



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2018 – 11:57 AM EST

PDB ID : 5WX2  
Title : Crystal structure of porcine kidney D-amino acid oxidase mutant (I230A/R283G)  
Authors : Motojima, F.; Yasukawa, K.; Ohno, A.; Asano, Y.  
Deposited on : 2017-01-06  
Resolution : 3.00 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

<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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

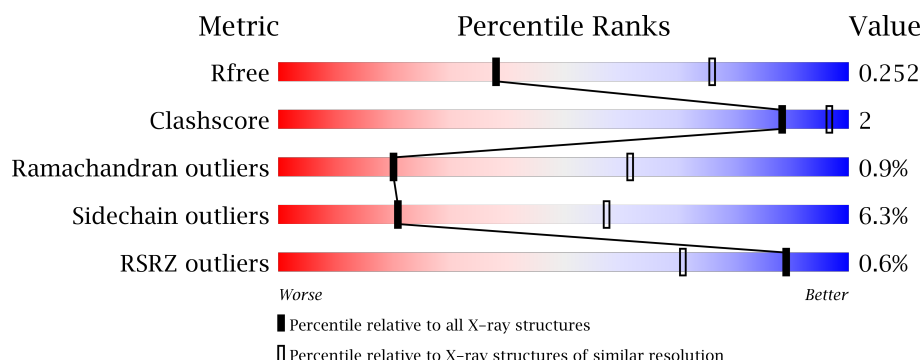
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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. 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	347	
1	B	347	
1	C	347	
1	D	347	
1	E	347	

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Mol	Chain	Length	Quality of chain
1	F	347	 2% 87% 10% ..
1	G	347	 82% 14% ..
1	H	347	 % 81% 15% ..

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
3	MPD	A	402	-	-	-	X
3	MPD	A	403	-	-	-	X
3	MPD	B	402	-	-	-	X
3	MPD	B	403	-	-	-	X
3	MPD	B	404	-	-	-	X
3	MPD	D	403	-	-	-	X
3	MPD	F	402	-	-	-	X
3	MPD	F	403	-	-	-	X
3	MPD	F	404	-	-	-	X
3	MPD	G	403	-	-	-	X
3	MPD	H	402	-	-	-	X
4	SO4	D	405	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22380 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 D-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	1	0
			2701	1737	469	486	9			
1	B	339	Total	C	N	O	S	0	0	0
			2710	1742	470	489	9			
1	C	339	Total	C	N	O	S	0	1	0
			2717	1747	472	489	9			
1	D	339	Total	C	N	O	S	0	0	0
			2710	1742	470	489	9			
1	E	339	Total	C	N	O	S	0	2	0
			2722	1750	473	490	9			
1	F	339	Total	C	N	O	S	0	0	0
			2710	1742	470	489	9			
1	G	338	Total	C	N	O	S	0	1	0
			2709	1741	471	488	9			
1	H	337	Total	C	N	O	S	0	1	0
			2701	1737	469	486	9			

There are 16 discrepancies between the modelled and reference sequences:

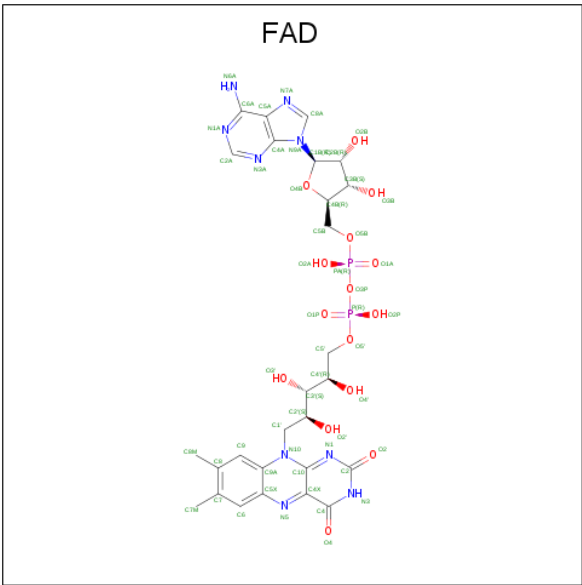
Chain	Residue	Modelled	Actual	Comment	Reference
A	230	ALA	ILE	engineered mutation	UNP P00371
A	283	GLY	ARG	engineered mutation	UNP P00371
B	230	ALA	ILE	engineered mutation	UNP P00371
B	283	GLY	ARG	engineered mutation	UNP P00371
C	230	ALA	ILE	engineered mutation	UNP P00371
C	283	GLY	ARG	engineered mutation	UNP P00371
D	230	ALA	ILE	engineered mutation	UNP P00371
D	283	GLY	ARG	engineered mutation	UNP P00371
E	230	ALA	ILE	engineered mutation	UNP P00371
E	283	GLY	ARG	engineered mutation	UNP P00371
F	230	ALA	ILE	engineered mutation	UNP P00371
F	283	GLY	ARG	engineered mutation	UNP P00371
G	230	ALA	ILE	engineered mutation	UNP P00371

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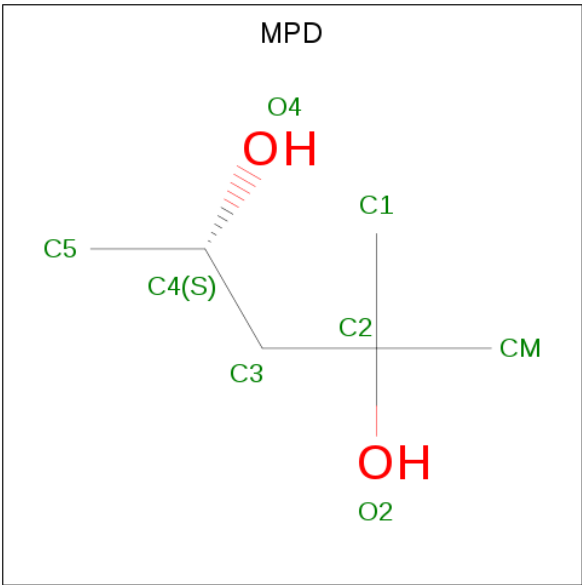
Chain	Residue	Modelled	Actual	Comment	Reference
G	283	GLY	ARG	engineered mutation	UNP P00371
H	230	ALA	ILE	engineered mutation	UNP P00371
H	283	GLY	ARG	engineered mutation	UNP P00371

- Molecule 2 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
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		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

