Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:05 PM GMT

PDB ID	:	1E0Y
Title	:	STRUCTURE OF THE D170S/T457E DOUBLE MUTANT OF VANILLYL-ALCOHOL OXIDASE
Authors	:	Van Der Heuvel, R.H.H.; Van Berkel, W.J.H.; Mattevi, A.
Deposited on	:	2000-04-11
Resolution	:	2.75 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

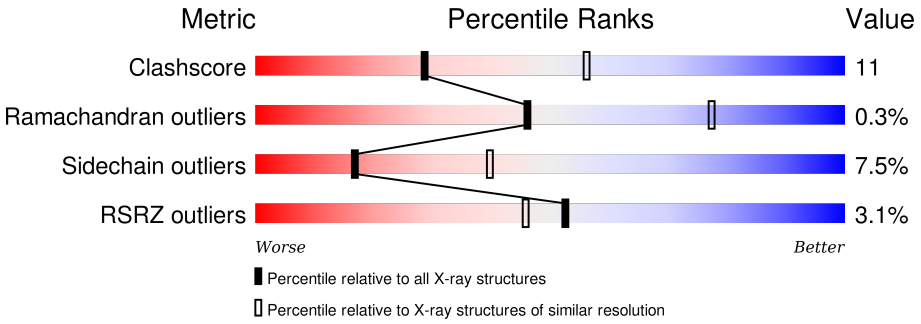
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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))
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 <=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	560	2% 68% 24%
1	B	560	4% 68% 25%

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	FCR	B	601	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8753 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.

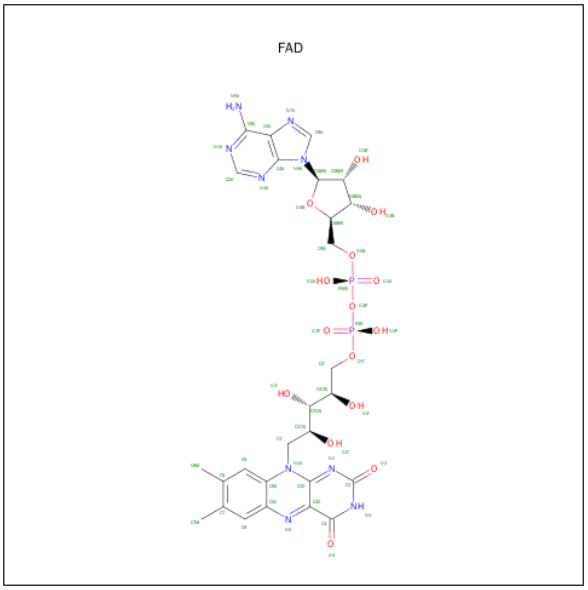
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	3	0	0
			4287	2753	730	781	23			
1	B	550	Total	C	N	O	S	0	0	0
			4269	2740	726	780	23			

There are 6 discrepancies between the modelled and reference sequences:

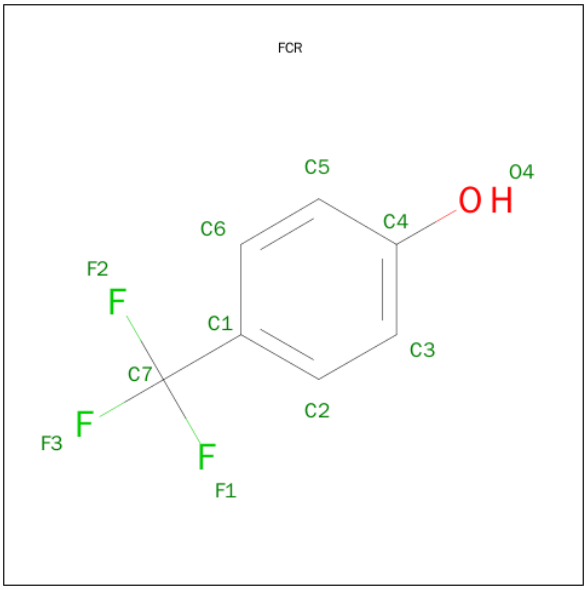
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	GLY	ARG	CONFLICT	UNP P56216
A	457	GLU	THR	ENGINEERED MUTATION	UNP P56216
A	170	SER	ASP	ENGINEERED MUTATION	UNP P56216
B	274	GLY	ARG	CONFLICT	UNP P56216
B	457	GLU	THR	ENGINEERED MUTATION	UNP P56216
B	170	SER	ASP	ENGINEERED MUTATION	UNP P56216

- 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		

- Molecule 3 is ALPHA,ALPHA,ALPHA-TRIFLUORO-P-CRESOL (three-letter code: FCR) (formula: $C_7H_5F_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	F	O	0	0
			11	7	3	1		

- Molecule 4 is water.

