



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 10:08 pm GMT

PDB ID : 2E4A
Title : Crystal Structure of Human D-Amino Acid Oxidase in complex with o-aminobenzoate
Authors : Kawazoe, T.; Tsuge, H.; Imagawa, T.; Fukui, K.
Deposited on : 2006-12-05
Resolution : 2.60 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

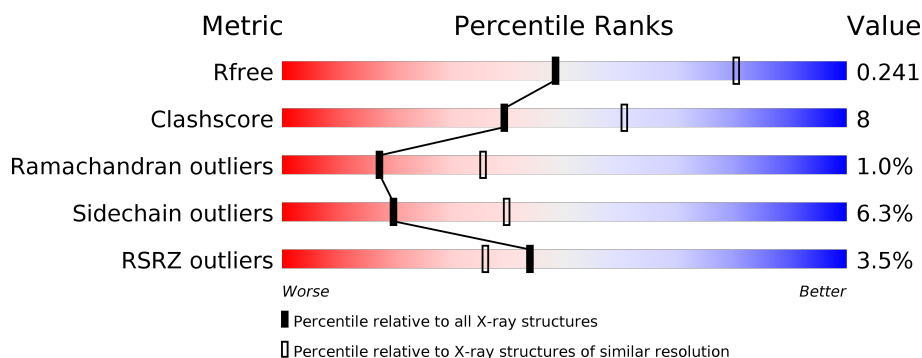
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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 ≥ 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.

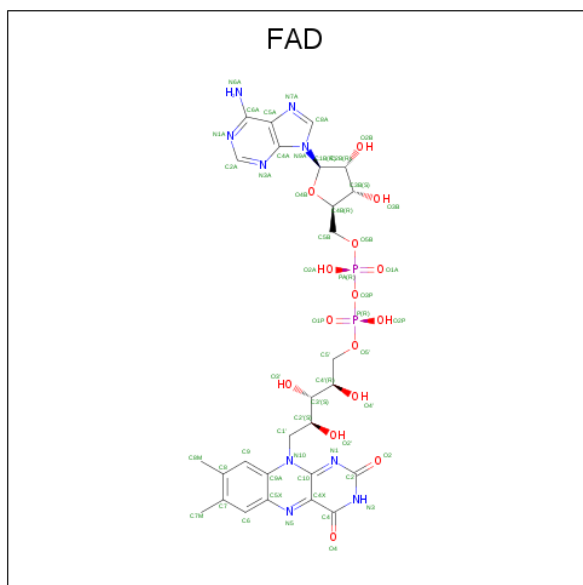
Mol	Chain	Length	Quality of chain
1	A	347	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 81%, yellow 16%, orange 3%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 81% 16% ... </div> </div>
1	B	347	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 78%, yellow 18%, orange 3%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 78% 18% .. </div> </div>
1	C	347	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, green 80%, yellow 16%, orange 3%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 6% 80% 16% .. </div> </div>
1	D	347	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, green 81%, yellow 15%, orange 3%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 6% 81% 15% .. </div> </div>

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	340	Total 2733	C 1751	N 479	O 494	S 9	0	0	0
1	B	340	Total 2733	C 1751	N 479	O 494	S 9	0	0	0
1	C	340	Total 2733	C 1751	N 479	O 494	S 9	0	0	0
1	D	340	Total 2733	C 1751	N 479	O 494	S 9	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



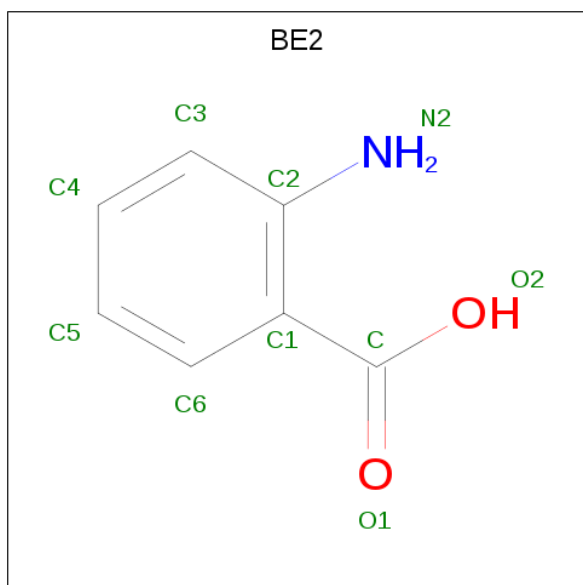
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 2-AMINOBENZOIC ACID (three-letter code: BE2) (formula: C₇H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	7	1	2		
3	B	1	Total	C	N	O	0	0
			10	7	1	2		
3	C	1	Total	C	N	O	0	0
			10	7	1	2		
3	D	1	Total	C	N	O	0	0
			10	7	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	33	Total	O	0	0
			33	33		
4	C	19	Total	O	0	0
			19	19		

