



# Full wwPDB X-ray Structure Validation Report

Nov 6, 2014 – 05:21 PM EST

PDB ID : 3K4C  
Title : Pyranose 2-oxidase H167A/T169G mutant  
Authors : Divne, C.; Tan, T.C.  
Deposited on : 2009-10-05  
Resolution : 1.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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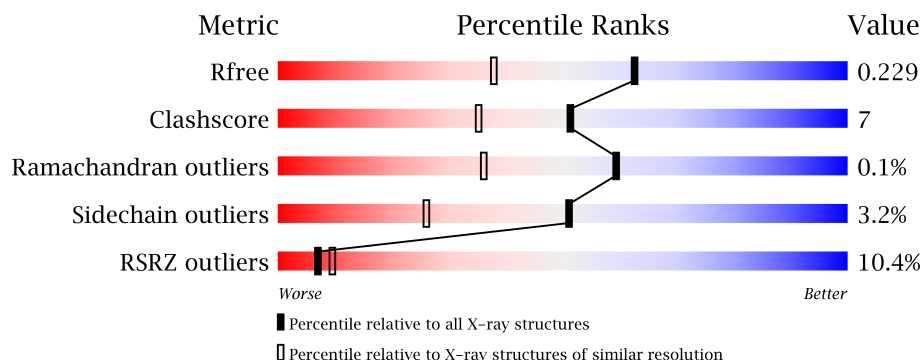
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24103

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	623	
1	B	623	
1	C	623	
1	D	623	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	FAD	A	801	-	X
2	FAD	B	801	-	X
2	FAD	D	801	-	X
3	1PE	A	905	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	1PE	B	902	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20305 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

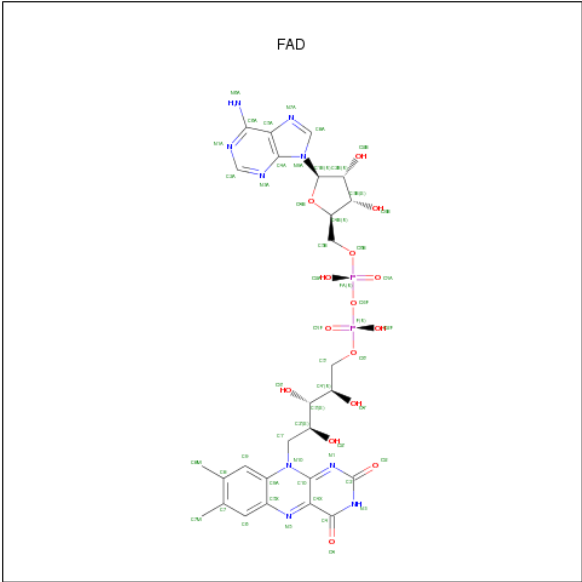
- Molecule 1 is a protein called Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4534	2863	775	871	25			
1	B	576	Total	C	N	O	S	0	0	0
			4534	2863	775	871	25			
1	C	575	Total	C	N	O	S	0	0	0
			4525	2858	774	869	24			
1	D	574	Total	C	N	O	S	0	0	0
			4518	2854	773	867	24			

There are 8 discrepancies between the modelled and reference sequences:

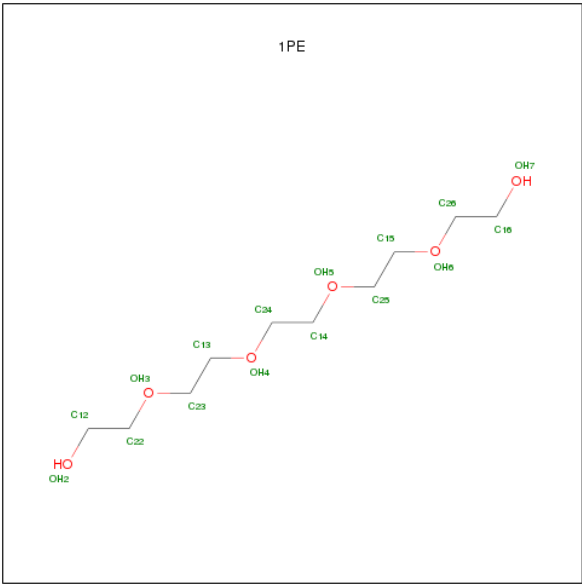
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	ALA	HIS	ENGINEERED	UNP Q7ZA32
A	169	GLY	THR	ENGINEERED	UNP Q7ZA32
B	167	ALA	HIS	ENGINEERED	UNP Q7ZA32
B	169	GLY	THR	ENGINEERED	UNP Q7ZA32
C	167	ALA	HIS	ENGINEERED	UNP Q7ZA32
C	169	GLY	THR	ENGINEERED	UNP Q7ZA32
D	167	ALA	HIS	ENGINEERED	UNP Q7ZA32
D	169	GLY	THR	ENGINEERED	UNP Q7ZA32

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



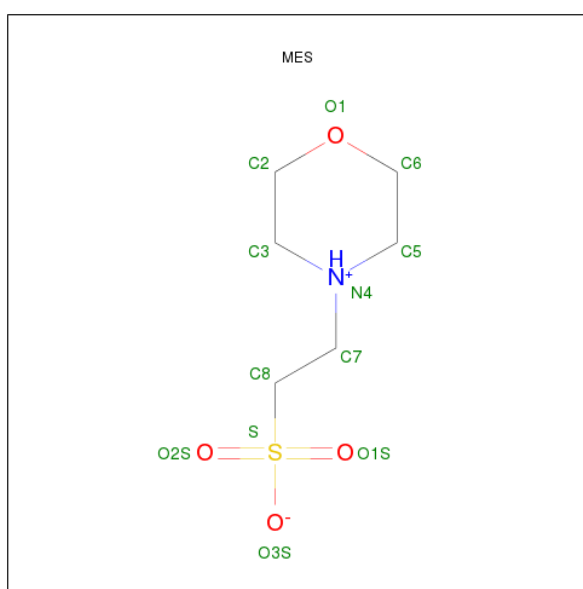
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	9	5		
3	A	1	Total	C	O	0	0
			12	8	4		
3	B	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	498	Total	O	0	0
			498	498		
5	B	554	Total	O	0	0
			554	554		
5	C	504	Total	O	0	0
			504	504		

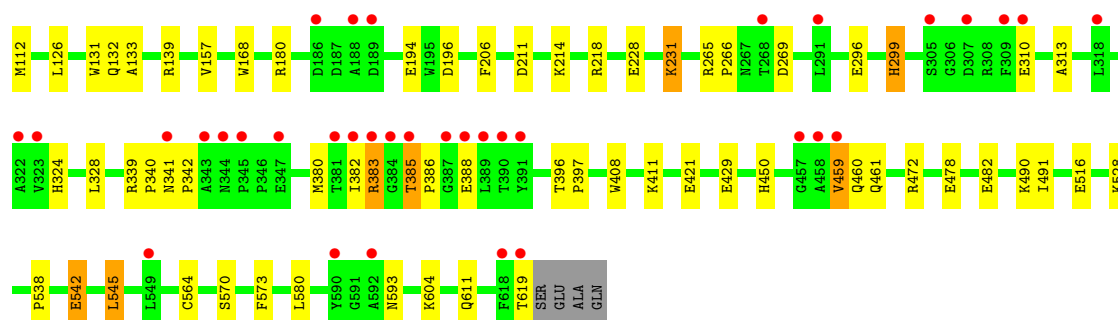
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	344	Total 344	O 344	0	0

