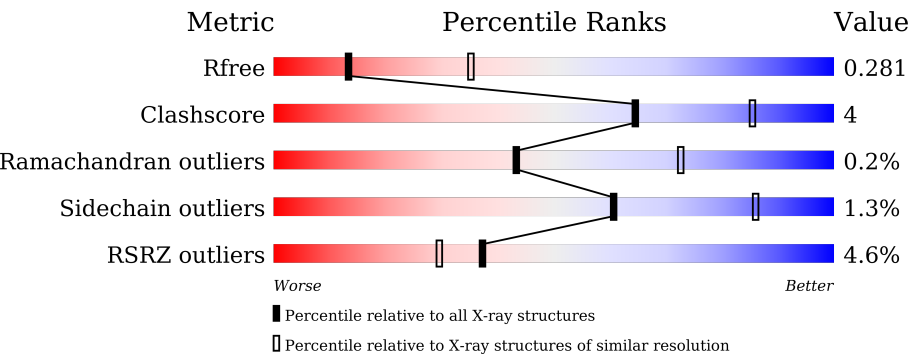
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	303	<div><div>2%</div><div>87%8%</div><div>••</div></div>
1	B	303	<div><div>2%</div><div>88%7%5%</div><div></div></div>
1	C	303	<div><div>6%</div><div>85%10%5%</div><div>•</div></div>
1	D	303	<div><div>2%</div><div>86%11%</div><div>•</div></div>
1	E	303	<div><div>3%</div><div>86%8%</div><div>••</div></div>
1	F	303	<div><div>3%</div><div>86%9%5%</div><div>•</div></div>

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Mol	Chain	Length	Quality of chain
1	G	303	 5% 81% 11% • 6%
1	H	303	 5% 88% 7% •
1	I	303	 5% 88% 8% • •
1	J	303	 9% 89% 6% • •

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	NPO	F	401	-	-	X	-

2 Entry composition

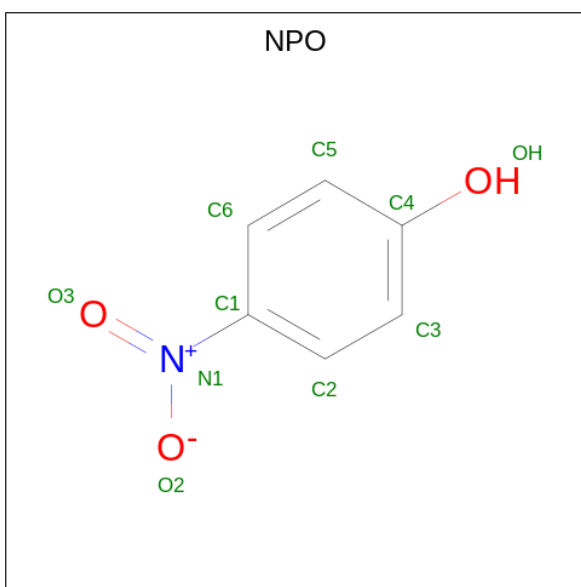
There are 3 unique types of molecules in this entry. The entry contains 44212 atoms, of which 22023 are hydrogens and 0 are deuteriums.

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 Mono-ethylhexylphthalate hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	292	Total	C	H	N	O	S	60	0	0
			4439	1418	2209	383	423	6			
1	B	289	Total	C	H	N	O	S	59	0	0
			4405	1408	2196	379	416	6			
1	C	289	Total	C	H	N	O	S	59	0	0
			4405	1408	2196	379	416	6			
1	D	292	Total	C	H	N	O	S	59	0	0
			4461	1427	2222	385	421	6			
1	E	291	Total	C	H	N	O	S	60	0	0
			4431	1416	2207	381	421	6			
1	F	289	Total	C	H	N	O	S	58	0	0
			4415	1410	2202	382	415	6			
1	G	284	Total	C	H	N	O	S	58	0	0
			4312	1374	2152	372	408	6			
1	H	291	Total	C	H	N	O	S	59	0	0
			4429	1416	2204	381	422	6			
1	I	293	Total	C	H	N	O	S	59	0	0
			4471	1430	2227	386	422	6			
1	J	291	Total	C	H	N	O	S	60	0	0
			4425	1414	2203	381	421	6			

- Molecule 2 is P-NITROPHENOL (CCD ID: NPO) (formula: C₆H₅NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	H	N	O	1	0
			15	6	5	1	3		

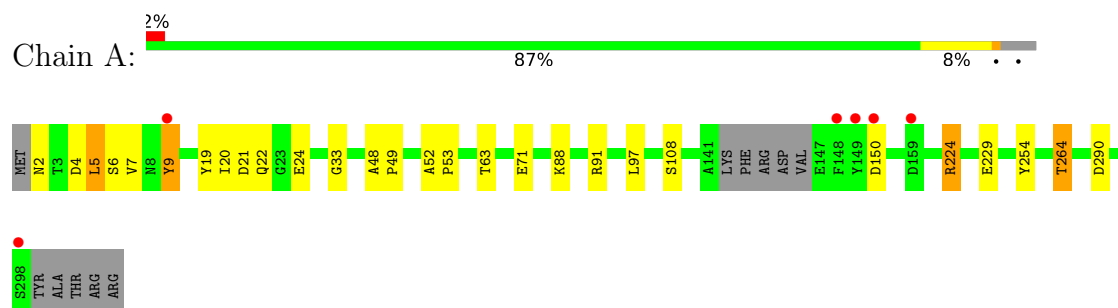
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			1	1		
3	F	1	Total	O	0	0
			1	1		
3	H	1	Total	O	0	0
			1	1		
3	I	1	Total	O	0	0
			1	1		

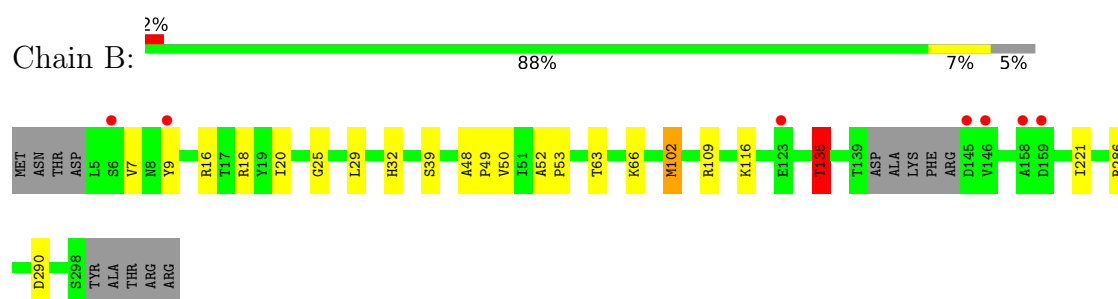
3 Residue-property plots [i](#)

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.