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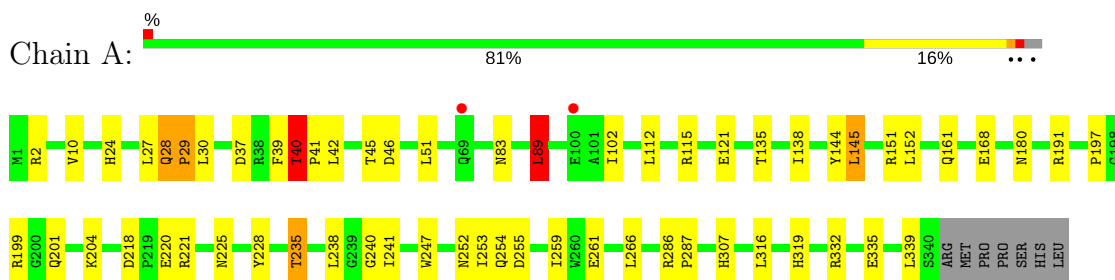
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	22	Total	O	0	0
			22	22		

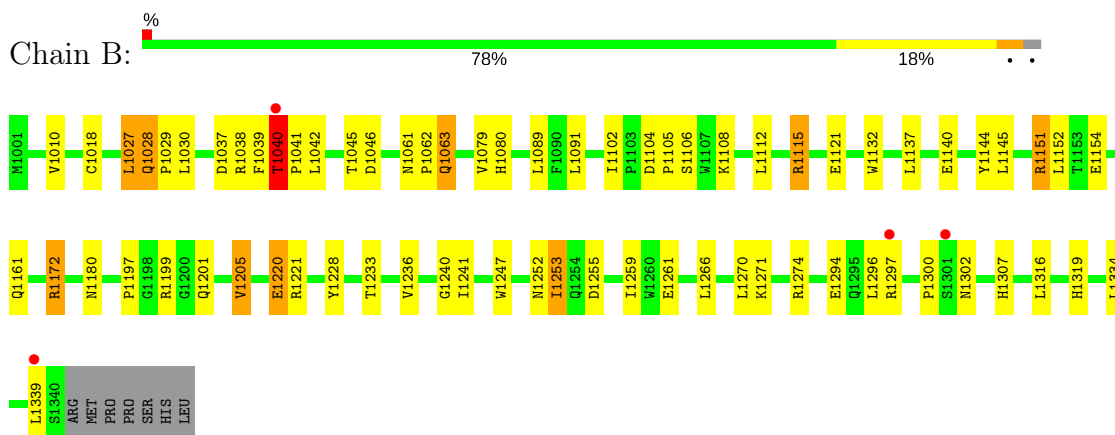
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

