



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:02 am BST

PDB ID : 5M21  
Title : Crystal structure of hydroquinone 1,2-dioxygenase from *Sphingomonas* sp. TTNP3 with 4-hydroxybenzoate bound  
Authors : Ferraroni, M.; Da Vela, S.; Scozzafava, A.; Kolvenbach, B.; Corvini, P.F.X.  
Deposited on : 2016-10-11  
Resolution : 1.99 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

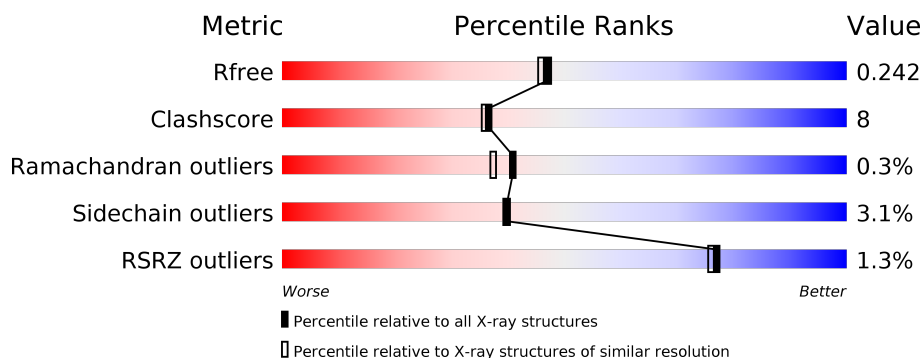
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	170	<div> <div>77%</div> <div>19%</div> <div>..</div> </div>
1	C	170	<div> <div>5%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	E	170	<div> <div>5%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	G	170	<div> <div>5%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
2	B	341	<div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
2	D	341	<div> <div>77%</div> <div>18%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	341	 81% 13% • •
2	H	341	 2% 84% 12% • •

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
4	PHB	D	402	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16580 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 Hydroquinone dioxygenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1275	808	216	245	6			
1	C	167	Total	C	N	O	S	0	0	0
			1284	813	217	248	6			
1	E	167	Total	C	N	O	S	0	0	0
			1275	808	213	248	6			
1	G	165	Total	C	N	O	S	0	0	0
			1251	796	209	240	6			

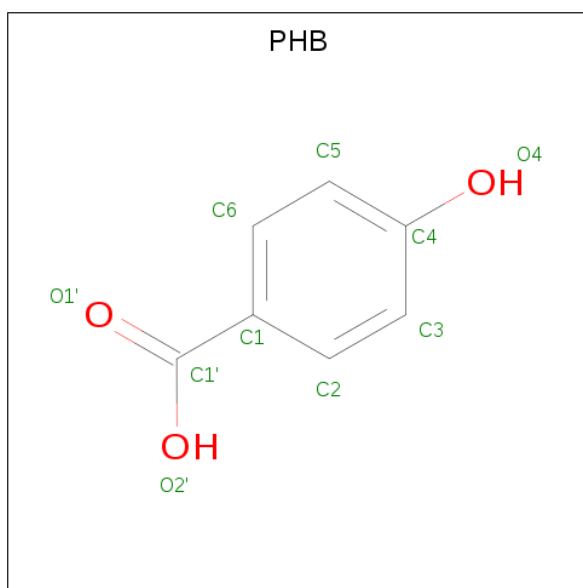
- Molecule 2 is a protein called Hydroquinone dioxygenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	325	Total	C	N	O	S	0	0	0
			2562	1624	448	476	14			
2	D	327	Total	C	N	O	S	0	2	0
			2572	1628	448	481	15			
2	F	326	Total	C	N	O	S	0	1	0
			2572	1630	449	478	15			
2	H	333	Total	C	N	O	S	0	0	0
			2604	1649	455	486	14			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		
3	F	1	Total	Fe	0	0
			1	1		

- Molecule 4 is P-HYDROXYBENZOIC ACID (three-letter code: PHB) (formula:  $C_7H_6O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	7	3		
4	D	1	Total	C	O	0	0
			10	7	3		
4	F	1	Total	C	O	0	0
			10	7	3		
4	H	1	Total	C	O	0	0
			10	7	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	97	Total	O	0	0
			97	97		
5	B	213	Total	O	0	0
			213	213		
5	C	117	Total	O	0	0
			117	117		
5	D	209	Total	O	0	0
			209	209		
5	E	89	Total	O	0	0
			89	89		
5	F	177	Total	O	0	0
			177	177		
5	G	50	Total	O	0	0
			50	50		

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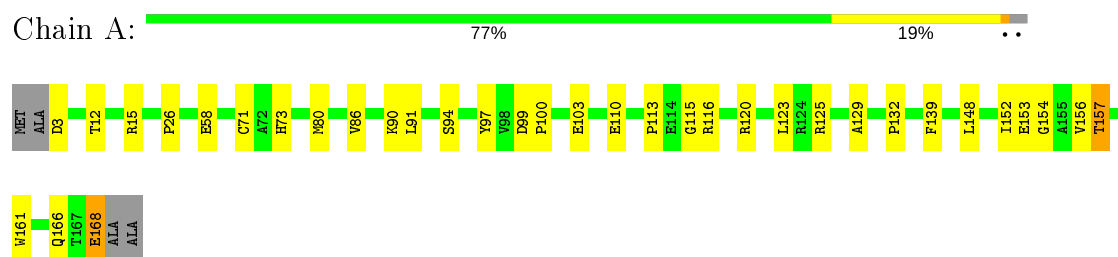
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	189	Total 189	O 189	0	0

