



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:35 PM GMT

PDB ID : 1PN0  
Title : Phenol hydroxylase from Trichosporon cutaneum  
Authors : Enroth, C.  
Deposited on : 2003-06-12  
Resolution : 1.70 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

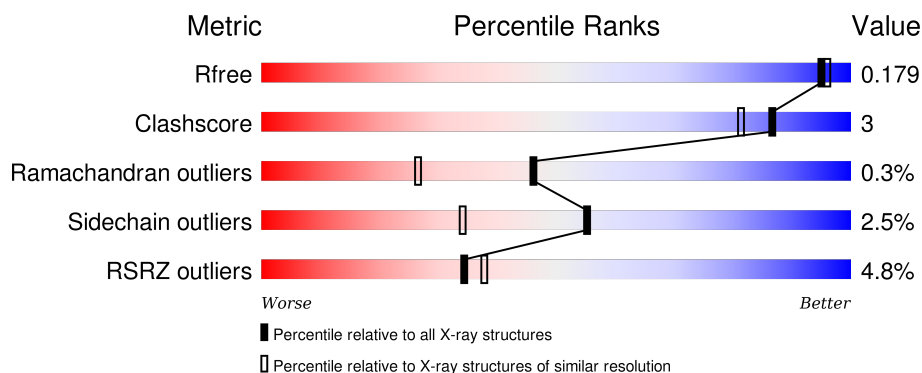
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	665	<div> <div>4%</div> <div>89% 8% ..</div> </div>
1	B	665	<div> <div>5%</div> <div>90% 8% .</div> </div>
1	C	665	<div> <div>5%</div> <div>90% 8% ..</div> </div>
1	D	665	<div> <div>5%</div> <div>90% 7% ..</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23772 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 Phenol 2-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	652	Total	C	N	O	S	15	0	0
			5187	3259	912	992	24			
1	B	652	Total	C	N	O	S	21	0	0
			5193	3263	913	993	24			
1	C	656	Total	C	N	O	S	5	0	0
			5230	3284	923	999	24			
1	D	656	Total	C	N	O	S	5	0	0
			5230	3284	923	999	24			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	ARG	HIS	SEE REMARK 999	UNP P15245
A	171	GLU	ASP	SEE REMARK 999	UNP P15245
A	172	ASP	HIS	SEE REMARK 999	UNP P15245
A	186	GLY	SER	SEE REMARK 999	UNP P15245
A	189	ARG	HIS	SEE REMARK 999	UNP P15245
A	265	ARG	PRO	SEE REMARK 999	UNP P15245
A	405	GLN	HIS	SEE REMARK 999	UNP P15245
A	406	PRO	ALA	SEE REMARK 999	UNP P15245
A	532	ALA	SER	SEE REMARK 999	UNP P15245
A	544	ARG	LEU	SEE REMARK 999	UNP P15245
A	549	GLY	VAL	SEE REMARK 999	UNP P15245
A	550	ALA	SER	SEE REMARK 999	UNP P15245
B	123	ARG	HIS	SEE REMARK 999	UNP P15245
B	171	GLU	ASP	SEE REMARK 999	UNP P15245
B	172	ASP	HIS	SEE REMARK 999	UNP P15245
B	186	GLY	SER	SEE REMARK 999	UNP P15245
B	189	ARG	HIS	SEE REMARK 999	UNP P15245
B	265	ARG	PRO	SEE REMARK 999	UNP P15245
B	405	GLN	HIS	SEE REMARK 999	UNP P15245
B	406	PRO	ALA	SEE REMARK 999	UNP P15245
B	532	ALA	SER	SEE REMARK 999	UNP P15245

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Chain	Residue	Modelled	Actual	Comment	Reference
B	544	ARG	LEU	SEE REMARK 999	UNP P15245
B	549	GLY	VAL	SEE REMARK 999	UNP P15245
B	550	ALA	SER	SEE REMARK 999	UNP P15245
C	123	ARG	HIS	SEE REMARK 999	UNP P15245
C	171	GLU	ASP	SEE REMARK 999	UNP P15245
C	172	ASP	HIS	SEE REMARK 999	UNP P15245
C	186	GLY	SER	SEE REMARK 999	UNP P15245
C	189	ARG	HIS	SEE REMARK 999	UNP P15245
C	265	ARG	PRO	SEE REMARK 999	UNP P15245
C	405	GLN	HIS	SEE REMARK 999	UNP P15245
C	406	PRO	ALA	SEE REMARK 999	UNP P15245
C	532	ALA	SER	SEE REMARK 999	UNP P15245
C	544	ARG	LEU	SEE REMARK 999	UNP P15245
C	549	GLY	VAL	SEE REMARK 999	UNP P15245
C	550	ALA	SER	SEE REMARK 999	UNP P15245
D	123	ARG	HIS	SEE REMARK 999	UNP P15245
D	171	GLU	ASP	SEE REMARK 999	UNP P15245
D	172	ASP	HIS	SEE REMARK 999	UNP P15245
D	186	GLY	SER	SEE REMARK 999	UNP P15245
D	189	ARG	HIS	SEE REMARK 999	UNP P15245
D	265	ARG	PRO	SEE REMARK 999	UNP P15245
D	405	GLN	HIS	SEE REMARK 999	UNP P15245
D	406	PRO	ALA	SEE REMARK 999	UNP P15245
D	532	ALA	SER	SEE REMARK 999	UNP P15245
D	544	ARG	LEU	SEE REMARK 999	UNP P15245
D	549	GLY	VAL	SEE REMARK 999	UNP P15245
D	550	ALA	SER	SEE REMARK 999	UNP P15245

