



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 09:11 am BST

PDB ID : 2B1X  
Title : Crystal structure of naphthalene 1,2-dioxygenase from *Rhodococcus* sp.  
Authors : Gakhar, L.; Malik, Z.A.; Allen, C.C.; Lipscomb, D.A.; Larkin, M.J.; Ramaswamy, S.  
Deposited on : 2005-09-16  
Resolution : 2.00 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

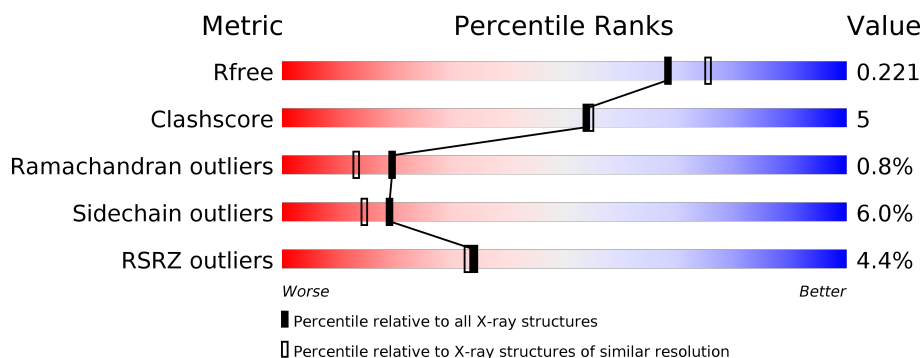
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	470	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>6%</div> </div> </div>
1	C	470	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>6%</div> </div> </div>
1	E	470	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>6%</div> </div> </div>
2	B	172	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>...</div> </div> </div>
2	D	172	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>...</div> </div> </div>
2	F	172	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>...</div> </div> </div>

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
5	MPD	C	1701	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15793 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 naphthalene dioxygenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3514	2238	606	650	20			
1	C	441	Total	C	N	O	S	0	0	0
			3514	2238	606	650	20			
1	E	441	Total	C	N	O	S	0	0	0
			3514	2238	606	650	20			

- Molecule 2 is a protein called naphthalene dioxygenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1340	833	231	268	8			
2	D	167	Total	C	N	O	S	0	0	0
			1340	833	231	268	8			
2	F	167	Total	C	N	O	S	0	0	0
			1340	833	231	268	8			

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

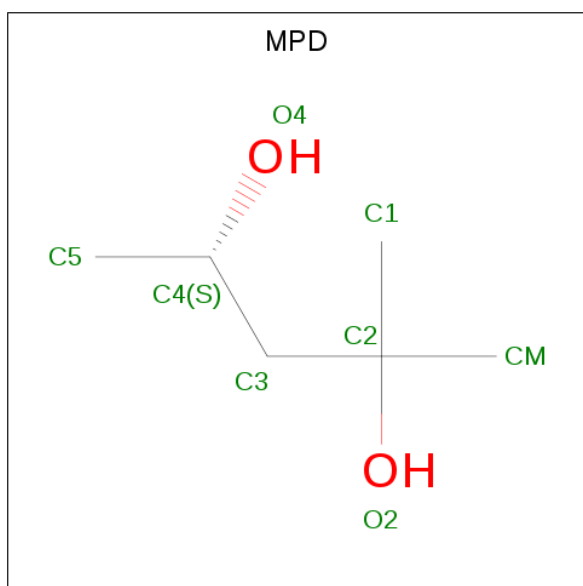
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0
5	E	1	Total C O 8 6 2	0	0

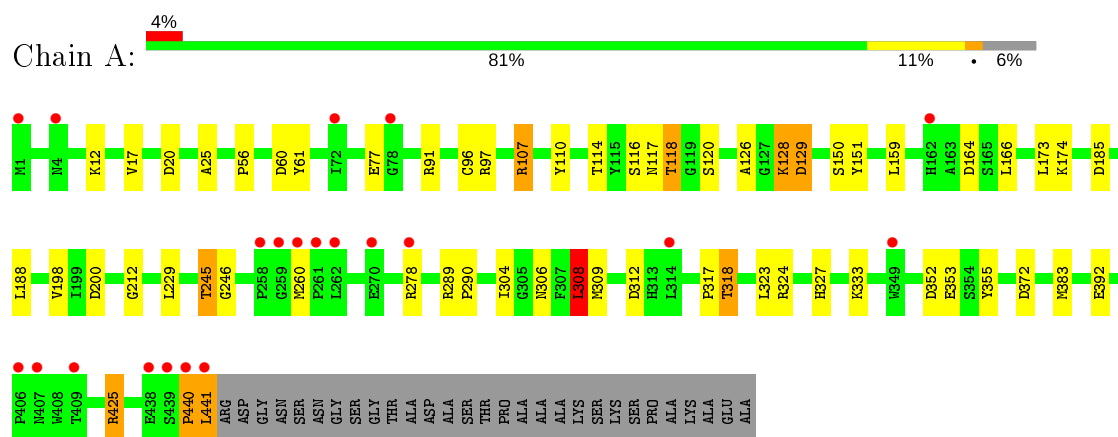
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	253	Total O 253 253	0	0
6	B	95	Total O 95 95	0	0
6	C	251	Total O 251 251	0	0
6	D	109	Total O 109 109	0	0
6	E	298	Total O 298 298	0	0
6	F	106	Total O 106 106	0	0