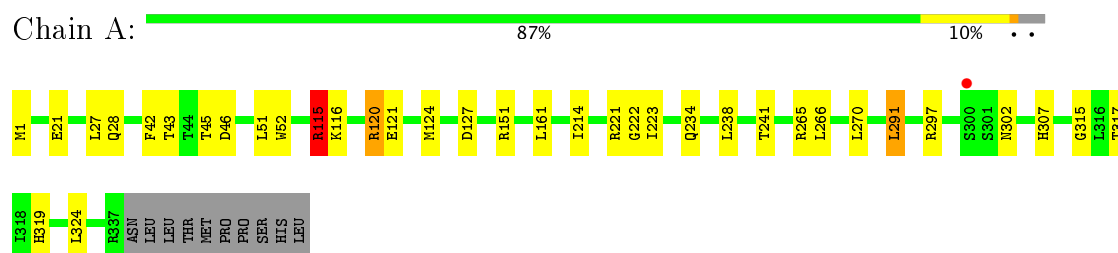
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	B	22	Total	O	0	0
			22	22		
5	C	5	Total	O	0	0
			5	5		
5	D	10	Total	O	0	0
			10	10		
5	E	4	Total	O	0	0
			4	4		
5	F	2	Total	O	0	0
			2	2		
5	G	4	Total	O	0	0
			4	4		
5	H	5	Total	O	0	0
			5	5		



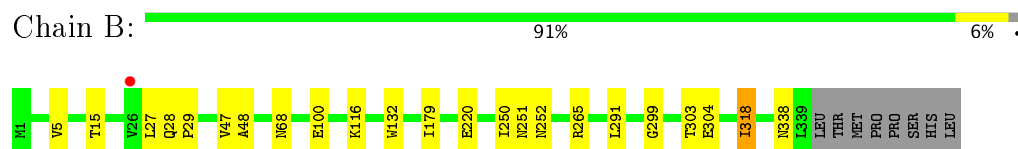
### 3 Residue-property plots

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.