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

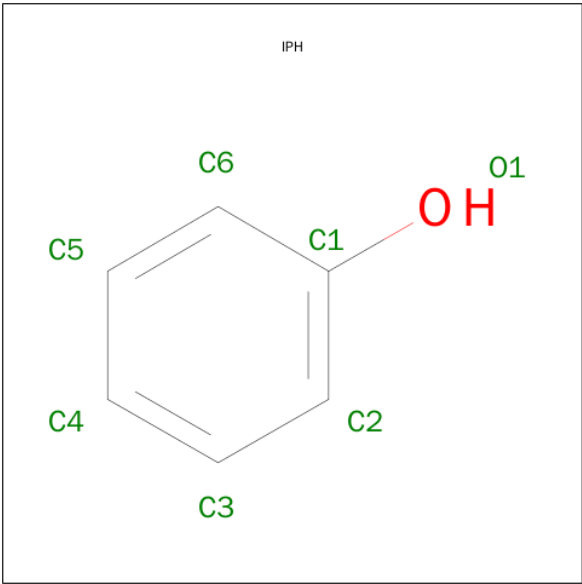
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is PHENOL (three-letter code: IPH) (formula: C<sub>6</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 6 1	0	0
4	B	1	Total C O 7 6 1	0	0
4	C	1	Total C O 7 6 1	0	0
4	D	1	Total C O 7 6 1	0	0

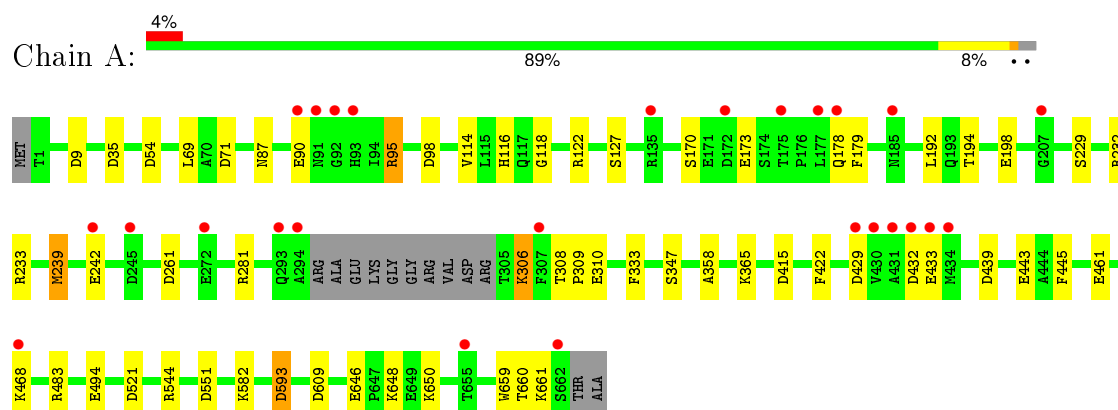
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	668	Total O 668 668	0	0
5	B	686	Total O 686 686	0	0
5	C	674	Total O 674 674	0	0
5	D	660	Total O 660 660	0	0

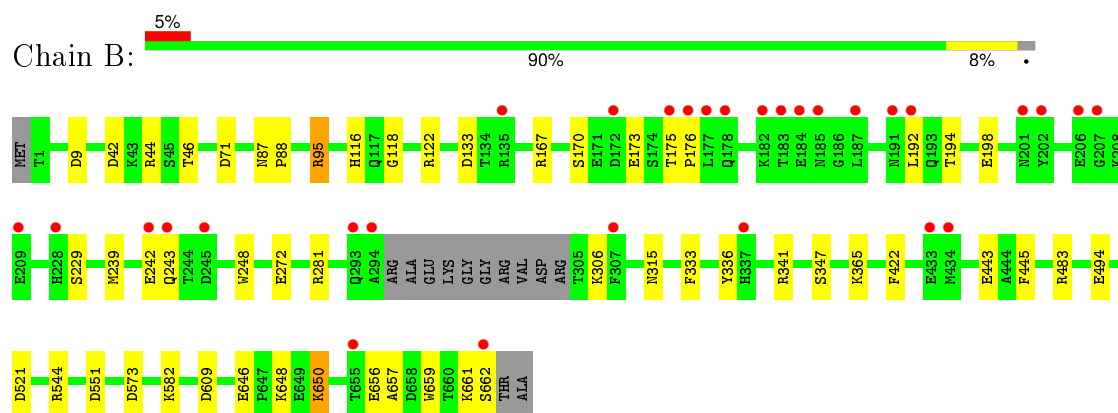
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