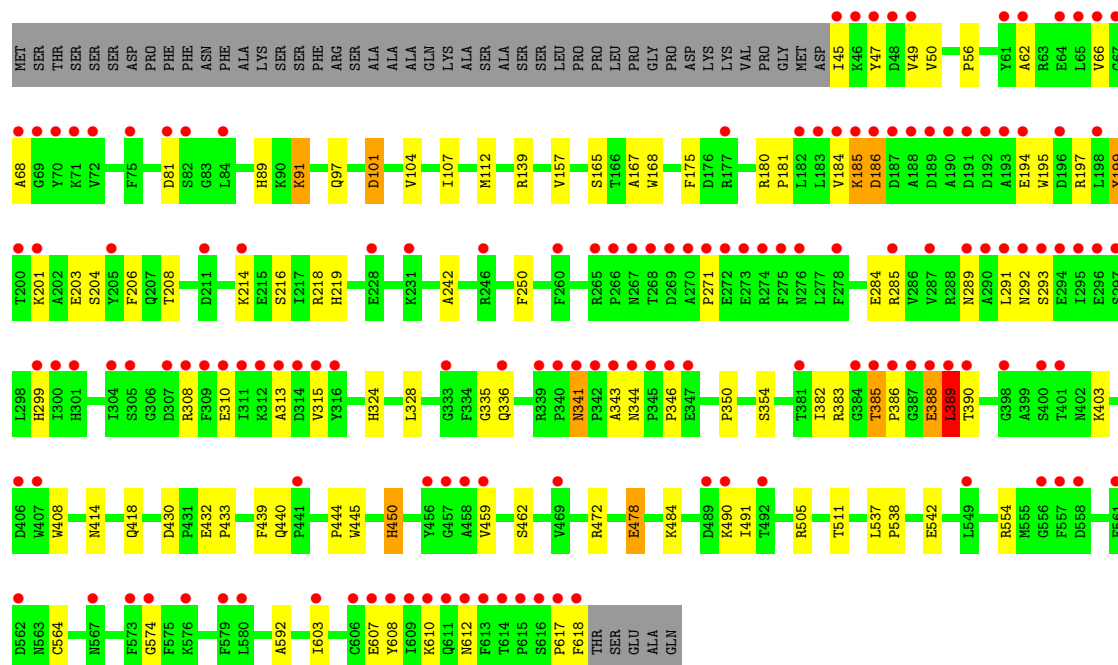






• Molecule 1: Pyranose 2-oxidase

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.21Å 102.96Å 137.12Å 90.00° 90.82° 90.00°	Depositor
Resolution (Å)	29.30 – 1.70 29.29 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.30-1.70) 96.8 (29.29-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.180 , 0.216 0.197 , 0.229	Depositor DCC
$R_{free}$ test set	3027 reflections (1.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 32.6	EDS
Estimated twinning fraction	0.014 for -k,-h,-l 0.008 for k,h,-l 0.022 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 295544 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20305	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: MES, FAD, 1PE

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	1.23	16/4649 (0.3%)	1.08	17/6320 (0.3%)
1	B	1.20	7/4649 (0.2%)	1.15	23/6320 (0.4%)
1	C	1.09	9/4640 (0.2%)	1.01	10/6309 (0.2%)
1	D	0.96	2/4633 (0.0%)	0.94	5/6299 (0.1%)
All	All	1.13	34/18571 (0.2%)	1.05	55/25248 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	SER	CB-OG	12.12	1.58	1.42
1	B	542	GLU	CD-OE1	8.97	1.35	1.25
1	A	82	SER	N-CA	8.77	1.63	1.46
1	B	481	GLU	CG-CD	8.40	1.64	1.51
1	A	542	GLU	CD-OE1	8.05	1.34	1.25
1	A	82	SER	CA-CB	7.04	1.63	1.52
1	C	542	GLU	CD-OE1	6.70	1.33	1.25
1	B	81	ASP	CB-CG	-6.40	1.38	1.51
1	A	316	TYR	CD1-CE1	6.26	1.48	1.39
1	A	383	ARG	CG-CD	6.24	1.67	1.51
1	D	542	GLU	CD-OE1	6.08	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	542	GLU	CD-OE2	6.08	1.32	1.25
1	C	542	GLU	CG-CD	6.05	1.61	1.51
1	A	542	GLU	CG-CD	5.91	1.60	1.51
1	A	91	LYS	CB-CG	-5.84	1.36	1.52
1	D	478	GLU	CD-OE1	5.79	1.32	1.25
1	C	296	GLU	CG-CD	5.76	1.60	1.51
1	A	228	GLU	CG-CD	5.60	1.60	1.51
1	A	421	GLU	CB-CG	5.56	1.62	1.52
1	B	559	GLU	CD-OE2	-5.54	1.19	1.25
1	C	542	GLU	CD-OE2	5.52	1.31	1.25
1	B	482	GLU	CD-OE1	5.49	1.31	1.25
1	A	516	GLU	CG-CD	5.49	1.60	1.51
1	B	104	VAL	CB-CG1	-5.41	1.41	1.52
1	A	358	GLU	CD-OE1	5.39	1.31	1.25
1	C	482	GLU	CD-OE2	5.38	1.31	1.25
1	C	482	GLU	CD-OE1	5.37	1.31	1.25
1	C	478	GLU	CD-OE2	5.27	1.31	1.25
1	A	330	VAL	CB-CG1	-5.11	1.42	1.52
1	C	194	GLU	CB-CG	-5.08	1.42	1.52
1	A	582	GLY	N-CA	-5.05	1.38	1.46
1	A	482	GLU	CG-CD	5.04	1.59	1.51
1	C	482	GLU	CG-CD	5.01	1.59	1.51
1	A	83	GLY	N-CA	5.00	1.53	1.46

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	NE-CZ-NH2	-19.20	110.70	120.30
1	B	139	ARG	NE-CZ-NH1	17.86	129.23	120.30
1	B	81	ASP	CB-CG-OD1	-16.86	103.13	118.30
1	C	139	ARG	NE-CZ-NH2	-16.04	112.28	120.30
1	C	139	ARG	NE-CZ-NH1	13.35	126.97	120.30
1	A	139	ARG	NE-CZ-NH1	12.41	126.51	120.30
1	D	139	ARG	NE-CZ-NH2	-10.43	115.09	120.30
1	C	81	ASP	CB-CG-OD1	-10.38	108.96	118.30
1	A	139	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	B	81	ASP	CB-CG-OD2	9.54	126.88	118.30
1	D	389	LEU	CB-CG-CD1	-9.35	95.10	111.00
1	B	308	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	A	314	ASP	CB-CG-OD1	8.59	126.03	118.30
1	B	211	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	B	211	ASP	CB-CG-OD1	8.43	125.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	C	180	ARG	NE-CZ-NH1	-7.40	116.60	120.30
1	B	159	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	B	175	PHE	CB-CG-CD1	6.89	125.62	120.80
1	A	503	ASP	CB-CG-OD1	6.84	124.45	118.30
1	D	139	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	374	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	261	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	554	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	349	LEU	CB-CG-CD2	6.34	121.78	111.00
1	D	180	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	B	175	PHE	CB-CG-CD2	-6.29	116.40	120.80
1	A	470	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	C	81	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	147	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	139	ARG	CD-NE-CZ	5.99	131.98	123.60
1	B	545	LEU	CB-CG-CD1	5.93	121.09	111.00
1	B	470	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	245	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	81	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	374	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	C	139	ARG	CG-CD-NE	-5.66	99.92	111.80
1	B	176	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	380	MET	CG-SD-CE	-5.51	91.38	100.20
1	B	91	LYS	CA-CB-CG	5.43	125.35	113.40
1	B	571	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	96	TYR	CB-CG-CD2	5.37	124.22	121.00
1	C	516	GLU	OE1-CD-OE2	-5.32	116.91	123.30
1	A	288	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	503	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	245	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	82	SER	CA-CB-OG	5.29	125.49	111.20
1	B	380	MET	CG-SD-CE	-5.29	91.74	100.20
1	B	481	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	A	261	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	C	545	LEU	CB-CG-CD1	5.20	119.84	111.00
1	D	389	LEU	CA-CB-CG	-5.19	103.36	115.30
1	C	211	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	554	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	198	LEU	CB-CG-CD2	5.01	119.51	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	ASP	Peptide
1	B	449	ILE	Peptide
1	D	388	GLU	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4534	0	4382	47	0
1	B	4534	0	4382	61	0
1	C	4525	0	4376	70	0
1	D	4518	0	4369	85	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	29	0	0
2	D	53	0	28	1	0
3	A	26	0	31	0	0
3	B	16	0	22	0	0
3	D	16	0	22	0	0
4	B	12	0	12	3	0
4	C	12	0	12	13	0
5	A	498	0	0	15	0
5	B	554	0	0	10	0
5	C	504	0	0	13	0
5	D	344	0	0	12	0
All	All	20305	0	17727	264	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (264) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:133:ALA:CB	4:C:901:MES:H71	1.40	1.50
1:C:299:HIS:CE1	1:C:310:GLU:HG2	1.60	1.36
1:C:383:ARG:HB2	1:C:383:ARG:NH1	1.45	1.31

