Full wwPDB X-ray Structure Validation Report (i)

Aug 24, 2026 – 10:15 AM JST

PDB ID	:	27CJ / pdb_000027cj
Title	:	Crystal structure of Cysteine-dependent hydrolase (CsdH) from Rhodococcus opacus in complex with degradation products of diethyl phthalate
Authors	:	Aggarwal, S.; Singh, S.; Aggarwal, D.; Sharma, A.K.; Kumar, P.
Deposited on	:	2026-05-26
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

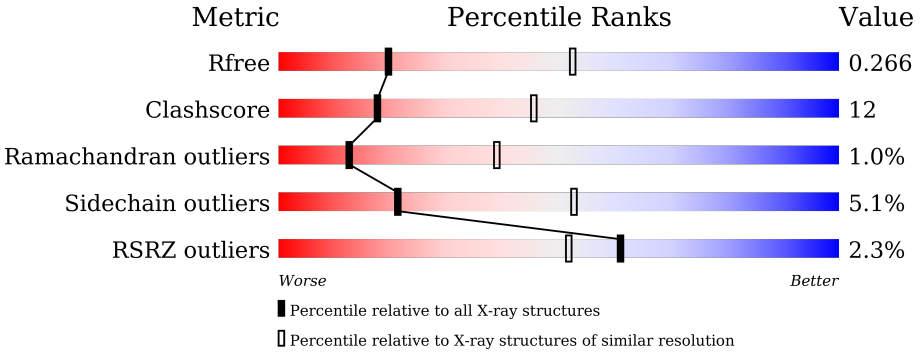
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 <=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	221	63% 31% • ••
1	B	221	67% 25% 5% ••
1	C	221	2% 76% 19% • •
1	D	221	6% 71% 24% • •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PHT	A	301	-	-	X	-
3	EOH	B	301	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6628 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.

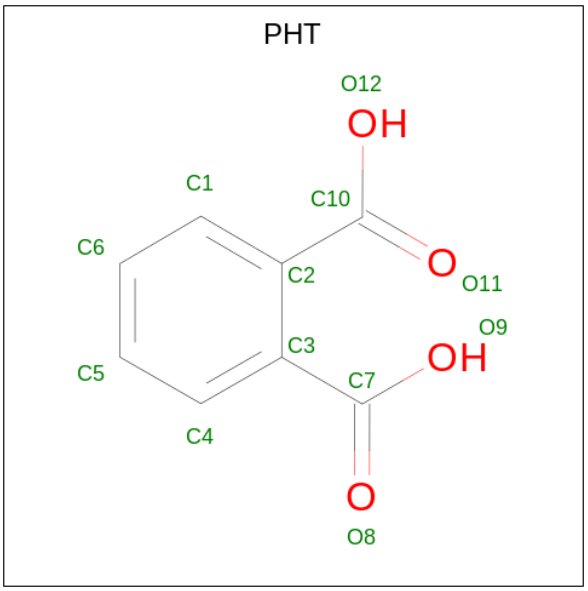
- Molecule 1 is a protein called N-carbamoylsarcosine amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1654	1045	282	322	5	0	0	0
1	B	218	1654	1045	282	322	5	0	0	0
1	C	216	1640	1037	280	319	4	0	0	0
1	D	217	1646	1040	281	321	4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

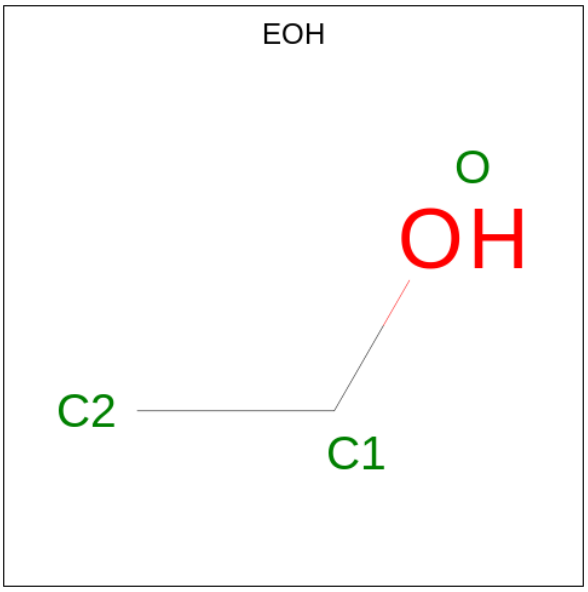
Chain	Residue	Modelled	Actual	Comment	Reference
A	220	SER	-	expression tag	UNP A0ABT4NK74
A	221	SER	-	expression tag	UNP A0ABT4NK74
B	220	SER	-	expression tag	UNP A0ABT4NK74
B	221	SER	-	expression tag	UNP A0ABT4NK74
C	220	SER	-	expression tag	UNP A0ABT4NK74
C	221	SER	-	expression tag	UNP A0ABT4NK74
D	220	SER	-	expression tag	UNP A0ABT4NK74
D	221	SER	-	expression tag	UNP A0ABT4NK74

- Molecule 2 is PHTHALIC ACID (CCD ID: PHT) (formula: $C_8H_6O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 8 4	0	0

- Molecule 3 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 3 2 1	0	0

- Molecule 4 is water.