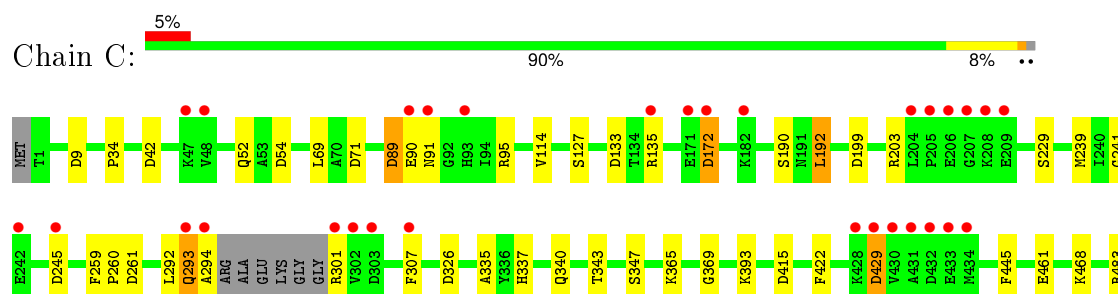
#### • Molecule 1: Phenol 2-monooxygenase

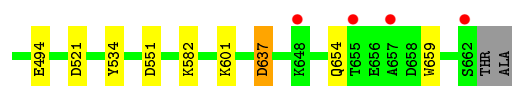


#### • Molecule 1: Phenol 2-monooxygenase

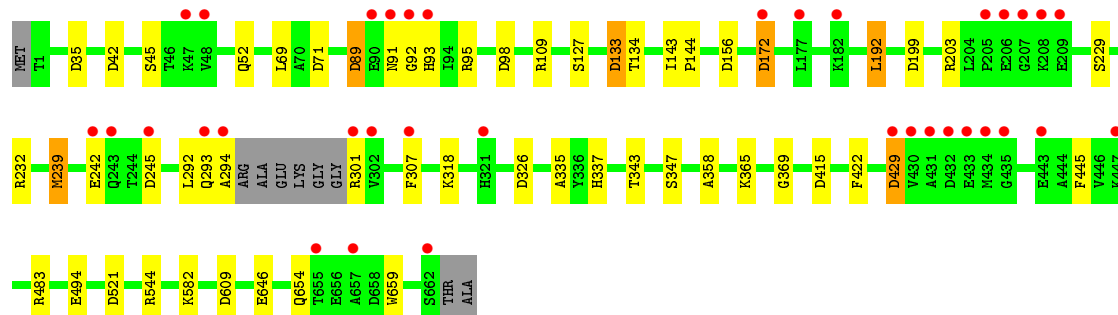
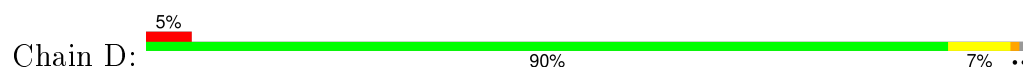


#### • Molecule 1: Phenol 2-monooxygenase





● Molecule 1: Phenol 2-monooxygenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.00Å 150.95Å 114.96Å 90.00° 114.63° 90.00°	Depositor
Resolution (Å)	19.96 – 1.70 18.64 – 1.70	Depositor EDS
% Data completeness (in resolution range)	86.1 (19.96-1.70) 86.1 (18.64-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.02	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.157 , 0.180 0.156 , 0.179	Depositor DCC
$R_{free}$ test set	14784 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.947	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.6	EDS
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 291840 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	23772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: IPH, FAD, CL

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	0.54	0/5302	0.81	12/7171 (0.2%)
1	B	0.56	0/5308	0.83	12/7178 (0.2%)
1	C	0.58	0/5345	0.81	13/7227 (0.2%)
1	D	0.56	1/5345 (0.0%)	0.82	17/7227 (0.2%)
All	All	0.56	1/21300 (0.0%)	0.82	54/28803 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	203	ARG	CG-CD	7.22	1.70	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	LYS	O-C-N	9.53	137.95	122.70
1	B	306	LYS	CA-C-N	-7.94	99.73	117.20
1	B	306	LYS	C-N-CA	-7.25	103.57	121.70
1	D	71	ASP	CB-CG-OD2	7.25	124.82	118.30
1	B	71	ASP	CB-CG-OD2	6.98	124.58	118.30
1	B	609	ASP	CB-CG-OD2	6.75	124.38	118.30
1	A	9	ASP	CB-CG-OD2	6.44	124.09	118.30
1	A	71	ASP	CB-CG-OD2	6.30	123.97	118.30
1	D	521	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	9	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	609	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	42	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	133	ASP	CB-CG-OD2	6.15	123.83	118.30
1	B	133	ASP	CB-CG-OD2	6.15	123.83	118.30
1	C	261	ASP	CB-CG-OD2	6.11	123.80	118.30
1	D	203	ARG	CB-CG-CD	6.10	127.46	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	9	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	306	LYS	O-C-N	-6.06	113.01	122.70
1	C	89	ASP	CB-CG-OD2	6.05	123.74	118.30
1	C	133	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	521	ASP	CB-CG-OD2	6.01	123.71	118.30
1	C	71	ASP	CB-CG-OD2	5.95	123.66	118.30
1	D	172	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	551	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	89	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	306	LYS	C-N-CA	5.80	136.19	121.70
1	D	415	ASP	CB-CG-OD2	5.79	123.52	118.30
1	C	42	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C	415	ASP	CB-CG-OD2	5.74	123.46	118.30
1	C	551	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	551	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	609	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	199	ASP	CB-CG-OD2	5.58	123.33	118.30
1	D	326	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	192	LEU	CA-CB-CG	5.53	128.03	115.30
1	C	172	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	203	ARG	CG-CD-NE	5.41	123.16	111.80
1	D	245	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	261	ASP	CB-CG-OD2	5.37	123.14	118.30
1	D	429	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	245	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	42	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	156	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	429	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	521	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	573	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	35	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	109	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	C	326	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	192	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	415	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	429	ASP	CB-CG-OD2	5.05	122.84	118.30
1	C	521	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	432	ASP	CB-CG-OD2	5.02	122.82	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	5187	0	5055	36	1
1	B	5193	0	5071	31	1
1	C	5230	0	5110	21	0
1	D	5230	0	5110	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
3	C	53	0	31	1	0
3	D	53	0	31	1	0
4	A	7	0	6	0	0
4	B	7	0	6	0	0
4	C	7	0	6	0	0
4	D	7	0	6	0	0
5	A	668	0	0	4	1
5	B	686	0	0	3	1
5	C	674	0	0	2	0
5	D	660	0	0	0	0
All	All	23772	0	20494	111	2