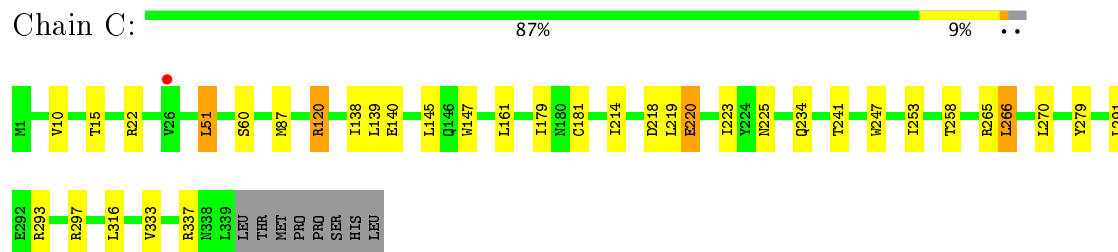
- Molecule 1: D-amino-acid oxidase



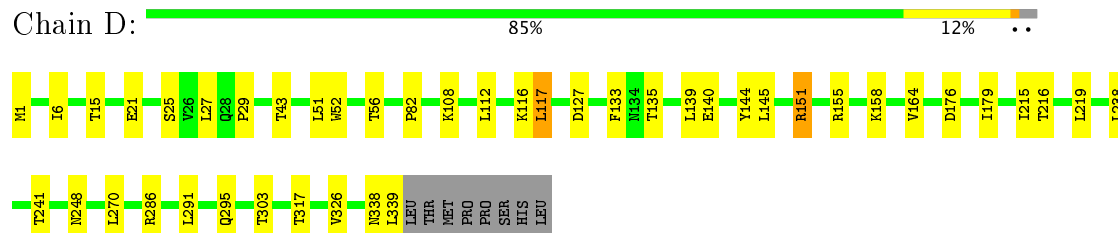
- Molecule 1: D-amino-acid oxidase



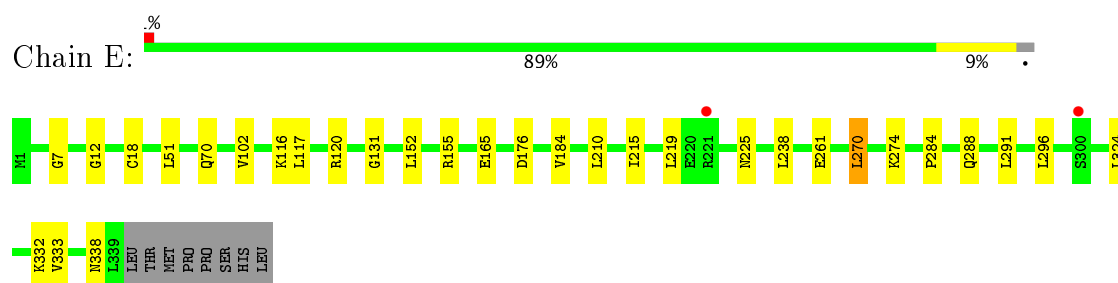
- Molecule 1: D-amino-acid oxidase



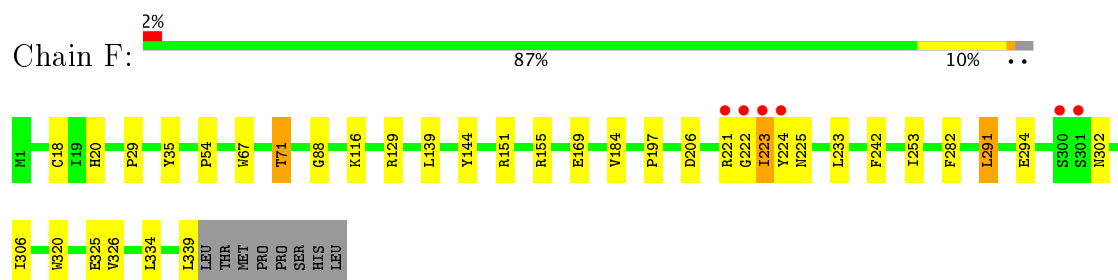
- Molecule 1: D-amino-acid oxidase



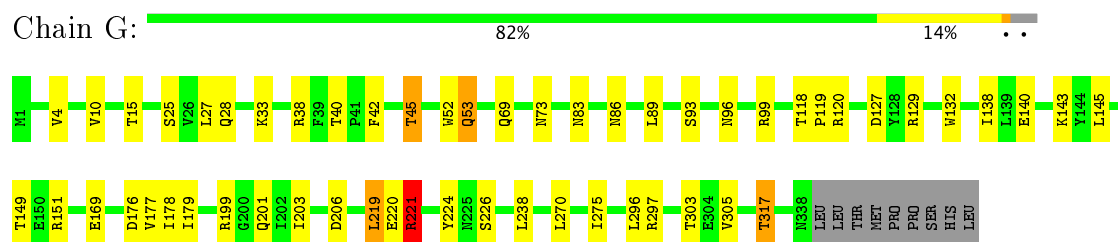
- Molecule 1: D-amino-acid oxidase



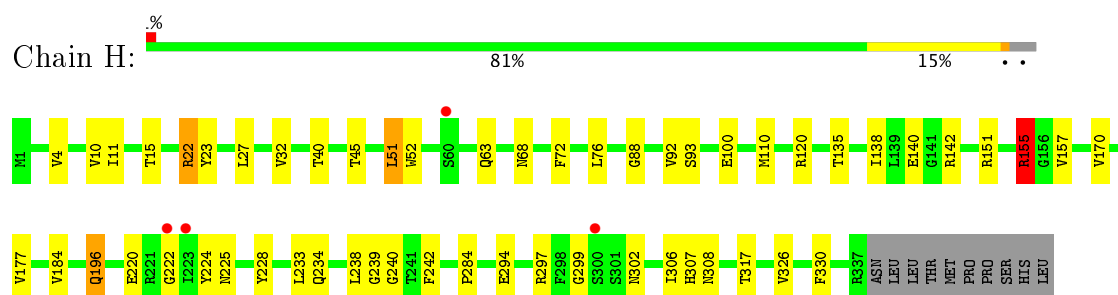
- Molecule 1: D-amino-acid oxidase



- Molecule 1: D-amino-acid oxidase



- Molecule 1: D-amino-acid oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.40 Å   270.90 Å   135.43 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.17 – 3.00 49.17 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.17-3.00) 100.0 (49.17-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.03 (at 3.01 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.165   ,   0.253 0.171   ,   0.252	Depositor DCC
$R_{free}$ test set	2943 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, SO4, FAD

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	0.58	0/2781	0.79	2/3788 (0.1%)
1	B	0.57	0/2786	0.74	0/3795
1	C	0.52	0/2797	0.70	1/3810 (0.0%)
1	D	0.54	0/2786	0.71	0/3795
1	E	0.53	0/2805	0.70	0/3821
1	F	0.53	0/2786	0.70	0/3795
1	G	0.50	0/2789	0.70	0/3799
1	H	0.55	0/2781	0.73	2/3788 (0.1%)
All	All	0.54	0/22311	0.72	5/30391 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	120	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	115	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	H	120	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	H	155	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	120	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2701	0	2649	11	0
1	B	2710	0	2659	9	0
1	C	2717	0	2666	12	0
1	D	2710	0	2659	11	0
1	E	2722	0	2672	8	1
1	F	2710	0	2659	9	1
1	G	2709	0	2655	22	0
1	H	2701	0	2649	22	1
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
2	E	53	0	31	0	0
2	F	53	0	31	0	0
2	G	53	0	31	0	0
2	H	53	0	31	0	0
3	A	32	0	56	2	0
3	B	32	0	56	0	0
3	C	8	0	14	2	0
3	D	24	0	42	0	0
3	E	8	0	14	0	0
3	F	32	0	56	0	0
3	G	24	0	42	2	0
3	H	16	0	28	0	0
4	A	5	0	0	1	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	1	0
4	F	5	0	0	0	0
4	H	5	0	0	0	0
5	A	18	0	0	0	0
5	B	22	0	0	1	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
5	E	4	0	0	0	0
5	F	2	0	0	0	0
5	G	4	0	0	0	0
5	H	5	0	0	0	2
All	All	22380	0	21824	103	4

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 2.