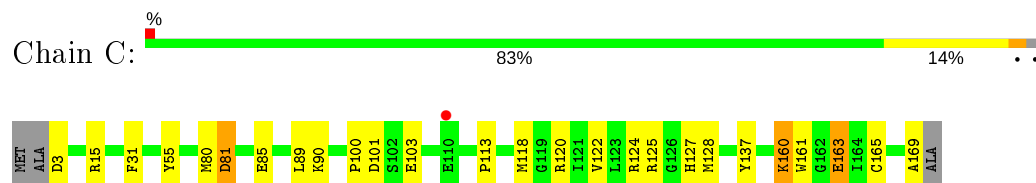
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

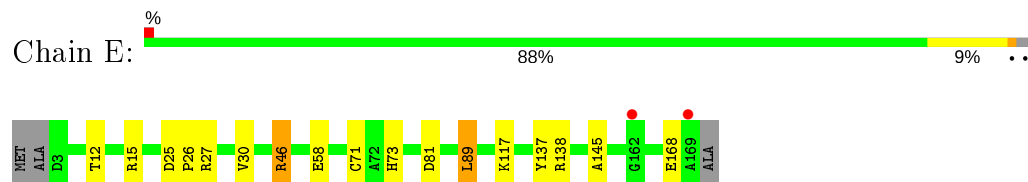
- Molecule 1: Hydroquinone dioxygenase small subunit



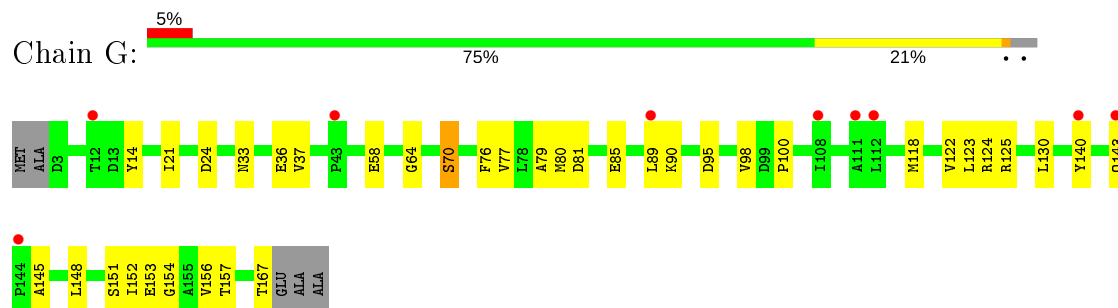
- Molecule 1: Hydroquinone dioxygenase small subunit




- Molecule 1: Hydroquinone dioxygenase small subunit

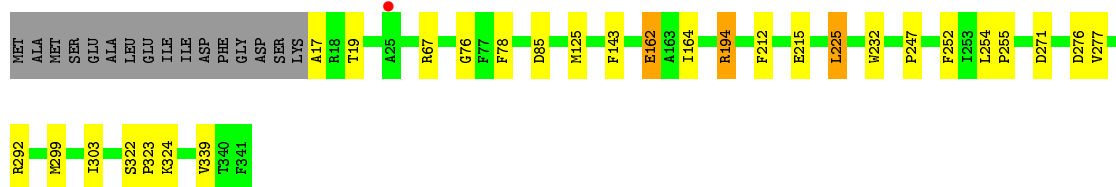


- Molecule 1: Hydroquinone dioxygenase small subunit




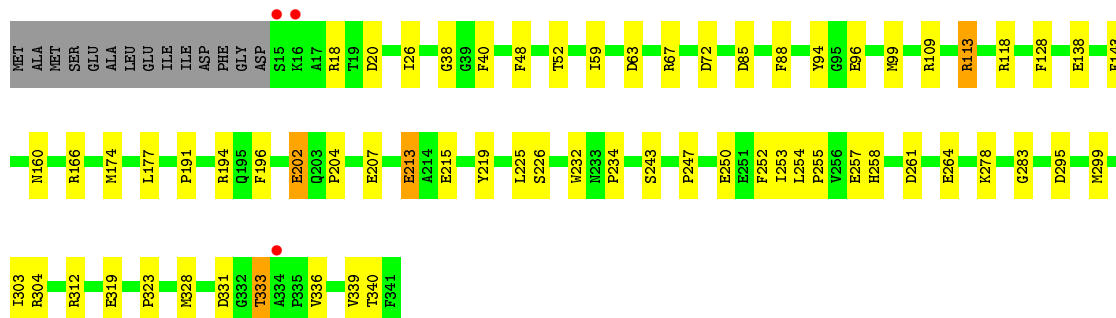
- Molecule 2: Hydroquinone dioxygenase large subunit