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 3.

All (111) 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:D:544:ARG:NE	1:D:646:GLU:OE2	1.96	0.98
1:A:95:ARG:HH11	1:A:95:ARG:HG3	1.25	0.97
1:B:95:ARG:HH11	1:B:95:ARG:HG3	1.27	0.97
1:A:646:GLU:OE1	1:A:650:LYS:HE2	1.70	0.92
1:A:87:ASN:O	1:A:95:ARG:HD3	1.72	0.90
1:B:87:ASN:O	1:B:95:ARG:HD3	1.73	0.88
1:B:95:ARG:HH11	1:B:95:ARG:CG	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ARG:NE	1:A:646:GLU:OE2	2.13	0.79
1:B:544:ARG:NE	1:B:646:GLU:OE2	2.14	0.79
1:B:656:GLU:OE1	5:B:938:HOH:O	2.03	0.77
1:A:95:ARG:HH11	1:A:95:ARG:CG	1.99	0.76
1:D:307:PHE:CE1	1:D:335:ALA:HB2	2.25	0.72
1:B:239:MET:HB3	1:B:341:ARG:HB3	1.77	0.67
1:B:116:HIS:HD2	1:B:118:GLY:H	1.42	0.66
1:C:307:PHE:CE1	1:C:335:ALA:HB2	2.30	0.65
1:D:544:ARG:HE	1:D:646:GLU:CD	1.98	0.64
1:D:192:LEU:O	1:D:301:ARG:NH1	2.32	0.59
1:B:242:GLU:HG3	1:B:243:GLN:N	2.18	0.58
1:A:116:HIS:HD2	1:A:118:GLY:H	1.50	0.58
1:A:660:THR:OG1	1:A:661:LYS:HE2	2.02	0.58
1:A:95:ARG:CG	1:A:95:ARG:NH1	2.65	0.56
1:C:461:GLU:OE1	1:C:468:LYS:HG3	2.05	0.56
1:D:89:ASP:OD1	1:D:92:GLY:N	2.38	0.56
1:B:87:ASN:O	1:B:95:ARG:CD	2.49	0.56
1:A:242:GLU:HG2	5:A:6439:HOH:O	2.05	0.56
1:A:646:GLU:OE1	1:A:650:LYS:CE	2.49	0.55
1:D:192:LEU:HD22	1:D:337:HIS:CD2	2.41	0.55
1:D:369:GLY:HA3	3:D:6041:FAD:H1'2	1.87	0.55
1:A:95:ARG:N	1:A:95:ARG:HD3	2.22	0.55
1:B:95:ARG:NH1	1:B:95:ARG:CG	2.63	0.54
1:A:170:SER:OG	1:A:173:GLU:HG3	2.07	0.54
1:C:369:GLY:HA3	3:C:6031:FAD:H1'2	1.89	0.54
1:C:293:GLN:O	1:C:294:ALA:HB2	2.07	0.54
1:A:648:LYS:HG3	5:A:6288:HOH:O	2.07	0.53
1:A:593:ASP:OD1	5:A:6310:HOH:O	2.18	0.53
1:D:544:ARG:CZ	1:D:646:GLU:OE2	2.57	0.53
1:D:89:ASP:OD1	1:D:91:ASN:N	2.42	0.53
1:D:239:MET:HG3	1:D:343:THR:HG22	1.91	0.52
1:B:648:LYS:HG3	5:B:932:HOH:O	2.10	0.52
1:B:443:GLU:OE1	1:B:443:GLU:HA	2.08	0.52
1:C:393:LYS:NZ	5:C:6555:HOH:O	2.32	0.51
1:A:308:THR:HB	1:A:309:PRO:HD2	1.93	0.51
1:B:582:LYS:HA	1:B:659:TRP:CE2	2.46	0.51
1:B:661:LYS:O	1:B:662:SER:C	2.50	0.51
1:C:601:LYS:HE2	5:C:6704:HOH:O	2.11	0.50
1:A:95:ARG:H	1:A:95:ARG:HD3	1.77	0.50
1:A:95:ARG:HG3	1:A:95:ARG:NH1	2.07	0.49
1:D:292:LEU:HD11	1:D:307:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:LEU:HD12	1:D:307:PHE:CE2	2.47	0.49
1:A:232:ARG:CZ	1:A:239:MET:HG2	2.43	0.48
1:C:199:ASP:O	1:C:203:ARG:HG2	2.13	0.48
1:D:582:LYS:HA	1:D:659:TRP:CE2	2.49	0.48
1:A:54:ASP:O	1:A:114:VAL:HA	2.14	0.48
1:A:582:LYS:HA	1:A:659:TRP:CE2	2.49	0.48