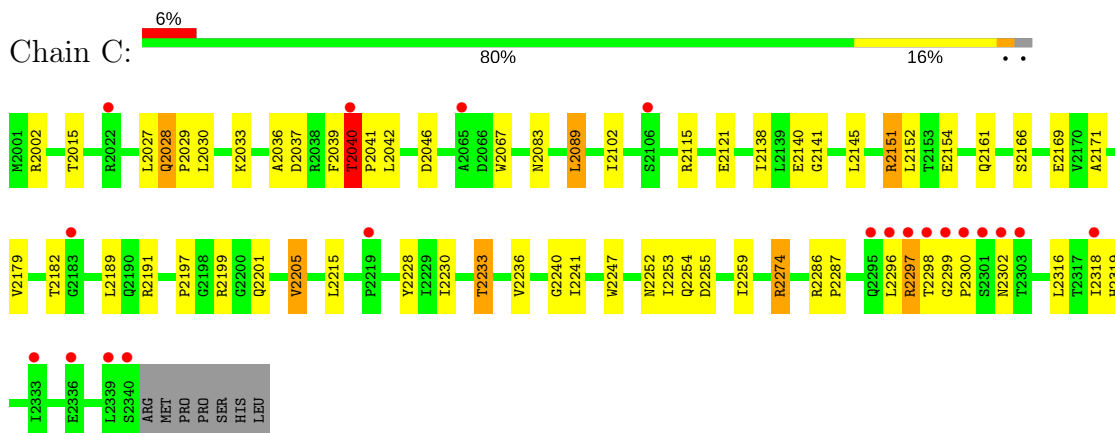
• Molecule 1: D-amino-acid oxidase



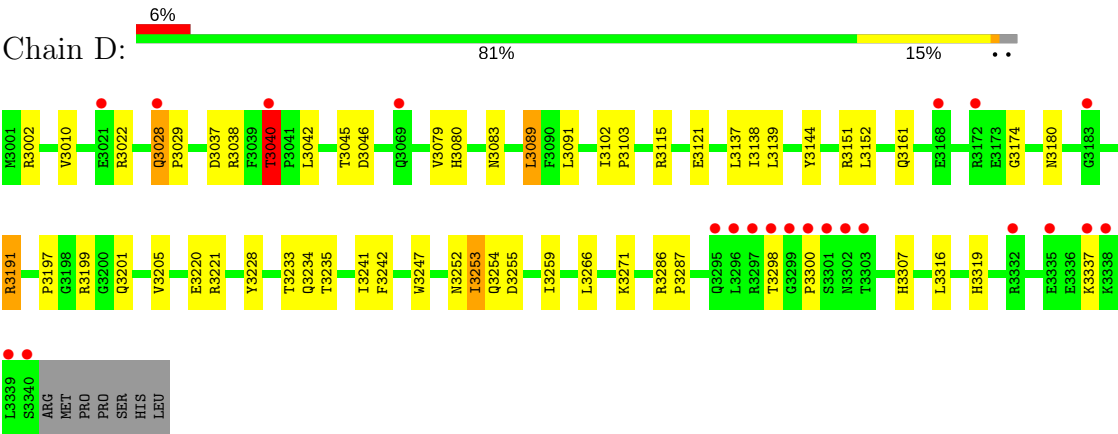
• Molecule 1: D-amino-acid oxidase



• Molecule 1: D-amino-acid oxidase



● Molecule 1: D-amino-acid oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.39Å 185.04Å 51.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.68 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.60) 98.8 (49.68-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.210 , 0.244 0.208 , 0.241	Depositor DCC
R_{free} test set	2287 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11290	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1598e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BE2, 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	0.51	0/2810	0.64	2/3824 (0.1%)
1	B	0.55	1/2810 (0.0%)	0.67	0/3824
1	C	0.49	0/2810	0.62	0/3824
1	D	0.51	0/2810	0.61	0/3824
All	All	0.51	1/11240 (0.0%)	0.64	2/15296 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1018	CYS	CB-SG	-5.34	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	40	THR	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2733	0	2680	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2733	0	2677	50	0
1	C	2733	0	2677	50	0
1	D	2733	0	2677	43	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
3	A	10	0	6	2	0
3	B	10	0	6	2	0
3	C	10	0	6	2	0
3	D	10	0	6	1	0
4	A	32	0	0	1	0
4	B	33	0	0	0	0
4	C	19	0	0	1	0
4	D	22	0	0	1	0
All	All	11290	0	10859	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (177) 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:C:2297:ARG:HA	1:C:2302:ASN:HB3	1.42	1.01
1:D:3028:GLN:HG2	1:D:3029:PRO:HD3	1.43	1.01
1:B:1241:ILE:HD12	1:B:1259:ILE:HD11	1.46	0.95
1:A:252:ASN:HD22	1:A:255:ASP:H	1.16	0.92
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.16	0.91
1:A:42:LEU:HD22	1:D:3042:LEU:HD22	1.53	0.89
1:D:3241:ILE:HD12	1:D:3259:ILE:HD11	1.53	0.89
1:C:2252:ASN:HD22	1:C:2255:ASP:H	1.22	0.87
1:C:2028:GLN:HB2	1:C:2029:PRO:HD3	1.57	0.86
1:A:28:GLN:HG2	1:A:29:PRO:HD3	1.58	0.85
1:C:2297:ARG:H	1:C:2297:ARG:HE	1.26	0.83
1:B:1297:ARG:HA	1:B:1302:ASN:HB3	1.61	0.82
1:B:1297:ARG:HG3	1:B:1302:ASN:HD22	1.44	0.81
1:B:1028:GLN:HB2	1:B:1029:PRO:HD2	1.65	0.79
1:C:2241:ILE:HD12	1:C:2259:ILE:HD11	1.67	0.77
1:C:2252:ASN:HD21	1:C:2254:GLN:HB3	1.49	0.77
1:D:3286:ARG:HG2	1:D:3287:PRO:HD2	1.67	0.76
1:A:180:ASN:HD22	1:A:307:HIS:CD2	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2201:GLN:HE22	1:C:2252:ASN:H	1.36	0.74
1:B:1028:GLN:HB2	1:B:1029:PRO:CD	2.18	0.74
1:D:3201:GLN:HE22	1:D:3252:ASN:H	1.34	0.73