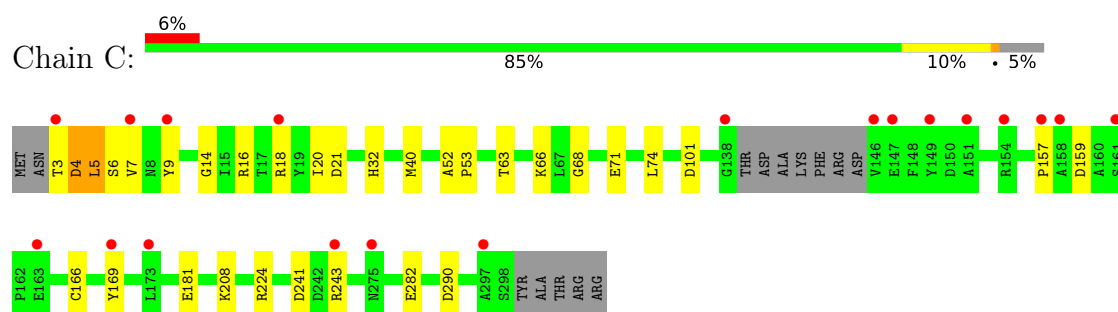
- Molecule 1: Mono-ethylhexylphthalate hydrolase



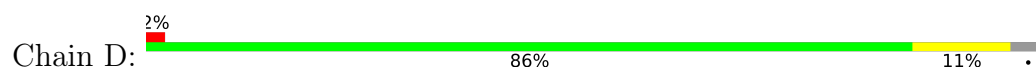
- Molecule 1: Mono-ethylhexylphthalate hydrolase

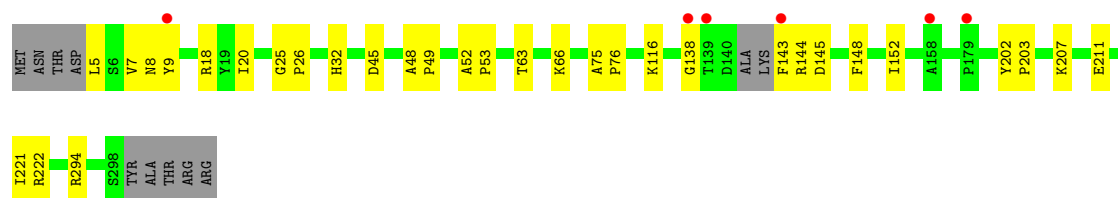


- Molecule 1: Mono-ethylhexylphthalate hydrolase

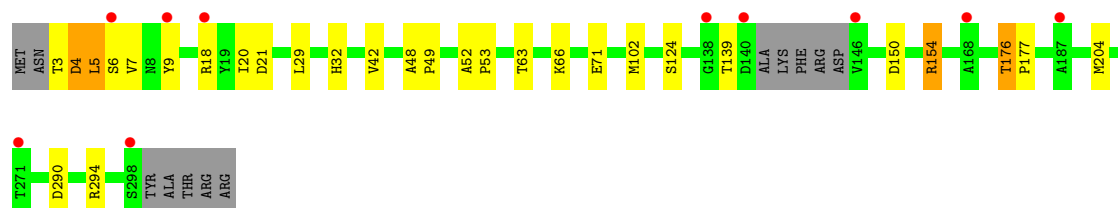
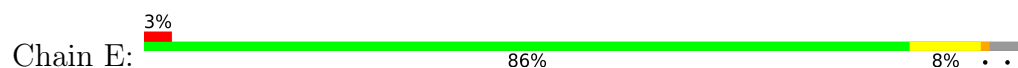


- Molecule 1: Mono-ethylhexylphthalate hydrolase

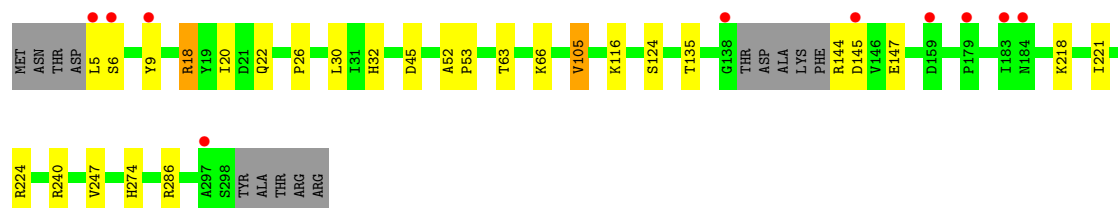
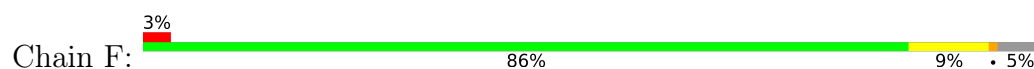




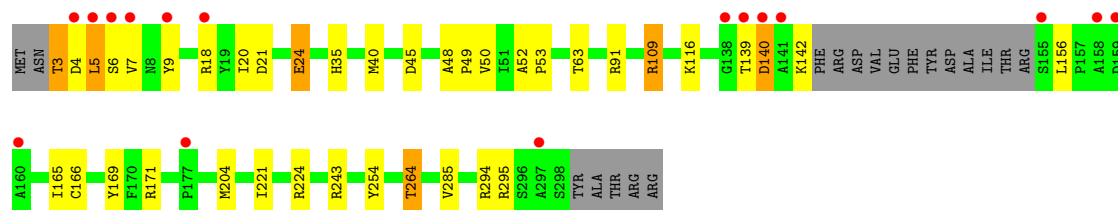
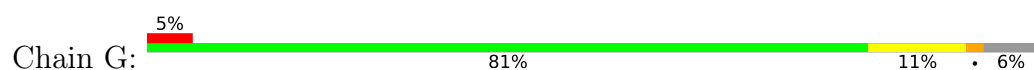
• Molecule 1: Mono-ethylhexylphthalate hydrolase