Chain B:  87% 8% 5%




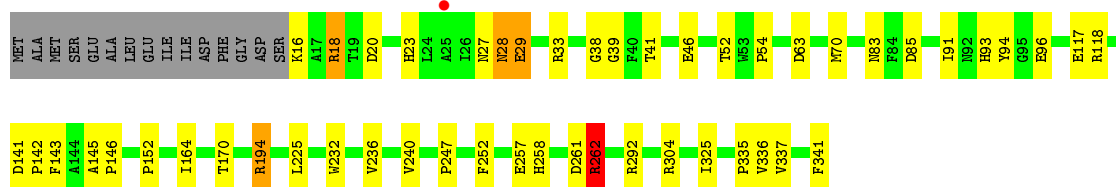
• Molecule 2: Hydroquinone dioxygenase large subunit

Chain D:  77% 18% 5%




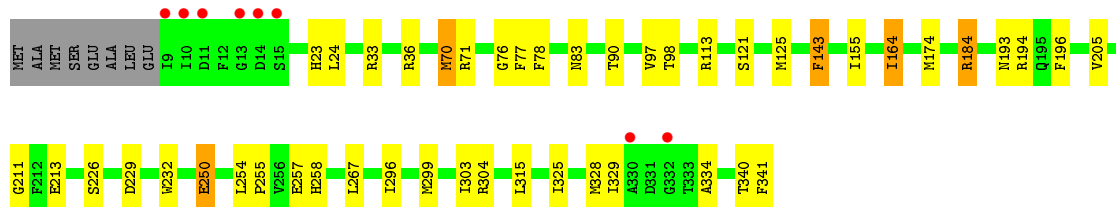
• Molecule 2: Hydroquinone dioxygenase large subunit

Chain F:  81% 13% 5%



• Molecule 2: Hydroquinone dioxygenase large subunit

Chain H:  84% 12% 5%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.78Å 124.87Å 92.37Å 90.00° 105.15° 90.00°	Depositor
Resolution (Å)	29.80 – 1.99 44.61 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.80-1.99) 98.6 (44.61-1.99)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.179 , 0.242 0.180 , 0.242	Depositor DCC
$R_{free}$ test set	6615 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PHB, FE

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	0.79	0/1302	0.88	2/1766 (0.1%)
1	C	0.79	0/1311	0.88	0/1778
1	E	0.73	0/1302	0.88	2/1768 (0.1%)
1	G	0.68	0/1278	0.82	1/1735 (0.1%)
2	B	0.85	0/2635	0.92	7/3583 (0.2%)
2	D	0.84	0/2651	0.92	3/3607 (0.1%)
2	F	0.81	0/2648	0.90	4/3599 (0.1%)
2	H	0.78	0/2677	0.88	4/3641 (0.1%)
All	All	0.80	0/15804	0.89	23/21477 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	276	ASP	CB-CG-OD1	7.68	125.21	118.30
2	D	85	ASP	CB-CG-OD1	7.63	125.17	118.30
2	H	184	ARG	NE-CZ-NH1	7.45	124.03	120.30
2	F	194	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	E	46	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	A	120	ARG	NE-CZ-NH2	-6.98	116.81	120.30
2	B	276	ASP	CB-CG-OD2	-6.48	112.47	118.30
2	B	194	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	H	184	ARG	NE-CZ-NH2	-6.36	117.12	120.30
2	D	63	ASP	CB-CG-OD1	6.35	124.02	118.30
2	D	113	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	B	225	LEU	CB-CG-CD1	-5.61	101.46	111.00
1	G	89	LEU	CA-CB-CG	5.40	127.73	115.30
1	E	89	LEU	CA-CB-CG	5.39	127.70	115.30
2	B	85	ASP	CB-CG-OD1	5.39	123.15	118.30
2	H	36	ARG	NE-CZ-NH1	5.36	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	262	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	H	71	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	B	271	ASP	CB-CG-OD1	-5.21	113.61	118.30
2	F	85	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	99	ASP	CB-CG-OD1	5.11	122.90	118.30
2	F	141	ASP	CB-CG-OD1	5.10	122.89	118.30
2	B	67	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1275	0	1220	29	0
1	C	1284	0	1229	27	0
1	E	1275	0	1209	15	0
1	G	1251	0	1188	33	0
2	B	2562	0	2426	15	0
2	D	2572	0	2424	67	0
2	F	2572	0	2430	40	0
2	H	2604	0	2443	45	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	B	10	0	4	1	0
4	D	10	0	5	5	0
4	F	10	0	4	1	0
4	H	10	0	4	1	0
5	A	97	0	0	4	0
5	B	213	0	0	1	0
5	C	117	0	0	6	0
5	D	209	0	0	15	0
5	E	89	0	0	3	0
5	F	177	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	50	0	0	5	0
5	H	189	0	0	14	0
All	All	16580	0	14586	238	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 8.