All (103) 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:27:LEU:HD13	1:D:339:LEU:HD11	1.73	0.69
1:A:46:ASP:HB3	3:A:403:MPD:H52	1.75	0.69
1:E:51:LEU:HD23	1:E:215:ILE:HD11	1.79	0.65
1:F:223:ILE:HG23	1:F:224:TYR:CE2	2.33	0.64
1:H:52:TRP:CE2	1:H:317:THR:HG23	2.36	0.60
1:C:51:LEU:HD12	1:C:138:ILE:HD13	1.85	0.58
1:A:214:ILE:HG21	1:A:266:LEU:HD22	1.86	0.57
1:A:115:ARG:NH2	1:A:121:GLU:OE2	2.38	0.57
1:C:293:ARG:NH1	1:C:333:VAL:HG22	2.20	0.56
1:H:4:VAL:HG11	1:H:170:VAL:HG13	1.87	0.56
1:E:51:LEU:CD2	1:E:215:ILE:HD11	2.36	0.56
1:C:218:ASP:O	1:C:220:GLU:N	2.39	0.56
1:G:52:TRP:HA	1:G:317:THR:HG22	1.88	0.55
1:B:68:ASN:ND2	1:B:318:ILE:HD12	2.21	0.55
1:G:296:LEU:HD12	1:G:305:VAL:HG21	1.88	0.55
1:H:92:VAL:HG11	1:H:138:ILE:HG13	1.89	0.55
1:C:15:THR:HG21	1:C:179:ILE:HG21	1.87	0.54
1:B:5:VAL:HG13	1:B:179:ILE:HB	1.89	0.54
1:A:291:LEU:HA	1:A:307:HIS:O	2.08	0.53
1:B:15:THR:HG21	1:B:179:ILE:HG21	1.90	0.53
1:G:238:LEU:HD21	1:G:270:LEU:HD13	1.90	0.53
1:E:120:ARG:NH1	4:E:403:SO4:O4	2.41	0.53
1:H:11:ILE:O	1:H:15:THR:HG23	2.09	0.53
1:H:10:VAL:HB	1:H:45:THR:HG21	1.90	0.52
1:H:177:VAL:HG11	1:H:330:PHE:HE1	1.74	0.52
1:F:67:TRP:O	1:F:71:THR:HG23	2.09	0.52
1:F:139:LEU:HD11	1:F:144:TYR:CG	2.45	0.52
1:D:112:LEU:HB2	1:D:135:THR:HB	1.92	0.52
1:D:139:LEU:HD21	1:D:144:TYR:CE2	2.45	0.52
1:D:139:LEU:HD21	1:D:144:TYR:CD2	2.45	0.52
1:A:124:MET:HG2	5:B:521:HOH:O	2.10	0.51
1:E:210:LEU:HD11	1:E:270:LEU:HD13	1.93	0.51
1:B:28:GLN:N	1:B:29:PRO:HD3	2.26	0.51
1:G:69:GLN:HE21	1:G:73:ASN:HD21	1.58	0.51
1:A:120:ARG:HD3	4:A:406:SO4:S	2.51	0.51
1:D:51:LEU:CD2	1:D:215:ILE:HD11	2.41	0.50
1:B:68:ASN:HD21	1:B:318:ILE:HD12	1.76	0.50
1:G:120:ARG:NH2	1:H:110:MET:O	2.45	0.50
1:C:279:TYR:CD1	3:C:402:MPD:H52	2.47	0.49
1:H:306:ILE:HG21	1:H:326:VAL:HG13	1.94	0.49
1:E:117:LEU:HD12	1:E:131:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ARG:NH1	4:C:403:SO4:O3	2.38	0.48
1:F:184:VAL:HG21	1:F:282:PHE:O	2.13	0.48
1:H:72:PHE:HE1	1:H:76:LEU:HD12	1.79	0.47
1:B:28:GLN:N	1:B:29:PRO:CD	2.78	0.47
1:F:306:ILE:HG21	1:F:326:VAL:HG13	1.97	0.47
1:G:42:PHE:CZ	3:G:404:MPD:H51	2.49	0.46
1:G:10:VAL:HG12	1:G:45:THR:HG21	1.97	0.46
1:G:52:TRP:CD1	1:G:317:THR:HG22	2.50	0.46
1:H:68:ASN:ND2	1:H:317:THR:HG22	2.31	0.46
1:D:52:TRP:CD1	1:D:317:THR:HA	2.50	0.46
1:H:15:THR:HG21	1:H:308:ASN:HD22	1.81	0.46
1:A:42:PHE:HA	3:A:404:MPD:H12	1.98	0.46
1:C:179:ILE:HG22	1:C:181:CYS:SG	2.55	0.45
1:H:151:ARG:O	1:H:155:ARG:HG2	2.16	0.45
1:G:15:THR:HG21	1:G:179:ILE:HG21	1.99	0.45
1:G:89:LEU:HA	1:G:138:ILE:O	2.17	0.45
1:E:70:GLN:HE21	1:E:324:LEU:HD12	1.81	0.45
1:D:6:ILE:HD13	1:D:164:VAL:HG21	1.98	0.45
1:H:88:GLY:HA2	1:H:233:LEU:HD11	1.99	0.45
1:B:303:THR:HG22	1:B:304:GLU:N	2.32	0.44
1:C:214:ILE:HG21	1:C:266:LEU:HD22	2.00	0.44
1:G:4:VAL:HB	1:G:178:ILE:HG22	2.00	0.44
1:G:83:ASN:OD1	1:G:86:ASN:ND2	2.50	0.44
1:A:52:TRP:CE2	1:A:317:THR:HG23	2.53	0.44
1:H:294:GLU:OE1	1:H:307:HIS:NE2	2.46	0.44
1:C:87:MET:HG2	1:C:147:TRP:CD2	2.53	0.44
1:H:184:VAL:N	1:H:284:PRO:HB3	2.33	0.44
1:F:88:GLY:HA2	1:F:233:LEU:HD11	2.00	0.43
1:C:225:ASN:HB3	1:C:258:THR:HG21	2.00	0.43
1:H:68:ASN:HD22	1:H:317:THR:HG22	1.83	0.43
1:G:53:GLN:HE22	1:G:96:ASN:HD21	1.67	0.43
1:C:279:TYR:CE1	3:C:402:MPD:H52	2.54	0.43
1:B:250:ILE:HG23	1:B:251:ASN:O	2.18	0.43
1:H:93:SER:HA	1:H:135:THR:HA	2.00	0.43
1:G:118:THR:HB	1:G:119:PRO:HD2	2.01	0.43
1:G:151:ARG:HA	1:G:151:ARG:NE	2.34	0.43
1:G:53:GLN:NE2	1:G:96:ASN:OD1	2.52	0.43
1:G:53:GLN:H	1:G:317:THR:HG21	1.84	0.42
1:A:43:THR:OG1	1:A:45:THR:HB	2.19	0.42
1:G:52:TRP:HA	1:G:317:THR:CG2	2.47	0.42
1:A:151:ARG:NE	1:A:151:ARG:HA	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:GLY:O	1:A:319:HIS:HB3	2.20	0.42
1:F:71:THR:HG22	1:F:320:TRP:HB3	2.01	0.42
1:E:7:GLY:O	1:E:12:GLY:HA3	2.19	0.42
1:H:51:LEU:HD12	1:H:52:TRP:N	2.35	0.41
1:G:221:ARG:NE	1:G:221:ARG:HA	2.34	0.41
1:B:47:VAL:O	1:B:48:ALA:C	2.57	0.41
1:F:291:LEU:HD21	1:F:325:GLU:HB3	2.02	0.41
1:H:22:ARG:HG2	1:H:23:TYR:CE2	2.56	0.41
1:C:10:VAL:HG21	1:C:316:LEU:HD23	2.03	0.41
1:D:15:THR:HG21	1:D:179:ILE:HG21	2.02	0.41
1:H:32:VAL:HB	1:H:157:VAL:HG13	2.03	0.41
1:D:151:ARG:O	1:D:155:ARG:HG2	2.21	0.41
1:F:20:HIS:ND1	1:F:155:ARG:NH1	2.69	0.40
1:H:52:TRP:CZ2	1:H:72:PHE:HB2	2.56	0.40
1:E:184:VAL:N	1:E:284:PRO:HB3	2.35	0.40
1:D:117:LEU:CD1	1:D:133:PHE:HB2	2.51	0.40
1:G:199:ARG:NH2	1:G:201:GLN:OE1	2.55	0.40
1:G:203:ILE:HG23	1:G:275:ILE:HG23	2.04	0.40
1:H:228:TYR:CZ	1:H:239:GLY:HA3	2.57	0.40
1:D:291:LEU:HD13	1:D:326:VAL:HG22	2.02	0.40
1:G:38:ARG:NH1	3:G:404:MPD:O2	2.55	0.40

All (4) 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)
5:H:503:HOH:O	5:H:503:HOH:O[4_556]	1.75	0.45
1:H:196:GLN:OE1	1:H:196:GLN:OE1[4_556]	2.10	0.10
5:H:502:HOH:O	5:H:502:HOH:O[4_556]	2.16	0.04
1:E:165:GLU:OE1	1:F:35:TYR:OH[6_544]	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	336/347 (97%)	317 (94%)	17 (5%)	2 (1%)	28	70
1	B	337/347 (97%)	317 (94%)	19 (6%)	1 (0%)	44	81
1	C	338/347 (97%)	312 (92%)	25 (7%)	1 (0%)	44	81
1	D	337/347 (97%)	309 (92%)	25 (7%)	3 (1%)	20	62
1	E	339/347 (98%)	322 (95%)	14 (4%)	3 (1%)	20	62
1	F	337/347 (97%)	307 (91%)	24 (7%)	6 (2%)	10	43
1	G	337/347 (97%)	305 (90%)	30 (9%)	2 (1%)	28	70
1	H	336/347 (97%)	300 (89%)	30 (9%)	6 (2%)	10	43
All	All	2697/2776 (97%)	2489 (92%)	184 (7%)	24 (1%)	20	62