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:383:ARG:CB	1:C:383:ARG:HH11	1.47	1.25
1:C:133:ALA:CB	4:C:901:MES:C7	2.20	1.18
1:A:45:ILE:H	1:A:45:ILE:HD12	1.01	1.13
1:C:133:ALA:HB2	4:C:901:MES:H71	1.18	1.12
1:C:133:ALA:HB3	4:C:901:MES:H71	1.15	1.11
1:C:101:ASP:O	1:C:104:VAL:HG12	1.50	1.07
1:C:133:ALA:HB2	4:C:901:MES:O1S	1.56	1.04
1:C:133:ALA:HB3	4:C:901:MES:C7	1.86	1.02
1:D:45:ILE:HA	5:D:2497:HOH:O	1.61	0.99
1:A:45:ILE:CD1	1:A:45:ILE:H	1.78	0.94
1:B:576:LYS:HD3	1:B:576:LYS:N	1.79	0.94
1:D:101:ASP:O	1:D:104:VAL:HG12	1.68	0.94
1:A:45:ILE:HD12	1:A:45:ILE:N	1.81	0.94
1:D:343:ALA:O	1:D:344:ASN:ND2	2.00	0.93
1:C:133:ALA:HB2	4:C:901:MES:C7	1.92	0.90
1:C:383:ARG:HB2	1:C:383:ARG:HH11	0.73	0.90
1:C:299:HIS:CE1	1:C:310:GLU:CG	2.54	0.89
1:C:490:LYS:HD3	1:C:491:ILE:HD13	1.55	0.88
1:B:347:GLU:HG3	1:B:348:LEU:HG	1.55	0.87
1:B:343:ALA:O	1:B:344:ASN:ND2	2.08	0.87
1:C:126:LEU:CD1	1:C:132:GLN:HG3	2.05	0.86
1:D:185:LYS:HD3	5:D:2678:HOH:O	1.75	0.85
1:B:101:ASP:O	1:B:104:VAL:HG12	1.77	0.85
1:D:285:ARG:HA	1:D:328:LEU:HD11	1.58	0.85
1:D:341:ASN:HD21	1:D:343:ALA:HB3	1.43	0.83
1:C:126:LEU:HD12	1:C:132:GLN:HG3	1.62	0.82
1:B:618:PHE:HD1	1:B:618:PHE:C	1.83	0.81
1:C:411:LYS:HE3	5:C:2449:HOH:O	1.79	0.81
1:D:343:ALA:C	1:D:344:ASN:HD22	1.84	0.81
1:A:101:ASP:OD2	1:A:459:VAL:HG13	1.82	0.80
1:A:84:LEU:HD23	5:B:2054:HOH:O	1.81	0.79
1:B:618:PHE:C	1:B:618:PHE:CD1	2.55	0.79
1:A:383:ARG:HB3	1:A:392:SER:HB3	1.65	0.78
1:D:185:LYS:HD2	1:D:185:LYS:H	1.49	0.77
1:B:385:THR:HG23	1:B:388:GLU:OE1	1.85	0.77
1:D:185:LYS:H	1:D:185:LYS:CD	1.95	0.77
1:D:341:ASN:HD22	1:D:343:ALA:H	1.36	0.73
1:B:450:HIS:CE1	1:B:472:ARG:HH11	2.07	0.73
1:D:341:ASN:ND2	1:D:343:ALA:H	1.86	0.73
1:B:341:ASN:HD22	1:B:341:ASN:C	1.92	0.72
1:D:608:TYR:CZ	1:D:612:ASN:OD1	2.42	0.72
1:A:450:HIS:HD2	5:A:1424:HOH:O	1.72	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:SER:HB2	5:A:1477:HOH:O	1.92	0.70
1:A:505:ARG:HD3	5:A:1785:HOH:O	1.92	0.70
1:D:157:VAL:HG21	1:D:324:HIS:HE1	1.56	0.69
1:B:450:HIS:HD2	5:B:1237:HOH:O	1.75	0.69
1:D:341:ASN:HD22	1:D:341:ASN:C	1.96	0.69
1:D:459:VAL:HG12	1:D:459:VAL:O	1.92	0.69
1:D:505:ARG:NH2	5:D:2273:HOH:O	2.25	0.68
1:D:285:ARG:HA	1:D:328:LEU:CD1	2.24	0.68
1:C:101:ASP:O	1:C:104:VAL:CG1	2.35	0.67
1:C:126:LEU:CD1	1:C:132:GLN:CG	2.72	0.67
1:A:157:VAL:HG21	1:A:324:HIS:HE1	1.60	0.66
1:B:450:HIS:HE1	1:B:472:ARG:HH11	1.42	0.66
1:A:344:ASN:HD22	1:A:345:PRO:HD2	1.60	0.65
1:B:489:ASP:O	1:B:490:LYS:HD2	1.96	0.65
1:D:617:PRO:O	1:D:618:PHE:C	2.35	0.65
1:D:389:LEU:C	1:D:389:LEU:HD12	2.00	0.65
1:D:308:ARG:HG3	1:D:308:ARG:HH11	1.62	0.65
1:C:132:GLN:OE1	4:C:901:MES:H31	1.97	0.64
1:A:132:GLN:HG2	5:A:2468:HOH:O	1.98	0.63
1:B:459:VAL:HG12	1:B:461:GLN:NE2	2.14	0.63
1:B:478:GLU:HG3	1:B:511:THR:OG1	2.00	0.62
1:B:459:VAL:HG22	5:B:2672:HOH:O	1.98	0.62
1:B:459:VAL:CG2	5:B:2672:HOH:O	2.48	0.62
1:D:389:LEU:HD12	1:D:389:LEU:O	1.99	0.61
1:D:450:HIS:HD2	5:D:2499:HOH:O	1.84	0.60
1:C:450:HIS:CE1	1:C:472:ARG:HH11	2.19	0.60
1:D:185:LYS:N	1:D:185:LYS:HD2	2.16	0.60
1:B:81:ASP:OD2	1:B:90:LYS:NZ	2.34	0.60
1:D:45:ILE:CA	5:D:2497:HOH:O	2.34	0.59
1:A:383:ARG:HD2	1:A:390:THR:O	2.02	0.59
1:B:308:ARG:HD2	5:B:2220:HOH:O	2.03	0.59
1:D:444:PRO:HD2	1:D:445:TRP:CZ3	2.38	0.59
1:D:291:LEU:O	1:D:292:ASN:HB2	2.03	0.58
1:D:382:ILE:HD13	5:D:2622:HOH:O	2.03	0.58
1:A:101:ASP:HB3	1:A:459:VAL:HG22	1.85	0.57
1:D:459:VAL:CG1	1:D:459:VAL:O	2.52	0.57
1:D:62:ALA:O	1:D:66:VAL:HG23	2.05	0.57
1:B:50:VAL:HG13	1:B:313:ALA:HB2	1.86	0.57
1:B:63:ARG:HD2	1:B:259:VAL:O	2.04	0.57
1:B:132:GLN:OE1	4:B:901:MES:H31	2.04	0.57
1:C:133:ALA:CB	4:C:901:MES:H72	2.28	0.56
1:C:450:HIS:HE1	1:C:472:ARG:HD2	1.70	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:414:ASN:O	1:D:418:GLN:HG3	2.06	0.56
1:A:457:GLY:HA2	5:A:2149:HOH:O	2.06	0.56
1:C:126:LEU:HD13	1:C:132:GLN:CG	2.35	0.56
1:D:478:GLU:HG3	1:D:511:THR:OG1	2.06	0.55
1:A:385:THR:O	1:A:388:GLU:HB2	2.06	0.55
1:B:542:GLU:HB2	1:B:545:LEU:HD22	1.88	0.55
1:C:382:ILE:HD13	5:C:2150:HOH:O	2.07	0.55
1:B:293:SER:O	1:B:576:LYS:HE2	2.06	0.55
1:C:131:TRP:O	1:C:132:GLN:HG2	2.06	0.55
1:B:100:ILE:HD13	1:B:100:ILE:O	2.07	0.55
1:D:308:ARG:CG	1:D:308:ARG:HH11	2.20	0.55
1:A:344:ASN:HD22	1:A:345:PRO:CD	2.20	0.54
1:C:604:LYS:NZ	5:C:1648:HOH:O	2.26	0.54
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.72	0.54
1:B:178:GLU:OE1	1:B:439:PHE:HE1	1.90	0.54
1:C:299:HIS:ND1	1:C:310:GLU:HG2	2.12	0.54
1:C:385:THR:OG1	1:C:388:GLU:CD	2.45	0.54
1:C:542:GLU:HB2	1:C:545:LEU:HD22	1.89	0.54
1:A:385:THR:HG22	1:A:386:PRO:HD2	1.89	0.54
1:A:411:LYS:HD3	5:A:2592:HOH:O	2.08	0.54
1:B:100:ILE:CD1	1:B:453:ALA:HB2	2.38	0.54
1:C:450:HIS:HD2	5:C:1651:HOH:O	1.89	0.54
1:B:342:PRO:C	1:B:344:ASN:H	2.11	0.54
1:C:47:TYR:O	1:C:313:ALA:HA	2.08	0.53
1:C:528:LYS:NZ	5:C:2436:HOH:O	2.40	0.53
1:A:104:VAL:HG13	1:A:454:PHE:O	2.07	0.53
1:C:383:ARG:CB	1:C:383:ARG:NH1	2.30	0.53
1:D:450:HIS:CE1	1:D:472:ARG:HH11	2.25	0.53
1:B:493:ASP:OD2	5:B:1303:HOH:O	2.19	0.53
1:C:328:LEU:HD23	1:C:328:LEU:C	2.28	0.53
1:B:284:GLU:OE1	1:B:308:ARG:NH2	2.42	0.52
1:A:450:HIS:CE1	1:A:472:ARG:HH11	2.27	0.52
1:A:478:GLU:CD	1:A:480:LYS:HE2	2.30	0.52
1:A:381:THR:HB	1:A:394:THR:OG1	2.09	0.52
1:D:216:SER:HB3	1:D:219:HIS:HB3	1.91	0.52
1:D:432:GLU:HB2	1:D:433:PRO:HD2	1.92	0.52
1:A:101:ASP:HB3	1:A:459:VAL:CG2	2.40	0.52
1:A:478:GLU:HG2	1:A:480:LYS:HE2	1.92	0.52
1:C:133:ALA:HB2	4:C:901:MES:C8	2.40	0.52
1:C:429:GLU:HG2	5:C:2850:HOH:O	2.09	0.52
1:B:100:ILE:HD11	1:B:453:ALA:HB2	1.92	0.52
1:D:185:LYS:O	1:D:186:ASP:C	2.46	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:341:ASN:C	1:B:341:ASN:ND2	2.63	0.51
1:D:335:GLY:O	1:D:346:PRO:HB3	2.10	0.51
1:D:50:VAL:HG23	1:D:50:VAL:O	2.11	0.51
1:A:178:GLU:OE1	1:A:441:PRO:HG3	2.11	0.51
1:B:538:PRO:HG2	1:C:538:PRO:HG2	1.92	0.51
1:D:385:THR:HG22	1:D:386:PRO:HD2	1.92	0.51
1:A:101:ASP:OD2	5:A:2823:HOH:O	2.19	0.51
1:C:132:GLN:OE1	4:C:901:MES:C3	2.59	0.51