All (238) 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:G:76:PHE:CD1	2:H:174:MET:CE	2.11	1.34
2:F:240:VAL:HB	5:F:658:HOH:O	1.13	1.30
1:C:128:MET:HG2	2:D:174:MET:CE	1.60	1.30
2:H:97:VAL:HB	5:H:648:HOH:O	1.07	1.25
1:G:76:PHE:CD1	2:H:174:MET:HE2	1.68	1.24
2:D:118:ARG:HG2	5:D:593:HOH:O	1.39	1.21
1:G:76:PHE:HD1	2:H:174:MET:CE	1.47	1.15
1:G:123:LEU:HD12	5:G:250:HOH:O	1.49	1.12
2:D:174:MET:SD	5:D:663:HOH:O	2.08	1.10
2:H:70:MET:SD	5:H:668:HOH:O	2.08	1.10
2:D:99:MET:HE3	2:D:128:PHE:CZ	1.89	1.07
1:G:140:TYR:HB3	5:G:226:HOH:O	1.57	1.02
2:D:99:MET:HE3	2:D:128:PHE:HZ	1.24	1.01
1:C:128:MET:CG	2:D:174:MET:CE	2.39	0.99
1:C:128:MET:HG2	2:D:174:MET:HE1	1.46	0.98
1:G:76:PHE:CE1	2:H:174:MET:CE	2.46	0.98
1:C:128:MET:SD	2:D:174:MET:HE2	2.07	0.95
1:G:58:GLU:OE2	1:G:157:THR:HG22	1.66	0.95
1:C:128:MET:HG2	2:D:174:MET:HE3	1.46	0.95
2:H:196:PHE:HB2	5:H:516:HOH:O	1.67	0.94
2:F:29:GLU:HG2	5:F:626:HOH:O	1.65	0.94
2:H:174:MET:SD	5:H:654:HOH:O	2.25	0.94
2:H:193:ASN:HB3	5:H:516:HOH:O	1.68	0.92
1:G:76:PHE:CE1	2:H:174:MET:HE2	2.05	0.91
2:D:99:MET:CE	2:D:128:PHE:HZ	1.84	0.90
2:H:267:LEU:HG	5:H:525:HOH:O	1.71	0.90
1:G:76:PHE:HD1	2:H:174:MET:HE1	1.36	0.87
2:D:99:MET:CE	2:D:128:PHE:CZ	2.57	0.86
1:G:76:PHE:CE1	2:H:174:MET:HE3	2.09	0.86
1:G:76:PHE:CD1	2:H:174:MET:HE3	2.09	0.85
1:A:80:MET:HE3	5:A:272:HOH:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:ARG:NE	5:D:501:HOH:O	2.09	0.81
2:F:70:MET:HE1	2:F:164:ILE:HG22	1.60	0.81
1:A:26:PRO:HG3	1:A:168:GLU:HB3	1.62	0.79
2:D:67:ARG:NH2	5:D:501:HOH:O	2.11	0.78
2:H:184:ARG:HD3	5:H:665:HOH:O	1.83	0.78
2:D:331:ASP:HB2	2:D:333:THR:HG22	1.66	0.77
1:A:125:ARG:HD3	5:A:221:HOH:O	1.86	0.76
2:F:93:HIS:HD2	5:F:567:HOH:O	1.66	0.76
1:A:100:PRO:HG3	2:D:323:PRO:HG2	1.69	0.74
1:A:110:GLU:CB	5:A:267:HOH:O	2.35	0.74
2:D:191:PRO:HD3	5:D:559:HOH:O	1.86	0.74
1:C:128:MET:SD	2:D:174:MET:CE	2.76	0.73
1:G:14:TYR:OH	1:G:36:GLU:HG3	1.88	0.73
1:C:128:MET:CG	2:D:174:MET:HE3	2.12	0.73
2:D:96:GLU:HB3	5:D:593:HOH:O	1.88	0.72
2:F:118:ARG:HB2	5:F:529:HOH:O	1.88	0.71
2:F:41:THR:HB	2:F:52:THR:OG1	1.90	0.71
2:D:234:PRO:HD3	4:D:402:PHB:H3	1.71	0.71
1:A:154:GLY:H	1:A:157:THR:HG23	1.56	0.71
1:A:166:GLN:HE21	1:A:168:GLU:HB2	1.57	0.69
2:F:23:HIS:ND1	5:F:502:HOH:O	2.25	0.68
2:F:46:GLU:HG3	5:H:609:HOH:O	1.93	0.68
2:F:18:ARG:NH2	2:F:20:ASP:OD2	2.27	0.67
2:F:41:THR:HG22	5:F:501:HOH:O	1.95	0.67
2:F:96:GLU:HB3	5:F:567:HOH:O	1.95	0.66
1:A:58:GLU:OE2	1:A:157:THR:HG22	1.95	0.66
2:H:267:LEU:HD12	2:H:296:ILE:HB	1.78	0.66
2:D:67:ARG:CZ	5:D:501:HOH:O	2.41	0.63
1:C:124:ARG:HD3	5:D:563:HOH:O	1.97	0.63
2:D:138:GLU:CB	5:D:700:HOH:O	2.46	0.63
2:D:166:ARG:HB2	5:D:607:HOH:O	1.99	0.63