1:B:1241:ILE:HD13	1:B:1255:ASP:HB3	1.70	0.73
1:B:1221:ARG:HG3	1:B:1221:ARG:HH21	1.55	0.72
1:B:1172:ARG:HH21	1:B:1172:ARG:HB2	1.53	0.71
1:C:2199:ARG:HH22	1:C:2201:GLN:NE2	1.89	0.70
1:C:2297:ARG:HA	1:C:2302:ASN:CB	2.20	0.70
1:A:180:ASN:ND2	1:A:307:HIS:HD2	1.90	0.67
1:C:2140:GLU:OE1	1:C:2233:THR:HG22	1.93	0.67
1:C:2027:LEU:HD23	1:C:2030:LEU:HD13	1.75	0.67
1:A:40:THR:O	1:A:46:ASP:OD2	2.13	0.67
1:B:1180:ASN:HD22	1:B:1307:HIS:HD2	1.43	0.66
1:A:24:HIS:HE1	4:A:357:HOH:O	1.79	0.66
1:D:3091:LEU:HD23	1:D:3137:LEU:HD23	1.78	0.66
1:B:1252:ASN:HD22	1:B:1255:ASP:H	1.44	0.66
1:D:3199:ARG:HH22	1:D:3201:GLN:HE21	1.43	0.65
1:B:1294:GLU:OE1	1:B:1307:HIS:HE1	1.79	0.65
1:A:201:GLN:HE22	1:A:252:ASN:H	1.44	0.64
1:D:3201:GLN:NE2	1:D:3252:ASN:H	1.96	0.63
1:B:1255:ASP:O	1:B:1259:ILE:HG12	1.98	0.63
1:C:2028:GLN:CB	1:C:2029:PRO:HD3	2.27	0.63
1:C:2274:ARG:HA	1:C:2274:ARG:NE	2.13	0.63
1:D:3316:LEU:O	1:D:3319:HIS:HD2	1.82	0.63
1:A:241:ILE:HD12	1:A:259:ILE:HD11	1.81	0.63
1:B:1140:GLU:OE1	1:B:1233:THR:HG22	1.99	0.63
1:C:2241:ILE:HD13	1:C:2255:ASP:HB3	1.81	0.62
1:D:3102:ILE:HG13	1:D:3103:PRO:HD2	1.81	0.62
1:D:3241:ILE:HD13	1:D:3255:ASP:HB3	1.81	0.62
1:D:3199:ARG:HH22	1:D:3201:GLN:NE2	1.98	0.62
1:B:1201:GLN:HE22	1:B:1252:ASN:H	1.47	0.62
1:A:252:ASN:HD21	1:A:254:GLN:HB3	1.64	0.62
1:C:2241:ILE:CD1	1:C:2259:ILE:HD11	2.29	0.62
1:D:3241:ILE:CD1	1:D:3255:ASP:HB3	2.30	0.62
1:C:2252:ASN:ND2	1:C:2255:ASP:H	1.93	0.61
1:C:2199:ARG:HH22	1:C:2201:GLN:HE21	1.48	0.61
1:D:3091:LEU:HD23	1:D:3137:LEU:CD2	2.31	0.60
1:C:2040:THR:O	1:C:2046:ASP:OD2	2.19	0.60
1:B:1028:GLN:CB	1:B:1029:PRO:CD	2.80	0.59
1:B:1241:ILE:CD1	1:B:1255:ASP:HB3	2.32	0.59
1:D:3233:THR:HG23	1:D:3234:GLN:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2151:ARG:NH1	1:C:2154:GLU:OE2	2.35	0.59
1:C:2252:ASN:ND2	1:C:2254:GLN:HB3	2.16	0.58
1:A:316:LEU:O	1:A:319:HIS:HD2	1.86	0.58
1:B:1220:GLU:OE1	1:B:1220:GLU:HA	2.04	0.57
1:C:2037:ASP:HB3	2:C:2351:FAD:O2B	2.04	0.57
1:A:252:ASN:ND2	1:A:255:ASP:H	1.96	0.57
1:D:3255:ASP:O	1:D:3259:ILE:HG12	2.05	0.56
1:D:3002:ARG:HB3	1:D:3002:ARG:HH11	1.70	0.56
1:B:1297:ARG:HA	1:B:1302:ASN:CB	2.33	0.56
1:C:2316:LEU:O	1:C:2319:HIS:HD2	1.89	0.56
1:C:2197:PRO:HG3	1:C:2247:TRP:CE2	2.41	0.55
1:B:1091:LEU:HD23	1:B:1137:LEU:HD23	1.88	0.55
1:C:2201:GLN:NE2	1:C:2252:ASN:H	2.03	0.55
1:B:1027:LEU:HD13	1:B:1030:LEU:HD13	1.89	0.55
1:A:89:LEU:HA	1:A:138:ILE:O	2.07	0.55
1:C:2028:GLN:HB2	1:C:2029:PRO:CD	2.33	0.54
1:C:2199:ARG:NH2	1:C:2201:GLN:HE21	2.05	0.54
1:A:42:LEU:HD22	1:D:3042:LEU:CD2	2.32	0.54
1:D:3115:ARG:NH2	1:D:3121:GLU:OE2	2.41	0.54
1:D:3253:ILE:O	1:D:3253:ILE:HD13	2.08	0.53