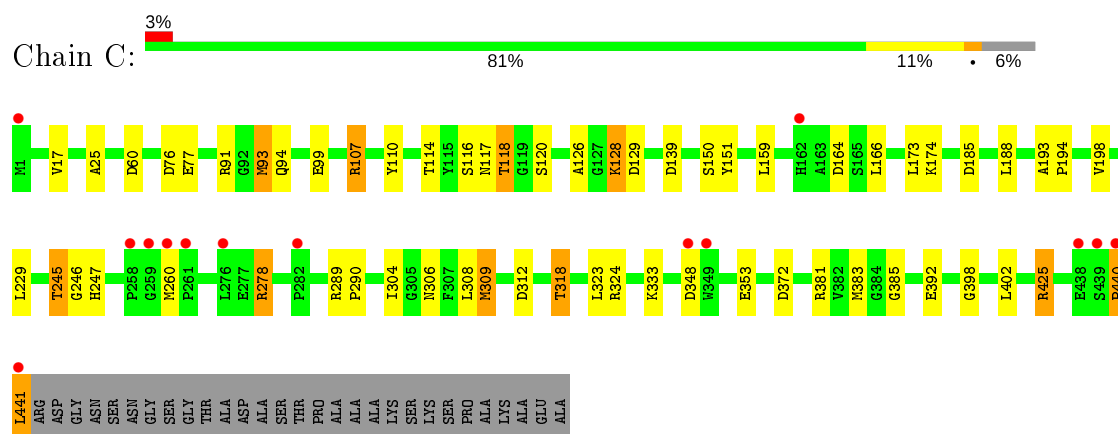
### 3 Residue-property plots [i](#)

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.

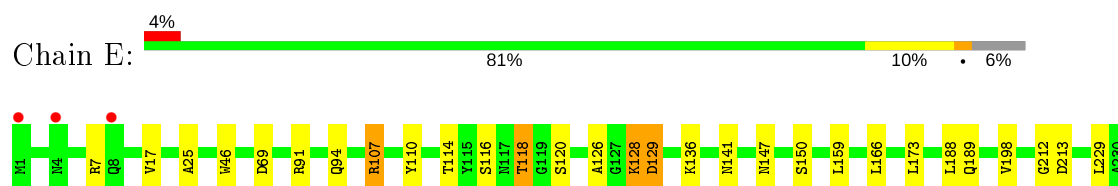
- Molecule 1: naphthalene dioxygenase large subunit



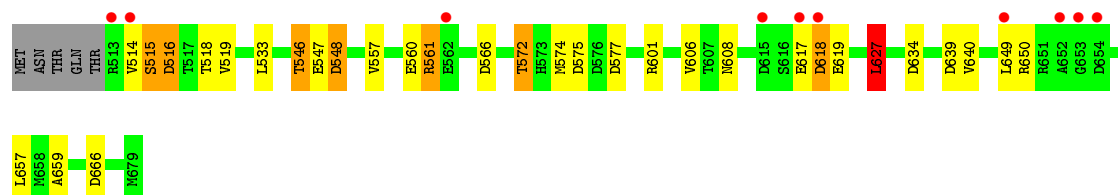
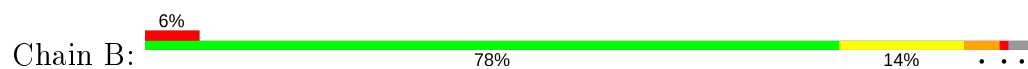
- Molecule 1: naphthalene dioxygenase large subunit



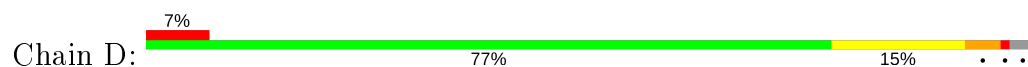
- Molecule 1: naphthalene dioxygenase large subunit



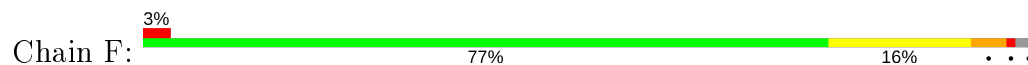
- Molecule 2: naphthalene dioxygenase small subunit



- Molecule 2: naphthalene dioxygenase small subunit



- Molecule 2: naphthalene dioxygenase small subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.74Å 144.25Å 186.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.80 – 2.00 19.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (20.80-2.00) 92.9 (19.96-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.191 , 0.224 0.222 , 0.221	Depositor DCC
$R_{free}$ test set	2949 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.2	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15793	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, FE, FES