1:D:285:ARG:CA	1:D:328:LEU:HD11	2.38	0.51
1:C:126:LEU:HD13	1:C:132:GLN:HG3	1.92	0.50
1:D:341:ASN:HD21	1:D:343:ALA:CB	2.20	0.50
1:D:341:ASN:ND2	1:D:343:ALA:HB3	2.18	0.50
1:A:558:ASP:OD2	5:A:2726:HOH:O	2.19	0.49
1:C:490:LYS:HD3	1:C:491:ILE:CD1	2.37	0.49
1:D:603:ILE:O	1:D:607:GLU:HG3	2.11	0.49
1:D:346:PRO:HG2	1:D:350:PRO:HA	1.94	0.49
1:D:289:ASN:OD1	1:D:292:ASN:N	2.46	0.49
1:C:450:HIS:HE1	1:C:472:ARG:HH11	1.60	0.49
1:D:181:PRO:HG2	1:D:195:TRP:HZ2	1.78	0.49
1:D:81:ASP:HB2	5:D:2214:HOH:O	2.13	0.49
1:C:133:ALA:HB2	4:C:901:MES:S	2.52	0.48
1:C:81:ASP:OD2	1:C:90:LYS:NZ	2.44	0.48
1:C:460:GLN:HB2	5:C:1928:HOH:O	2.13	0.48
1:D:385:THR:O	1:D:388:GLU:HG3	2.13	0.48
1:B:178:GLU:HB2	5:B:1867:HOH:O	2.13	0.48
1:B:459:VAL:HG12	1:B:461:GLN:HE22	1.78	0.48
1:C:81:ASP:OD1	1:C:81:ASP:N	2.47	0.48
1:D:308:ARG:NH1	1:D:308:ARG:CG	2.77	0.48
1:C:46:LYS:HG3	1:C:47:TYR:N	2.26	0.48
1:D:341:ASN:ND2	1:D:341:ASN:C	2.67	0.48
1:B:81:ASP:C	1:B:81:ASP:OD1	2.47	0.47
1:D:194:GLU:OE1	5:D:2796:HOH:O	2.20	0.47
1:A:460:GLN:HB2	5:A:1838:HOH:O	2.14	0.47
1:D:389:LEU:HD12	1:D:389:LEU:HA	1.16	0.47
1:C:385:THR:O	1:C:386:PRO:C	2.50	0.47
1:B:47:TYR:O	1:B:313:ALA:HA	2.15	0.47
1:A:505:ARG:HD2	5:A:2693:HOH:O	2.14	0.47
1:C:101:ASP:OD2	1:C:459:VAL:HG23	2.15	0.47
1:D:184:VAL:HG13	5:D:2678:HOH:O	2.15	0.47
1:D:199:TYR:O	1:D:203:GLU:HG3	2.14	0.47
1:B:91:LYS:NZ	1:B:452:ASP:OD1	2.46	0.46
1:B:537:LEU:HB3	1:B:538:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:SER:HB3	5:A:2308:HOH:O	2.16	0.46
1:A:158:THR:HG22	1:A:160:VAL:HG22	1.97	0.46
1:D:450:HIS:HE1	1:D:472:ARG:HH11	1.62	0.46
1:C:564:CYS:HG	1:C:573:PHE:HE2	1.64	0.46
1:A:44:ASP:HB2	1:A:47:TYR:CZ	2.51	0.45
1:C:231:LYS:HE2	1:C:231:LYS:HB2	1.48	0.45
1:D:89:HIS:CE1	1:D:91:LYS:HB3	2.50	0.45
1:B:81:ASP:N	1:B:81:ASP:OD1	2.45	0.45
1:C:450:HIS:CE1	1:C:472:ARG:HD2	2.51	0.45
1:D:385:THR:OG1	1:D:388:GLU:OE1	2.20	0.45
1:D:439:PHE:C	1:D:440:GLN:HG2	2.37	0.45
1:B:104:VAL:HG13	1:B:105:ASN:N	2.32	0.45
1:C:196:ASP:OD1	5:C:2646:HOH:O	2.21	0.45
1:D:47:TYR:O	1:D:313:ALA:HA	2.17	0.45
1:D:218:ARG:HD2	5:D:1256:HOH:O	2.16	0.45
1:A:126:LEU:HD12	1:A:132:GLN:HG3	1.99	0.44
1:A:342:PRO:C	1:A:344:ASN:N	2.71	0.44
1:B:450:HIS:HE1	1:B:472:ARG:HD2	1.83	0.44
1:B:481:GLU:OE2	1:B:484:LYS:NZ	2.48	0.44
1:C:459:VAL:HG13	1:C:461:GLN:NE2	2.32	0.44
5:C:2186:HOH:O	1:D:462:SER:HB2	2.17	0.44
1:C:570:SER:HB3	1:C:580:LEU:O	2.18	0.44
1:D:56:PRO:HD3	1:D:165:SER:HB3	1.99	0.44
1:D:208:THR:HA	1:D:242:ALA:HA	1.99	0.44
1:A:89:HIS:CE1	1:A:91:LYS:HB2	2.53	0.44
1:C:341:ASN:HA	1:C:342:PRO:HD2	1.90	0.44
1:A:450:HIS:HE1	1:A:472:ARG:HH11	1.64	0.44
1:C:214:LYS:O	5:C:2277:HOH:O	2.21	0.44
1:C:460:GLN:OE1	5:C:1928:HOH:O	2.21	0.44
1:D:107:ILE:HG12	1:D:167:ALA:HB1	1.99	0.44
1:B:607:GLU:HG3	5:B:2890:HOH:O	2.17	0.44
1:D:490:LYS:HG3	1:D:491:ILE:HD13	2.00	0.44
1:A:478:GLU:CG	1:A:480:LYS:HE2	2.48	0.44
1:D:45:ILE:N	5:D:2497:HOH:O	2.50	0.43
1:C:265:ARG:HA	1:C:266:PRO:C	2.38	0.43
4:C:901:MES:H82	4:C:901:MES:H51	1.78	0.43
1:D:343:ALA:C	1:D:344:ASN:ND2	2.55	0.43
1:D:68:ALA:HB2	1:D:610:LYS:NZ	2.33	0.43
1:B:218:ARG:HD2	5:B:1188:HOH:O	2.18	0.43
1:A:64:GLU:OE2	1:A:205:TYR:OH	2.29	0.43
1:D:197:ARG:NH2	1:D:607:GLU:OE1	2.47	0.43
1:A:432:GLU:H	1:A:432:GLU:CD	2.20	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:339:ARG:HA	1:C:340:PRO:HD3	1.85	0.43
1:B:158:THR:HG22	1:B:160:VAL:HG22	2.01	0.42
1:B:139:ARG:HD3	4:B:901:MES:O2S	2.19	0.42
1:C:228:GLU:HG3	1:C:231:LYS:NZ	2.33	0.42
1:A:505:ARG:NH1	5:A:2693:HOH:O	2.29	0.42
1:D:554:ARG:O	1:D:564:CYS:HB2	2.19	0.42
1:A:462:SER:OG	4:B:901:MES:H61	2.20	0.42
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.83	0.42
1:B:487:PHE:HB3	1:B:498:PRO:HB2	2.01	0.42
1:B:564:CYS:HG	1:B:573:PHE:HE2	1.67	0.42
1:C:218:ARG:HD2	5:C:1133:HOH:O	2.20	0.42
1:B:104:VAL:HG23	1:B:454:PHE:O	2.20	0.42
1:B:513:LYS:NZ	1:B:517:ASP:OD2	2.53	0.42
1:C:396:THR:HA	1:C:397:PRO:HD3	1.90	0.42
1:C:45:ILE:HB	1:C:46:LYS:H	1.20	0.42
1:C:385:THR:N	1:C:388:GLU:OE1	2.47	0.42
1:A:450:HIS:HE1	1:A:472:ARG:HD2	1.85	0.42
1:C:383:ARG:CG	1:C:383:ARG:NH1	2.83	0.42
1:D:299:HIS:CD2	1:D:310:GLU:HG2	2.55	0.42
1:D:201:LYS:HD3	1:D:603:ILE:HG21	2.01	0.42
1:A:218:ARG:HD2	5:A:1396:HOH:O	2.20	0.41
1:A:375:SER:HA	5:A:2923:HOH:O	2.19	0.41
1:B:471:TRP:CH2	1:B:526:SER:HA	2.55	0.41
1:D:293:SER:HA	1:D:574:GLY:O	2.20	0.41
1:D:175:PHE:CE1	1:D:592:ALA:HB3	2.55	0.41
1:B:328:LEU:C	1:B:328:LEU:HD23	2.40	0.41
1:D:284:GLU:O	1:D:285:ARG:HB3	2.21	0.41
1:B:56:PRO:HD3	1:B:165:SER:HB3	2.03	0.41
1:B:590:TYR:CE2	1:B:594:PRO:HB3	2.55	0.41
1:D:299:HIS:NE2	1:D:310:GLU:CD	2.74	0.41
1:B:344:ASN:O	1:B:345:PRO:C	2.58	0.41
1:C:611:GLN:HG2	5:C:2779:HOH:O	2.21	0.41
1:D:385:THR:H	1:D:388:GLU:CD	2.24	0.41
1:B:385:THR:CG2	1:B:388:GLU:OE1	2.62	0.41
1:B:460:GLN:HB2	5:B:2241:HOH:O	2.21	0.41
1:B:185:LYS:H	1:B:185:LYS:HG2	1.68	0.41
5:A:2721:HOH:O	1:B:461:GLN:HB3	2.20	0.41
1:C:101:ASP:CG	1:C:459:VAL:HG23	2.40	0.41
1:A:107:ILE:HG12	1:A:167:ALA:HB1	2.02	0.41
1:D:336:GLN:NE2	1:D:344:ASN:O	2.53	0.41
1:D:390:THR:HB	5:D:2845:HOH:O	2.20	0.41
1:D:537:LEU:HB3	1:D:538:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:608:TYR:CD1	1:D:608:TYR:C	2.94	0.41
1:D:97:GLN:HG3	1:D:250:PHE:CE2	2.56	0.41
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.20	0.41
1:A:408:TRP:C	1:A:408:TRP:CD1	2.95	0.40
1:D:354:SER:OG	1:D:484:LYS:NZ	2.53	0.40
1:B:576:LYS:CD	1:B:576:LYS:N	2.65	0.40
1:D:49:VAL:HG22	1:D:315:VAL:HB	2.03	0.40
1:C:47:TYR:CD2	1:C:73:ALA:HB2	2.56	0.40
2:D:801:FAD:H9	2:D:801:FAD:H1'1	1.87	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	574/623 (92%)	559 (97%)	15 (3%)	0	100	100
1	B	574/623 (92%)	557 (97%)	16 (3%)	1 (0%)	56	33
1	C	573/623 (92%)	558 (97%)	15 (3%)	0	100	100
1	D	572/623 (92%)	551 (96%)	19 (3%)	2 (0%)	50	27
All	All	2293/2492 (92%)	2225 (97%)	65 (3%)	3 (0%)	59	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	389	LEU
1	D	186	ASP
1	B	345	PRO