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	219	LEU
1	E	219	LEU
1	F	29	PRO
1	F	197	PRO
1	F	222	GLY
1	H	225	ASN
1	B	299	GLY
1	D	338	ASN
1	E	338	ASN
1	F	223	ILE
1	H	220	GLU
1	A	223	ILE
1	G	221	ARG
1	H	240	GLY
1	D	25	SER
1	E	225	ASN
1	F	221	ARG
1	G	219	LEU
1	H	222	GLY
1	H	100	GLU
1	D	29	PRO
1	F	54	PRO
1	H	299	GLY
1	A	222	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	287/296 (97%)	268 (93%)	19 (7%)	19	55
1	B	288/296 (97%)	278 (96%)	10 (4%)	41	78
1	C	289/296 (98%)	270 (93%)	19 (7%)	19	55
1	D	288/296 (97%)	265 (92%)	23 (8%)	14	45
1	E	290/296 (98%)	275 (95%)	15 (5%)	27	65
1	F	288/296 (97%)	273 (95%)	15 (5%)	27	65
1	G	288/296 (97%)	260 (90%)	28 (10%)	9	35
1	H	287/296 (97%)	272 (95%)	15 (5%)	27	65
All	All	2305/2368 (97%)	2161 (94%)	144 (6%)	21	58

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	21	GLU
1	A	27	LEU
1	A	28	GLN
1	A	51	LEU
1	A	115	ARG
1	A	116	LYS
1	A	127	ASP
1	A	161	LEU
1	A	221	ARG
1	A	234	GLN
1	A	238	LEU
1	A	241	THR
1	A	265	ARG
1	A	270	LEU
1	A	291	LEU
1	A	297	ARG
1	A	302	ASN
1	A	324	LEU

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Mol	Chain	Res	Type
1	B	27	LEU
1	B	100	GLU
1	B	116	LYS
1	B	132	TRP
1	B	220	GLU
1	B	252	ASN
1	B	265	ARG
1	B	291	LEU
1	B	318	ILE
1	B	338	ASN
1	C	22	ARG
1	C	51	LEU
1	C	60	SER
1	C	139	LEU
1	C	140	GLU
1	C	145	LEU
1	C	161	LEU
1	C	220	GLU
1	C	223	ILE
1	C	234	GLN
1	C	241	THR
1	C	247	TRP
1	C	253	ILE
1	C	265	ARG
1	C	266	LEU
1	C	270	LEU
1	C	291	LEU
1	C	297	ARG
1	C	337	ARG
1	D	1	MET
1	D	21	GLU
1	D	43	THR
1	D	56	THR
1	D	82	PRO
1	D	108	LYS
1	D	116	LYS
1	D	117	LEU
1	D	127	ASP
1	D	140	GLU
1	D	145	LEU
1	D	151	ARG
1	D	158	LYS

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Mol	Chain	Res	Type
1	D	176	ASP
1	D	216	THR
1	D	219	LEU
1	D	238	LEU
1	D	241	THR
1	D	248	ASN
1	D	270	LEU
1	D	286	ARG
1	D	295	GLN
1	D	303	THR
1	E	18	CYS
1	E	102	VAL
1	E	116	LYS
1	E	152	LEU
1	E	155	ARG
1	E	176	ASP
1	E	238	LEU
1	E	261	GLU
1	E	270	LEU
1	E	274	LYS
1	E	288	GLN
1	E	291	LEU
1	E	296	LEU
1	E	332	LYS
1	E	333	VAL
1	F	18	CYS
1	F	71	THR
1	F	116	LYS
1	F	129	ARG
1	F	151	ARG
1	F	169	GLU
1	F	206	ASP
1	F	225	ASN
1	F	242	PHE
1	F	253	ILE
1	F	291	LEU
1	F	294	GLU
1	F	302	ASN
1	F	334	LEU
1	F	339	LEU
1	G	25	SER
1	G	27	LEU

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Mol	Chain	Res	Type
1	G	28	GLN
1	G	33	LYS
1	G	40	THR
1	G	45	THR
1	G	53	GLN
1	G	93	SER
1	G	99	ARG
1	G	127	ASP
1	G	129	ARG
1	G	132	TRP
1	G	140	GLU
1	G	143	LYS
1	G	145	LEU
1	G	149	THR
1	G	169	GLU
1	G	176	ASP
1	G	177	VAL
1	G	206	ASP
1	G	219	LEU
1	G	220	GLU
1	G	221	ARG
1	G	224	TYR
1	G	226	SER
1	G	297	ARG
1	G	303	THR
1	G	317	THR
1	H	22	ARG
1	H	27	LEU
1	H	40	THR
1	H	51	LEU
1	H	63	GLN
1	H	140	GLU
1	H	142	ARG
1	H	155	ARG
1	H	196	GLN
1	H	224	TYR
1	H	234	GLN
1	H	238	LEU
1	H	242	PHE
1	H	297	ARG
1	H	302	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	68	ASN
1	B	53	GLN
1	B	68	ASN
1	B	73	ASN
1	B	96	ASN
1	B	190	GLN
1	C	68	ASN
1	C	69	GLN
1	C	70	GLN
1	D	68	ASN
1	D	70	GLN
1	D	234	GLN
1	E	68	ASN
1	E	69	GLN
1	E	70	GLN
1	E	134	ASN
1	F	66	ASN
1	F	70	GLN
1	F	78	HIS
1	F	83	ASN
1	F	86	ASN
1	F	243	GLN
1	G	53	GLN
1	G	68	ASN
1	G	69	GLN
1	G	70	GLN
1	G	83	ASN
1	G	86	ASN
1	G	96	ASN
1	G	248	ASN
1	G	295	GLN
1	H	63	GLN
1	H	68	ASN
1	H	78	HIS
1	H	225	ASN
1	H	302	ASN
1	H	308	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