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	0.71	0/3620	0.84	11/4919 (0.2%)
1	C	0.71	1/3620 (0.0%)	0.83	9/4919 (0.2%)
1	E	0.81	0/3620	0.86	10/4919 (0.2%)
2	B	0.68	0/1360	0.95	9/1845 (0.5%)
2	D	0.73	0/1360	0.97	9/1845 (0.5%)
2	F	0.74	0/1360	0.99	10/1845 (0.5%)
All	All	0.74	1/14940 (0.0%)	0.88	58/20292 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	93	MET	CG-SD	-5.06	1.68	1.81

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ARG	NE-CZ-NH2	-8.76	115.92	120.30
2	F	618	ASP	CB-CG-OD2	7.93	125.43	118.30
1	A	425	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	E	345	ASP	CB-CG-OD2	7.15	124.74	118.30
1	C	425	ARG	NE-CZ-NH2	-6.99	116.80	120.30
2	D	618	ASP	CB-CG-OD2	6.95	124.55	118.30
2	D	627	LEU	CA-CB-CG	6.86	131.07	115.30
2	B	618	ASP	CB-CG-OD2	6.83	124.45	118.30
2	D	639	ASP	CB-CG-OD2	6.83	124.44	118.30
2	B	627	LEU	CA-CB-CG	6.79	130.91	115.30
1	E	129	ASP	CB-CG-OD2	6.70	124.33	118.30
1	E	425	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	F	627	LEU	CA-CB-CG	6.54	130.35	115.30
1	A	97	ARG	NE-CZ-NH1	6.39	123.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	516	ASP	CB-CG-OD2	6.33	124.00	118.30
2	D	516	ASP	CB-CG-OD2	6.30	123.97	118.30
2	B	516	ASP	CB-CG-OD2	6.29	123.96	118.30
1	C	139	ASP	CB-CG-OD2	6.24	123.92	118.30
2	F	666	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	352	ASP	CB-CG-OD2	6.12	123.81	118.30
2	F	534	ASP	CB-CG-OD2	6.07	123.77	118.30
2	B	639	ASP	CB-CG-OD2	6.02	123.72	118.30
2	B	666	ASP	CB-CG-OD2	6.01	123.71	118.30
1	E	213	ASP	CB-CG-OD2	6.00	123.69	118.30
1	A	129	ASP	CB-CG-OD2	5.97	123.67	118.30
2	F	597	ASP	CB-CG-OD2	5.95	123.65	118.30
2	D	548	ASP	CB-CG-OD2	5.93	123.64	118.30
1	E	312	ASP	CB-CG-OD2	5.89	123.60	118.30
1	E	372	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	372	ASP	CB-CG-OD2	5.73	123.46	118.30
2	F	561	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	312	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	76	ASP	CB-CG-OD1	5.66	123.40	118.30
2	D	647	ASP	CB-CG-OD2	5.55	123.30	118.30
2	F	647	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	308	LEU	CA-CB-CG	5.51	127.97	115.30
2	D	572	THR	N-CA-CB	-5.49	99.86	110.30
1	A	20	ASP	CB-CG-OD2	5.47	123.22	118.30
1	C	425	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	F	548	ASP	CB-CG-OD2	5.45	123.21	118.30
2	D	666	ASP	CB-CG-OD2	5.45	123.21	118.30
2	B	561	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	F	615	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	97	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	C	372	ASP	CB-CG-OD2	5.37	123.13	118.30
1	E	245	THR	N-CA-CB	-5.37	100.11	110.30
1	A	164	ASP	CB-CG-OD2	5.35	123.11	118.30
1	E	348	ASP	CB-CG-OD2	5.27	123.04	118.30
2	B	548	ASP	CB-CG-OD2	5.15	122.93	118.30
2	B	634	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	60	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	312	ASP	CB-CG-OD2	5.10	122.89	118.30
1	E	308	LEU	CA-CB-CG	5.08	126.98	115.30
1	C	348	ASP	CB-CG-OD2	5.07	122.87	118.30
2	D	534	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	164	ASP	CB-CG-OD2	5.05	122.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	332	ASP	CB-CG-OD2	5.04	122.84	118.30
2	B	577	ASP	CB-CG-OD1	5.03	122.83	118.30

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	3514	0	3344	30	0
1	C	3514	0	3344	33	0
1	E	3514	0	3344	39	0
2	B	1340	0	1307	19	0
2	D	1340	0	1307	19	0
2	F	1340	0	1307	19	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	4	0	0	0	0
4	C	4	0	0	0	0
4	E	4	0	0	0	0
5	A	32	0	56	0	0
5	C	24	0	42	5	0
5	E	48	0	84	2	0
6	A	253	0	0	3	0
6	B	95	0	0	1	0
6	C	251	0	0	3	0
6	D	109	0	0	0	0
6	E	298	0	0	11	0
6	F	106	0	0	2	0
All	All	15793	0	14135	154	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 5.