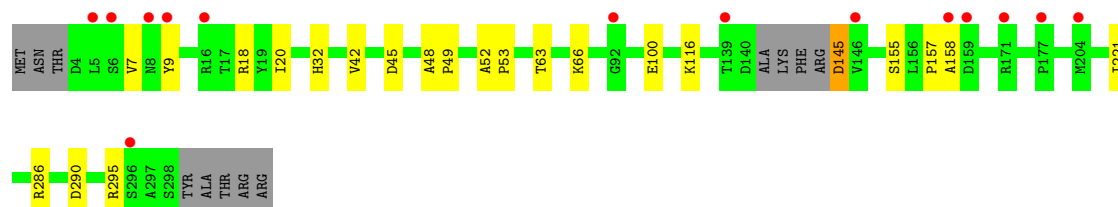
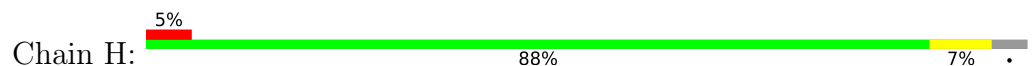
• Molecule 1: Mono-ethylhexylphthalate hydrolase



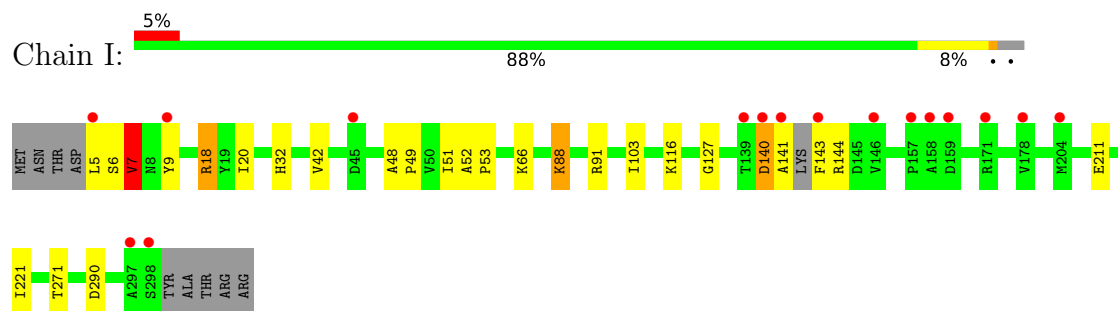
• Molecule 1: Mono-ethylhexylphthalate hydrolase



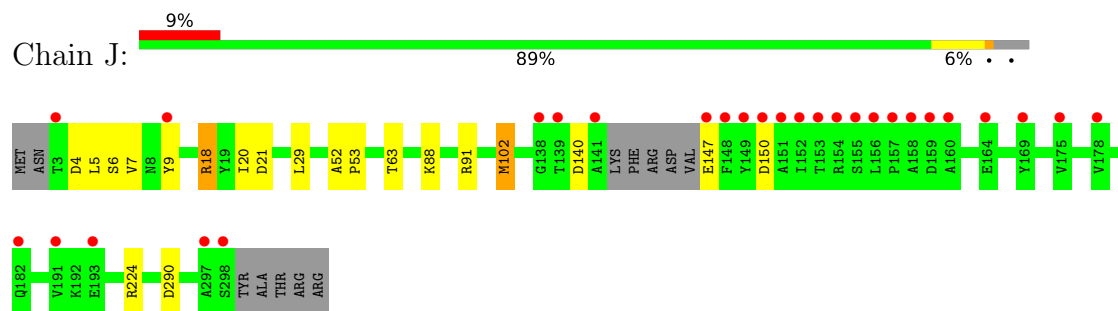
• Molecule 1: Mono-ethylhexylphthalate hydrolase



- Molecule 1: Mono-ethylhexylphthalate hydrolase



- Molecule 1: Mono-ethylhexylphthalate hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	176.31Å 244.89Å 192.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.29 – 2.80 24.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.29-2.80) 99.7 (24.29-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.272 , 0.294 0.260 , 0.281	Depositor DCC
R_{free} test set	5006 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	44212	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: NPO

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	0.67	0/2279	1.00	4/3097 (0.1%)
1	B	0.67	0/2258	1.00	3/3068 (0.1%)
1	C	0.69	0/2258	1.00	4/3068 (0.1%)
1	D	0.68	0/2289	0.98	3/3109 (0.1%)
1	E	0.68	0/2273	0.99	3/3089 (0.1%)
1	F	0.67	0/2262	0.97	0/3072
1	G	0.70	0/2207	1.01	5/2998 (0.2%)
1	H	0.65	0/2274	0.98	2/3090 (0.1%)
1	I	0.65	0/2294	0.99	3/3116 (0.1%)
1	J	0.65	0/2271	0.96	3/3086 (0.1%)
All	All	0.67	0/22665	0.99	30/30793 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	E	0	1
1	F	0	1
1	G	0	4
1	I	0	1
1	J	0	2
All	All	0	13

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	145	ASP	CA-CB-CG	7.22	119.82	112.60
1	A	150	ASP	CA-CB-CG	6.94	119.54	112.60
1	G	3	THR	CA-CB-OG1	-6.87	99.30	109.60
1	A	264	THR	CA-CB-OG1	-6.67	99.60	109.60
1	J	290	ASP	CA-CB-CG	6.35	118.95	112.60
1	E	204	MET	CG-SD-CE	6.18	114.50	100.90
1	C	208	LYS	CB-CG-CD	6.16	125.46	111.30
1	E	290	ASP	CA-CB-CG	6.03	118.63	112.60
1	G	204	MET	CG-SD-CE	5.99	114.07	100.90
1	C	290	ASP	CA-CB-CG	5.93	118.53	112.60
1	I	140	ASP	CA-CB-CG	5.77	118.37	112.60
1	B	135	THR	OG1-CB-CG2	5.71	120.72	109.30
1	I	290	ASP	CA-CB-CG	5.60	118.20	112.60
1	G	24	GLU	CB-CG-CD	5.58	122.08	112.60
1	C	282	GLU	CG-CD-OE2	-5.51	105.72	118.40
1	J	102	MET	CG-SD-CE	-5.51	88.78	100.90
1	G	140	ASP	CB-CA-C	5.37	118.34	109.70
1	D	145	ASP	CA-CB-CG	5.34	117.94	112.60
1	G	264	THR	CA-CB-OG1	-5.24	101.74	109.60
1	E	139	THR	OG1-CB-CG2	-5.24	98.82	109.30
1	C	101	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	102	MET	CG-SD-CE	-5.19	89.48	100.90
1	D	143	PHE	CA-CB-CG	5.18	118.98	113.80
1	I	88	LYS	CB-CG-CD	5.17	123.19	111.30
1	A	290	ASP	CA-CB-CG	5.16	117.76	112.60
1	J	140	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	290	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	2	ASN	CB-CA-C	5.13	119.85	110.10
1	D	294	ARG	CA-CB-CG	5.12	124.34	114.10
1	H	290	ASP	CA-CB-CG	5.05	117.65	112.60