36 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	401	-	51,58,58	1.51	8 (15%)	54,89,89	2.07	9 (16%)
3	MPD	A	402	-	7,7,7	0.30	0	9,10,10	0.60	0
3	MPD	A	403	-	7,7,7	0.20	0	9,10,10	0.50	0
3	MPD	A	404	-	7,7,7	0.44	0	9,10,10	1.00	0
3	MPD	A	405	-	7,7,7	0.56	0	9,10,10	0.68	0
4	SO4	A	406	-	4,4,4	0.48	0	6,6,6	0.48	0
2	FAD	B	401	-	51,58,58	1.32	7 (13%)	54,89,89	2.00	9 (16%)
3	MPD	B	402	-	7,7,7	0.22	0	9,10,10	0.76	0
3	MPD	B	403	-	7,7,7	0.30	0	9,10,10	0.44	0
3	MPD	B	404	-	7,7,7	0.42	0	9,10,10	0.34	0
3	MPD	B	405	-	7,7,7	0.38	0	9,10,10	0.42	0
2	FAD	C	401	-	51,58,58	1.44	7 (13%)	54,89,89	1.93	11 (20%)
3	MPD	C	402	-	7,7,7	0.45	0	9,10,10	0.62	0
4	SO4	C	403	-	4,4,4	0.43	0	6,6,6	0.58	0
2	FAD	D	401	-	51,58,58	1.39	8 (15%)	54,89,89	1.99	11 (20%)
3	MPD	D	402	-	7,7,7	0.24	0	9,10,10	0.65	0
3	MPD	D	403	-	7,7,7	0.41	0	9,10,10	0.55	0
3	MPD	D	404	-	7,7,7	0.37	0	9,10,10	0.63	0
4	SO4	D	405	-	4,4,4	0.44	0	6,6,6	0.37	0
2	FAD	E	401	-	51,58,58	1.36	6 (11%)	54,89,89	2.03	9 (16%)
3	MPD	E	402	-	7,7,7	0.29	0	9,10,10	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	E	403	-	4,4,4	0.51	0	6,6,6	0.24	0
2	FAD	F	401	-	51,58,58	1.40	6 (11%)	54,89,89	1.84	7 (12%)
3	MPD	F	402	-	7,7,7	0.27	0	9,10,10	0.38	0
3	MPD	F	403	-	7,7,7	0.46	0	9,10,10	0.53	0
3	MPD	F	404	-	7,7,7	0.27	0	9,10,10	0.31	0
3	MPD	F	405	-	7,7,7	0.40	0	9,10,10	0.39	0
4	SO4	F	406	-	4,4,4	0.44	0	6,6,6	0.27	0
2	FAD	G	401	-	51,58,58	1.45	7 (13%)	54,89,89	2.17	9 (16%)
3	MPD	G	402	-	7,7,7	0.31	0	9,10,10	0.24	0
3	MPD	G	403	-	7,7,7	0.29	0	9,10,10	0.32	0
3	MPD	G	404	-	7,7,7	0.32	0	9,10,10	0.64	0
2	FAD	H	401	-	51,58,58	1.32	7 (13%)	54,89,89	2.04	6 (11%)
3	MPD	H	402	-	7,7,7	0.24	0	9,10,10	0.52	0
3	MPD	H	403	-	7,7,7	0.33	0	9,10,10	0.71	0
4	SO4	H	404	-	4,4,4	0.45	0	6,6,6	0.33	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	401	-	-	0/28/50/50	0/6/6/6
3	MPD	A	402	-	-	0/5/5/5	0/0/0/0
3	MPD	A	403	-	-	0/5/5/5	0/0/0/0
3	MPD	A	404	-	-	0/5/5/5	0/0/0/0
3	MPD	A	405	-	-	0/5/5/5	0/0/0/0
4	SO4	A	406	-	-	0/0/0/0	0/0/0/0
2	FAD	B	401	-	-	0/28/50/50	0/6/6/6
3	MPD	B	402	-	-	0/5/5/5	0/0/0/0
3	MPD	B	403	-	-	0/5/5/5	0/0/0/0
3	MPD	B	404	-	-	0/5/5/5	0/0/0/0
3	MPD	B	405	-	-	0/5/5/5	0/0/0/0
2	FAD	C	401	-	-	0/28/50/50	0/6/6/6
3	MPD	C	402	-	-	0/5/5/5	0/0/0/0
4	SO4	C	403	-	-	0/0/0/0	0/0/0/0
2	FAD	D	401	-	-	0/28/50/50	0/6/6/6
3	MPD	D	402	-	-	0/5/5/5	0/0/0/0
3	MPD	D	403	-	-	0/5/5/5	0/0/0/0
3	MPD	D	404	-	-	0/5/5/5	0/0/0/0
4	SO4	D	405	-	-	0/0/0/0	0/0/0/0
2	FAD	E	401	-	-	0/28/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	E	402	-	-	0/5/5/5	0/0/0/0
4	SO4	E	403	-	-	0/0/0/0	0/0/0/0
2	FAD	F	401	-	-	0/28/50/50	0/6/6/6
3	MPD	F	402	-	-	0/5/5/5	0/0/0/0
3	MPD	F	403	-	-	0/5/5/5	0/0/0/0
3	MPD	F	404	-	-	0/5/5/5	0/0/0/0
3	MPD	F	405	-	-	0/5/5/5	0/0/0/0
4	SO4	F	406	-	-	0/0/0/0	0/0/0/0
2	FAD	G	401	-	-	0/28/50/50	0/6/6/6
3	MPD	G	402	-	-	0/5/5/5	0/0/0/0
3	MPD	G	403	-	-	0/5/5/5	0/0/0/0
3	MPD	G	404	-	-	0/5/5/5	0/0/0/0
2	FAD	H	401	-	-	0/28/50/50	0/6/6/6
3	MPD	H	402	-	-	0/5/5/5	0/0/0/0
3	MPD	H	403	-	-	0/5/5/5	0/0/0/0
4	SO4	H	404	-	-	0/0/0/0	0/0/0/0