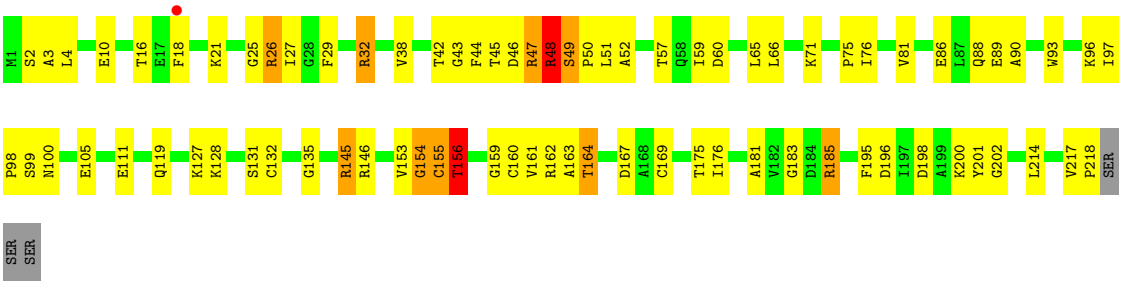
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	6	6	6	0	0
			Total	O		
4	B	8	8	8	0	0
			Total	O		
4	C	3	3	3	0	0
			Total	O		
4	D	2	2	2	0	0

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.

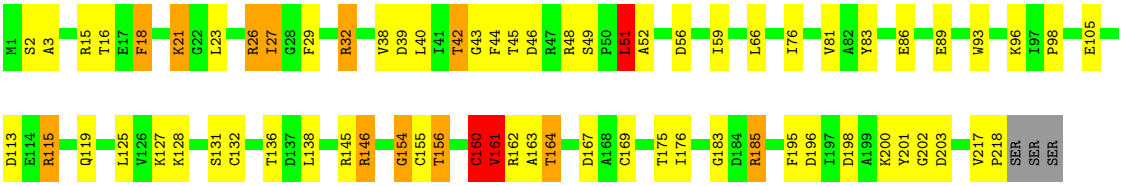
• Molecule 1: N-carbamoylsarcosine amidohydrolase

Chain A:



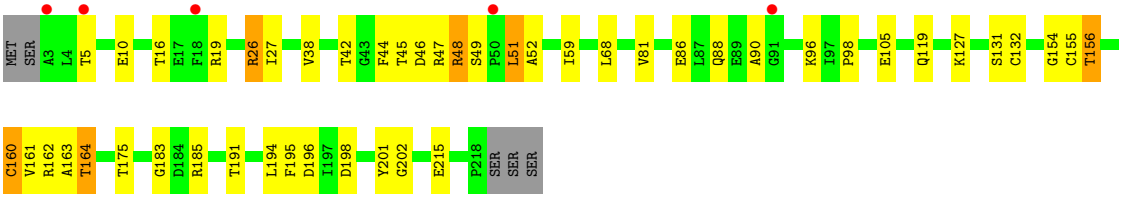
• Molecule 1: N-carbamoylsarcosine amidohydrolase

Chain B:



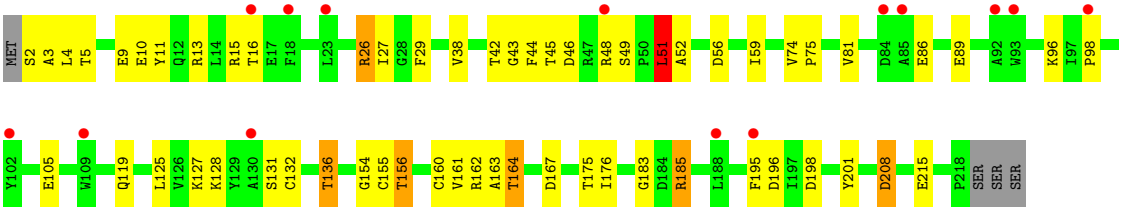
• Molecule 1: N-carbamoylsarcosine amidohydrolase

Chain C:



• Molecule 1: N-carbamoylsarcosine amidohydrolase

Chain D:


MET
S2
A3
L4
T5
E9
E10
Y11
Q12
R13
L14
R15
T16
E17
F18
L23
R26
I27
G28
F29
V38
T42
G43
F44
T45
D46
R47
R48
S49
P50
L51
A52
D56
I59
V74
P75
V81
D84
A85
E86
E89
A92
W93
K96
I97
P98
Y102
E105
W109
Q119
L125
V126
K127
K128
Y129
A130
S131
C132
T136
G154
C155
T156
C160
V161
R162
A163
T164
D167
T175
I176
G183
D184
R185
L188
F195
D196
I197
D198
Y201
D208
E215
P218
SER
SER
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	62.71Å 137.45Å 190.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.11 – 2.90 28.11 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.11-2.90) 99.7 (28.11-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.82 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.239 , 0.263 0.238 , 0.266	Depositor DCC
R_{free} test set	531 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6628	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PHT, EOH

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	0.65	0/1681	1.44	19/2284 (0.8%)
1	B	0.63	0/1681	1.41	15/2284 (0.7%)
1	C	0.55	0/1667	1.30	7/2266 (0.3%)
1	D	0.54	0/1673	1.29	10/2274 (0.4%)
All	All	0.60	0/6702	1.36	51/9108 (0.6%)

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	4
1	B	0	5
1	C	0	1
1	D	0	1
All	All	0	11