All (154) 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)
2:B:572:THR:HG21	2:B:575:ASP:HB2	1.45	0.98
2:F:572:THR:HG21	2:F:575:ASP:HB2	1.43	0.98
2:D:572:THR:HG21	2:D:575:ASP:HB2	1.46	0.96
2:B:608:ASN:HD21	2:F:606:VAL:H	1.26	0.84
1:E:128:LYS:HD2	1:E:129:ASP:H	1.42	0.81
5:C:1707:MPD:H13	1:E:94:GLN:OE1	1.81	0.81
1:A:118:THR:HG22	1:A:120:SER:H	1.46	0.80
1:A:128:LYS:HD2	1:A:129:ASP:H	1.47	0.79
1:C:118:THR:HG22	1:C:120:SER:H	1.47	0.77
1:E:118:THR:HG22	1:E:120:SER:H	1.51	0.76
2:F:619:GLU:HG2	2:F:650:ARG:HG2	1.67	0.76
2:D:619:GLU:HG2	2:D:650:ARG:HG2	1.66	0.75
1:E:128:LYS:CD	1:E:129:ASP:H	1.99	0.75
2:B:606:VAL:H	2:D:608:ASN:HD21	1.34	0.74
2:D:606:VAL:H	2:F:608:ASN:HD21	1.34	0.74
1:E:141:ASN:HB2	6:E:1829:HOH:O	1.86	0.74
2:B:619:GLU:HG2	2:B:650:ARG:HG2	1.69	0.74
1:E:107:ARG:HD2	1:E:114:THR:OG1	1.87	0.73
1:C:128:LYS:HD2	1:C:129:ASP:H	1.54	0.71
2:F:572:THR:HG23	2:F:574:MET:H	1.58	0.68
1:E:189:GLN:HB2	6:E:1740:HOH:O	1.94	0.68
2:D:546:THR:HG23	2:D:548:ASP:OD1	1.94	0.68
1:E:118:THR:HG21	6:E:1874:HOH:O	1.94	0.67
1:A:128:LYS:CD	1:A:129:ASP:H	2.09	0.65
1:A:107:ARG:HD2	1:A:114:THR:OG1	1.97	0.65
1:C:25:ALA:HB1	1:C:383:MET:CE	2.27	0.65
1:A:304:ILE:HG12	1:A:323:LEU:HD22	1.79	0.65
1:A:185:ASP:OD2	1:A:278:ARG:NH2	2.29	0.64
1:C:128:LYS:CD	1:C:129:ASP:H	2.11	0.64
1:E:25:ALA:HB1	1:E:383:MET:HE1	1.80	0.64
1:C:107:ARG:HD2	1:C:114:THR:OG1	1.98	0.63
1:C:304:ILE:HG12	1:C:323:LEU:HD22	1.81	0.62
1:C:25:ALA:HB1	1:C:383:MET:HE1	1.80	0.62
1:E:128:LYS:HD2	1:E:128:LYS:H	1.63	0.62
1:E:25:ALA:HB1	1:E:383:MET:CE	2.29	0.62
2:F:547:GLU:CD	2:F:547:GLU:H	2.02	0.62
2:F:679:MET:HE2	6:F:737:HOH:O	1.99	0.62
2:D:546:THR:CG2	2:D:548:ASP:OD1	2.49	0.61
2:B:515:SER:HB3	2:B:518:THR:HB	1.83	0.60
1:C:381:ARG:HH11	5:C:1707:MPD:H11	1.67	0.60
1:C:17:VAL:O	1:C:425:ARG:HD2	2.01	0.59
1:E:126:ALA:HA	1:E:128:LYS:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:547:GLU:CD	2:B:547:GLU:H	2.08	0.57
1:E:128:LYS:CD	1:E:128:LYS:H	2.16	0.57
1:E:116:SER:OG	1:E:118:THR:HB	2.03	0.57
2:F:515:SER:HB3	2:F:518:THR:HB	1.85	0.57
1:E:231:PRO:HB3	5:E:1712:MPD:H13	1.87	0.57
1:E:189:GLN:CB	6:E:1740:HOH:O	2.53	0.56
1:C:185:ASP:OD2	1:C:278:ARG:NH2	2.37	0.56
2:D:547:GLU:CD	2:D:547:GLU:H	2.08	0.56
2:B:546:THR:CG2	2:B:659:ALA:HA	2.36	0.55
1:C:77:GLU:HG2	1:C:117:ASN:HD21	1.71	0.55
2:F:627:LEU:HD13	2:F:640:VAL:HG13	1.88	0.55
1:E:308:LEU:HD22	1:E:317:PRO:HB2	1.88	0.55
1:E:318:THR:HG23	6:E:1720:HOH:O	2.04	0.55
2:D:627:LEU:HD13	2:D:640:VAL:HG13	1.89	0.55
1:C:381:ARG:HD3	5:C:1707:MPD:H12	1.89	0.55
1:E:304:ILE:HG12	1:E:323:LEU:HD22	1.88	0.55
2:F:546:THR:HG23	2:F:548:ASP:OD1	2.07	0.54
2:D:515:SER:HB3	2:D:518:THR:HB	1.88	0.54
2:F:619:GLU:OE2	2:F:650:ARG:HD3	2.08	0.54
1:E:17:VAL:O	1:E:425:ARG:HD2	2.08	0.54
1:A:198:VAL:HG11	1:A:333:LYS:HE3	1.90	0.53
1:E:7:ARG:NH2	6:E:1980:HOH:O	2.42	0.53
1:A:25:ALA:HB1	1:A:383:MET:CE	2.39	0.52
1:A:25:ALA:HB1	1:A:383:MET:HE1	1.91	0.52
1:E:327:HIS:HD2	6:E:1725:HOH:O	1.92	0.52
1:E:128:LYS:HD2	1:E:129:ASP:N	2.20	0.52
2:B:515:SER:HB2	2:B:519:VAL:HG23	1.92	0.52
1:E:128:LYS:HD2	1:E:128:LYS:N	2.25	0.52
1:C:318:THR:HG23	6:C:1715:HOH:O	2.09	0.52
1:C:99:GLU:HG3	2:D:558:THR:HB	1.92	0.51
1:E:245:THR:HG22	1:E:246:GLY:O	2.10	0.51
1:A:383:MET:HE3	1:A:383:MET:HA	1.92	0.51
1:A:126:ALA:HA	1:A:128:LYS:HE2	1.92	0.51
2:F:572:THR:HG23	2:F:574:MET:N	2.23	0.51
1:A:12:LYS:NZ	6:A:1813:HOH:O	2.43	0.51
2:B:546:THR:HG23	2:B:548:ASP:OD1	2.11	0.50
1:C:318:THR:HG21	1:C:353:GLU:HB3	1.91	0.50
2:F:546:THR:HG23	2:F:548:ASP:H	1.75	0.50
2:B:546:THR:HG21	2:B:659:ALA:HA	1.92	0.50