### 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	502/540 (93%)	487 (97%)	15 (3%)	53	29
1	B	502/540 (93%)	484 (96%)	18 (4%)	47	22
1	C	501/540 (93%)	486 (97%)	15 (3%)	53	29
1	D	500/540 (93%)	484 (97%)	16 (3%)	51	26
All	All	2005/2160 (93%)	1941 (97%)	64 (3%)	51	26

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	112	MET
1	A	168	TRP
1	A	206	PHE
1	A	269	ASP
1	A	299	HIS
1	A	344	ASN
1	A	385	THR
1	A	388	GLU
1	A	408	TRP
1	A	429	GLU
1	A	445	TRP
1	A	490	LYS
1	A	496	ASN
1	A	593	ASN
1	B	45	ILE
1	B	46	LYS
1	B	100	ILE
1	B	168	TRP
1	B	206	PHE
1	B	310	GLU
1	B	341	ASN
1	B	344	ASN
1	B	347	GLU
1	B	385	THR
1	B	400	SER

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Mol	Chain	Res	Type
1	B	408	TRP
1	B	441	PRO
1	B	460	GLN
1	B	545	LEU
1	B	576	LYS
1	B	593	ASN
1	B	618	PHE
1	C	45	ILE
1	C	46	LYS
1	C	112	MET
1	C	168	TRP
1	C	206	PHE
1	C	231	LYS
1	C	269	ASP
1	C	299	HIS
1	C	383	ARG
1	C	385	THR
1	C	408	TRP
1	C	421	GLU
1	C	459	VAL
1	C	593	ASN
1	C	619	THR
1	D	91	LYS
1	D	101	ASP
1	D	112	MET
1	D	168	TRP
1	D	185	LYS
1	D	199	TYR
1	D	204	SER
1	D	206	PHE
1	D	214	LYS
1	D	271	PRO
1	D	341	ASN
1	D	383	ARG
1	D	385	THR
1	D	403	LYS
1	D	408	TRP
1	D	450	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	299	HIS
1	A	324	HIS
1	A	341	ASN
1	A	344	ASN
1	A	450	HIS
1	B	341	ASN
1	B	450	HIS
1	B	461	GLN
1	B	611	GLN
1	C	224	ASN
1	C	263	GLN
1	C	299	HIS
1	C	341	ASN
1	C	344	ASN
1	C	450	HIS
1	C	461	GLN
1	D	132	GLN
1	D	207	GLN
1	D	324	HIS
1	D	341	ASN
1	D	344	ASN
1	D	450	HIS
1	D	612	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

10 ligands are modelled in this entry.