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	161	VAL	N-CA-CB	14.02	134.37	111.23
1	A	156	THR	CA-CB-OG1	-13.29	89.67	109.60
1	A	105	GLU	CB-CA-C	-11.19	93.06	109.84
1	A	57	THR	CA-CB-OG1	-9.67	95.10	109.60
1	B	201	TYR	CB-CA-C	7.88	121.56	109.34
1	D	56	ASP	CB-CA-C	7.75	123.05	110.88
1	B	16	THR	CA-CB-OG1	-7.51	98.34	109.60
1	D	16	THR	CA-CB-OG1	-7.17	98.84	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	105	GLU	CB-CA-C	-7.12	97.90	109.72
1	A	21	LYS	CA-CB-CG	6.99	128.09	114.10
1	A	47	ARG	CB-CA-C	6.87	124.10	110.42
1	A	119	GLN	CB-CA-C	-6.80	98.56	109.37
1	A	16	THR	CA-CB-OG1	-6.76	99.46	109.60
1	C	119	GLN	CB-CA-C	-6.70	98.72	109.37
1	D	208	ASP	CA-CB-CG	6.56	119.16	112.60
1	B	56	ASP	CB-CA-C	6.51	121.11	110.88
1	B	119	GLN	CB-CA-C	-6.33	99.30	109.37
1	C	16	THR	CA-CB-OG1	-6.25	100.23	109.60
1	D	119	GLN	CB-CA-C	-6.25	99.44	109.37
1	B	185	ARG	CB-CA-C	-6.01	97.43	109.99
1	C	10	GLU	CB-CG-CD	5.88	122.60	112.60
1	B	21	LYS	CG-CD-CE	5.83	124.72	111.30
1	A	60	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	167	ASP	CB-CA-C	5.78	120.38	110.79
1	A	145	ARG	CG-CD-NE	5.76	124.67	112.00
1	D	167	ASP	CB-CA-C	5.74	120.32	110.79
1	A	111	GLU	CB-CG-CD	5.63	122.18	112.60
1	D	201	TYR	CB-CA-C	5.59	119.04	109.65
1	C	201	TYR	CB-CA-C	5.46	118.88	109.15
1	A	201	TYR	CB-CA-C	5.44	118.79	109.65
1	B	42	THR	CA-CB-OG1	-5.44	101.44	109.60
1	B	39	ASP	CB-CA-C	-5.43	104.17	111.89
1	B	105	GLU	CB-CA-C	-5.41	100.73	109.72
1	A	167	ASP	CB-CA-C	5.40	119.75	110.79
1	B	51	LEU	CA-C-N	5.40	131.85	121.54
1	B	51	LEU	C-N-CA	5.40	131.85	121.54
1	C	119	GLN	N-CA-CB	5.39	115.99	109.74
1	A	155	CYS	CA-CB-SG	-5.34	102.12	114.40
1	B	160	CYS	N-CA-C	-5.31	101.79	109.59
1	D	51	LEU	CA-C-N	5.29	131.64	121.54
1	D	51	LEU	C-N-CA	5.29	131.64	121.54
1	A	119	GLN	N-CA-CB	5.28	115.86	109.74
1	A	18	PHE	CA-CB-CG	5.21	119.02	113.80
1	A	155	CYS	N-CA-CB	5.21	119.30	110.49
1	C	19	ARG	CA-CB-CG	5.16	124.43	114.10
1	C	191	THR	CA-CB-OG1	-5.03	102.05	109.60
1	B	18	PHE	CA-CB-CG	5.02	118.82	113.80
1	D	215	GLU	CB-CA-C	-5.01	102.33	110.85
1	A	154	GLY	CA-C-N	-5.01	111.97	121.54
1	A	154	GLY	C-N-CA	-5.01	111.97	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	GLU	CB-CA-C	5.01	119.37	110.85

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	GLY	Peptide
1	A	32	ARG	Sidechain
1	A	47	ARG	Sidechain
1	A	48	ARG	Sidechain
1	B	115	ARG	Sidechain
1	B	145	ARG	Sidechain
1	B	15	ARG	Sidechain
1	B	154	GLY	Peptide
1	B	32	ARG	Sidechain
1	C	154	GLY	Peptide
1	D	154	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1654	0	1656	60	1
1	B	1654	0	1656	51	0
1	C	1640	0	1639	35	0
1	D	1646	0	1644	32	0
2	A	12	0	4	8	0
3	B	3	0	6	2	0
4	A	6	0	0	1	0
4	B	8	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
All	All	6628	0	6605	164	1