1:A:87:ASN:O	1:A:95:ARG:CD	2.52	0.47
1:C:292:LEU:HD12	1:C:307:PHE:CE2	2.49	0.47
1:C:582:LYS:HA	1:C:659:TRP:CE2	2.49	0.47
1:A:544:ARG:HE	1:A:646:GLU:CD	2.17	0.47
1:B:116:HIS:HB3	1:B:281:ARG:NH2	2.30	0.47
1:C:89:ASP:OD1	1:C:89:ASP:C	2.53	0.47
1:D:239:MET:HG3	1:D:343:THR:CG2	2.44	0.47
1:B:116:HIS:HD2	1:B:118:GLY:N	2.11	0.46
1:C:192:LEU:HD22	1:C:337:HIS:CD2	2.50	0.46
1:A:308:THR:HB	1:A:310:GLU:OE1	2.15	0.46
1:A:232:ARG:HD3	1:A:358:ALA:O	2.16	0.45
1:B:194:THR:O	1:B:198:GLU:HG3	2.17	0.45
1:C:534:TYR:OH	1:C:637:ASP:OD1	2.27	0.45
1:B:167:ARG:NH1	5:B:747:HOH:O	2.36	0.45
1:B:650:LYS:HE2	1:B:650:LYS:HB2	1.47	0.45
1:D:133:ASP:O	1:D:134:THR:OG1	2.21	0.44
1:B:95:ARG:H	1:B:95:ARG:HD3	1.82	0.44
1:A:178:GLN:HG2	1:A:179:PHE:CE1	2.53	0.44
1:A:194:THR:O	1:A:198:GLU:HG3	2.17	0.44
1:D:232:ARG:HD3	1:D:358:ALA:O	2.18	0.44
1:B:656:GLU:HG2	1:B:657:ALA:O	2.18	0.43
1:B:87:ASN:HB2	1:B:88:PRO:CD	2.48	0.43
1:A:116:HIS:HB3	1:A:281:ARG:NH2	2.33	0.43
1:A:178:GLN:HG2	1:A:179:PHE:CD1	2.53	0.43
1:D:292:LEU:CD1	1:D:307:PHE:CE2	3.01	0.43
1:D:544:ARG:NH2	1:D:646:GLU:OE2	2.51	0.43
1:A:439:ASP:O	1:A:443:GLU:HG3	2.18	0.43
1:A:116:HIS:HD2	1:A:118:GLY:N	2.14	0.43
1:D:89:ASP:OD2	1:D:93:HIS:HB2	2.19	0.42
1:B:95:ARG:N	1:B:95:ARG:HD3	2.35	0.42
1:C:292:LEU:HD11	1:C:307:PHE:CZ	2.54	0.42
1:D:293:GLN:HA	1:D:294:ALA:HA	1.66	0.42
1:C:241:GLY:HA3	1:C:340:GLN:O	2.19	0.42
1:B:170:SER:OG	1:B:173:GLU:HG3	2.19	0.42
1:C:54:ASP:O	1:C:114:VAL:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:LEU:HD21	1:D:127:SER:HB2	2.01	0.42
1:A:308:THR:HB	1:A:309:PRO:CD	2.50	0.41
1:C:89:ASP:OD1	1:C:91:ASN:N	2.53	0.41
1:A:544:ARG:HG3	1:A:646:GLU:HG2	2.01	0.41
1:B:544:ARG:HE	1:B:646:GLU:CD	2.19	0.41
1:B:544:ARG:HG3	1:B:646:GLU:HG2	2.01	0.41
1:A:310:GLU:CD	1:A:310:GLU:H	2.24	0.41
1:B:248:TRP:HB2	1:B:336:TYR:CZ	2.56	0.41
1:A:461:GLU:OE1	1:A:468:LYS:HG3	2.21	0.41
1:A:35:ASP:OD1	5:A:6086:HOH:O	2.22	0.41
1:C:239:MET:HG3	1:C:343:THR:HG22	2.02	0.41
1:C:69:LEU:HD21	1:C:127:SER:HB2	2.03	0.40
1:A:69:LEU:HD21	1:A:127:SER:HB2	2.03	0.40
1:C:34:PRO:O	1:C:135:ARG:NH2	2.49	0.40
1:B:544:ARG:HE	1:B:646:GLU:CG	2.35	0.40
1:D:143:ILE:HA	1:D:144:PRO:HD3	1.97	0.40
1:C:190:SER:HB2	1:C:335:ALA:O	2.21	0.40
1:B:175:THR:HA	1:B:176:PRO:HD3	1.86	0.40
1:C:259:PHE:HA	1:C:260:PRO:HD3	1.93	0.40
1:B:44:ARG:HD2	1:B:46:THR:O	2.21	0.40
1:D:192:LEU:O	1:D:301:ARG:NH2	2.54	0.40
1:B:242:GLU:CG	1:B:243:GLN:N	2.84	0.40