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	B	286	ARG	Sidechain
1	C	16	ARG	Sidechain
1	C	224	ARG	Sidechain
1	E	154	ARG	Sidechain
1	F	224	ARG	Sidechain
1	G	109	ARG	Sidechain
1	G	224	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	G	243	ARG	Sidechain
1	G	91	ARG	Sidechain
1	I	91	ARG	Sidechain
1	J	18	ARG	Sidechain
1	J	224	ARG	Sidechain

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	2230	2209	2199	17	0
1	B	2209	2196	2186	12	0
1	C	2209	2196	2186	22	0
1	D	2239	2222	2212	19	0
1	E	2224	2207	2197	19	0
1	F	2213	2202	2192	26	0
1	G	2160	2152	2142	30	0
1	H	2225	2204	2194	13	0
1	I	2244	2227	2217	14	0
1	J	2222	2203	2193	14	0
2	F	10	5	5	5	0
3	B	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
All	All	22189	22023	21923	174	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 4.

All (174) 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:A:254:TYR:CE1	1:A:264:THR:HG22	1.88	1.08
1:B:109:ARG:HA	1:B:135:THR:HG21	1.37	1.06
1:G:254:TYR:CE1	1:G:264:THR:HG22	1.90	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:254:TYR:HE1	1:G:264:THR:HG22	1.27	0.97
1:A:254:TYR:HE1	1:A:264:THR:HG22	1.30	0.93
1:F:30:LEU:HD23	1:F:105:VAL:CG1	2.03	0.88
1:H:9:TYR:CZ	1:H:18:ARG:HG3	2.08	0.88
1:D:9:TYR:CZ	1:D:18:ARG:HG3	2.09	0.87
1:C:9:TYR:CZ	1:C:18:ARG:HG3	2.13	0.83
1:B:9:TYR:CZ	1:B:18:ARG:HG3	2.13	0.83
1:E:6:SER:OG	1:E:21:ASP:O	1.97	0.82
1:E:9:TYR:CZ	1:E:18:ARG:HG3	2.16	0.80
1:D:138:GLY:HA2	1:D:222:ARG:NH2	1.97	0.79
1:D:26:PRO:HD3	1:G:5:LEU:HA	1.64	0.79
1:D:148:PHE:O	1:D:152:ILE:HD12	1.84	0.78
1:F:30:LEU:HD23	1:F:105:VAL:HG11	1.65	0.78
1:F:240:ARG:O	1:F:247:VAL:HG21	1.83	0.77
1:G:9:TYR:CZ	1:G:18:ARG:HG3	2.20	0.77
1:G:50:VAL:HG13	1:G:285:VAL:HG22	1.66	0.76
1:A:254:TYR:CE1	1:A:264:THR:CG2	2.71	0.74
1:G:156:LEU:HD13	1:G:165:ILE:HD13	1.69	0.71
1:C:40:MET:HA	1:C:40:MET:HE2	1.74	0.69
1:G:40:MET:HE1	1:G:166:CYS:HA	1.75	0.68
1:F:30:LEU:HD23	1:F:105:VAL:HG13	1.73	0.68
1:A:33:GLY:HA3	1:A:108:SER:OG	1.94	0.68
1:F:9:TYR:CZ	1:F:18:ARG:HG3	2.27	0.68
1:E:176:THR:HG22	1:E:177:PRO:HD2	1.76	0.67
1:A:4:ASP:O	1:A:7:VAL:HG13	1.93	0.67
1:A:6:SER:HB2	1:A:21:ASP:O	1.94	0.67
1:G:254:TYR:CE1	1:G:264:THR:CG2	2.73	0.67
1:J:9:TYR:CZ	1:J:18:ARG:HG3	2.30	0.66
1:I:9:TYR:CZ	1:I:18:ARG:HG3	2.30	0.66
1:E:3:THR:O	1:E:4:ASP:OD2	2.15	0.65
1:F:30:LEU:CD2	1:F:105:VAL:HG11	2.26	0.65
1:C:40:MET:HE1	1:C:166:CYS:HA	1.80	0.64
1:H:9:TYR:CE2	1:H:18:ARG:HG3	2.34	0.63
1:B:29:LEU:HD22	1:B:102:MET:HE1	1.80	0.62
1:C:40:MET:HE3	1:C:169:TYR:HB2	1.82	0.60
1:D:9:TYR:CE2	1:D:18:ARG:HG3	2.36	0.60
1:I:144:ARG:NH1	1:I:211:GLU:OE2	2.34	0.60
1:C:3:THR:O	1:C:4:ASP:HB2	2.02	0.59
1:G:40:MET:HA	1:G:40:MET:HE2	1.82	0.59
1:G:6:SER:HB3	1:G:21:ASP:O	2.02	0.59
1:B:9:TYR:CE2	1:B:18:ARG:HG3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:7:VAL:HG12	1:J:20:ILE:HG12	1.85	0.58
1:D:144:ARG:NH1	1:D:211:GLU:OE2	2.37	0.58
1:G:3:THR:OG1	1:G:4:ASP:N	2.35	0.58
1:E:3:THR:O	1:E:4:ASP:CG	2.47	0.57
1:C:9:TYR:CE2	1:C:18:ARG:HG3	2.39	0.57
1:I:103:ILE:HD12	1:I:127:GLY:HA3	1.86	0.57
1:E:9:TYR:CE2	1:E:18:ARG:HG3	2.40	0.57
1:G:40:MET:HE3	1:G:169:TYR:HB2	1.86	0.57
1:C:6:SER:HB3	1:C:21:ASP:O	2.06	0.55