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 12.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ARG:HH11	1:C:48:ARG:HG3	1.17	1.05
1:A:100:ASN:HD21	2:A:301:PHT:H6	1.24	0.98
1:D:160:CYS:O	1:D:164:THR:HG23	1.69	0.91
1:A:160:CYS:O	1:A:164:THR:HG23	1.72	0.90
1:C:160:CYS:O	1:C:164:THR:HG23	1.72	0.89
1:A:160:CYS:SG	2:A:301:PHT:C7	2.61	0.88
1:A:160:CYS:SG	2:A:301:PHT:O8	2.32	0.87
1:C:48:ARG:HG3	1:C:48:ARG:NH1	1.75	0.87
1:C:48:ARG:HH11	1:C:48:ARG:CG	1.89	0.84
1:A:100:ASN:ND2	2:A:301:PHT:H6	1.94	0.81
1:A:200:LYS:HD3	3:B:301:EOH:H21	1.65	0.78
1:D:51:LEU:HD13	1:D:185:ARG:HE	1.48	0.77
1:A:145:ARG:HD3	4:A:403:HOH:O	1.84	0.77
1:A:156:THR:HG21	1:B:200:LYS:HZ2	1.49	0.76
1:B:113:ASP:OD2	1:B:115:ARG:NH2	2.16	0.76
1:A:156:THR:HG21	1:B:200:LYS:NZ	2.01	0.74
1:A:156:THR:HG22	1:A:159:GLY:N	2.09	0.68
1:B:66:LEU:HD22	1:B:76:ILE:HD13	1.76	0.67
1:A:100:ASN:HD21	2:A:301:PHT:C6	2.03	0.67
1:B:27:ILE:HD12	1:B:175:THR:H	1.60	0.67
1:A:132:CYS:SG	1:A:164:THR:HG21	2.34	0.66
1:A:97:ILE:HD13	2:A:301:PHT:H1	1.78	0.65
1:A:50:PRO:O	1:B:21:LYS:HB3	1.97	0.65
1:A:96:LYS:NZ	1:B:203:ASP:OD1	2.30	0.64
1:B:160:CYS:SG	3:B:301:EOH:O	2.42	0.64
1:D:89:GLU:HB3	1:D:128:LYS:HE3	1.81	0.63
1:B:40:LEU:HD21	1:B:154:GLY:HA2	1.81	0.63
1:D:132:CYS:H	1:D:164:THR:HG22	1.63	0.63
1:A:45:THR:HG21	1:A:59:ILE:HD11	1.82	0.61
1:A:89:GLU:HB3	1:A:128:LYS:HE3	1.82	0.61
1:B:89:GLU:HB3	1:B:128:LYS:HE3	1.81	0.61
1:B:132:CYS:H	1:B:164:THR:HG22	1.66	0.61
1:A:27:ILE:HD12	1:A:175:THR:H	1.65	0.61
1:C:132:CYS:H	1:C:164:THR:HG22	1.66	0.61
1:A:132:CYS:H	1:A:164:THR:HG22	1.66	0.60
1:A:26:ARG:HH22	1:A:198:ASP:CG	2.08	0.60
1:C:27:ILE:HD12	1:C:175:THR:H	1.65	0.60
1:D:27:ILE:HD12	1:D:175:THR:H	1.66	0.60
1:C:51:LEU:HD11	1:C:185:ARG:HH21	1.67	0.60
1:C:26:ARG:HH22	1:C:198:ASP:CG	2.10	0.59
1:D:26:ARG:HH22	1:D:198:ASP:CG	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:THR:O	1:B:161:VAL:HB	2.03	0.58
1:C:132:CYS:SG	1:C:164:THR:HG21	2.43	0.58
1:A:26:ARG:N	1:A:26:ARG:HD2	2.19	0.58
1:D:132:CYS:SG	1:D:164:THR:HG21	2.45	0.57
1:D:26:ARG:N	1:D:26:ARG:HD2	2.19	0.56
1:B:26:ARG:HD2	1:B:26:ARG:N	2.19	0.56
1:C:26:ARG:N	1:C:26:ARG:HD2	2.19	0.56
1:A:51:LEU:HD13	1:A:99:SER:HB2	1.87	0.56
1:B:26:ARG:HH22	1:B:198:ASP:CG	2.13	0.56
1:A:96:LYS:HD3	1:B:202:GLY:HA2	1.89	0.54
1:C:51:LEU:HD13	1:C:185:ARG:HE	1.73	0.54
1:C:68:LEU:HD22	1:C:215:GLU:HG2	1.89	0.53
1:B:132:CYS:SG	1:B:164:THR:HG21	2.49	0.53
1:D:11:TYR:O	1:D:15:ARG:HG3	2.09	0.52
1:D:132:CYS:H	1:D:164:THR:CG2	2.22	0.52
1:C:46:ASP:C	1:C:48:ARG:H	2.17	0.52
1:C:156:THR:O	1:C:161:VAL:HB	2.10	0.52
1:D:125:LEU:HD11	1:D:136:THR:HB	1.92	0.52
1:A:46:ASP:C	1:A:48:ARG:H	2.18	0.52
1:B:132:CYS:H	1:B:164:THR:CG2	2.23	0.52
1:A:25:GLY:O	1:B:96:LYS:NZ	2.43	0.51
1:B:125:LEU:HD11	1:B:136:THR:HB	1.92	0.51
1:A:97:ILE:HG23	1:B:23:LEU:HG	1.92	0.51
1:C:45:THR:HG21	1:C:59:ILE:HD11	1.93	0.51
1:C:51:LEU:CD1	1:C:185:ARG:HE	2.23	0.51
1:A:2:SER:O	1:A:3:ALA:C	2.54	0.50
1:A:162:ARG:CZ	1:B:162:ARG:HD3	2.41	0.50
1:A:160:CYS:HG	2:A:301:PHT:C7	2.08	0.50
1:B:2:SER:O	1:B:3:ALA:C	2.54	0.50
1:B:46:ASP:C	1:B:48:ARG:H	2.20	0.50
1:C:46:ASP:CG	1:C:48:ARG:HD2	2.37	0.49
1:B:96:LYS:O	1:B:98:PRO:HD3	2.12	0.49
1:D:156:THR:O	1:D:161:VAL:HB	2.11	0.49
1:C:155:CYS:O	1:C:183:GLY:O	2.30	0.49
1:C:132:CYS:H	1:C:164:THR:CG2	2.25	0.49
1:D:2:SER:O	1:D:3:ALA:C	2.56	0.49
1:A:132:CYS:H	1:A:164:THR:CG2	2.25	0.49
1:B:156:THR:O	1:B:160:CYS:O	2.31	0.49
1:D:155:CYS:O	1:D:183:GLY:O	2.30	0.49
1:A:93:TRP:CD1	1:B:169:CYS:SG	3.06	0.48