1:A:37:ASP:HB3	2:A:351:FAD:O2B	2.08	0.53
1:A:115:ARG:NH2	1:A:121:GLU:OE2	2.41	0.53
1:D:3180:ASN:HD22	1:D:3307:HIS:HD2	1.56	0.53
1:D:3252:ASN:HD22	1:D:3255:ASP:H	1.57	0.52
1:A:39:PHE:O	1:A:41:PRO:HD2	2.08	0.52
1:D:3028:GLN:CG	1:D:3029:PRO:HD3	2.29	0.52
1:B:1042:LEU:HD22	1:C:2042:LEU:HB3	1.92	0.51
1:A:241:ILE:CD1	1:A:259:ILE:HD11	2.41	0.51
1:B:1228:TYR:CE2	3:B:1352:BE2:H6	2.46	0.51
1:D:3197:PRO:HG3	1:D:3247:TRP:CE2	2.46	0.51
1:B:1042:LEU:CD2	1:C:2042:LEU:HD22	2.40	0.51
1:B:1201:GLN:NE2	1:B:1252:ASN:H	2.06	0.51
1:D:3038:ARG:O	2:D:3351:FAD:O3B	2.29	0.51
1:A:199:ARG:HH22	1:A:201:GLN:NE2	2.10	0.50
1:C:2297:ARG:NE	1:C:2297:ARG:H	2.03	0.50
1:A:197:PRO:HG3	1:A:247:TRP:CE2	2.47	0.49
1:D:3002:ARG:HB3	1:D:3002:ARG:NH1	2.27	0.49
1:D:3221:ARG:HH21	1:D:3221:ARG:HG3	1.77	0.49
1:D:3241:ILE:CD1	1:D:3259:ILE:HD11	2.35	0.49
1:A:332:ARG:O	1:A:335:GLU:HG2	2.13	0.49
1:B:1205:VAL:HG12	1:B:1236:VAL:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2115:ARG:NH2	1:C:2121:GLU:OE2	2.45	0.49
1:A:241:ILE:HD13	1:A:255:ASP:HB3	1.95	0.49
1:B:1115:ARG:NH2	1:B:1121:GLU:OE2	2.45	0.48
1:C:2036:ALA:HB3	1:C:2039:PHE:CZ	2.47	0.48
1:C:2297:ARG:N	1:C:2297:ARG:HE	2.04	0.48
1:B:1228:TYR:CZ	3:B:1352:BE2:H6	2.48	0.48
1:B:1027:LEU:HD11	1:B:1334:LEU:HD21	1.96	0.48
1:B:1042:LEU:HD22	1:C:2042:LEU:HD22	1.96	0.48
1:B:1221:ARG:NH2	1:B:1221:ARG:HG3	2.24	0.48
1:C:2141:GLY:O	1:C:2145:LEU:HB2	2.13	0.48
1:C:2171:ALA:HB1	1:C:2298:THR:HG21	1.96	0.47
1:D:3235:THR:HG22	4:D:23:HOH:O	2.14	0.47
1:B:1040:THR:O	1:B:1046:ASP:OD2	2.33	0.47
1:D:3115:ARG:HH22	1:D:3121:GLU:CD	2.18	0.47
1:A:115:ARG:HH22	1:A:121:GLU:CD	2.17	0.47
1:D:3252:ASN:ND2	1:D:3254:GLN:HB3	2.30	0.47
1:B:1091:LEU:HD23	1:B:1137:LEU:CD2	2.44	0.46
1:C:2205:VAL:HG12	1:C:2236:VAL:HB	1.98	0.46
1:B:1316:LEU:O	1:B:1319:HIS:HD2	1.97	0.46
1:A:201:GLN:NE2	1:A:252:ASN:H	2.13	0.46
1:A:252:ASN:HB3	1:A:255:ASP:HB2	1.98	0.46
1:D:3010:VAL:HB	1:D:3045:THR:HG21	1.98	0.46
1:A:199:ARG:HH22	1:A:201:GLN:HE21	1.63	0.46
1:A:27:LEU:HD13	1:A:30:LEU:HD13	1.98	0.46
1:A:286:ARG:HG2	1:A:287:PRO:HD2	1.97	0.45
1:B:1061:ASN:OD1	1:B:1063:GLN:HB2	2.16	0.45
1:A:144:TYR:OH	1:A:319:HIS:HE1	1.99	0.45
1:C:2002:ARG:HH22	1:C:2033:LYS:NZ	2.13	0.45
1:D:3040:THR:O	1:D:3046:ASP:OD2	2.35	0.45
1:B:1199:ARG:HH22	1:B:1201:GLN:NE2	2.15	0.45
1:C:2228:TYR:CZ	3:C:2352:BE2:H6	2.52	0.45
1:D:3298:THR:HG23	1:D:3298:THR:O	2.16	0.45
1:A:42:LEU:CD2	1:D:3042:LEU:HD22	2.37	0.45
1:D:3079:VAL:HG23	1:D:3089:LEU:HD22	1.99	0.45
1:B:1027:LEU:O	1:B:1028:GLN:O	2.33	0.44
1:C:2286:ARG:HG2	1:C:2287:PRO:HD2	1.98	0.44
1:D:3022:ARG:HG3	1:D:3022:ARG:O	2.17	0.44