1:A:318:THR:HG23	6:A:1714:HOH:O	2.10	0.50
1:C:128:LYS:HD2	1:C:128:LYS:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:557:VAL:O	2:F:566:ASP:HB2	2.11	0.50
1:A:151:TYR:CE2	1:A:174:LYS:HD2	2.47	0.50
1:C:318:THR:CG2	6:C:1715:HOH:O	2.60	0.49
1:A:128:LYS:HD2	1:A:128:LYS:H	1.78	0.49
2:F:644:GLU:OE1	6:F:715:HOH:O	2.20	0.49
1:E:46:TRP:CH2	1:E:147:ASN:HB3	2.48	0.49
2:D:546:THR:HG23	2:D:548:ASP:H	1.78	0.48
1:A:77:GLU:HG2	1:A:117:ASN:HD21	1.78	0.48
2:B:572:THR:HG23	2:B:574:MET:H	1.77	0.48
2:F:515:SER:HB2	2:F:519:VAL:HG23	1.96	0.48
1:A:128:LYS:CD	1:A:128:LYS:H	2.27	0.48
2:D:515:SER:HB2	2:D:519:VAL:HG23	1.96	0.48
1:E:107:ARG:CD	1:E:114:THR:OG1	2.60	0.48
1:A:327:HIS:HD2	6:A:1959:HOH:O	1.97	0.47
1:C:107:ARG:HH12	5:C:1701:MPD:HM1	1.79	0.47
1:C:128:LYS:H	1:C:128:LYS:CD	2.26	0.47
2:D:619:GLU:OE2	2:D:650:ARG:HD3	2.15	0.47
2:D:546:THR:CG2	2:D:659:ALA:HA	2.45	0.47
1:C:126:ALA:HA	1:C:128:LYS:HE2	1.97	0.47
2:D:572:THR:HG23	2:D:574:MET:H	1.79	0.46
1:A:308:LEU:HD22	1:A:317:PRO:HB2	1.97	0.46
1:E:318:THR:HG21	1:E:353:GLU:HB3	1.97	0.46
2:B:627:LEU:HD13	2:B:640:VAL:HG13	1.97	0.46
2:B:619:GLU:OE2	2:B:650:ARG:HD3	2.15	0.46
2:D:608:ASN:N	2:D:608:ASN:HD22	2.14	0.46
2:B:560:GLU:OE1	6:B:773:HOH:O	2.21	0.46
1:C:247:HIS:HD2	6:C:1805:HOH:O	1.99	0.46
1:C:116:SER:OG	1:C:118:THR:HB	2.15	0.46
1:C:107:ARG:HH22	5:C:1701:MPD:H31	1.80	0.46
1:E:318:THR:CG2	6:E:1720:HOH:O	2.61	0.46
2:B:546:THR:HG23	2:B:548:ASP:H	1.80	0.46
1:E:327:HIS:HE1	6:E:1841:HOH:O	1.99	0.45
1:A:17:VAL:O	1:A:425:ARG:HD2	2.16	0.45
1:A:61:TYR:CE1	1:A:96:CYS:SG	3.10	0.45
1:E:309:MET:HE2	1:E:309:MET:HB2	1.87	0.45
1:C:245:THR:HG22	1:C:246:GLY:O	2.16	0.45
2:F:546:THR:CG2	2:F:548:ASP:OD1	2.64	0.45
1:C:198:VAL:HG11	1:C:333:LYS:HE3	1.99	0.45
2:D:622:VAL:HG21	2:D:649:LEU:HD22	1.98	0.45
2:B:572:THR:HG23	2:B:574:MET:N	2.32	0.44
2:D:557:VAL:O	2:D:566:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:546:THR:CG2	2:F:659:ALA:HA	2.47	0.44
2:D:546:THR:HG21	2:D:659:ALA:HA	1.99	0.44
1:E:198:VAL:HG11	1:E:333:LYS:HE3	2.00	0.44
1:E:440:PRO:O	1:E:441:LEU:HB2	2.18	0.44
1:A:318:THR:HG21	1:A:353:GLU:HB3	2.00	0.43
1:E:136:LYS:HE2	6:E:1910:HOH:O	2.19	0.43
1:E:128:LYS:CD	1:E:129:ASP:N	2.75	0.43
1:E:341:LEU:HD12	1:E:341:LEU:N	2.34	0.43
1:A:116:SER:OG	1:A:118:THR:HB	2.19	0.43
1:A:440:PRO:O	1:A:441:LEU:HB2	2.18	0.43
2:F:602:SER:HA	2:F:629:TYR:O	2.19	0.42
1:A:245:THR:HG22	1:A:246:GLY:O	2.19	0.42
1:C:309:MET:HE2	1:C:309:MET:HB2	1.96	0.42
1:A:56:PRO:HD2	1:A:60:ASP:OD2	2.20	0.42
1:C:151:TYR:CE2	1:C:174:LYS:HD2	2.55	0.41
1:C:289:ARG:HB3	1:C:290:PRO:HD3	2.02	0.41
1:C:385:GLY:HA3	1:E:69:ASP:OD1	2.20	0.41
1:C:398:GLY:HA3	1:C:402:LEU:HG	2.02	0.41
1:C:440:PRO:O	1:C:441:LEU:HB2	2.21	0.41
1:C:93:MET:HG2	1:C:94:GLN:N	2.36	0.41
1:A:355:TYR:OH	2:B:572:THR:HB	2.21	0.41
1:E:383:MET:HE3	1:E:383:MET:HA	2.03	0.41
1:A:289:ARG:HB3	1:A:290:PRO:HD3	2.02	0.41
1:C:193:ALA:HB1	1:C:194:PRO:HD2	2.03	0.41
1:A:200:ASP:OD1	1:A:200:ASP:N	2.51	0.41
1:E:382:VAL:HG22	6:E:1745:HOH:O	2.21	0.41
2:B:546:THR:CG2	2:B:548:ASP:OD1	2.69	0.40
2:B:557:VAL:O	2:B:566:ASP:HB2	2.21	0.40
1:A:128:LYS:HD2	1:A:129:ASP:N	2.26	0.40
5:E:1711:MPD:O4	5:E:1711:MPD:HM3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/470 (93%)	425 (97%)	12 (3%)	2 (0%)	29	23
1	C	439/470 (93%)	423 (96%)	15 (3%)	1 (0%)	47	44
1	E	439/470 (93%)	428 (98%)	9 (2%)	2 (0%)	29	23
2	B	165/172 (96%)	155 (94%)	7 (4%)	3 (2%)	8	3
2	D	165/172 (96%)	156 (94%)	6 (4%)	3 (2%)	8	3
2	F	165/172 (96%)	155 (94%)	7 (4%)	3 (2%)	8	3
All	All	1812/1926 (94%)	1742 (96%)	56 (3%)	14 (1%)	19	13