1:D:46:ASP:C	1:D:48:ARG:H	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:CYS:O	1:A:183:GLY:O	2.31	0.47
1:B:113:ASP:CG	1:B:115:ARG:HH21	2.18	0.47
1:B:27:ILE:HD11	1:B:202:GLY:HA2	1.97	0.47
1:B:38:VAL:O	1:B:155:CYS:HB2	2.15	0.47
1:A:29:PHE:CE2	1:A:176:ILE:HG13	2.50	0.47
1:D:10:GLU:CD	1:D:13:ARG:HH21	2.23	0.46
1:D:46:ASP:OD2	1:D:48:ARG:HD2	2.16	0.46
1:B:42:THR:C	1:B:44:PHE:H	2.24	0.46
1:C:45:THR:CG2	1:C:59:ILE:HD11	2.46	0.46
1:A:93:TRP:CD1	1:B:169:CYS:HG	2.33	0.46
1:C:38:VAL:O	1:C:155:CYS:HB2	2.15	0.46
1:D:38:VAL:O	1:D:155:CYS:HB2	2.16	0.46
1:B:26:ARG:NH2	1:B:198:ASP:OD2	2.48	0.46
1:D:5:THR:O	1:D:9:GLU:HB2	2.15	0.45
1:D:49:SER:C	1:D:51:LEU:H	2.24	0.45
1:A:162:ARG:O	1:A:163:ALA:C	2.60	0.45
1:A:32:ARG:HD2	1:A:146:ARG:O	2.16	0.45
1:D:42:THR:C	1:D:44:PHE:H	2.24	0.45
1:B:83:TYR:HE1	1:B:128:LYS:HB3	1.82	0.45
1:B:45:THR:HG22	1:B:59:ILE:HD11	1.98	0.45
1:B:217:VAL:HA	1:B:218:PRO:HD3	1.83	0.45
1:A:162:ARG:NH1	1:B:162:ARG:HD3	2.32	0.45
1:A:169:CYS:HG	1:B:93:TRP:CD1	2.35	0.45
1:D:29:PHE:CE2	1:D:176:ILE:HG13	2.52	0.45
1:A:26:ARG:NH2	1:A:198:ASP:OD1	2.50	0.44
1:A:81:VAL:HA	1:A:127:LYS:O	2.17	0.44
1:A:38:VAL:O	1:A:155:CYS:HB2	2.17	0.44
1:A:131:SER:HA	1:A:164:THR:HG22	2.00	0.44
1:C:27:ILE:HD11	1:C:202:GLY:HA2	1.99	0.44
1:D:81:VAL:HA	1:D:127:LYS:O	2.17	0.44
1:D:45:THR:HG21	1:D:59:ILE:HD11	2.00	0.44
1:A:65:LEU:HD22	1:A:214:LEU:HD12	2.00	0.44
1:D:45:THR:CG2	1:D:59:ILE:HD11	2.48	0.44
1:A:66:LEU:HD22	1:A:76:ILE:HD13	2.00	0.43
1:A:27:ILE:HD11	1:A:202:GLY:HA2	2.00	0.43
1:A:96:LYS:O	1:A:98:PRO:HD3	2.17	0.43
1:C:131:SER:HA	1:C:164:THR:HG22	1.99	0.43
1:C:46:ASP:C	1:C:48:ARG:N	2.76	0.43
1:A:217:VAL:HA	1:A:218:PRO:HD2	1.83	0.43
1:C:81:VAL:HA	1:C:127:LYS:O	2.19	0.43
1:C:162:ARG:O	1:C:163:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:VAL:HA	1:B:127:LYS:O	2.18	0.43
1:D:26:ARG:NH2	1:D:198:ASP:OD1	2.52	0.42
1:D:96:LYS:O	1:D:98:PRO:HD3	2.19	0.42
1:B:131:SER:HA	1:B:164:THR:HG22	2.00	0.42
1:B:155:CYS:O	1:B:183:GLY:O	2.36	0.42
1:D:162:ARG:O	1:D:163:ALA:C	2.62	0.42
1:B:29:PHE:CE2	1:B:176:ILE:HG13	2.54	0.42
1:C:26:ARG:NH2	1:C:198:ASP:OD1	2.52	0.42
1:A:153:VAL:HG12	1:A:181:ALA:HB3	2.02	0.42
1:D:131:SER:HA	1:D:164:THR:HG22	2.02	0.42
1:B:162:ARG:O	1:B:163:ALA:C	2.61	0.42
1:A:42:THR:C	1:A:44:PHE:H	2.27	0.42
1:D:46:ASP:C	1:D:48:ARG:N	2.77	0.42
1:A:46:ASP:C	1:A:48:ARG:N	2.77	0.42
1:A:75:PRO:HG2	1:A:145:ARG:HD2	2.02	0.42
1:B:32:ARG:HD2	1:B:146:ARG:O	2.19	0.42
1:C:49:SER:C	1:C:51:LEU:H	2.28	0.42
1:A:97:ILE:CD1	2:A:301:PHT:H1	2.49	0.41
1:B:138:LEU:HD12	1:B:138:LEU:O	2.20	0.41
1:B:46:ASP:C	1:B:48:ARG:N	2.78	0.41
1:A:45:THR:CG2	1:A:59:ILE:HD11	2.50	0.41
1:A:49:SER:C	1:A:51:LEU:H	2.28	0.41
1:D:74:VAL:HA	1:D:75:PRO:HD3	1.84	0.41
1:A:156:THR:O	1:A:161:VAL:HB	2.20	0.41
1:C:46:ASP:OD2	1:C:48:ARG:CD	2.69	0.41
1:A:195:PHE:O	1:A:196:ASP:C	2.64	0.41
1:B:27:ILE:CD1	1:B:175:THR:H	2.32	0.41
1:C:96:LYS:O	1:C:98:PRO:HD3	2.21	0.41
1:C:195:PHE:O	1:C:196:ASP:C	2.64	0.41
1:D:195:PHE:O	1:D:196:ASP:C	2.64	0.41
1:C:42:THR:C	1:C:44:PHE:H	2.28	0.41
1:C:88:GLN:C	1:C:90:ALA:H	2.28	0.41
1:B:49:SER:C	1:B:51:LEU:H	2.28	0.40
1:A:2:SER:O	1:A:4:LEU:N	2.55	0.40
1:A:88:GLN:C	1:A:90:ALA:H	2.29	0.40
1:A:93:TRP:HD1	1:B:169:CYS:SG	2.43	0.40
1:A:185:ARG:HD2	1:B:18:PHE:CZ	2.57	0.40
1:B:42:THR:O	1:B:44:PHE:N	2.55	0.40
1:C:194:LEU:HD23	1:C:194:LEU:HA	1.93	0.40
1:B:195:PHE:O	1:B:196:ASP:C	2.64	0.40
1:C:46:ASP:OD2	1:C:48:ARG:HD3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLY:O	1:A:135:GLY:O[4_555]	2.14	0.06