2:F:27:ASN:OD1	2:F:29:GLU:HG3	1.99	0.62
1:G:85:GLU:HB2	5:G:226:HOH:O	1.98	0.62
2:H:24:LEU:O	2:H:33:ARG:NH1	2.34	0.60
2:D:99:MET:HE3	2:D:128:PHE:CE1	2.35	0.60
1:A:12:THR:O	1:A:12:THR:CG2	2.50	0.59
1:E:27:ARG:HH12	2:F:341:PHE:C	2.05	0.59
2:D:18:ARG:HD3	2:D:20:ASP:OD1	2.03	0.59
2:F:93:HIS:CD2	5:F:567:HOH:O	2.49	0.59
2:B:323:PRO:HG3	1:C:100:PRO:HG3	1.85	0.58
1:C:15:ARG:HG3	1:C:15:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:109:ARG:NE	5:D:503:HOH:O	2.28	0.58
2:D:234:PRO:CD	4:D:402:PHB:H3	2.33	0.57
2:H:196:PHE:CB	5:H:516:HOH:O	2.40	0.57
2:D:331:ASP:HB2	2:D:333:THR:CG2	2.35	0.57
1:C:169:ALA:HB1	5:C:255:HOH:O	2.05	0.57
2:H:196:PHE:CD2	5:H:516:HOH:O	2.51	0.57
2:F:16:LYS:N	5:F:506:HOH:O	2.36	0.57
1:G:90:LYS:HB2	1:G:118:MET:HG3	1.86	0.57
1:A:12:THR:O	1:A:12:THR:HG22	2.03	0.57
1:E:81:ASP:O	1:E:145:ALA:HB1	2.05	0.56
1:G:64:GLY:O	1:G:140:TYR:HA	2.04	0.56
1:C:3:ASP:HB2	5:C:279:HOH:O	2.06	0.56
1:C:127:HIS:ND1	2:D:204:PRO:HB3	2.21	0.56
1:A:154:GLY:H	1:A:157:THR:CG2	2.18	0.56
2:B:232:TRP:HA	4:B:402:PHB:O4	2.06	0.56
2:B:322:SER:OG	2:B:324:LYS:HG2	2.05	0.56
2:D:174:MET:HE2	2:D:219:TYR:HE1	1.70	0.55
2:D:331:ASP:CB	2:D:333:THR:HG22	2.36	0.55
2:D:99:MET:CE	2:D:128:PHE:CE1	2.89	0.55
1:E:117:LYS:HG2	5:E:277:HOH:O	2.06	0.55
1:G:76:PHE:HE1	2:H:174:MET:HE3	1.65	0.55
2:F:39:GLY:O	2:F:54:PRO:HD3	2.07	0.55
2:F:240:VAL:HG13	2:F:240:VAL:O	2.07	0.55
1:C:163:GLU:HB3	5:C:292:HOH:O	2.07	0.55
1:A:26:PRO:CG	1:A:168:GLU:HB3	2.37	0.54
2:D:88:PHE:CZ	2:D:99:MET:HE2	2.42	0.54
2:F:18:ARG:NE	5:F:503:HOH:O	2.27	0.54
2:F:18:ARG:HB3	2:F:20:ASP:OD1	2.08	0.52
2:B:225:LEU:HD21	2:B:247:PRO:HB2	1.90	0.52
1:C:31:PHE:O	1:C:165:CYS:HA	2.09	0.52
2:H:70:MET:HE2	2:H:143:PHE:HB2	1.90	0.52
1:E:46:ARG:NH1	1:E:137:TYR:OH	2.40	0.52
2:D:328:MET:HA	2:D:333:THR:HG23	1.91	0.52
2:F:94:TYR:OH	2:F:261:ASP:OD2	2.17	0.52
2:D:196:PHE:CD2	2:D:226:SER:HA	2.45	0.51
1:G:21:ILE:HD12	1:G:24:ASP:O	2.09	0.51
2:F:70:MET:CE	2:F:164:ILE:HA	2.40	0.51
1:C:160:LYS:HB2	1:C:163:GLU:HG3	1.93	0.51
2:F:232:TRP:HA	4:F:402:PHB:O4	2.11	0.51
1:A:153:GLU:HA	1:A:157:THR:HG21	1.92	0.50
2:F:335:PRO:HB2	2:F:337:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLU:HB3	1:A:152:ILE:HG21	1.93	0.50
2:B:162:GLU:H	2:B:162:GLU:CD	2.15	0.50
2:H:77:PHE:CD2	2:H:97:VAL:HG21	2.47	0.49
1:A:97:TYR:CZ	1:A:113:PRO:HB3	2.47	0.49
2:D:48:PHE:HB3	2:D:59:ILE:HG23	1.94	0.49
1:G:153:GLU:HA	1:G:157:THR:HG21	1.94	0.49
1:E:46:ARG:CD	1:E:58:GLU:OE1	2.60	0.49
2:B:254:LEU:HD12	2:B:255:PRO:CD	2.43	0.49
1:G:154:GLY:H	1:G:157:THR:HG23	1.78	0.49
1:C:90:LYS:HE2	5:C:266:HOH:O	2.12	0.49
2:D:257:GLU:OE1	2:D:304:ARG:HD2	2.13	0.49
1:G:80:MET:O	1:G:125:ARG:HG3	2.13	0.49
2:H:97:VAL:HG23	2:H:121:SER:OG	2.12	0.49