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	514	VAL
2	B	516	ASP
2	D	514	VAL
2	D	516	ASP
2	F	514	VAL
2	F	516	ASP
1	E	440	PRO
2	B	515	SER
1	C	440	PRO
2	D	515	SER
2	F	515	SER
1	A	440	PRO
1	E	212	GLY
1	A	212	GLY

### 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	371/389 (95%)	351 (95%)	20 (5%)	22	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	371/389 (95%)	350 (94%)	21 (6%)	20	16
1	E	371/389 (95%)	349 (94%)	22 (6%)	19	15
2	B	147/154 (96%)	137 (93%)	10 (7%)	16	11
2	D	147/154 (96%)	135 (92%)	12 (8%)	11	7
2	F	147/154 (96%)	138 (94%)	9 (6%)	18	14
All	All	1554/1629 (95%)	1460 (94%)	94 (6%)	19	14

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	107	ARG
1	A	110	TYR
1	A	118	THR
1	A	128	LYS
1	A	150	SER
1	A	159	LEU
1	A	166	LEU
1	A	173	LEU
1	A	188	LEU
1	A	229	LEU
1	A	245	THR
1	A	260	MET
1	A	306	ASN
1	A	308	LEU
1	A	309	MET
1	A	318	THR
1	A	324	ARG
1	A	392	GLU
1	A	441	LEU
2	B	533	LEU
2	B	546	THR
2	B	561	ARG
2	B	572	THR
2	B	601	ARG
2	B	617	GLU
2	B	618	ASP
2	B	627	LEU
2	B	649	LEU
2	B	657	LEU