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	216/221 (98%)	201 (93%)	13 (6%)	2 (1%)	14	41
1	B	216/221 (98%)	200 (93%)	13 (6%)	3 (1%)	9	30
1	C	214/221 (97%)	201 (94%)	11 (5%)	2 (1%)	14	41
1	D	215/221 (97%)	201 (94%)	12 (6%)	2 (1%)	14	41
All	All	861/884 (97%)	803 (93%)	49 (6%)	9 (1%)	12	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	ALA
1	B	161	VAL
1	C	52	ALA
1	D	52	ALA
1	A	52	ALA
1	C	47	ARG
1	D	43	GLY
1	A	43	GLY
1	B	43	GLY

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	173/176 (98%)	165 (95%)	8 (5%)	24	57
1	B	173/176 (98%)	164 (95%)	9 (5%)	21	52
1	C	171/176 (97%)	162 (95%)	9 (5%)	20	52
1	D	172/176 (98%)	163 (95%)	9 (5%)	21	52
All	All	689/704 (98%)	654 (95%)	35 (5%)	21	53

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	48	ARG
1	A	49	SER
1	A	71	LYS
1	A	86	GLU
1	A	156	THR
1	A	164	THR
1	A	185	ARG
1	B	26	ARG
1	B	27	ILE
1	B	51	LEU
1	B	86	GLU
1	B	146	ARG
1	B	156	THR
1	B	160	CYS
1	B	164	THR
1	B	185	ARG
1	C	5	THR
1	C	26	ARG
1	C	48	ARG
1	C	51	LEU
1	C	86	GLU
1	C	105	GLU
1	C	156	THR
1	C	160	CYS
1	C	164	THR
1	D	4	LEU
1	D	26	ARG

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Mol	Chain	Res	Type
1	D	51	LEU
1	D	86	GLU
1	D	136	THR
1	D	156	THR
1	D	164	THR
1	D	185	ARG
1	D	208	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	C	73	GLN

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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EOH	B	301	-	2,2,2	0.20	0	1,1,1	0.05	0
2	PHT	A	301	-	12,12,12	1.18	1 (8%)	16,16,16	1.22	3 (18%)

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	PHT	A	301	-	-	0/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	PHT	O9-C7	-3.35	1.20	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	PHT	C4-C3-C7	-2.29	113.37	118.63
2	A	301	PHT	C1-C2-C10	-2.10	113.81	118.63
2	A	301	PHT	O8-C7-C3	-2.05	116.95	121.94

There are no chirality outliers.

There are no torsion outliers.

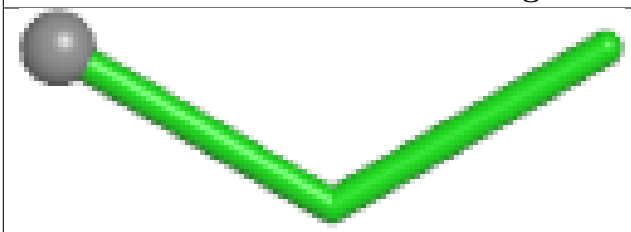
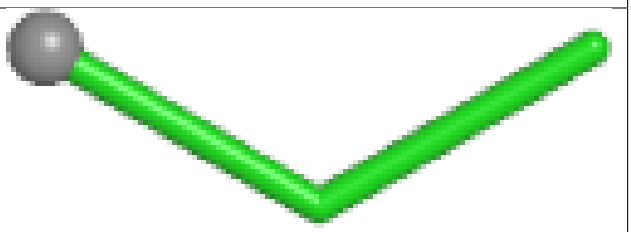
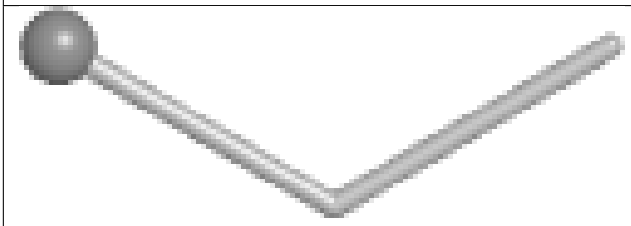
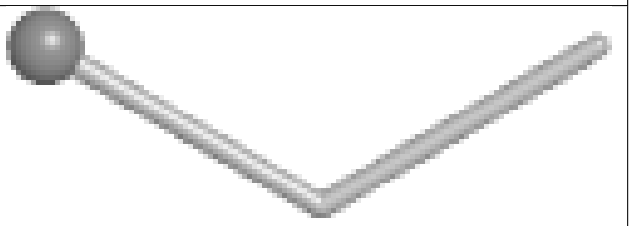
There are no ring outliers.