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FAD	A	801	-	58,58,58	1.45	8 (13%)	85,89,89	2.08	21 (24%)
3	1PE	A	904	-	12,13,15	0.75	0	11,12,14	0.37	0
3	1PE	A	905	-	11,11,15	2.40	1 (9%)	9,10,14	0.71	0
2	FAD	B	801	-	58,58,58	1.67	12 (20%)	85,89,89	2.16	21 (24%)
4	MES	B	901	-	12,12,12	2.27	3 (25%)	16,16,16	3.21	8 (50%)
3	1PE	B	902	-	15,15,15	0.62	0	14,14,14	0.27	0
2	FAD	C	801	-	58,58,58	1.37	10 (17%)	85,89,89	2.37	26 (30%)
4	MES	C	901	-	12,12,12	1.94	2 (16%)	16,16,16	3.90	8 (50%)
2	FAD	D	801	-	58,58,58	1.89	13 (22%)	85,89,89	2.63	32 (37%)
3	1PE	D	903	-	15,15,15	0.72	0	14,14,14	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	801	-	-	0/34/50/50	0/6/6/6
3	1PE	A	904	-	-	0/11/11/13	0/0/0/0
3	1PE	A	905	-	-	0/9/9/13	0/0/0/0
2	FAD	B	801	-	-	0/34/50/50	0/6/6/6
4	MES	B	901	-	-	0/6/14/14	0/1/1/1
3	1PE	B	902	-	-	0/13/13/13	0/0/0/0
2	FAD	C	801	-	-	0/34/50/50	0/6/6/6
4	MES	C	901	-	-	0/6/14/14	0/1/1/1
2	FAD	D	801	-	-	0/34/50/50	0/6/6/6
3	1PE	D	903	-	-	0/13/13/13	0/0/0/0

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	905	1PE	C12-C22	7.44	1.58	1.55
2	D	801	FAD	O2-C2	6.91	1.30	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	MES	C8-S	-6.81	1.66	1.78
4	C	901	MES	C8-S	-5.84	1.68	1.78
2	B	801	FAD	C1'-N10	4.85	1.53	1.48
2	D	801	FAD	C6-C5X	4.76	1.48	1.41
2	A	801	FAD	C4A-N3A	-4.59	1.28	1.35
2	B	801	FAD	C8A-N9A	-4.45	1.29	1.36
2	D	801	FAD	C8A-N9A	-4.43	1.30	1.36
2	B	801	FAD	O4B-C1B	4.00	1.46	1.41
2	A	801	FAD	C8M-C8	3.71	1.58	1.51
2	B	801	FAD	C4A-N3A	-3.68	1.29	1.35
2	C	801	FAD	C2B-C1B	-3.42	1.48	1.53
2	B	801	FAD	C5A-C4A	-3.20	1.33	1.40
2	B	801	FAD	C1B-N9A	-3.13	1.38	1.48
2	A	801	FAD	O2-C2	3.10	1.25	1.21
2	A	801	FAD	C4X-N5	3.09	1.38	1.33
2	D	801	FAD	C10-N1	3.06	1.41	1.35
2	B	801	FAD	C2B-C1B	-3.05	1.49	1.53
2	D	801	FAD	O4B-C4B	-2.75	1.38	1.45
2	D	801	FAD	C2B-C3B	-2.72	1.45	1.53
2	C	801	FAD	O3B-C3B	-2.66	1.36	1.43
2	D	801	FAD	O2B-C2B	-2.65	1.36	1.43
2	A	801	FAD	C2A-N3A	2.63	1.36	1.32
2	C	801	FAD	C4'-C3'	2.60	1.58	1.53
2	A	801	FAD	C2A-N1A	-2.56	1.28	1.33
2	A	801	FAD	C8A-N9A	-2.55	1.32	1.36
2	B	801	FAD	C8M-C8	2.45	1.55	1.51
4	B	901	MES	O2S-S	2.43	1.51	1.45
2	D	801	FAD	C1'-N10	-2.42	1.45	1.48
2	C	801	FAD	C4-N3	-2.39	1.33	1.36
2	B	801	FAD	O3B-C3B	-2.38	1.37	1.43
2	C	801	FAD	C4A-N9A	-2.32	1.34	1.37
2	D	801	FAD	O3B-C3B	-2.31	1.37	1.43
2	C	801	FAD	PA-O2A	-2.31	1.44	1.55
2	D	801	FAD	PA-O3P	2.30	1.64	1.59
2	D	801	FAD	C5'-C4'	2.29	1.55	1.51
2	B	801	FAD	P-O3P	2.25	1.63	1.59
4	B	901	MES	O1S-S	2.23	1.51	1.45
2	D	801	FAD	C1B-N9A	-2.22	1.41	1.48
2	C	801	FAD	O4B-C4B	-2.21	1.39	1.45
2	B	801	FAD	C2A-N3A	2.17	1.35	1.32
2	D	801	FAD	C2A-N3A	2.12	1.35	1.32
2	C	801	FAD	C2A-N1A	2.11	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	C9-C9A	2.04	1.45	1.40
2	C	801	FAD	C9-C8	2.03	1.43	1.37
4	C	901	MES	C5-C6	2.02	1.55	1.51
2	B	801	FAD	O4B-C4B	-2.02	1.40	1.45
2	C	801	FAD	C2B-C3B	-2.00	1.47	1.53