1:A:58:GLU:OE2	1:A:157:THR:CG2	2.60	0.48
2:B:254:LEU:HD12	2:B:255:PRO:HD2	1.95	0.48
2:D:20:ASP:OD2	2:D:38:GLY:HA2	2.13	0.48
1:A:3:ASP:N	5:A:202:HOH:O	2.46	0.48
2:D:113:ARG:HD2	5:D:628:HOH:O	2.13	0.48
1:E:27:ARG:NH1	2:F:341:PHE:C	2.66	0.48
2:F:70:MET:CE	2:F:142:PRO:HG2	2.44	0.48
2:H:340:THR:O	2:H:341:PHE:CB	2.61	0.48
2:H:329:ILE:HG13	2:H:334:ALA:HB3	1.94	0.48
2:H:76:GLY:HA2	2:H:125:MET:HE3	1.95	0.48
1:A:123:LEU:HD21	1:A:129:ALA:HB2	1.96	0.48
2:H:258:HIS:O	2:H:304:ARG:HA	2.13	0.48
2:F:240:VAL:CG1	5:F:658:HOH:O	2.51	0.48
2:B:17:ALA:HA	5:B:650:HOH:O	2.13	0.47
2:D:213:GLU:CD	2:D:213:GLU:H	2.17	0.47
2:D:250:GLU:O	2:D:312:ARG:HA	2.14	0.47
2:D:109:ARG:HD3	5:D:510:HOH:O	2.14	0.47
2:D:323:PRO:HD3	5:D:504:HOH:O	2.15	0.47
2:D:234:PRO:HD3	4:D:402:PHB:C3	2.41	0.47
1:C:80:MET:O	1:C:125:ARG:HG3	2.14	0.47
1:C:55:TYR:CD1	2:D:243:SER:HB2	2.49	0.47
1:G:77:VAL:HA	1:G:148:LEU:O	2.15	0.47
1:G:154:GLY:H	1:G:157:THR:CG2	2.28	0.47
1:C:89:LEU:HD22	1:C:113:PRO:HG2	1.96	0.47
1:A:90:LYS:O	1:A:115:GLY:HA3	2.15	0.46
1:E:117:LYS:CD	5:E:289:HOH:O	2.63	0.46
2:F:23:HIS:HB3	2:F:33:ARG:HD3	1.97	0.46
1:A:116:ARG:NH1	2:B:212:PHE:HZ	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:258:HIS:O	2:F:304:ARG:HA	2.16	0.46
1:G:70:SER:HB3	1:G:98:VAL:HG21	1.97	0.46
2:D:174:MET:CE	2:D:219:TYR:HE1	2.29	0.46
2:D:40:PHE:HA	2:D:52:THR:O	2.16	0.46
1:E:46:ARG:HD2	1:E:58:GLU:OE1	2.16	0.46
1:G:122:VAL:HB	2:H:205:VAL:HB	1.98	0.45
2:H:267:LEU:CD1	5:H:525:HOH:O	2.64	0.45
2:F:38:GLY:HA3	2:F:117:GLU:OE1	2.16	0.45
2:H:196:PHE:CD2	2:H:226:SER:HA	2.52	0.45
1:E:71:CYS:SG	1:E:73:HIS:CE1	3.10	0.45
1:C:137:TYR:HD1	5:C:280:HOH:O	1.99	0.45
2:H:113:ARG:HA	2:H:113:ARG:HD2	1.83	0.45
1:E:15:ARG:O	2:F:292:ARG:HD2	2.17	0.45
2:H:90:THR:HA	2:H:98:THR:O	2.17	0.45
2:H:232:TRP:HA	4:H:402:PHB:O4	2.17	0.45
1:A:80:MET:O	1:A:125:ARG:HG3	2.17	0.45
1:E:25:ASP:OD1	1:E:26:PRO:HD2	2.17	0.45
2:H:267:LEU:CG	5:H:525:HOH:O	2.46	0.45
2:B:76:GLY:HA2	2:B:125:MET:HE1	1.98	0.44
2:F:83:ASN:HB2	2:F:257:GLU:HB2	1.99	0.44
1:G:167:THR:C	5:G:232:HOH:O	2.55	0.44
1:G:130:LEU:HB2	2:H:174:MET:HE3	1.98	0.44
2:F:225:LEU:HD11	2:F:247:PRO:HB2	1.99	0.44
1:A:161:TRP:CD2	2:B:339:VAL:HG11	2.52	0.44
2:H:250:GLU:OE2	2:H:315:LEU:HD23	2.17	0.44
1:C:85:GLU:HG3	1:C:122:VAL:HG22	1.99	0.44
2:H:325:ILE:HA	2:H:328:MET:HE2	1.98	0.44
1:G:58:GLU:OE2	1:G:157:THR:CG2	2.52	0.44
1:G:125:ARG:HD3	5:G:212:HOH:O	2.18	0.44
2:H:196:PHE:HD2	5:H:516:HOH:O	1.95	0.44
1:C:3:ASP:CB	5:C:279:HOH:O	2.65	0.44
2:D:253:ILE:HG22	2:D:254:LEU:O	2.17	0.44
2:D:264:GLU:OE2	2:D:319:GLU:OE2	2.36	0.44
2:F:28:ASN:OD1	2:F:28:ASN:N	2.51	0.44
1:E:117:LYS:HB3	5:F:673:HOH:O	2.17	0.44