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Mol	Chain	Res	Type
1	C	91	ARG
1	C	107	ARG
1	C	110	TYR
1	C	118	THR
1	C	128	LYS
1	C	150	SER
1	C	159	LEU
1	C	166	LEU
1	C	173	LEU
1	C	188	LEU
1	C	229	LEU
1	C	245	THR
1	C	260	MET
1	C	278	ARG
1	C	306	ASN
1	C	308	LEU
1	C	309	MET
1	C	318	THR
1	C	324	ARG
1	C	392	GLU
1	C	441	LEU
2	D	533	LEU
2	D	546	THR
2	D	552	VAL
2	D	561	ARG
2	D	572	THR
2	D	601	ARG
2	D	608	ASN
2	D	617	GLU
2	D	618	ASP
2	D	627	LEU
2	D	649	LEU
2	D	657	LEU
1	E	91	ARG
1	E	107	ARG
1	E	110	TYR
1	E	118	THR
1	E	128	LYS
1	E	150	SER
1	E	159	LEU
1	E	166	LEU
1	E	173	LEU

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Mol	Chain	Res	Type
1	E	188	LEU
1	E	229	LEU
1	E	245	THR
1	E	260	MET
1	E	276	LEU
1	E	278	ARG
1	E	306	ASN
1	E	308	LEU
1	E	309	MET
1	E	318	THR
1	E	324	ARG
1	E	392	GLU
1	E	441	LEU
2	F	533	LEU
2	F	546	THR
2	F	561	ARG
2	F	572	THR
2	F	601	ARG
2	F	618	ASP
2	F	627	LEU
2	F	649	LEU
2	F	657	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	HIS
2	B	608	ASN
1	C	327	HIS
2	D	608	ASN
1	E	327	HIS
2	F	608	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 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	$\# Z  > 2$
5	MPD	A	1709	-	7,7,7	0.31	0	9,10,10	0.32	0
4	FES	E	501	1	0,4,4	0.00	-	-		
5	MPD	A	1703	-	7,7,7	0.63	0	9,10,10	0.52	0
5	MPD	C	1707	-	7,7,7	0.83	0	9,10,10	0.87	1 (11%)
4	FES	A	501	1	0,4,4	0.00	-	-		
5	MPD	E	1711	-	7,7,7	0.59	0	9,10,10	0.25	0
5	MPD	E	1708	-	7,7,7	0.37	0	9,10,10	0.57	0
5	MPD	A	1702	-	7,7,7	0.33	0	9,10,10	0.35	0
5	MPD	C	1701	-	7,7,7	0.29	0	9,10,10	0.44	0
5	MPD	E	1712	-	7,7,7	0.22	0	9,10,10	0.71	0
5	MPD	E	1713	-	7,7,7	0.36	0	9,10,10	0.93	0
5	MPD	E	1705	-	7,7,7	0.39	0	9,10,10	0.35	0
5	MPD	C	1704	-	7,7,7	0.44	0	9,10,10	1.00	1 (11%)
5	MPD	A	1700	-	7,7,7	0.54	0	9,10,10	0.75	0
5	MPD	E	1710	-	7,7,7	0.27	0	9,10,10	0.38	0
4	FES	C	501	1	0,4,4	0.00	-	-		

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
5	MPD	A	1709	-	-	2/5/5/5	-
4	FES	E	501	1	-	-	0/1/1/1
5	MPD	A	1703	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	C	1707	-	-	0/5/5/5	-
4	FES	A	501	1	-	-	0/1/1/1
5	MPD	E	1711	-	-	0/5/5/5	-
5	MPD	A	1702	-	-	1/5/5/5	-
4	FES	C	501	1	-	-	0/1/1/1
5	MPD	C	1701	-	-	0/5/5/5	-
5	MPD	E	1712	-	-	1/5/5/5	-
5	MPD	E	1713	-	-	1/5/5/5	-
5	MPD	E	1705	-	-	3/5/5/5	-
5	MPD	C	1704	-	-	1/5/5/5	-
5	MPD	A	1700	-	-	0/5/5/5	-
5	MPD	E	1710	-	-	1/5/5/5	-
5	MPD	E	1708	-	-	0/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1704	MPD	CM-C2-C1	-2.65	105.06	110.57
5	C	1707	MPD	CM-C2-C1	-2.17	106.05	110.57

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1709	MPD	C2-C3-C4-O4
5	E	1713	MPD	C2-C3-C4-O4
5	E	1705	MPD	C2-C3-C4-O4
5	C	1704	MPD	O2-C2-C3-C4
5	A	1709	MPD	C2-C3-C4-C5
5	A	1702	MPD	C2-C3-C4-C5
5	E	1712	MPD	C2-C3-C4-C5
5	E	1705	MPD	C2-C3-C4-C5
5	E	1705	MPD	O2-C2-C3-C4
5	E	1710	MPD	C2-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1707	MPD	3	0
5	E	1711	MPD	1	0
5	C	1701	MPD	2	0
5	E	1712	MPD	1	0