All (2) 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:233:ARG:NH2	1:B:272:GLU:OE2[2_746]	2.15	0.05
5:A:6078:HOH:O	5:B:733:HOH:O[1_454]	2.17	0.03

## 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	648/665 (97%)	631 (97%)	15 (2%)	2 (0%)	46	26
1	B	648/665 (97%)	633 (98%)	14 (2%)	1 (0%)	52	32
1	C	652/665 (98%)	637 (98%)	13 (2%)	2 (0%)	46	26
1	D	652/665 (98%)	636 (98%)	14 (2%)	2 (0%)	46	26
All	All	2600/2660 (98%)	2537 (98%)	56 (2%)	7 (0%)	46	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	LYS
1	C	52	GLN
1	D	52	GLN
1	A	229	SER
1	C	229	SER
1	D	229	SER
1	B	229	SER

### 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	560/571 (98%)	546 (98%)	14 (2%)	55	34
1	B	562/571 (98%)	551 (98%)	11 (2%)	63	44
1	C	566/571 (99%)	551 (97%)	15 (3%)	52	31
1	D	566/571 (99%)	550 (97%)	16 (3%)	51	29
All	All	2254/2284 (99%)	2198 (98%)	56 (2%)	55	34

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLU
1	A	95	ARG
1	A	98	ASP
1	A	122	ARG

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Mol	Chain	Res	Type
1	A	239	MET
1	A	333	PHE
1	A	347	SER
1	A	365	LYS
1	A	422	PHE
1	A	433	GLU
1	A	445	PHE
1	A	483	ARG
1	A	494	GLU
1	A	593	ASP
1	B	95	ARG
1	B	122	ARG
1	B	315	ASN
1	B	333	PHE
1	B	347	SER
1	B	365	LYS
1	B	422	PHE
1	B	445	PHE
1	B	483	ARG
1	B	494	GLU
1	B	650	LYS
1	C	90	GLU
1	C	95	ARG
1	C	172	ASP
1	C	192	LEU
1	C	293	GLN
1	C	301	ARG
1	C	347	SER
1	C	365	LYS
1	C	422	PHE
1	C	429	ASP
1	C	445	PHE
1	C	483	ARG
1	C	494	GLU
1	C	637	ASP
1	C	654	GLN
1	D	45	SER
1	D	95	ARG
1	D	98	ASP
1	D	172	ASP
1	D	192	LEU
1	D	239	MET