1:A:71:CYS:SG	1:A:73:HIS:CE1	3.11	0.43
2:D:177:LEU:HA	2:D:177:LEU:HD23	1.89	0.43
2:F:118:ARG:HG3	5:F:567:HOH:O	2.17	0.43
1:A:100:PRO:HG3	2:D:323:PRO:CG	2.44	0.43
2:D:258:HIS:O	2:D:304:ARG:HA	2.18	0.43
1:E:168:GLU:N	5:E:202:HOH:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ARG:O	2:B:292:ARG:HD2	2.19	0.43
2:B:299:MET:HB3	2:B:303:ILE:HD11	2.00	0.43
1:G:151:SER:OG	1:G:152:ILE:N	2.47	0.43
2:H:23:HIS:HB3	2:H:33:ARG:HD3	2.00	0.43
2:D:299:MET:HB3	2:D:303:ILE:HD11	2.01	0.43
1:A:58:GLU:O	1:A:148:LEU:HA	2.19	0.43
2:D:88:PHE:HZ	2:D:99:MET:CE	2.30	0.43
2:F:63:ASP:HB3	2:F:152:PRO:HG3	1.99	0.43
1:G:81:ASP:O	1:G:145:ALA:HB1	2.18	0.43
2:F:170:THR:HG23	2:F:236:VAL:HB	2.01	0.43
2:D:109:ARG:NH2	5:D:503:HOH:O	2.52	0.43
2:H:70:MET:CE	2:H:164:ILE:HA	2.49	0.43
1:A:91:LEU:HD13	1:A:94:SER:HA	2.00	0.42
2:D:94:TYR:OH	2:D:261:ASP:OD2	2.26	0.42
1:E:46:ARG:HD3	1:E:58:GLU:OE1	2.18	0.42
2:H:229:ASP:HB2	5:H:662:HOH:O	2.18	0.42
2:F:39:GLY:H	2:F:117:GLU:CD	2.23	0.42
2:D:278:LYS:HD3	2:D:283:GLY:O	2.20	0.42
2:D:234:PRO:CG	4:D:402:PHB:C3	2.97	0.42
2:F:261:ASP:OD1	2:F:262:ARG:HD2	2.20	0.42
1:G:33:ASN:O	1:G:37:VAL:HG23	2.20	0.42
2:D:303:ILE:C	2:D:303:ILE:HD12	2.40	0.41
2:F:145:ALA:O	2:F:146:PRO:C	2.58	0.41
2:H:211:GLY:N	2:H:213:GLU:OE1	2.53	0.41
1:A:86:VAL:HG22	1:A:139:PHE:CD1	2.55	0.41
2:H:83:ASN:HB2	2:H:257:GLU:HB2	2.02	0.41
1:E:117:LYS:CB	5:F:673:HOH:O	2.69	0.41
1:G:79:ALA:HB3	1:G:124:ARG:O	2.20	0.41
2:H:299:MET:HB3	2:H:303:ILE:HD11	2.02	0.41
2:B:277:VAL:HG13	2:B:303:ILE:HD13	2.02	0.41
2:D:254:LEU:HA	2:D:255:PRO:HD3	1.91	0.41
1:C:120:ARG:HD3	2:D:207:GLU:OE1	2.20	0.41
2:D:202:GLU:HG3	2:D:202:GLU:H	1.64	0.40
2:D:225:LEU:HA	2:D:225:LEU:HD23	1.82	0.40
2:H:254:LEU:HD12	2:H:255:PRO:HD2	2.03	0.40
1:C:161:TRP:CD2	2:D:339:VAL:HG11	2.56	0.40
2:D:88:PHE:CZ	2:D:99:MET:CE	3.04	0.40
2:F:240:VAL:CB	5:F:658:HOH:O	2.00	0.40
2:D:232:TRP:HA	4:D:402:PHB:O4	2.21	0.40
1:G:95:ASP:OD1	1:G:100:PRO:HG3	2.21	0.40
1:C:31:PHE:CZ	2:D:295:ASP:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PRO:HG3	2:B:215:GLU:HG3	2.02	0.40
1:C:15:ARG:NH1	1:C:15:ARG:HG3	2.35	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	164/170 (96%)	158 (96%)	6 (4%)	0	100	100
1	C	165/170 (97%)	154 (93%)	10 (6%)	1 (1%)	25	19
1	E	165/170 (97%)	156 (94%)	8 (5%)	1 (1%)	25	19
1	G	163/170 (96%)	149 (91%)	14 (9%)	0	100	100
2	B	323/341 (95%)	307 (95%)	15 (5%)	1 (0%)	41	37
2	D	327/341 (96%)	310 (95%)	16 (5%)	1 (0%)	41	37
2	F	325/341 (95%)	309 (95%)	15 (5%)	1 (0%)	41	37
2	H	331/341 (97%)	312 (94%)	19 (6%)	0	100	100
All	All	1963/2044 (96%)	1855 (94%)	103 (5%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	252	PHE
2	F	252	PHE
1	C	81	ASP
2	B	252	PHE
1	E	30	VAL