4:C:46:HOH:O	1:D:3080:HIS:HE1	2.00	0.44
1:D:3286:ARG:CG	1:D:3287:PRO:HD2	2.44	0.44
1:C:2015:THR:HG21	1:C:2179:VAL:HG11	2.00	0.44
1:B:1039:PHE:O	1:B:1041:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1197:PRO:HG3	1:B:1247:TRP:CE2	2.52	0.44
1:C:2040:THR:HG23	1:C:2145:LEU:HB3	2.00	0.43
1:C:2182:THR:HG21	1:C:2189:LEU:HD11	2.00	0.43
1:A:228:TYR:CE2	3:A:352:BE2:H6	2.53	0.43
1:A:10:VAL:HB	1:A:45:THR:HG21	1.99	0.43
1:B:1115:ARG:HH22	1:B:1121:GLU:CD	2.22	0.43
1:B:1144:TYR:OH	1:B:1319:HIS:HE1	2.01	0.43
1:B:1104:ASP:HB3	1:B:1108:LYS:HD2	2.01	0.43
1:B:1038:ARG:O	2:B:1351:FAD:O3B	2.37	0.43
1:A:40:THR:HG23	1:A:145:LEU:HB3	2.01	0.42
1:B:1151:ARG:O	1:B:1154:GLU:HG2	2.20	0.42
1:B:1241:ILE:HD12	1:B:1259:ILE:CD1	2.33	0.42
1:C:2067:TRP:HB2	1:C:2318:ILE:HD11	2.00	0.42
1:C:2241:ILE:CD1	1:C:2255:ASP:HB3	2.46	0.42
1:C:2089:LEU:HA	1:C:2138:ILE:O	2.19	0.42
1:A:218:ASP:OD2	1:A:221:ARG:NH2	2.52	0.42
1:A:228:TYR:CZ	3:A:352:BE2:H6	2.54	0.42
1:A:112:LEU:HB2	1:A:135:THR:HB	2.02	0.41
1:B:1105:PRO:HD3	1:B:1132:TRP:CZ2	2.56	0.41
1:A:204:LYS:HD2	1:A:235:THR:HG21	2.02	0.41
1:C:2166:SER:O	1:C:2169:GLU:HB3	2.20	0.41
1:B:1010:VAL:HB	1:B:1045:THR:HG21	2.02	0.41
1:A:51:LEU:HA	1:A:138:ILE:HD13	2.03	0.41
1:A:252:ASN:ND2	1:A:254:GLN:HB3	2.32	0.41
1:B:1061:ASN:HA	1:B:1062:PRO:HD2	1.88	0.41
1:B:1253:ILE:HD13	1:B:1253:ILE:O	2.20	0.41
1:B:1079:VAL:HG13	1:B:1080:HIS:CD2	2.56	0.41
1:C:2274:ARG:HA	1:C:2274:ARG:HE	1.85	0.41
1:C:2230:ILE:HD11	3:C:2352:BE2:H5	2.02	0.41
1:D:3089:LEU:HA	1:D:3138:ILE:O	2.21	0.41
1:B:1199:ARG:HH22	1:B:1201:GLN:HE21	1.68	0.40
1:C:2299:GLY:HA3	1:C:2300:PRO:HD2	1.82	0.40
1:D:3139:LEU:HD11	1:D:3144:TYR:CD1	2.55	0.40
1:D:3191:ARG:HE	1:D:3191:ARG:HB3	1.73	0.40
1:C:2039:PHE:O	1:C:2041:PRO:HD2	2.21	0.40
1:D:3228:TYR:CZ	3:D:3352:BE2:H6	2.56	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	338/347 (97%)	318 (94%)	17 (5%)	3 (1%)	19	38
1	B	338/347 (97%)	320 (95%)	13 (4%)	5 (2%)	11	23
1	C	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	27	51
1	D	338/347 (97%)	324 (96%)	11 (3%)	3 (1%)	19	38
All	All	1352/1388 (97%)	1279 (95%)	60 (4%)	13 (1%)	17	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	B	1028	GLN
1	B	1040	THR
1	B	1300	PRO
1	D	3040	THR
1	B	1339	LEU
1	C	2040	THR
1	D	3174	GLY
1	A	240	GLY
1	B	1240	GLY
1	D	3300	PRO
1	A	29	PRO
1	C	2240	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	292/299 (98%)	273 (94%)	19 (6%)	19	38
1	B	292/299 (98%)	269 (92%)	23 (8%)	13	27
1	C	292/299 (98%)	276 (94%)	16 (6%)	24	47
1	D	292/299 (98%)	276 (94%)	16 (6%)	24	47
All	All	1168/1196 (98%)	1094 (94%)	74 (6%)	20	40