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	FAD	C6-C5X	-2.51	1.38	1.41
2	A	401	FAD	C1'-N10	-2.01	1.46	1.48
2	D	401	FAD	C2A-N3A	2.05	1.35	1.32
2	G	401	FAD	C10-N1	2.19	1.36	1.33
2	D	401	FAD	C10-N1	2.23	1.36	1.33
2	D	401	FAD	C9A-N10	2.31	1.41	1.38
2	C	401	FAD	C10-N1	2.33	1.36	1.33
2	E	401	FAD	C5A-C4A	2.37	1.45	1.40
2	B	401	FAD	C5A-C4A	2.41	1.45	1.40
2	B	401	FAD	O4B-C1B	2.41	1.44	1.41
2	H	401	FAD	C5A-C4A	2.51	1.46	1.40
2	B	401	FAD	C4-C4X	2.62	1.46	1.41
2	B	401	FAD	C8-C7	2.70	1.47	1.41
2	D	401	FAD	C8-C7	2.73	1.47	1.41
2	A	401	FAD	C5A-C4A	2.75	1.46	1.40
2	F	401	FAD	C9A-N10	2.82	1.42	1.38
2	C	401	FAD	C4-C4X	2.85	1.46	1.41
2	A	401	FAD	C2A-N3A	2.86	1.36	1.32
2	B	401	FAD	C9A-N10	2.89	1.42	1.38
2	G	401	FAD	C9A-N10	2.96	1.42	1.38
2	H	401	FAD	C8-C7	2.99	1.48	1.41
2	H	401	FAD	C9A-C5X	2.99	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	FAD	C5A-C4A	3.00	1.47	1.40
2	A	401	FAD	C8-C7	3.01	1.48	1.41
2	F	401	FAD	C8-C7	3.03	1.48	1.41
2	H	401	FAD	C4-C4X	3.12	1.47	1.41
2	A	401	FAD	C9A-N10	3.22	1.43	1.38
2	B	401	FAD	C9A-C5X	3.22	1.49	1.42
2	E	401	FAD	C9A-N10	3.23	1.43	1.38
2	G	401	FAD	C8-C7	3.24	1.49	1.41
2	D	401	FAD	C9A-C5X	3.29	1.49	1.42
2	E	401	FAD	C9A-C5X	3.29	1.49	1.42
2	C	401	FAD	C5A-C4A	3.32	1.48	1.40
2	G	401	FAD	C5A-C4A	3.34	1.48	1.40
2	D	401	FAD	C5A-C4A	3.36	1.48	1.40
2	E	401	FAD	C8-C7	3.37	1.49	1.41
2	E	401	FAD	C4-C4X	3.41	1.47	1.41
2	C	401	FAD	C4X-C10	3.45	1.47	1.41
2	C	401	FAD	C9A-N10	3.51	1.43	1.38
2	H	401	FAD	C9A-N10	3.53	1.43	1.38
2	G	401	FAD	C4-C4X	3.57	1.48	1.41
2	H	401	FAD	C4X-C10	3.67	1.47	1.41
2	F	401	FAD	C4-C4X	3.69	1.48	1.41
2	D	401	FAD	C4X-C10	3.70	1.47	1.41
2	G	401	FAD	C9A-C5X	3.72	1.50	1.42
2	D	401	FAD	C4-C4X	3.78	1.48	1.41
2	A	401	FAD	C9A-C5X	3.79	1.50	1.42
2	B	401	FAD	C4X-C10	3.83	1.47	1.41
2	C	401	FAD	C8-C7	3.90	1.50	1.41
2	E	401	FAD	C4X-C10	3.91	1.47	1.41
2	A	401	FAD	C4-C4X	3.95	1.48	1.41
2	F	401	FAD	C9A-C5X	3.97	1.50	1.42
2	G	401	FAD	C4X-C10	4.05	1.48	1.41
2	C	401	FAD	C9A-C5X	4.08	1.51	1.42
2	F	401	FAD	C4X-C10	4.08	1.48	1.41
2	A	401	FAD	C4X-C10	4.32	1.48	1.41