1:B:29:LEU:HD22	1:B:102:MET:CE	2.37	0.55
1:E:294:ARG:HD3	1:H:286:ARG:HD3	1.88	0.55
1:J:6:SER:HB3	1:J:21:ASP:O	2.07	0.55
1:A:52:ALA:HB3	1:A:53:PRO:HD3	1.90	0.54
1:E:52:ALA:HB3	1:E:53:PRO:HD3	1.90	0.54
1:C:40:MET:HE2	1:C:40:MET:CA	2.35	0.54
1:I:52:ALA:HB3	1:I:53:PRO:HD3	1.90	0.54
1:F:274:HIS:NE2	2:F:401:NPO:H5	2.23	0.53
1:A:7:VAL:HG12	1:A:20:ILE:HG12	1.88	0.53
1:G:35:HIS:HD2	1:G:109:ARG:HE	1.56	0.53
1:B:52:ALA:HB3	1:B:53:PRO:HD3	1.91	0.53
1:C:52:ALA:HB3	1:C:53:PRO:HD3	1.91	0.53
1:D:25:GLY:HA2	1:G:4:ASP:O	2.09	0.53
1:D:7:VAL:O	1:D:8:ASN:ND2	2.42	0.53
1:G:52:ALA:HB3	1:G:53:PRO:HD3	1.91	0.53
1:A:9:TYR:OH	1:A:71:GLU:HB3	2.09	0.52
1:H:52:ALA:HB3	1:H:53:PRO:HD3	1.91	0.52
1:F:144:ARG:HD2	1:F:147:GLU:HG3	1.92	0.52
1:G:5:LEU:O	1:G:6:SER:HB2	2.08	0.52
1:A:33:GLY:HA3	1:A:108:SER:HG	1.75	0.52
1:B:109:ARG:CA	1:B:135:THR:HG21	2.25	0.52
1:I:6:SER:O	1:I:7:VAL:O	2.27	0.52
1:D:52:ALA:HB3	1:D:53:PRO:HD3	1.92	0.51
1:C:5:LEU:O	1:C:6:SER:HB2	2.09	0.51
1:G:9:TYR:CE2	1:G:18:ARG:HG3	2.46	0.51
1:G:40:MET:HE3	1:G:169:TYR:CB	2.41	0.51
1:J:52:ALA:HB3	1:J:53:PRO:HD3	1.92	0.50
1:F:52:ALA:HB3	1:F:53:PRO:HD3	1.94	0.50
1:C:241:ASP:HB3	1:C:243:ARG:HH12	1.76	0.50
1:F:274:HIS:CE1	2:F:401:NPO:H5	2.47	0.50
1:I:5:LEU:HD23	1:I:20:ILE:HG21	1.94	0.49
1:E:29:LEU:HD22	1:E:102:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:TYR:CE2	1:A:97:LEU:HD21	2.48	0.49
1:E:7:VAL:HG12	1:E:20:ILE:HG12	1.93	0.49
1:G:140:ASP:C	1:G:142:LYS:H	2.21	0.49
1:A:20:ILE:HB	1:A:63:THR:HG22	1.96	0.48
1:A:88:LYS:HE3	1:H:157:PRO:HA	1.95	0.48
1:J:147:GLU:HG2	1:J:150:ASP:HB2	1.93	0.48
1:J:29:LEU:HD22	1:J:102:MET:CE	2.43	0.48
1:C:20:ILE:HB	1:C:63:THR:HG22	1.96	0.48
1:C:40:MET:HE3	1:C:169:TYR:CB	2.43	0.48
1:I:5:LEU:HD21	1:I:51:ILE:HG21	1.96	0.48
1:J:5:LEU:O	1:J:6:SER:HB2	2.12	0.47
1:E:150:ASP:O	1:E:154:ARG:HG2	2.13	0.47
1:F:9:TYR:CE2	1:F:18:ARG:HG3	2.50	0.47
1:J:20:ILE:HB	1:J:63:THR:HG22	1.97	0.47
1:D:5:LEU:HG	1:D:7:VAL:HG13	1.97	0.47
1:F:135:THR:H	2:F:401:NPO:H3	1.80	0.47
1:B:16:ARG:NH2	1:C:14:GLY:O	2.47	0.47
1:F:286:ARG:HD2	1:G:294:ARG:HD3	1.96	0.47
1:I:18:ARG:C	1:I:18:ARG:HE	2.23	0.47
1:J:9:TYR:CZ	1:J:18:ARG:CG	2.96	0.47
1:G:7:VAL:HG22	1:G:20:ILE:HG12	1.96	0.46
1:E:294:ARG:HD3	1:H:286:ARG:CD	2.44	0.46
1:C:157:PRO:HB2	1:C:159:ASP:OD1	2.14	0.46
1:F:5:LEU:HD13	1:F:20:ILE:HD13	1.98	0.46
1:F:18:ARG:HE	1:F:18:ARG:C	2.24	0.46
1:F:30:LEU:HA	1:F:105:VAL:HG13	1.96	0.46
1:G:20:ILE:HB	1:G:63:THR:HG22	1.99	0.45
1:J:29:LEU:HD22	1:J:102:MET:HE1	1.98	0.45
1:C:3:THR:O	1:C:4:ASP:CB	2.64	0.45
1:C:7:VAL:HG22	1:C:20:ILE:HG12	1.97	0.45
1:B:20:ILE:HB	1:B:63:THR:HG22	1.99	0.45
1:H:157:PRO:O	1:H:158:ALA:HB3	2.17	0.45
1:D:20:ILE:HB	1:D:63:THR:HG22	1.98	0.44
1:F:6:SER:OG	1:F:22:GLN:CD	2.61	0.44
1:E:3:THR:O	1:E:4:ASP:CB	2.65	0.44
1:F:116:LYS:HD3	1:F:221:ILE:HD11	1.98	0.44
1:G:139:THR:O	1:G:140:ASP:C	2.59	0.44
1:I:9:TYR:CE2	1:I:18:ARG:HG3	2.53	0.44
1:J:88:LYS:HA	1:J:91:ARG:HH11	1.83	0.44
1:C:18:ARG:HD2	1:C:71:GLU:OE1	2.18	0.43
1:E:29:LEU:HD22	1:E:102:MET:HE1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:ILE:HB	1:H:63:THR:HG22	1.99	0.43
1:H:48:ALA:N	1:H:49:PRO:CD	2.82	0.43