2 monomers are involved in 10 short contacts:

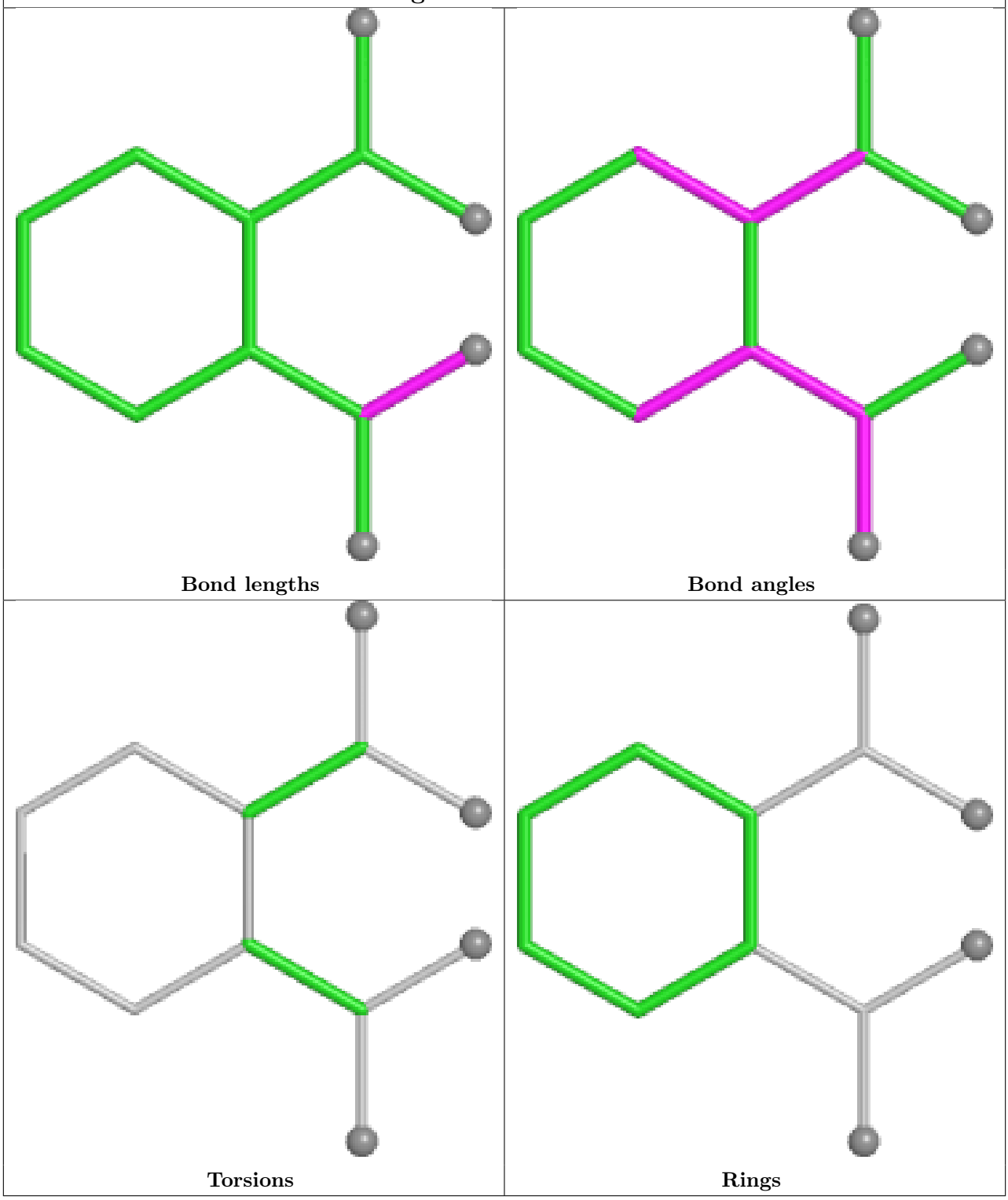
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	EOH	2	0
2	A	301	PHT	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand EOH B 301	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand PHT A 301



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	218/221 (98%)	-0.13	1 (0%) 87 83	10, 30, 62, 88	0
1	B	218/221 (98%)	-0.14	0 100 100	12, 31, 55, 77	0
1	C	216/221 (97%)	0.34	5 (2%) 61 52	37, 61, 107, 142	0
1	D	217/221 (98%)	0.78	14 (6%) 25 20	40, 75, 117, 142	0
All	All	869/884 (98%)	0.21	20 (2%) 61 52	10, 47, 105, 142	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	18	PHE	4.6
1	D	195	PHE	3.2
1	D	102	TYR	3.0
1	C	3	ALA	3.0
1	D	85	ALA	2.8
1	A	18	PHE	2.7
1	D	18	PHE	2.7
1	D	48	ARG	2.7
1	D	84	ASP	2.6
1	D	188	LEU	2.6
1	D	93	TRP	2.5
1	C	91	GLY	2.4
1	D	109	TRP	2.4
1	D	130	ALA	2.4
1	C	5	THR	2.4
1	D	23	LEU	2.3
1	D	16	THR	2.2
1	D	98	PRO	2.2
1	C	50	PRO	2.1
1	D	92	ALA	2.1

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)