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	28	GLN
1	A	83	ASN
1	A	89	LEU
1	A	102	ILE
1	A	145	LEU
1	A	151	ARG
1	A	152	LEU
1	A	161	GLN
1	A	168	GLU
1	A	191	ARG
1	A	220	GLU
1	A	225	ASN
1	A	235	THR
1	A	238	LEU
1	A	253	ILE
1	A	261	GLU
1	A	266	LEU
1	A	339	LEU
1	B	1027	LEU
1	B	1037	ASP
1	B	1040	THR
1	B	1063	GLN
1	B	1089	LEU
1	B	1102	ILE
1	B	1106	SER
1	B	1112	LEU
1	B	1115	ARG
1	B	1145	LEU
1	B	1151	ARG
1	B	1152	LEU
1	B	1161	GLN
1	B	1172	ARG

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Mol	Chain	Res	Type
1	B	1205	VAL
1	B	1220	GLU
1	B	1253	ILE
1	B	1261	GLU
1	B	1266	LEU
1	B	1270	LEU
1	B	1271	LYS
1	B	1274	ARG
1	B	1296	LEU
1	C	2028	GLN
1	C	2040	THR
1	C	2083	ASN
1	C	2089	LEU
1	C	2102	ILE
1	C	2151	ARG
1	C	2152	LEU
1	C	2161	GLN
1	C	2191	ARG
1	C	2205	VAL
1	C	2215	LEU
1	C	2233	THR
1	C	2253	ILE
1	C	2274	ARG
1	C	2296	LEU
1	C	2297	ARG
1	D	3028	GLN
1	D	3037	ASP
1	D	3040	THR
1	D	3083	ASN
1	D	3089	LEU
1	D	3151	ARG
1	D	3152	LEU
1	D	3161	GLN
1	D	3191	ARG
1	D	3205	VAL
1	D	3220	GLU
1	D	3242	PHE
1	D	3253	ILE
1	D	3266	LEU
1	D	3271	LYS
1	D	3337	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	69	GLN
1	A	161	GLN
1	A	201	GLN
1	A	243	GLN
1	A	252	ASN
1	A	288	GLN
1	A	307	HIS
1	A	319	HIS
1	B	1024	HIS
1	B	1063	GLN
1	B	1080	HIS
1	B	1146	GLN
1	B	1161	GLN
1	B	1201	GLN
1	B	1243	GLN
1	B	1252	ASN
1	B	1302	ASN
1	B	1307	HIS
1	B	1319	HIS
1	C	2069	GLN
1	C	2080	HIS
1	C	2161	GLN
1	C	2201	GLN
1	C	2243	GLN
1	C	2252	ASN
1	C	2288	GLN
1	C	2307	HIS
1	C	2319	HIS
1	D	3024	HIS
1	D	3060	ASN
1	D	3080	HIS
1	D	3083	ASN
1	D	3143	ASN
1	D	3161	GLN
1	D	3201	GLN
1	D	3225	ASN
1	D	3243	GLN
1	D	3252	ASN
1	D	3307	HIS
1	D	3319	HIS