1:I:116:LYS:HD3	1:I:221:ILE:HD11	2.00	0.43
1:J:9:TYR:CE2	1:J:18:ARG:HG3	2.53	0.43
1:F:135:THR:N	2:F:401:NPO:H3	2.33	0.43
1:H:116:LYS:HD3	1:H:221:ILE:HD11	2.01	0.43
1:G:116:LYS:HD3	1:G:221:ILE:HD11	2.01	0.43
1:A:91:ARG:HH21	1:H:155:SER:HB3	1.83	0.42
1:D:148:PHE:O	1:D:152:ILE:CD1	2.63	0.42
1:B:48:ALA:N	1:B:49:PRO:CD	2.82	0.42
1:C:5:LEU:HD23	1:F:26:PRO:HG2	2.01	0.42
1:E:48:ALA:N	1:E:49:PRO:CD	2.83	0.42
1:F:32:HIS:CE1	1:F:66:LYS:HE2	2.54	0.42
1:F:286:ARG:CD	1:G:294:ARG:HD3	2.48	0.42
1:D:26:PRO:HG3	1:G:5:LEU:HD23	2.00	0.42
1:D:116:LYS:HD3	1:D:221:ILE:HD11	2.02	0.42
1:C:32:HIS:CE1	1:C:66:LYS:HE2	2.54	0.42
1:G:9:TYR:OH	1:G:18:ARG:HG3	2.20	0.42
1:D:5:LEU:HD21	1:D:45:ASP:OD1	2.20	0.42
1:G:45:ASP:OD1	1:G:45:ASP:N	2.52	0.42
1:A:5:LEU:HB3	1:A:22:GLN:NE2	2.34	0.42
1:A:48:ALA:N	1:A:49:PRO:CD	2.83	0.42
1:C:5:LEU:HA	1:F:26:PRO:HD3	2.01	0.42
1:D:48:ALA:N	1:D:49:PRO:CD	2.83	0.42
1:H:18:ARG:NH2	1:H:45:ASP:OD1	2.53	0.42
1:G:140:ASP:C	1:G:142:LYS:N	2.76	0.42
1:E:18:ARG:HD3	1:E:71:GLU:OE1	2.21	0.41
1:E:20:ILE:HB	1:E:63:THR:HG22	2.02	0.41
1:J:147:GLU:CG	1:J:150:ASP:HB2	2.50	0.41
1:A:224:ARG:O	1:A:229:GLU:HB2	2.20	0.41
1:H:32:HIS:CE1	1:H:66:LYS:HE2	2.54	0.41
1:B:32:HIS:CE1	1:B:66:LYS:HE2	2.55	0.41
1:I:9:TYR:OH	1:I:18:ARG:HG3	2.20	0.41
1:F:145:ASP:OD2	1:F:218:LYS:NZ	2.45	0.41
1:E:5:LEU:O	1:E:6:SER:HB3	2.19	0.41
1:F:20:ILE:HB	1:F:63:THR:HG22	2.03	0.41
1:F:274:HIS:HE2	2:F:401:NPO:H5	1.86	0.41
1:G:48:ALA:N	1:G:49:PRO:CD	2.84	0.41
1:C:68:GLY:HA2	1:C:74:LEU:HA	2.03	0.41
1:I:32:HIS:CE1	1:I:66:LYS:HE2	2.56	0.41
1:D:32:HIS:CE1	1:D:66:LYS:HE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:HIS:CE1	1:E:66:LYS:HE2	2.56	0.40
1:J:4:ASP:O	1:J:7:VAL:HG13	2.21	0.40
1:B:116:LYS:HD3	1:B:221:ILE:HD11	2.03	0.40
1:D:75:ALA:HA	1:D:76:PRO:HD3	1.97	0.40
1:D:202:TYR:HB3	1:D:203:PRO:HD3	2.03	0.40
1:I:141:ALA:HB3	1:I:143:PHE:CE1	2.57	0.40
1:I:48:ALA:N	1:I:49:PRO:CD	2.85	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	288/303 (95%)	281 (98%)	6 (2%)	1 (0%)	36	66
1	B	285/303 (94%)	277 (97%)	7 (2%)	1 (0%)	30	60
1	C	285/303 (94%)	276 (97%)	7 (2%)	2 (1%)	18	47
1	D	288/303 (95%)	281 (98%)	7 (2%)	0	100	100
1	E	287/303 (95%)	279 (97%)	6 (2%)	2 (1%)	18	47
1	F	285/303 (94%)	277 (97%)	8 (3%)	0	100	100
1	G	280/303 (92%)	272 (97%)	8 (3%)	0	100	100
1	H	287/303 (95%)	279 (97%)	8 (3%)	0	100	100
1	I	289/303 (95%)	280 (97%)	8 (3%)	1 (0%)	36	66
1	J	287/303 (95%)	279 (97%)	8 (3%)	0	100	100
All	All	2861/3030 (94%)	2781 (97%)	73 (3%)	7 (0%)	43	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	C	5	LEU
1	E	4	ASP
1	E	5	LEU
1	I	7	VAL
1	B	25	GLY
1	C	4	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/241 (96%)	229 (99%)	2 (1%)	70	89
1	B	229/241 (95%)	225 (98%)	4 (2%)	53	83
1	C	229/241 (95%)	228 (100%)	1 (0%)	84	94
1	D	232/241 (96%)	231 (100%)	1 (0%)	84	94
1	E	231/241 (96%)	228 (99%)	3 (1%)	61	86
1	F	229/241 (95%)	225 (98%)	4 (2%)	53	83
1	G	224/241 (93%)	220 (98%)	4 (2%)	51	82
1	H	231/241 (96%)	226 (98%)	5 (2%)	45	78
1	I	232/241 (96%)	226 (97%)	6 (3%)	40	75
1	J	230/241 (95%)	230 (100%)	0	100	100
All	All	2298/2410 (95%)	2268 (99%)	30 (1%)	61	86