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Mol	Chain	Res	Type
1	D	242	GLU
1	D	318	LYS
1	D	347	SER
1	D	365	LYS
1	D	422	PHE
1	D	429	ASP
1	D	445	PHE
1	D	483	ARG
1	D	494	GLU
1	D	654	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	93	HIS
1	A	116	HIS
1	A	315	ASN
1	A	449	ASN
1	B	116	HIS
1	B	449	ASN
1	C	337	HIS
1	C	449	ASN
1	C	604	GLN
1	D	243	GLN
1	D	337	HIS
1	D	449	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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FAD	A	6011	-	48,58,58	1.07	5 (10%)	54,89,89	2.22	8 (14%)
4	IPH	A	6012	-	7,7,7	0.67	0	8,8,8	1.21	0
3	FAD	B	6021	-	48,58,58	1.08	4 (8%)	54,89,89	2.53	7 (12%)
4	IPH	B	6022	-	7,7,7	0.49	0	8,8,8	1.12	1 (12%)
3	FAD	C	6031	-	48,58,58	1.20	5 (10%)	54,89,89	2.53	9 (16%)
4	IPH	C	6032	-	7,7,7	0.70	0	8,8,8	0.58	0
3	FAD	D	6041	-	48,58,58	1.21	5 (10%)	54,89,89	2.24	6 (11%)
4	IPH	D	6042	-	7,7,7	0.75	0	8,8,8	0.43	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
3	FAD	A	6011	-	-	0/30/50/50	0/6/6/6
4	IPH	A	6012	-	-	0/0/0/0	0/1/1/1
3	FAD	B	6021	-	-	0/30/50/50	0/6/6/6
4	IPH	B	6022	-	-	0/0/0/0	0/1/1/1
3	FAD	C	6031	-	-	0/30/50/50	0/6/6/6
4	IPH	C	6032	-	-	0/0/0/0	0/1/1/1
3	FAD	D	6041	-	-	0/30/50/50	0/6/6/6
4	IPH	D	6042	-	-	0/0/0/0	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	6011	FAD	C5X-N5	2.01	1.38	1.35
3	A	6011	FAD	C2A-N1A	2.22	1.38	1.33
3	C	6031	FAD	C5X-N5	2.22	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	6021	FAD	C2A-N1A	2.27	1.38	1.33
3	B	6021	FAD	C10-N1	2.28	1.39	1.35
3	C	6031	FAD	C10-N1	2.41	1.39	1.35
3	A	6011	FAD	C4-N3	2.51	1.37	1.33
3	D	6041	FAD	C2A-N1A	2.53	1.38	1.33
3	B	6021	FAD	C4X-N5	2.88	1.37	1.33
3	D	6041	FAD	C4X-N5	2.90	1.37	1.33
3	D	6041	FAD	C1'-N10	2.91	1.51	1.48
3	D	6041	FAD	C4-N3	3.00	1.38	1.33
3	A	6011	FAD	C4X-N5	3.03	1.38	1.33
3	C	6031	FAD	C4-N3	3.16	1.39	1.33
3	A	6011	FAD	C2A-N3A	3.31	1.38	1.32
3	B	6021	FAD	C2A-N3A	3.35	1.38	1.32
3	C	6031	FAD	C2A-N3A	3.43	1.38	1.32
3	D	6041	FAD	C2A-N3A	3.52	1.38	1.32
3	C	6031	FAD	C4X-N5	3.96	1.39	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6031	FAD	N3A-C2A-N1A	-14.62	117.70	128.89
3	B	6021	FAD	N3A-C2A-N1A	-13.94	118.22	128.89
3	D	6041	FAD	N3A-C2A-N1A	-13.44	118.60	128.89
3	A	6011	FAD	N3A-C2A-N1A	-12.18	119.57	128.89
3	B	6021	FAD	C4X-C4-N3	-3.78	118.42	123.59
3	A	6011	FAD	C4X-C4-N3	-3.38	118.97	123.59
3	C	6031	FAD	C4X-C4-N3	-2.80	119.76	123.59
3	A	6011	FAD	P-O3P-PA	-2.57	125.51	132.73
3	B	6021	FAD	C1B-N9A-C4A	-2.38	123.35	126.94
3	C	6031	FAD	C4X-C10-N10	-2.28	119.17	120.52
3	A	6011	FAD	C1B-N9A-C4A	-2.21	123.60	126.94
4	B	6022	IPH	C4-C3-C2	-2.15	117.04	120.19
3	D	6041	FAD	C4X-C4-N3	-2.15	120.65	123.59
3	D	6041	FAD	C1B-N9A-C4A	-2.07	123.82	126.94
3	C	6031	FAD	C4-C4X-C10	-2.04	118.64	119.94
3	D	6041	FAD	C4X-N5-C5X	2.10	119.17	116.76
3	B	6021	FAD	C2A-N1A-C6A	2.11	122.53	118.77
3	A	6011	FAD	C1'-N10-C9A	2.11	121.23	118.86
3	C	6031	FAD	C1'-N10-C9A	2.17	121.30	118.86
3	B	6021	FAD	C4X-N5-C5X	2.46	119.59	116.76
3	C	6031	FAD	C2A-N1A-C6A	2.47	123.17	118.77
3	C	6031	FAD	C4X-N5-C5X	2.51	119.65	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	6011	FAD	C4X-N5-C5X	2.90	120.10	116.76
3	D	6041	FAD	C5X-C9A-N10	3.38	120.19	117.62
3	C	6031	FAD	C5X-C9A-N10	3.64	120.39	117.62
3	B	6021	FAD	C5X-C9A-N10	4.19	120.80	117.62
3	A	6011	FAD	C5X-C9A-N10	4.47	121.02	117.62
3	A	6011	FAD	C4-N3-C2	5.82	120.28	115.25
3	D	6041	FAD	C4-N3-C2	5.90	120.34	115.25