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 ⓘ

8 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	351	-	51,58,58	1.10	4 (7%)	57,89,89	2.55	14 (24%)
3	BE2	A	352	-	7,10,10	0.50	0	9,13,13	1.05	0
2	FAD	B	1351	-	51,58,58	1.19	5 (9%)	57,89,89	2.46	18 (31%)
3	BE2	B	1352	-	7,10,10	0.56	0	9,13,13	1.20	0
2	FAD	C	2351	-	51,58,58	1.15	4 (7%)	57,89,89	2.42	10 (17%)
3	BE2	C	2352	-	7,10,10	0.52	0	9,13,13	1.44	2 (22%)
2	FAD	D	3351	-	51,58,58	1.21	4 (7%)	57,89,89	2.38	12 (21%)
3	BE2	D	3352	-	7,10,10	0.70	0	9,13,13	0.93	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	351	-	-	0/28/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BE2	A	352	-	-	0/0/4/4	0/1/1/1
2	FAD	B	1351	-	-	0/28/50/50	0/6/6/6
3	BE2	B	1352	-	-	0/0/4/4	0/1/1/1
2	FAD	C	2351	-	-	0/28/50/50	0/6/6/6
3	BE2	C	2352	-	-	0/0/4/4	0/1/1/1
2	FAD	D	3351	-	-	0/28/50/50	0/6/6/6
3	BE2	D	3352	-	-	0/0/4/4	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3351	FAD	C9A-N10	-3.09	1.35	1.38
2	C	2351	FAD	C9A-N10	-2.77	1.35	1.38
2	C	2351	FAD	C8A-N9A	-2.70	1.33	1.36
2	A	351	FAD	C8A-N9A	-2.64	1.33	1.36
2	B	1351	FAD	C8A-N9A	-2.59	1.33	1.36
2	D	3351	FAD	C8A-N9A	-2.28	1.34	1.36
2	B	1351	FAD	C9A-N10	-2.22	1.36	1.38
2	A	351	FAD	C2A-N3A	2.03	1.35	1.32
2	B	1351	FAD	C10-N1	2.10	1.36	1.33
2	A	351	FAD	C4-C4X	2.20	1.45	1.41
2	C	2351	FAD	C4-C4X	2.63	1.46	1.41
2	B	1351	FAD	C4-C4X	3.02	1.46	1.41
2	A	351	FAD	C4X-C10	3.65	1.47	1.41
2	B	1351	FAD	C4X-C10	3.84	1.47	1.41
2	D	3351	FAD	C4-C4X	3.85	1.48	1.41
2	D	3351	FAD	C4X-C10	4.32	1.48	1.41
2	C	2351	FAD	C4X-C10	4.42	1.48	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2351	FAD	N3A-C2A-N1A	-9.83	120.45	128.86
2	D	3351	FAD	N3A-C2A-N1A	-9.71	120.55	128.86
2	A	351	FAD	N3A-C2A-N1A	-9.48	120.75	128.86
2	B	1351	FAD	N3A-C2A-N1A	-9.30	120.90	128.86
2	B	1351	FAD	P-O3P-PA	-7.98	105.80	132.63
2	A	351	FAD	P-O3P-PA	-7.64	106.96	132.63
2	C	2351	FAD	P-O3P-PA	-5.59	113.83	132.63
2	D	3351	FAD	P-O3P-PA	-5.56	113.93	132.63
2	C	2351	FAD	C4X-C4-N3	-4.71	116.77	123.47
2	D	3351	FAD	C4X-C4-N3	-4.42	117.18	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	351	FAD	C4X-C4-N3	-3.23	118.87	123.47
2	B	1351	FAD	C1B-N9A-C4A	-3.22	121.08	126.64
2	B	1351	FAD	C4X-C4-N3	-3.20	118.92	123.47
2	D	3351	FAD	C1B-N9A-C4A	-3.14	121.22	126.64
2	A	351	FAD	C4-C4X-C10	-3.07	117.66	119.95
2	C	2351	FAD	O2P-P-O5'	-2.89	94.35	107.75
2	C	2351	FAD	C4'-C3'-C2'	-2.70	107.72	113.40
2	A	351	FAD	O2P-P-O5'	-2.68	95.29	107.75
3	C	2352	BE2	C6-C1-C	-2.63	116.18	120.23
2	D	3351	FAD	C4-C4X-C10	-2.54	118.05	119.95
2	A	351	FAD	C4B-O4B-C1B	-2.46	107.26	109.83
2	B	1351	FAD	C4B-O4B-C1B	-2.45	107.27	109.83
2	B	1351	FAD	C4-C4X-C10	-2.41	118.15	119.95
2	B	1351	FAD	C5B-C4B-C3B	-2.35	106.45	115.29
2	A	351	FAD	C9A-N10-C10	-2.31	118.69	121.77
2	B	1351	FAD	C4A-C5A-N7A	-2.22	107.27	109.41
3	C	2352	BE2	C3-C2-N2	-2.20	115.77	120.16
2	B	1351	FAD	C4X-C10-N10	-2.19	118.36	120.40
2	B	1351	FAD	O2P-P-O5'	-2.19	97.56	107.75
2	A	351	FAD	C1B-N9A-C4A	-2.16	122.90	126.64
2	C	2351	FAD	C4A-C5A-N7A	-2.10	107.38	109.41
2	C	2351	FAD	C9A-N10-C10	-2.10	118.97	121.77
2	D	3351	FAD	C4B-O4B-C1B	-2.08	107.66	109.83
2	D	3351	FAD	O2P-P-O5'	-2.08	98.11	107.75
2	A	351	FAD	C4X-C10-N10	-2.06	118.48	120.40
2	B	1351	FAD	P-O5'-C5'	-2.05	109.65	121.68
2	B	1351	FAD	C2B-C3B-C4B	2.03	106.52	102.62
2	A	351	FAD	C6-C5X-C9A	2.19	121.95	119.01
2	D	3351	FAD	C1'-N10-C10	2.22	120.68	118.46
2	A	351	FAD	C2B-C3B-C4B	2.22	106.88	102.62
2	B	1351	FAD	C6-C5X-C9A	2.25	122.03	119.01
2	D	3351	FAD	C4X-N5-C5X	2.26	119.13	116.76
2	B	1351	FAD	C4-C4X-N5	2.70	121.74	118.70
2	D	3351	FAD	C4-C4X-N5	2.99	122.07	118.70
2	C	2351	FAD	C1'-N10-C9A	3.15	121.11	118.31
2	B	1351	FAD	C4X-N5-C5X	3.16	120.07	116.76
2	B	1351	FAD	C1'-N10-C9A	3.31	121.26	118.31
2	B	1351	FAD	C5X-C9A-N10	4.35	121.03	117.71
2	D	3351	FAD	C5X-C9A-N10	4.67	121.28	117.71
2	A	351	FAD	C1'-N10-C9A	4.90	122.67	118.31
2	C	2351	FAD	C5X-C9A-N10	5.08	121.59	117.71
2	A	351	FAD	C5X-C9A-N10	6.19	122.44	117.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1351	FAD	C4-N3-C2	6.43	120.61	115.14
2	A	351	FAD	C4-N3-C2	6.91	121.03	115.14
2	D	3351	FAD	C4-N3-C2	7.96	121.92	115.14
2	C	2351	FAD	C4-N3-C2	8.39	122.28	115.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	351	FAD	1	0
3	A	352	BE2	2	0
2	B	1351	FAD	1	0
3	B	1352	BE2	2	0
2	C	2351	FAD	1	0
3	C	2352	BE2	2	0
2	D	3351	FAD	1	0
3	D	3352	BE2	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, 95th 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 ²)	Q<0.9
1	A	340/347 (97%)	-0.13	2 (0%) 89 88	21, 36, 55, 73	0
1	B	340/347 (97%)	-0.17	4 (1%) 79 75	18, 33, 53, 79	0
1	C	340/347 (97%)	0.13	20 (5%) 22 16	27, 41, 61, 84	0
1	D	340/347 (97%)	0.14	22 (6%) 19 14	28, 42, 67, 89	0
All	All	1360/1388 (97%)	-0.01	48 (3%) 44 36	18, 38, 61, 89	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2298	THR	8.1
1	C	2339	LEU	7.6
1	D	3298	THR	6.6
1	D	3297	ARG	5.6
1	D	3302	ASN	5.2
1	C	2300	PRO	4.7
1	D	3300	PRO	4.7
1	C	2340	SER	4.6
1	D	3301	SER	4.4
1	C	2299	GLY	4.3
1	C	2301	SER	3.9
1	D	3028	GLN	3.7
1	D	3340	SER	3.6
1	D	3296	LEU	3.5
1	C	2318	ILE	3.5
1	D	3303	THR	3.5
1	D	3295	GLN	3.3
1	C	2297	ARG	3.0
1	C	2296	LEU	3.0
1	D	3299	GLY	2.9
1	C	2303	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1297	ARG	2.9
1	B	1040	THR	2.8
1	D	3040	THR	2.7
1	D	3338	LYS	2.6
1	C	2106	SER	2.6
1	C	2302	ASN	2.5
1	C	2295	GLN	2.4
1	C	2219	PRO	2.4
1	C	2040	THR	2.4
1	D	3183	GLY	2.3
1	D	3339	LEU	2.3
1	D	3337	LYS	2.3
1	C	2022	ARG	2.3
1	D	3172	ARG	2.3
1	B	1301	SER	2.3
1	C	2336	GLU	2.3
1	D	3335	GLU	2.3
1	D	3332	ARG	2.3
1	C	2183	GLY	2.2
1	A	69	GLN	2.2
1	D	3069	GLN	2.2
1	C	2333	ILE	2.2
1	D	3021	GLU	2.2
1	D	3168	GLU	2.1
1	C	2065	ALA	2.1
1	B	1339	LEU	2.0
1	A	100	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	D	3351	53/53	0.91	0.20	27,38,46,47	0
2	FAD	B	1351	53/53	0.92	0.18	19,24,38,41	0
2	FAD	C	2351	53/53	0.93	0.17	22,31,40,44	0
2	FAD	A	351	53/53	0.94	0.19	21,27,35,40	0
3	BE2	A	352	10/10	0.95	0.15	29,30,31,31	0
3	BE2	C	2352	10/10	0.96	0.12	29,30,30,30	0
3	BE2	D	3352	10/10	0.96	0.13	29,30,31,32	0
3	BE2	B	1352	10/10	0.98	0.14	21,23,24,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.