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	C4-N3-C2	-8.78	107.36	125.39
2	C	801	FAD	N3A-C2A-N1A	-8.74	121.20	128.89
4	C	901	MES	O1-C2-C3	-8.64	101.25	111.35
4	C	901	MES	O3S-S-C8	-8.21	85.21	105.98
2	C	801	FAD	C8A-N9A-C4A	8.02	113.48	106.96
2	B	801	FAD	N3A-C2A-N1A	-7.48	122.31	128.89
2	D	801	FAD	O4B-C1B-N9A	7.19	123.75	108.10
4	B	901	MES	O3S-S-C8	-7.04	88.17	105.98
2	A	801	FAD	C2-N1-C10	6.85	121.55	114.95
2	D	801	FAD	C2-N1-C10	6.82	121.52	114.95
4	B	901	MES	C5-N4-C3	6.68	124.18	109.77
2	D	801	FAD	C8A-N9A-C4A	6.68	112.39	106.96
2	A	801	FAD	N3A-C2A-N1A	-6.48	123.19	128.89
2	B	801	FAD	C2-N1-C10	6.47	121.17	114.95
2	D	801	FAD	N3A-C2A-N1A	-6.25	123.39	128.89
4	C	901	MES	C5-N4-C3	5.97	122.64	109.77
2	D	801	FAD	C4-C4X-C10	-5.77	107.58	117.18
2	D	801	FAD	C4X-C4-N3	5.60	134.25	116.21
2	C	801	FAD	N3A-C4A-N9A	5.13	134.18	125.39
2	B	801	FAD	C5A-C4A-N3A	-5.04	121.07	125.98
2	C	801	FAD	C2-N1-C10	5.03	119.79	114.95
2	B	801	FAD	N3A-C4A-N9A	5.01	133.99	125.39
2	B	801	FAD	C1'-N10-C9A	4.98	123.91	118.67
2	C	801	FAD	C1'-N10-C9A	4.91	123.83	118.67
2	A	801	FAD	C6A-C5A-C4A	4.83	122.97	117.55
2	B	801	FAD	C4-N3-C2	-4.58	116.00	125.39
2	D	801	FAD	C4X-C10-N10	-4.53	117.78	120.53
2	B	801	FAD	O4B-C1B-C2B	4.37	113.05	106.69
2	B	801	FAD	C8A-N9A-C4A	4.16	110.34	106.96
4	B	901	MES	O2S-S-C8	-4.16	93.51	106.37
4	B	901	MES	O3S-S-O2S	4.14	123.32	112.50
2	A	801	FAD	C2A-N1A-C6A	4.13	126.11	118.76
2	C	801	FAD	C1'-N10-C10	-4.10	114.36	118.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	N3A-C4A-N9A	4.05	132.33	125.39
2	A	801	FAD	C4A-C5A-N7A	-4.02	105.52	109.41
2	A	801	FAD	C1'-N10-C9A	3.99	122.86	118.67
2	A	801	FAD	C4X-C10-N10	-3.99	118.11	120.53
2	C	801	FAD	C2B-C1B-N9A	3.89	123.94	113.35
2	C	801	FAD	O2'-C2'-C3'	3.83	118.69	109.04
4	C	901	MES	C2-C3-N4	3.79	114.80	109.97
2	D	801	FAD	O2B-C2B-C3B	3.76	124.00	111.83
2	D	801	FAD	O4B-C4B-C5B	3.75	122.68	109.37
2	B	801	FAD	C9A-N10-C10	-3.73	118.09	121.77
2	C	801	FAD	C8A-N9A-C1B	-3.66	119.26	126.15
2	D	801	FAD	O2A-PA-O1A	3.63	132.22	112.14
2	B	801	FAD	C2B-C3B-C4B	3.56	109.74	102.64
2	B	801	FAD	C4B-O4B-C1B	-3.52	105.85	109.72
2	C	801	FAD	C5A-C6A-N6A	3.50	128.64	120.72
2	A	801	FAD	N6A-C6A-N1A	3.47	126.47	119.11
4	C	901	MES	O2S-S-O1S	3.45	120.45	112.39
4	C	901	MES	C7-N4-C5	3.36	120.10	111.65
2	A	801	FAD	C2B-C1B-N9A	3.35	122.47	113.35
2	A	801	FAD	O4B-C1B-N9A	3.25	115.17	108.10
2	B	801	FAD	C4-C4X-C10	-3.22	111.82	117.18
2	C	801	FAD	C5A-C4A-N9A	-3.20	102.65	107.09
2	A	801	FAD	C5A-C4A-N3A	-3.20	122.87	125.98
2	D	801	FAD	O2B-C2B-C1B	3.19	121.59	111.49
2	C	801	FAD	C10-C4X-N5	-3.17	119.16	122.57
2	D	801	FAD	N3-C2-N1	3.14	127.79	121.11
2	C	801	FAD	O2B-C2B-C3B	3.12	121.92	111.83
2	C	801	FAD	O4B-C1B-N9A	3.09	114.82	108.10
4	B	901	MES	O2S-S-O1S	3.07	119.57	112.39
2	A	801	FAD	O3B-C3B-C4B	3.06	120.07	111.07
2	D	801	FAD	C4-C4X-N5	3.04	131.30	117.77
2	D	801	FAD	O5'-P-O1P	-3.02	97.54	109.37
2	C	801	FAD	C4X-N5-C5X	2.97	120.14	116.68
2	D	801	FAD	C5B-C4B-C3B	2.93	126.92	115.19
2	D	801	FAD	C5A-C4A-N9A	-2.92	103.04	107.09
2	C	801	FAD	O2B-C2B-C1B	2.92	120.72	111.49
2	B	801	FAD	C4X-C4-N3	2.90	125.57	116.21
2	C	801	FAD	C5A-C4A-N3A	-2.89	123.17	125.98
2	A	801	FAD	C8A-N9A-C4A	2.83	109.26	106.96
2	D	801	FAD	C8A-N9A-C1B	-2.82	120.84	126.15
2	C	801	FAD	N7A-C8A-N9A	-2.82	105.81	112.20
2	D	801	FAD	C7-C6-C5X	-2.76	116.28	120.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	C9A-N10-C10	-2.74	119.06	121.77
2	A	801	FAD	C5A-C6A-N1A	-2.74	110.06	119.27
2	D	801	FAD	O5B-PA-O1A	-2.69	98.84	109.37
2	B	801	FAD	C5X-C9A-N10	2.67	119.60	117.63
2	C	801	FAD	N6A-C6A-N1A	-2.66	113.48	119.11
2	D	801	FAD	C2B-C1B-N9A	2.61	120.45	113.35
2	C	801	FAD	O4B-C4B-C3B	2.58	110.41	105.16
2	B	801	FAD	C6A-C5A-C4A	2.56	120.42	117.55
2	B	801	FAD	C5A-C6A-N6A	2.56	126.51	120.72
2	A	801	FAD	C7M-C7-C6	-2.53	113.49	120.25
2	A	801	FAD	O4'-C4'-C3'	2.47	115.26	109.04
4	B	901	MES	C7-N4-C3	2.46	117.83	111.65
2	C	801	FAD	C3B-C2B-C1B	2.44	104.74	100.92
2	B	801	FAD	O3B-C3B-C4B	2.43	118.22	111.07
4	B	901	MES	C7-N4-C5	2.39	117.67	111.65
4	C	901	MES	O3S-S-O1S	2.39	118.76	112.50
2	C	801	FAD	O4B-C1B-C2B	2.39	110.17	106.69
2	A	801	FAD	C4B-O4B-C1B	2.37	112.32	109.72
2	D	801	FAD	C4X-N5-C5X	2.36	119.44	116.68
2	B	801	FAD	O2B-C2B-C3B	2.33	119.38	111.83
2	D	801	FAD	C6A-C5A-C4A	2.30	120.13	117.55
2	A	801	FAD	C5X-C9A-N10	2.25	119.29	117.63
2	D	801	FAD	C1'-N10-C9A	2.25	121.03	118.67
2	B	801	FAD	C4X-C10-N10	-2.25	119.17	120.53
2	A	801	FAD	N3A-C4A-N9A	2.22	129.20	125.39
2	A	801	FAD	O2B-C2B-C3B	2.21	118.96	111.83
2	B	801	FAD	C2B-C1B-N9A	2.18	119.28	113.35
2	D	801	FAD	O3P-PA-O5B	-2.17	97.15	102.91
2	A	801	FAD	O2B-C2B-C1B	2.17	118.36	111.49
2	D	801	FAD	O4'-C4'-C5'	-2.16	105.70	110.13
2	C	801	FAD	C4-N3-C2	-2.14	121.00	125.39
2	D	801	FAD	C10-C4X-N5	-2.14	120.27	122.57
4	B	901	MES	C2-C3-N4	2.11	112.65	109.97
2	C	801	FAD	C4B-O4B-C1B	-2.08	107.43	109.72
2	D	801	FAD	O3B-C3B-C4B	2.05	117.11	111.07
2	B	801	FAD	C2A-N3A-C4A	2.02	119.09	113.27
2	D	801	FAD	O2A-PA-O3P	2.02	114.71	105.14
2	C	801	FAD	P-O3P-PA	2.02	137.52	131.93
2	D	801	FAD	C4X-C10-N1	-2.01	120.16	123.00