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	24	GLU
1	B	7	VAL
1	B	39	SER
1	B	50	VAL
1	B	135	THR
1	C	181	GLU

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Mol	Chain	Res	Type
1	D	207	LYS
1	E	42	VAL
1	E	124	SER
1	E	176	THR
1	F	18	ARG
1	F	45	ASP
1	F	105	VAL
1	F	124	SER
1	G	5	LEU
1	G	24	GLU
1	G	171	ARG
1	G	295	ARG
1	H	7	VAL
1	H	42	VAL
1	H	100	GLU
1	H	145	ASP
1	H	295	ARG
1	I	7	VAL
1	I	18	ARG
1	I	42	VAL
1	I	88	LYS
1	I	140	ASP
1	I	271	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	GLN
1	C	22	GLN
1	D	8	ASN
1	E	255	GLN
1	G	255	GLN
1	I	22	GLN
1	I	78	HIS
1	J	8	ASN
1	J	255	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	NPO	F	401	-	9,10,10	0.38	0	11,13,13	1.20	0

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	NPO	F	401	-	-	2/2/4/4	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

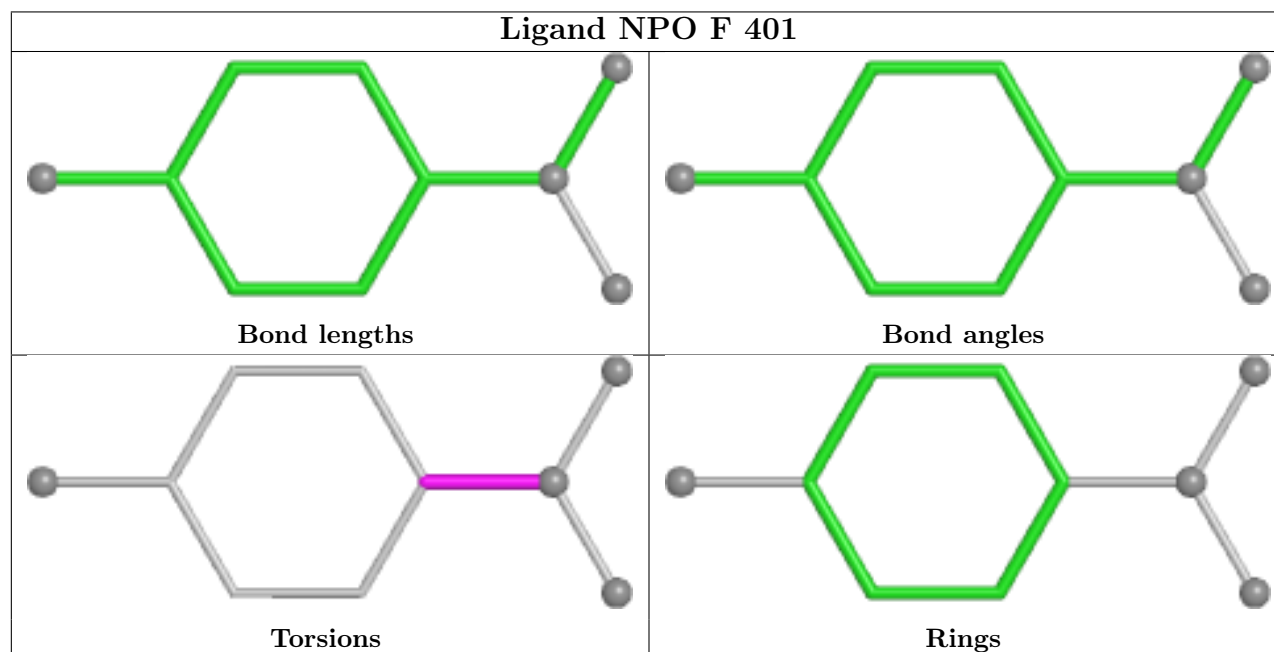
Mol	Chain	Res	Type	Atoms
2	F	401	NPO	C2-C1-N1-O3
2	F	401	NPO	C6-C1-N1-O3

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	NPO	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [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	292/303 (96%)	0.43	6 (2%) 63 54	22, 30, 42, 52	0
1	B	289/303 (95%)	0.36	7 (2%) 59 49	21, 29, 37, 47	0
1	C	289/303 (95%)	0.47	19 (6%) 24 18	21, 29, 42, 56	0
1	D	292/303 (96%)	0.28	6 (2%) 63 54	20, 27, 40, 51	0
1	E	291/303 (96%)	0.37	10 (3%) 48 39	21, 29, 42, 51	0
1	F	289/303 (95%)	0.32	10 (3%) 47 38	20, 27, 39, 52	0
1	G	284/303 (93%)	0.45	16 (5%) 30 23	21, 29, 40, 55	0
1	H	291/303 (96%)	0.43	14 (4%) 35 28	21, 30, 42, 55	0
1	I	293/303 (96%)	0.57	16 (5%) 30 23	25, 34, 42, 53	0
1	J	291/303 (96%)	0.66	28 (9%) 13 10	23, 34, 56, 76	0
All	All	2901/3030 (95%)	0.43	132 (4%) 37 29	20, 30, 43, 76	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	153	THR	5.4
1	C	173	LEU	4.7
1	J	151	ALA	4.6
1	C	146	VAL	4.4
1	J	150	ASP	4.4
1	J	9	TYR	4.3
1	J	149	TYR	4.3
1	E	146	VAL	4.2
1	J	155	SER	4.1
1	I	298	SER	4.0
1	J	148	PHE	4.0
1	C	147	GLU	3.8
1	G	9	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	158	ALA	3.8
1	J	156	LEU	3.8
1	J	154	ARG	3.7
1	D	143	PHE	3.6
1	H	171	ARG	3.6
1	H	139	THR	3.6
1	J	3	THR	3.5
1	G	177	PRO	3.5
1	B	6	SER	3.4
1	F	9	TYR	3.4
1	G	138	GLY	3.3
1	F	5	LEU	3.3
1	C	9	TYR	3.2
1	J	169	TYR	3.2
1	C	3	THR	3.2
1	A	298	SER	3.2
1	J	298	SER	3.2
1	I	5	LEU	3.1
1	A	150	ASP	3.1
1	H	159	ASP	3.1
1	I	139	THR	3.1
1	H	6	SER	3.1
1	I	159	ASP	3.1
1	H	177	PRO	3.0
1	I	141	ALA	3.0
1	I	143	PHE	3.0
1	A	149	TYR	3.0
1	F	6	SER	3.0
1	H	158	ALA	2.9
1	F	159	ASP	2.9
1	E	271	THR	2.9
1	G	158	ALA	2.9
1	A	9	TYR	2.8
1	C	154	ARG	2.8
1	J	152	ILE	2.8
1	E	140	ASP	2.8
1	F	138	GLY	2.8
1	C	151	ALA	2.8
1	C	297	ALA	2.7
1	D	158	ALA	2.7
1	D	139	THR	2.7
1	D	138	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	193	GLU	2.6
1	E	168	ALA	2.6
1	J	141	ALA	2.6
1	J	297	ALA	2.6
1	C	157	PRO	2.6
1	D	179	PRO	2.6
1	H	5	LEU	2.6
1	I	178	VAL	2.6
1	I	140	ASP	2.6
1	J	159	ASP	2.6
1	E	187	ALA	2.5
1	I	297	ALA	2.5
1	C	275	ASN	2.5
1	F	179	PRO	2.5
1	F	183	ILE	2.5
1	H	9	TYR	2.5
1	H	146	VAL	2.5
1	G	297	ALA	2.5
1	F	184	ASN	2.5
1	H	296	SER	2.5
1	J	175	VAL	2.5
1	C	138	GLY	2.5
1	G	4	ASP	2.4
1	C	149	TYR	2.4
1	D	9	TYR	2.4
1	I	9	TYR	2.4
1	G	139	THR	2.4
1	E	6	SER	2.4
1	B	158	ALA	2.4
1	J	160	ALA	2.4
1	G	140	ASP	2.4
1	G	160	ALA	2.4
1	J	164	GLU	2.4
1	A	159	ASP	2.3
1	C	169	TYR	2.3
1	E	18	ARG	2.3
1	J	158	ALA	2.3
1	J	182	GLN	2.3
1	B	123	GLU	2.3
1	G	155	SER	2.3
1	J	147	GLU	2.2
1	F	145	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	159	ASP	2.2
1	B	146	VAL	2.2
1	G	6	SER	2.2
1	H	16	ARG	2.2
1	E	9	TYR	2.2
1	C	158	ALA	2.2
1	C	7	VAL	2.2
1	G	7	VAL	2.2
1	I	146	VAL	2.2
1	E	298	SER	2.2
1	G	141	ALA	2.2
1	C	243	ARG	2.2
1	I	171	ARG	2.2
1	B	159	ASP	2.1
1	J	178	VAL	2.1
1	I	45	ASP	2.1
1	H	92	GLY	2.1
1	J	191	VAL	2.1
1	E	138	GLY	2.1
1	C	18	ARG	2.1
1	G	18	ARG	2.1
1	G	5	LEU	2.1
1	B	145	ASP	2.1
1	B	9	TYR	2.1
1	I	204	MET	2.0
1	H	8	ASN	2.0
1	J	138	GLY	2.0
1	F	297	ALA	2.0
1	C	163	GLU	2.0
1	H	204	MET	2.0
1	C	161	SER	2.0
1	I	157	PRO	2.0
1	J	157	PRO	2.0
1	A	148	PHE	2.0
1	J	139	THR	2.0