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	FAD	N3A-C2A-N1A	-7.90	121.98	128.86
2	H	401	FAD	N3A-C2A-N1A	-7.05	122.72	128.86
2	B	401	FAD	N3A-C2A-N1A	-6.95	122.80	128.86
2	G	401	FAD	N3A-C2A-N1A	-6.69	123.03	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FAD	N3A-C2A-N1A	-6.54	123.16	128.86
2	F	401	FAD	N3A-C2A-N1A	-6.48	123.21	128.86
2	D	401	FAD	N3A-C2A-N1A	-6.17	123.48	128.86
2	G	401	FAD	C4-C4X-C10	-6.05	115.07	119.96
2	C	401	FAD	N3A-C2A-N1A	-5.54	124.03	128.86
2	H	401	FAD	C4X-C4-N3	-4.74	116.73	123.48
2	C	401	FAD	C4X-C10-N10	-4.23	117.58	120.52
2	A	401	FAD	C4X-C4-N3	-4.11	117.64	123.48
2	D	401	FAD	C4-C4X-C10	-4.09	116.65	119.96
2	B	401	FAD	C4-C4X-C10	-3.76	116.92	119.96
2	F	401	FAD	C4X-C4-N3	-3.60	118.36	123.48
2	E	401	FAD	C4X-C4-N3	-3.12	119.04	123.48
2	B	401	FAD	C4A-C5A-N7A	-3.05	106.47	109.41
2	A	401	FAD	C4-C4X-C10	-3.03	117.51	119.96
2	D	401	FAD	C4A-C5A-N7A	-3.02	106.50	109.41
2	B	401	FAD	C4X-C10-N10	-2.82	118.56	120.52
2	E	401	FAD	C1B-N9A-C4A	-2.79	121.81	126.64
2	E	401	FAD	C4-C4X-C10	-2.79	117.71	119.96
2	C	401	FAD	C4-C4X-C10	-2.76	117.73	119.96
2	H	401	FAD	C4A-C5A-N7A	-2.70	106.80	109.41
2	B	401	FAD	C4X-C4-N3	-2.69	119.65	123.48
2	C	401	FAD	C4A-C5A-N7A	-2.59	106.91	109.41
2	E	401	FAD	C4A-C5A-N7A	-2.59	106.91	109.41
2	C	401	FAD	C4X-C4-N3	-2.57	119.82	123.48
2	D	401	FAD	C4X-C4-N3	-2.55	119.86	123.48
2	A	401	FAD	C4A-C5A-N7A	-2.43	107.06	109.41
2	G	401	FAD	C4X-C4-N3	-2.35	120.13	123.48
2	D	401	FAD	C4B-O4B-C1B	-2.33	107.29	109.77
2	B	401	FAD	C1B-N9A-C4A	-2.18	122.87	126.64
2	F	401	FAD	C4-C4X-C10	-2.13	118.24	119.96
2	A	401	FAD	O5'-P-O1P	-2.02	101.11	109.25
2	G	401	FAD	O2A-PA-O1A	2.02	122.72	112.28
2	F	401	FAD	N6A-C6A-N1A	2.05	122.83	118.77
2	D	401	FAD	O2A-PA-O1A	2.06	122.92	112.28
2	C	401	FAD	C2A-N1A-C6A	2.06	122.37	118.77
2	G	401	FAD	C2A-N1A-C6A	2.26	122.72	118.77
2	C	401	FAD	N6A-C6A-N1A	2.45	123.63	118.77
2	E	401	FAD	C4-C4X-N5	2.59	121.52	118.68
2	C	401	FAD	C6-C5X-C9A	2.63	122.41	119.00
2	D	401	FAD	O3'-C3'-C2'	2.78	115.71	108.82
2	A	401	FAD	C4-C4X-N5	2.87	121.82	118.68
2	F	401	FAD	C4X-N5-C5X	3.36	120.31	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	FAD	C4X-N5-C5X	3.60	120.56	116.76
2	B	401	FAD	C4X-N5-C5X	3.64	120.60	116.76
2	D	401	FAD	C1'-N10-C9A	3.71	121.75	118.35
2	C	401	FAD	C1'-N10-C9A	3.82	121.84	118.35
2	F	401	FAD	C1'-N10-C9A	3.83	121.86	118.35
2	D	401	FAD	C4-C4X-N5	3.96	123.02	118.68
2	E	401	FAD	C4X-N5-C5X	4.22	121.22	116.76
2	D	401	FAD	C4X-N5-C5X	4.39	121.39	116.76
2	G	401	FAD	C4-C4X-N5	4.43	123.53	118.68
2	H	401	FAD	C4X-N5-C5X	4.58	121.60	116.76
2	A	401	FAD	C4X-N5-C5X	4.71	121.74	116.76
2	A	401	FAD	C1'-N10-C9A	4.79	122.74	118.35
2	C	401	FAD	C4X-N5-C5X	4.97	122.01	116.76
2	B	401	FAD	C1'-N10-C9A	5.09	123.01	118.35
2	H	401	FAD	C1'-N10-C9A	5.24	123.15	118.35
2	G	401	FAD	C1'-N10-C9A	5.31	123.22	118.35
2	E	401	FAD	C1'-N10-C9A	5.78	123.64	118.35
2	C	401	FAD	C4-N3-C2	6.50	120.84	115.16
2	E	401	FAD	C4-N3-C2	6.82	121.12	115.16
2	F	401	FAD	C4-N3-C2	7.26	121.51	115.16
2	D	401	FAD	C4-N3-C2	7.31	121.56	115.16
2	B	401	FAD	C4-N3-C2	7.33	121.57	115.16
2	H	401	FAD	C4-N3-C2	7.74	121.93	115.16
2	G	401	FAD	C4-N3-C2	8.14	122.28	115.16
2	A	401	FAD	C4-N3-C2	8.64	122.72	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	MPD	1	0
3	A	404	MPD	1	0
4	A	406	SO4	1	0
3	C	402	MPD	2	0
4	C	403	SO4	1	0
4	E	403	SO4	1	0
3	G	404	MPD	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	337/347 (97%)	-0.63	1 (0%) 93 82	28, 44, 91, 128	0
1	B	339/347 (97%)	-0.60	1 (0%) 93 82	26, 49, 85, 114	0
1	C	339/347 (97%)	-0.51	1 (0%) 93 82	36, 53, 100, 133	0
1	D	339/347 (97%)	-0.49	0 100 100	35, 54, 100, 135	0
1	E	339/347 (97%)	-0.39	2 (0%) 89 71	37, 65, 110, 157	0
1	F	339/347 (97%)	-0.28	6 (1%) 69 40	41, 73, 115, 140	0
1	G	338/347 (97%)	-0.39	0 100 100	41, 67, 113, 137	0
1	H	337/347 (97%)	-0.34	4 (1%) 79 53	46, 69, 112, 155	0
All	All	2707/2776 (97%)	-0.45	15 (0%) 89 71	26, 60, 106, 157	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	223	ILE	4.5
1	H	222	GLY	4.2
1	F	222	GLY	4.0
1	F	301	SER	3.4
1	F	221	ARG	3.3
1	E	221	ARG	2.9
1	F	223	ILE	2.9
1	E	300	SER	2.8
1	H	60	SER	2.6
1	F	224	TYR	2.4
1	F	300	SER	2.4
1	H	300	SER	2.2
1	A	300	SER	2.1
1	C	26	VAL	2.0
1	B	26	VAL	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
3	MPD	H	402	8/8	0.89	0.29	7.64	82,86,89,92	0
3	MPD	D	403	8/8	0.89	0.45	6.50	87,92,95,96	0
3	MPD	B	402	8/8	0.91	0.25	5.05	52,63,67,68	0
3	MPD	A	402	8/8	0.93	0.26	4.66	72,76,80,85	0
3	MPD	F	402	8/8	0.93	0.24	4.12	77,84,90,94	0
3	MPD	A	403	8/8	0.97	0.24	3.74	51,63,69,70	0
3	MPD	G	403	8/8	0.93	0.27	3.56	79,83,86,89	0
3	MPD	F	404	8/8	0.94	0.24	3.50	55,64,72,73	0
3	MPD	B	404	8/8	0.93	0.21	3.42	64,74,79,86	0
3	MPD	B	403	8/8	0.93	0.24	3.21	78,86,90,95	0
3	MPD	F	403	8/8	0.93	0.22	2.84	74,77,78,80	0
4	SO4	D	405	5/5	0.92	0.24	2.68	102,106,108,111	0
3	MPD	B	405	8/8	0.92	0.22	1.97	73,78,83,84	0
3	MPD	G	404	8/8	0.90	0.24	1.94	83,91,93,93	0
3	MPD	G	402	8/8	0.91	0.23	1.92	58,65,68,71	0
3	MPD	C	402	8/8	0.94	0.21	1.85	47,51,52,55	0
3	MPD	H	403	8/8	0.93	0.24	1.82	53,64,69,73	0
3	MPD	D	402	8/8	0.96	0.21	1.74	53,61,64,65	0
3	MPD	A	404	8/8	0.97	0.18	1.17	39,42,43,45	0
3	MPD	F	405	8/8	0.92	0.21	1.15	84,89,90,92	0
3	MPD	E	402	8/8	0.96	0.18	0.22	79,83,85,86	0
2	FAD	B	401	53/53	0.98	0.15	-0.32	33,37,45,47	0
2	FAD	H	401	53/53	0.97	0.15	-0.32	41,46,52,56	0
2	FAD	G	401	53/53	0.97	0.14	-0.69	44,54,60,63	0
2	FAD	D	401	53/53	0.98	0.14	-0.72	29,40,47,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	E	401	53/53	0.98	0.13	-0.82	41,49,54,58	0
2	FAD	F	401	53/53	0.97	0.13	-0.92	43,52,59,60	0
2	FAD	C	401	53/53	0.98	0.12	-1.03	35,42,46,49	0
4	SO4	H	404	5/5	0.96	0.13	-1.06	83,87,91,96	0
2	FAD	A	401	53/53	0.98	0.12	-1.19	28,32,35,36	0
4	SO4	F	406	5/5	0.92	0.13	-1.19	98,99,105,107	0
4	SO4	C	403	5/5	0.96	0.09	-2.09	62,71,76,76	0
4	SO4	E	403	5/5	0.97	0.08	-2.48	93,98,105,105	0
3	MPD	D	404	8/8	0.89	0.27	-	101,111,113,115	0
4	SO4	A	406	5/5	0.96	0.12	-	54,55,58,60	0
3	MPD	A	405	8/8	0.93	0.18	-	64,73,75,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.