## 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, 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	441/470 (93%)	0.15	21 (4%) 30 29	9, 15, 27, 60	0
1	C	441/470 (93%)	0.09	14 (3%) 47 46	9, 15, 27, 60	0
1	E	441/470 (93%)	0.03	18 (4%) 37 36	9, 15, 27, 60	0
2	B	167/172 (97%)	0.15	10 (5%) 21 20	10, 17, 38, 63	0
2	D	167/172 (97%)	0.14	12 (7%) 15 14	10, 17, 38, 63	0
2	F	167/172 (97%)	0.07	6 (3%) 42 42	10, 17, 38, 63	0
All	All	1824/1926 (94%)	0.10	81 (4%) 34 33	9, 15, 32, 63	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	441	LEU	9.8
1	E	439	SER	8.0
1	E	1	MET	7.8
1	E	440	PRO	6.9
2	F	514	VAL	6.4
1	A	258	PRO	6.2
2	D	514	VAL	6.2
1	C	440	PRO	5.7
2	D	617	GLU	5.7
1	E	259	GLY	5.6
1	C	1	MET	5.4
1	A	1	MET	5.4
1	A	441	LEU	5.3
1	C	258	PRO	5.2
1	C	439	SER	5.2
1	A	259	GLY	5.2
1	E	261	PRO	5.2
2	D	654	ASP	5.1
1	E	441	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	259	GLY	4.8
1	E	260	MET	4.6
1	A	261	PRO	4.5
1	E	258	PRO	4.5
1	C	260	MET	4.4
1	A	439	SER	4.3
2	B	513	ARG	4.1
2	D	649	LEU	4.0
2	F	617	GLU	4.0
2	F	564	VAL	3.9
2	D	564	VAL	3.9
2	B	654	ASP	3.8
1	E	406	PRO	3.8
2	F	654	ASP	3.7
1	A	260	MET	3.7
1	A	440	PRO	3.5
2	B	649	LEU	3.5
2	B	514	VAL	3.5
2	B	653	GLY	3.4
2	D	618	ASP	3.3
1	C	261	PRO	3.2
2	D	653	GLY	3.1
1	A	349	TRP	3.1
2	B	617	GLU	3.0
1	A	262	LEU	3.0
2	B	562	GLU	3.0
1	A	4	ASN	2.9
2	D	562	GLU	2.7
1	E	407	ASN	2.6
1	C	348	ASP	2.6
2	F	513	ARG	2.5
1	A	438	GLU	2.5
2	D	652	ALA	2.5
1	A	162	HIS	2.5
2	F	649	LEU	2.4
1	A	407	ASN	2.4
1	A	406	PRO	2.4
1	C	276	LEU	2.4
1	E	403	GLU	2.4
1	E	401	VAL	2.4
1	C	349	TRP	2.4
1	E	4	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	270	GLU	2.3
1	E	402	LEU	2.3
2	B	618	ASP	2.3
2	D	513	ARG	2.3
2	B	652	ALA	2.3
1	E	400	GLY	2.3
1	C	162	HIS	2.2
1	A	278	ARG	2.2
1	A	72	ILE	2.2
1	E	262	LEU	2.2
1	A	409	THR	2.2
1	C	282	PRO	2.2
2	B	615	ASP	2.2
1	A	78	GLY	2.1
2	D	517	THR	2.1
1	E	276	LEU	2.1
2	D	547	GLU	2.1
1	E	8	GLN	2.1
1	C	438	GLU	2.0
1	A	314	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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
5	MPD	A	1709	8/8	0.52	0.39	71,72,73,73	0
5	MPD	C	1701	8/8	0.58	0.40	75,76,79,79	0
5	MPD	E	1713	8/8	0.71	0.35	41,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MPD	E	1705	8/8	0.73	0.28	56,59,61,61	0
5	MPD	E	1712	8/8	0.76	0.28	63,64,65,65	0
5	MPD	A	1703	8/8	0.78	0.25	30,33,36,38	0
5	MPD	E	1710	8/8	0.78	0.34	97,97,97,97	0
5	MPD	A	1702	8/8	0.81	0.23	68,68,70,70	0
5	MPD	E	1711	8/8	0.84	0.22	33,34,35,36	0
5	MPD	C	1704	8/8	0.89	0.22	26,29,34,34	0
5	MPD	C	1707	8/8	0.91	0.14	20,24,28,28	0
5	MPD	E	1708	8/8	0.93	0.13	24,30,34,39	0
5	MPD	A	1700	8/8	0.95	0.12	25,28,32,33	0
3	FE	A	502	1/1	0.99	0.05	19,19,19,19	0
4	FES	A	501	4/4	0.99	0.04	20,20,20,22	0
3	FE	E	502	1/1	0.99	0.02	21,21,21,21	0
4	FES	E	501	4/4	0.99	0.03	19,19,19,20	0
3	FE	C	502	1/1	0.99	0.05	21,21,21,21	0
4	FES	C	501	4/4	0.99	0.04	20,20,21,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.