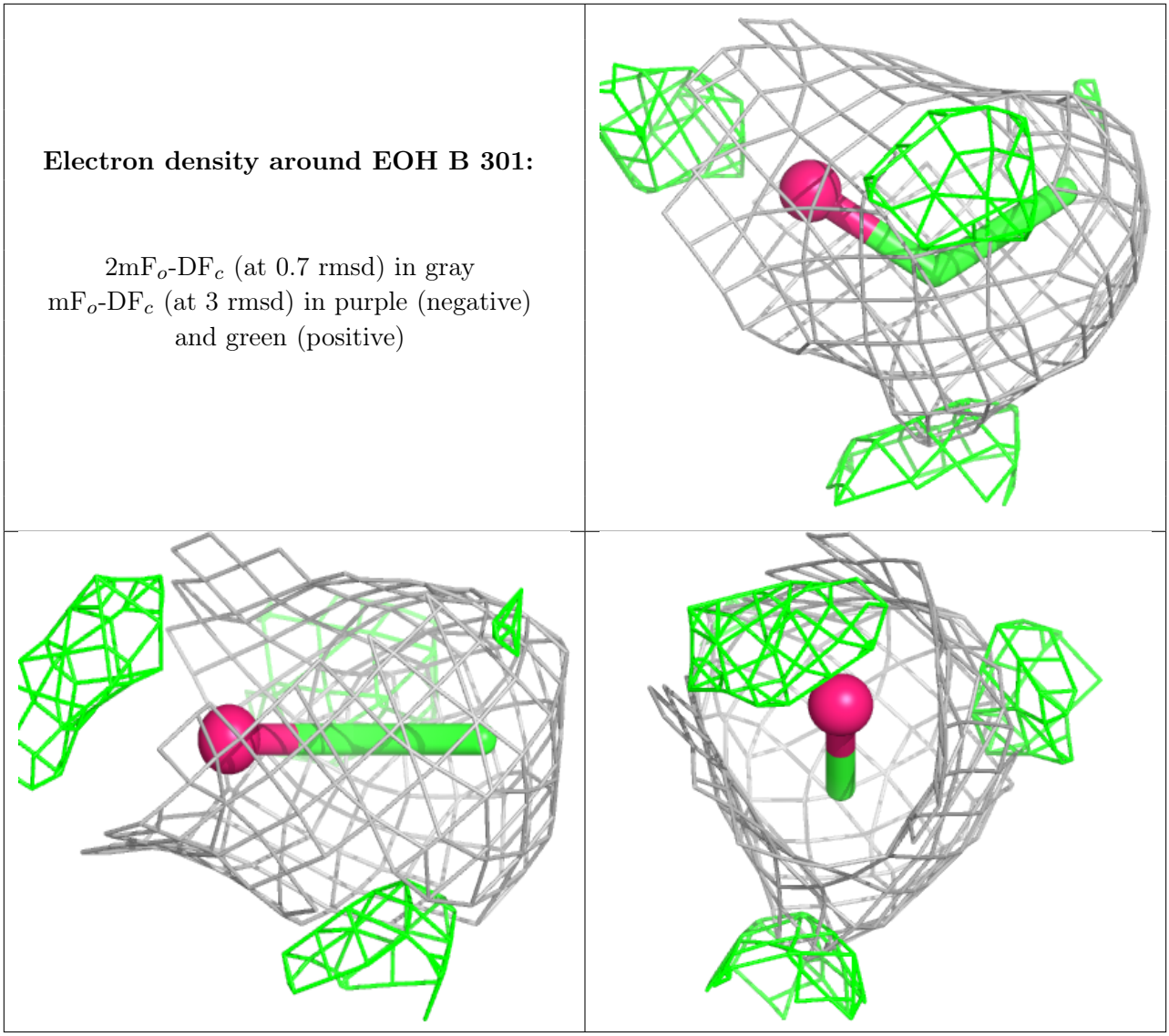
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EOH	B	301	3/3	0.92	0.22	22,22,22,23	0
2	PHT	A	301	12/12	0.96	0.09	15,22,25,29	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.

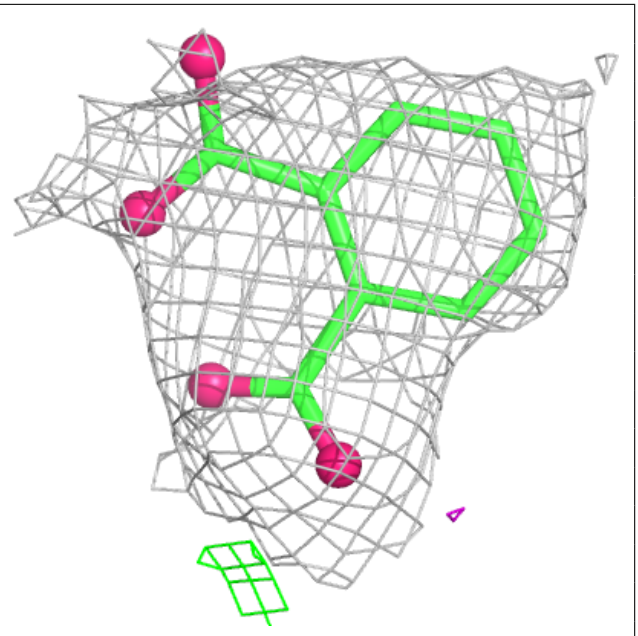
Electron density around EOH B 301:

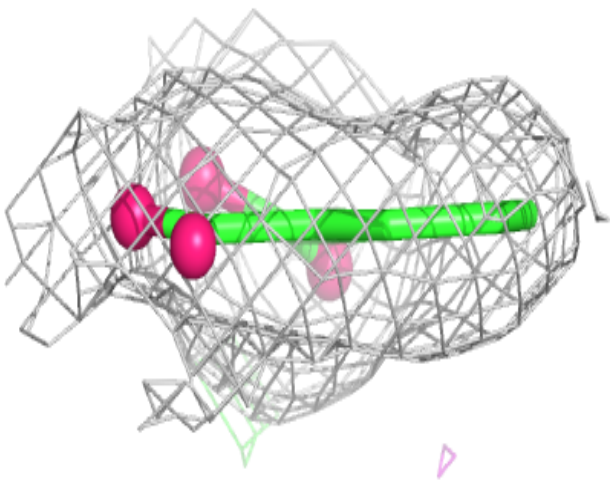
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

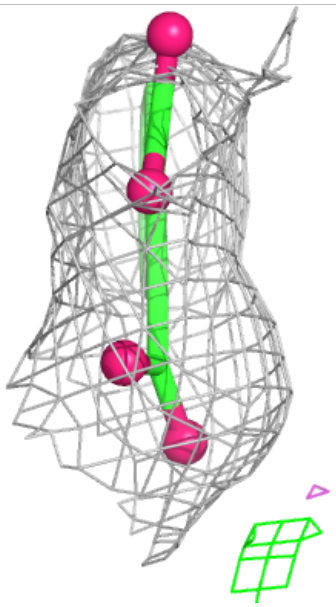


Electron density around PHT A 301:

$2mF_o$-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.