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

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

6.3 Carbohydrates [i](#)

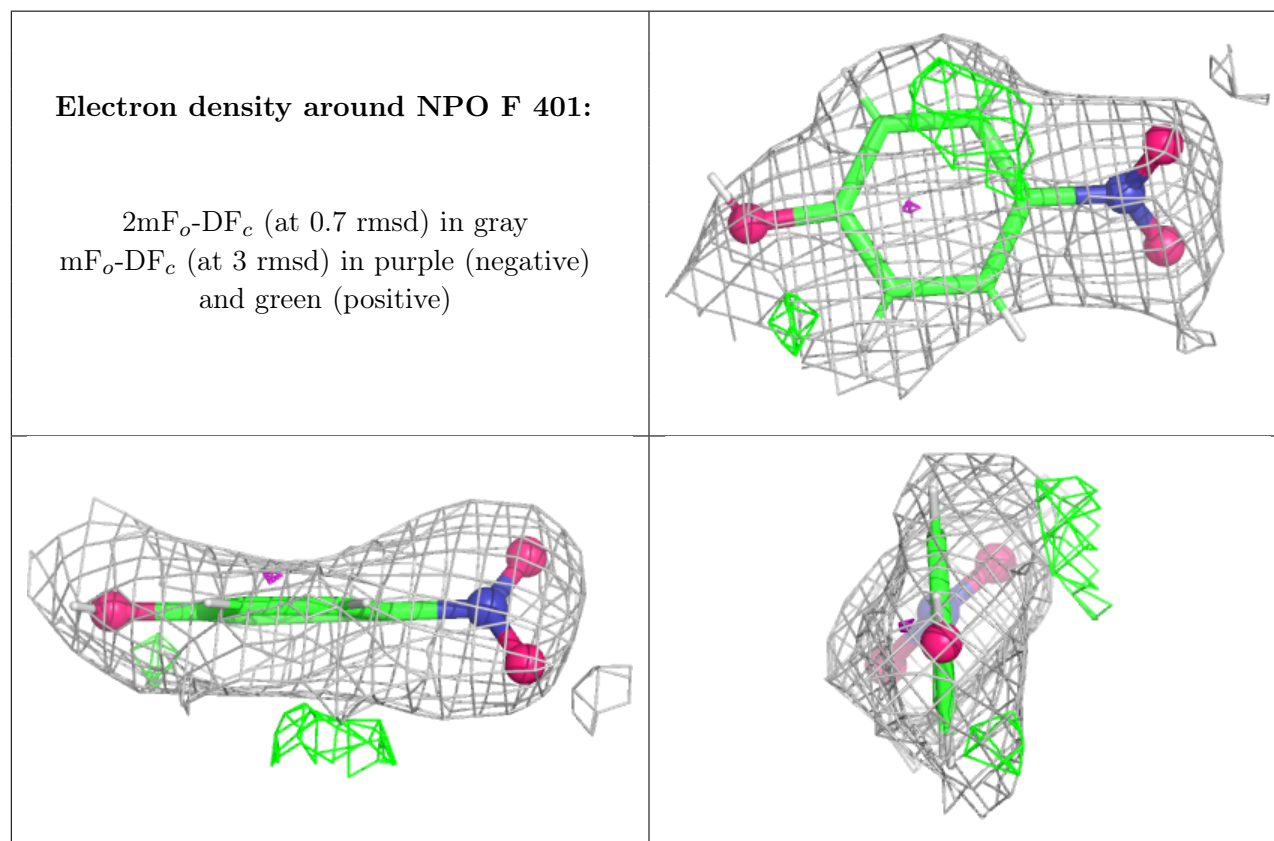
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
2	NPO	F	401	10/10	0.91	0.15	26,27,29,30	1

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.



6.5 Other polymers [i](#)

There are no such residues in this entry.