2	C	801	FAD	O3B-C3B-C4B	2.00	116.97	111.07
4	C	901	MES	C6-O1-C2	-2.00	103.08	109.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	576/623 (92%)	0.34	34 (5%) 22 26	4, 10, 24, 40	0
1	B	576/623 (92%)	0.28	25 (4%) 34 38	4, 10, 22, 45	0
1	C	575/623 (92%)	0.42	37 (6%) 19 23	6, 13, 28, 39	0
1	D	574/623 (92%)	1.19	143 (24%) 1 2	3, 14, 24, 40	0
All	All	2301/2492 (92%)	0.56	239 (10%) 7 9	3, 12, 25, 45	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	618	PHE	9.4
1	D	45	ILE	8.1
1	D	459	VAL	7.6
1	C	389	LEU	7.5
1	D	184	VAL	7.0
1	D	617	PRO	6.7
1	D	343	ALA	6.6
1	A	381	THR	6.3
1	C	619	THR	6.3
1	D	345	PRO	6.0
1	C	390	THR	5.8
1	D	290	ALA	5.8
1	D	268	THR	5.7
1	D	458	ALA	5.4
1	A	459	VAL	5.4
1	D	190	ALA	5.4
1	A	343	ALA	5.2
1	D	309	PHE	5.1
1	A	344	ASN	5.0
1	B	458	ALA	4.9
1	C	382	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	45	ILE	4.9
1	D	187	ASP	4.8
1	D	556	GLY	4.7
1	D	611	GLN	4.7
1	D	616	SER	4.7
1	A	401	THR	4.7
1	D	385	THR	4.7
1	D	342	PRO	4.7
1	A	345	PRO	4.7
1	D	272	GLU	4.7
1	D	186	ASP	4.7
1	D	269	ASP	4.6
1	C	383	ARG	4.6
1	C	343	ALA	4.6
1	C	458	ALA	4.6
1	D	67	GLY	4.5
1	D	557	PHE	4.5
1	D	68	ALA	4.5
1	D	69	GLY	4.5
1	D	193	ALA	4.4
1	C	45	ILE	4.4
1	D	271	PRO	4.4
1	D	49	VAL	4.4
1	D	267	ASN	4.3
1	A	45	ILE	4.2
1	D	183	LEU	4.2
1	D	188	ALA	4.2
1	D	291	LEU	4.2
1	D	315	VAL	4.2
1	D	278	PHE	4.1
1	D	304	ILE	4.1
1	D	46	LYS	4.1
1	D	606	CYS	4.1
1	D	400	SER	4.1
1	D	398	GLY	4.0
1	B	618	PHE	3.9
1	D	47	TYR	3.9
1	D	266	PRO	3.9
1	C	344	ASN	3.8
1	C	618	PHE	3.8
1	D	189	ASP	3.8
1	C	388	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	188	ALA	3.8
1	D	70	TYR	3.8
1	B	44	ASP	3.7
1	D	48	ASP	3.7
1	B	345	PRO	3.6
1	D	65	LEU	3.6
1	D	344	ASN	3.5
1	A	457	GLY	3.5
1	D	314	ASP	3.5
1	D	613	PHE	3.5
1	B	185	LYS	3.4
1	A	458	ALA	3.4
1	D	66	VAL	3.4
1	D	341	ASN	3.4
1	C	385	THR	3.4
1	C	391	TYR	3.4
1	D	312	LYS	3.4
1	D	182	LEU	3.4
1	D	307	ASP	3.3
1	B	344	ASN	3.3
1	D	614	THR	3.3
1	D	347	GLU	3.3
1	D	75	PHE	3.3
1	D	609	ILE	3.3
1	A	342	PRO	3.2
1	D	198	LEU	3.2
1	B	343	ALA	3.2
1	D	270	ALA	3.2
1	D	574	GLY	3.2
1	D	205	TYR	3.2
1	A	382	ILE	3.2
1	D	191	ASP	3.2
1	A	385	THR	3.2
1	D	457	GLY	3.2
1	D	311	ILE	3.2
1	D	573	PHE	3.2
1	D	289	ASN	3.1
1	D	310	GLU	3.1
1	A	400	SER	3.1
1	D	192	ASP	3.1
1	D	346	PRO	3.1
1	D	401	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	287	VAL	3.1
1	A	394	THR	3.1
1	A	397	PRO	3.1
1	D	561	GLU	3.1
1	A	341	ASN	3.1
1	D	456	TYR	3.0
1	D	406	ASP	3.0
1	D	316	TYR	3.0
1	D	579	PHE	3.0
1	D	185	LYS	3.0
1	A	396	THR	3.0
1	D	490	LYS	2.9
1	A	383	ARG	2.9
1	C	387	GLY	2.9
1	C	384	GLY	2.9
1	D	300	ILE	2.9
1	C	322	ALA	2.8
1	D	211	ASP	2.8
1	D	386	PRO	2.8
1	B	232	GLY	2.8
1	D	72	VAL	2.8
1	D	407	TRP	2.8
1	B	583	CYS	2.8
1	D	390	THR	2.8
1	B	580	LEU	2.8
1	C	291	LEU	2.8
1	D	308	ARG	2.7
1	B	186	ASP	2.7
1	D	608	TYR	2.7
1	D	84	LEU	2.7
1	C	381	THR	2.7
1	C	323	VAL	2.7
1	D	301	HIS	2.7
1	D	194	GLU	2.6
1	D	273	GLU	2.6
1	D	274	ARG	2.6
1	B	457	GLY	2.6
1	B	318	LEU	2.6
1	D	81	ASP	2.6
1	A	186	ASP	2.6
1	D	200	THR	2.6
1	D	305	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	341	ASN	2.5
1	D	340	PRO	2.5
1	D	615	PRO	2.5
1	D	296	GLU	2.5
1	D	387	GLY	2.5
1	D	297	SER	2.5
1	B	459	VAL	2.5
1	A	398	GLY	2.5
1	D	567	ASN	2.5
1	C	309	PHE	2.5
1	D	388	GLU	2.5
1	D	603	ILE	2.5
1	A	268	THR	2.5
1	D	201	LYS	2.5
1	D	339	ARG	2.4
1	D	275	PHE	2.4
1	D	441	PRO	2.4
1	D	276	ASN	2.4
1	B	52	VAL	2.4
1	D	576	LYS	2.4
1	C	186	ASP	2.4
1	B	43	MET	2.4
1	D	260	PHE	2.4
1	C	189	ASP	2.4
1	C	307	ASP	2.4
1	C	549	LEU	2.3
1	A	44	ASP	2.3
1	D	558	ASP	2.3
1	B	400	SER	2.3
1	C	592	ALA	2.3
1	D	71	LYS	2.3
1	D	293	SER	2.3
1	C	268	THR	2.3
1	D	384	GLY	2.3
1	D	610	LYS	2.3
1	C	57	ILE	2.3
1	D	62	ALA	2.3
1	A	389	LEU	2.3
1	D	549	LEU	2.3
1	D	177	ARG	2.3
1	A	618	PHE	2.3
1	D	333	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	265	ARG	2.2
1	D	607	GLU	2.2
1	D	469	VAL	2.2
1	A	361	LEU	2.2
1	D	580	LEU	2.2
1	D	612	ASN	2.2
1	D	64	GLU	2.2
1	A	390	THR	2.2
1	D	82	SER	2.2
1	D	313	ALA	2.2
1	A	388	GLU	2.2
1	A	362	VAL	2.2
1	C	457	GLY	2.2
1	B	601	LEU	2.2
1	D	389	LEU	2.1
1	C	305	SER	2.1
1	D	231	LYS	2.1
1	A	474	PHE	2.1
1	C	345	PRO	2.1
1	D	246	ARG	2.1
1	B	268	THR	2.1
1	D	562	ASP	2.1
1	B	322	ALA	2.1
1	A	583	CYS	2.1
1	D	292	ASN	2.1
1	D	61	TYR	2.1
1	A	317	VAL	2.1
1	B	323	VAL	2.1
1	D	228	GLU	2.1
1	C	347	GLU	2.1
1	D	299	HIS	2.1
1	D	381	THR	2.1
1	A	469	VAL	2.1
1	C	459	VAL	2.1
1	D	196	ASP	2.1
1	D	214	LYS	2.1
1	D	336	GLN	2.1
1	D	489	ASP	2.0
1	C	310	GLU	2.0
1	D	294	GLU	2.0
1	A	82	SER	2.0
1	C	590	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	285	ARG	2.0
1	B	57	ILE	2.0
1	B	449	ILE	2.0
1	A	393	VAL	2.0
1	D	492	THR	2.0
1	B	51	ILE	2.0
1	D	295	ILE	2.0
1	C	318	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	1PE	A	905	12/16	0.14	3.33	29,31,36,38	0
3	1PE	B	902	16/16	0.14	3.10	35,38,48,55	0
2	FAD	D	801	53/53	0.21	3.01	19,24,29,31	0
2	FAD	A	801	53/53	0.20	2.82	8,12,16,19	0
2	FAD	B	801	53/53	0.21	2.25	10,12,15,18	0
2	FAD	C	801	53/53	0.19	1.97	13,17,21,23	0
3	1PE	A	904	14/16	0.13	1.82	30,35,39,42	0
4	MES	C	901	12/12	0.14	0.86	26,30,32,33	0
3	1PE	D	903	16/16	0.13	0.46	37,45,51,55	0
4	MES	B	901	12/12	0.11	0.44	24,28,31,31	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.