### 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	128/131 (98%)	125 (98%)	3 (2%)	50	53
1	C	129/131 (98%)	123 (95%)	6 (5%)	26	22
1	E	127/131 (97%)	124 (98%)	3 (2%)	49	51
1	G	124/131 (95%)	121 (98%)	3 (2%)	49	51
2	B	268/284 (94%)	262 (98%)	6 (2%)	52	55
2	D	270/284 (95%)	258 (96%)	12 (4%)	28	25
2	F	268/284 (94%)	259 (97%)	9 (3%)	37	36
2	H	269/284 (95%)	262 (97%)	7 (3%)	46	48
All	All	1583/1660 (95%)	1534 (97%)	49 (3%)	40	40

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	VAL
1	A	157	THR
1	A	168	GLU
2	B	19	THR
2	B	78	PHE
2	B	143	PHE
2	B	162	GLU
2	B	164	ILE
2	B	194	ARG
1	C	81	ASP
1	C	101	ASP
1	C	103	GLU
1	C	118	MET
1	C	160	LYS
1	C	163	GLU
2	D	26	ILE
2	D	72	ASP
2	D	143	PHE
2	D	160	ASN

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Mol	Chain	Res	Type
2	D	194	ARG
2	D	202	GLU
2	D	213	GLU
2	D	215	GLU
2	D	247	PRO
2	D	333	THR
2	D	336	VAL
2	D	340	THR
1	E	12	THR
1	E	89	LEU
1	E	138	ARG
2	F	18	ARG
2	F	28	ASN
2	F	29	GLU
2	F	91	ILE
2	F	143	PHE
2	F	194	ARG
2	F	262	ARG
2	F	325	ILE
2	F	336	VAL
1	G	70	SER
1	G	143	GLN
1	G	156	VAL
2	H	70	MET
2	H	78	PHE
2	H	143	PHE
2	H	155	ILE
2	H	164	ILE
2	H	194	ARG
2	H	250	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	160	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PHB	B	402	3	8,10,10	1.18	1 (12%)	10,13,13	0.33	0
4	PHB	D	402	3	8,10,10	1.45	1 (12%)	10,13,13	0.22	0
4	PHB	F	402	3	8,10,10	0.98	1 (12%)	10,13,13	0.44	0
4	PHB	H	402	3	8,10,10	1.09	1 (12%)	10,13,13	0.36	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
4	PHB	B	402	3	-	0/0/4/4	0/1/1/1
4	PHB	D	402	3	-	0/0/4/4	0/1/1/1
4	PHB	F	402	3	-	0/0/4/4	0/1/1/1
4	PHB	H	402	3	-	0/0/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	402	PHB	C1-C1'	4.09	1.51	1.47
4	B	402	PHB	C1-C1'	3.21	1.50	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	402	PHB	C1-C1'	2.96	1.50	1.47
4	F	402	PHB	C1-C1'	2.72	1.50	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	PHB	1	0
4	D	402	PHB	5	0
4	F	402	PHB	1	0
4	H	402	PHB	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	166/170 (97%)	-0.29	0 100 100	14, 25, 40, 52	0
1	C	167/170 (98%)	-0.31	1 (0%) 89 88	16, 26, 39, 55	0
1	E	167/170 (98%)	-0.18	2 (1%) 79 78	17, 27, 44, 61	0
1	G	165/170 (97%)	0.26	9 (5%) 25 24	24, 37, 49, 59	0
2	B	325/341 (95%)	-0.18	1 (0%) 94 93	15, 21, 34, 54	0
2	D	327/341 (95%)	-0.19	3 (0%) 84 83	15, 22, 41, 69	0
2	F	326/341 (95%)	-0.04	1 (0%) 94 93	15, 26, 44, 67	0
2	H	333/341 (97%)	-0.04	8 (2%) 59 57	15, 26, 50, 70	0
All	All	1976/2044 (96%)	-0.12	25 (1%) 77 76	14, 25, 45, 70	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	169	ALA	5.4
2	H	9	ILE	4.8
2	H	10	ILE	4.5
2	H	14	ASP	4.4
2	H	332	GLY	3.7
1	G	108	ILE	3.7
2	H	13	GLY	3.7
2	H	11	ASP	3.1
1	G	140	TYR	3.0
1	G	112	LEU	2.9
1	G	43	PRO	2.9
1	G	111	ALA	2.6
2	H	15	SER	2.6
2	F	25	ALA	2.5
1	G	12	THR	2.5
2	D	15	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	143	GLN	2.4
2	H	330	ALA	2.4
2	D	16	LYS	2.3
1	G	144	PRO	2.2
1	G	89	LEU	2.2
1	E	162	GLY	2.2
1	C	110	GLU	2.2
2	D	334	ALA	2.1
2	B	25	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 carbohydrates 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PHB	D	402	10/10	0.90	0.18	23,28,44,46	0
4	PHB	B	402	10/10	0.95	0.13	24,26,28,36	0
4	PHB	H	402	10/10	0.95	0.13	27,32,36,40	0
4	PHB	F	402	10/10	0.96	0.12	29,33,55,58	0
3	FE	H	401	1/1	0.99	0.06	35,35,35,35	0
3	FE	D	401	1/1	0.99	0.07	32,32,32,32	0
3	FE	F	401	1/1	0.99	0.06	35,35,35,35	0
3	FE	B	401	1/1	1.00	0.06	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.