3	C	6031	FAD	C4-N3-C2	7.57	121.79	115.25
3	B	6021	FAD	C4-N3-C2	8.57	122.65	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	6031	FAD	1	0
3	D	6041	FAD	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	650/665 (97%)	-0.12	26 (4%)	42	46	3, 9, 25, 40	1 (0%)
1	B	650/665 (97%)	-0.08	30 (4%)	36	40	3, 9, 23, 40	1 (0%)
1	C	656/665 (98%)	-0.07	34 (5%)	31	33	3, 9, 26, 44	1 (0%)
1	D	656/665 (98%)	0.04	35 (5%)	30	32	3, 9, 25, 40	1 (0%)
All	All	2612/2660 (98%)	-0.06	125 (4%)	34	38	3, 9, 25, 44	4 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	294	ALA	9.7
1	C	430	VAL	8.9
1	D	430	VAL	8.6
1	C	662	SER	8.3
1	D	294	ALA	8.2
1	D	662	SER	7.8
1	B	662	SER	7.7
1	A	662	SER	7.6
1	B	177	LEU	7.6
1	A	434	MET	7.6
1	B	307	PHE	6.9
1	C	207	GLY	6.8
1	B	185	ASN	6.3
1	B	294	ALA	6.2
1	D	302	VAL	6.2
1	A	294	ALA	6.1
1	D	434	MET	6.0
1	A	430	VAL	5.9
1	C	302	VAL	5.9
1	D	431	ALA	5.7
1	C	434	MET	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	90	GLU	5.3
1	A	307	PHE	5.3
1	D	207	GLY	5.2
1	C	433	GLU	5.1
1	C	206	GLU	5.0
1	D	433	GLU	5.0
1	D	206	GLU	4.9
1	B	175	THR	4.9
1	D	93	HIS	4.8
1	A	431	ALA	4.7
1	A	207	GLY	4.7
1	D	242	GLU	4.6
1	C	91	ASN	4.5
1	D	429	ASP	4.5
1	B	176	PRO	4.4
1	B	207	GLY	4.4
1	D	91	ASN	4.4
1	C	431	ALA	4.4
1	D	293	GLN	4.3
1	B	655	THR	4.3
1	A	175	THR	4.3
1	C	293	GLN	4.2
1	C	90	GLU	4.0
1	C	209	GLU	4.0
1	A	93	HIS	3.9
1	B	135	ARG	3.9
1	A	90	GLU	3.8
1	B	242	GLU	3.8
1	A	433	GLU	3.7
1	B	206	GLU	3.7
1	B	243	GLN	3.7
1	D	432	ASP	3.6
1	C	47	LYS	3.6
1	B	434	MET	3.4
1	D	301	ARG	3.4
1	B	433	GLU	3.4
1	C	301	ARG	3.3
1	B	192	LEU	3.3
1	C	182	LYS	3.3
1	C	208	LYS	3.3
1	D	208	LYS	3.3
1	A	172	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	182	LYS	3.2
1	C	171	GLU	3.1
1	A	242	GLU	3.1
1	C	655	THR	3.1
1	A	432	ASP	3.1
1	C	245	ASP	3.0
1	C	93	HIS	3.0
1	D	243	GLN	3.0
1	B	293	GLN	3.0
1	C	48	VAL	3.0
1	D	177	LEU	2.9
1	B	209	GLU	2.9
1	A	293	GLN	2.9
1	B	182	LYS	2.8
1	C	432	ASP	2.8
1	D	48	VAL	2.8
1	A	177	LEU	2.8
1	D	209	GLU	2.7
1	B	337	HIS	2.7
1	A	92	GLY	2.7
1	A	185	ASN	2.7
1	B	201	ASN	2.7
1	B	178	GLN	2.7
1	B	228	HIS	2.7
1	D	307	PHE	2.6
1	C	429	ASP	2.6
1	A	655	THR	2.6
1	C	172	ASP	2.6
1	B	191	ASN	2.6
1	D	435	GLY	2.6
1	C	657	ALA	2.5
1	C	307	PHE	2.5
1	D	321	HIS	2.5
1	A	91	ASN	2.5
1	D	172	ASP	2.5
1	D	92	GLY	2.5
1	C	428	LYS	2.4
1	A	135	ARG	2.4
1	D	47	LYS	2.4
1	C	648	LYS	2.4
1	D	245	ASP	2.4
1	A	272	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	205	PRO	2.3
1	B	183	THR	2.3
1	A	245	ASP	2.3
1	B	187	LEU	2.3
1	A	429	ASP	2.2
1	B	172	ASP	2.2
1	A	468	LYS	2.2
1	B	184	GLU	2.2
1	D	655	THR	2.1
1	C	205	PRO	2.1
1	D	657	ALA	2.1
1	C	242	GLU	2.1
1	D	447	LYS	2.1
1	C	204	LEU	2.1
1	C	135	ARG	2.1
1	B	202	TYR	2.1
1	B	245	ASP	2.1
1	D	443	GLU	2.1
1	A	178	GLN	2.0
1	C	303	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	IPH	A	6012	7/7	0.94	0.08	1.53	22,24,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	IPH	C	6032	7/7	0.94	0.09	1.51	23,28,31,32	0
4	IPH	B	6022	7/7	0.95	0.08	1.37	22,27,29,30	0
4	IPH	D	6042	7/7	0.92	0.09	1.29	29,33,35,35	0
3	FAD	D	6041	53/53	0.94	0.12	1.21	6,11,14,15	0
3	FAD	C	6031	53/53	0.97	0.10	1.11	7,11,14,15	0
2	CL	C	6003	1/1	0.99	0.09	1.01	13,13,13,13	0
3	FAD	B	6021	53/53	0.96	0.10	0.89	4,8,13,17	0
2	CL	D	6004	1/1	1.00	0.08	0.39	13,13,13,13	0
2	CL	B	6002	1/1	0.99	0.07	-0.38	12,12,12,12	0
3	FAD	A	6011	53/53	0.98	0.06	-0.47	4,8,11,13	0
2	CL	A	6001	1/1	0.99	0.06	-0.54	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.