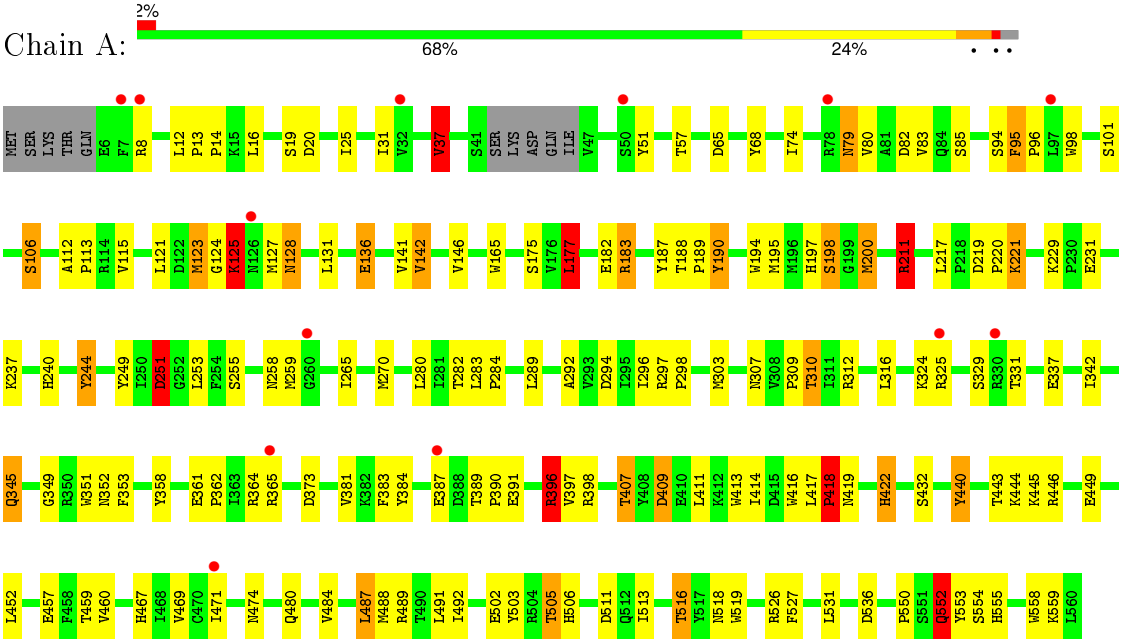
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	38	Total	O	0	0
			38	38		

3 Residue-property plots (i)

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

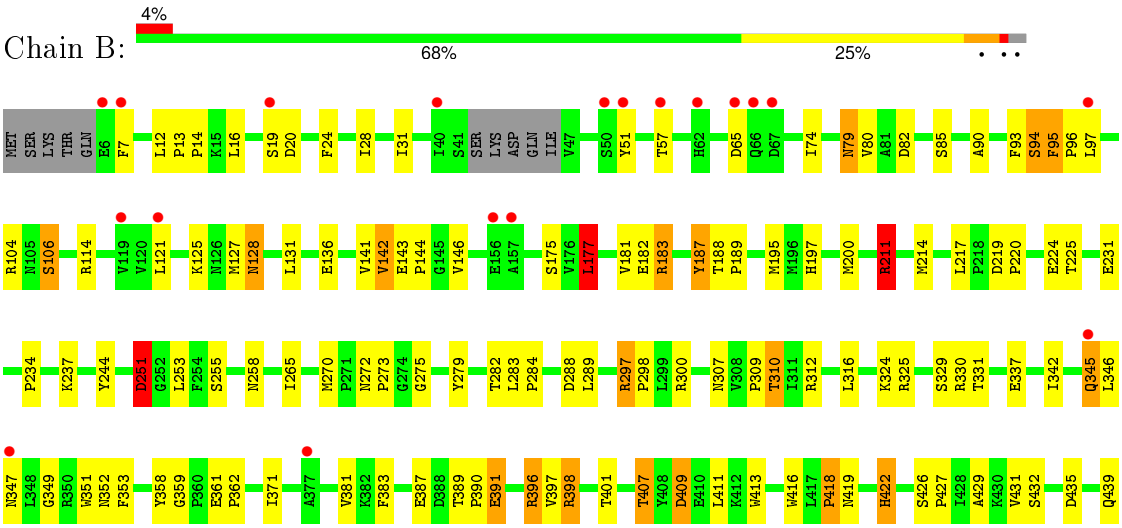
- Molecule 1: VANILLYL-ALCOHOL OXIDASE

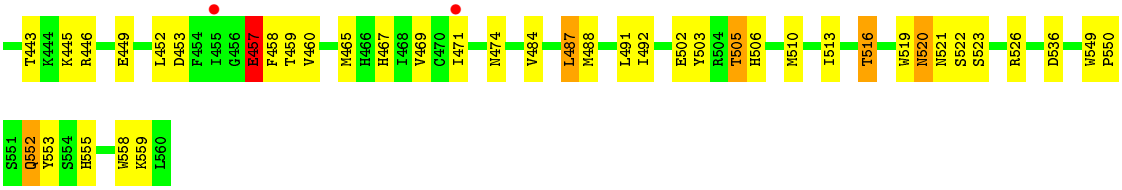
Chain A:



- Molecule 1: VANILLYL-ALCOHOL OXIDASE

Chain B:




T443
K444
K445
R446
E449
L452
D453
F454
T455
G456
E457
F458
T459
V460
M465
H466
H467
I468
V469
C470
I471
N474
V484
L487
M488
L491
I492
E502
Y503
R504
T505
H506
M510
I513
T516
W519
N520
N521
S522
S523
R526
D536
W549
P550
S551
Q552
Y553
S554
H555
W558
K559
L560

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	131.28Å 131.28Å 134.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 24.04 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-2.75) 97.1 (24.04-2.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.76Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.287 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.0	EDS
Estimated twinning fraction	0.006 for l,-k,h 0.017 for -l,-k,-h 0.025 for -h,-l,-k 0.006 for -h,l,k 0.038 for -h,k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 28714 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8753	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FCR, 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	0.52	1/4406 (0.0%)	1.52	58/5997 (1.0%)
1	B	0.49	0/4387	1.52	50/5972 (0.8%)
All	All	0.51	1/8793 (0.0%)	1.52	108/11969 (0.9%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	LYS	CG-CD	9.88	1.86	1.52

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	211	ARG	CD-NE-CZ	20.72	152.61	123.60
1	A	211	ARG	CD-NE-CZ	18.02	148.83	123.60
1	B	398	ARG	NE-CZ-NH1	15.28	127.94	120.30
1	B	211	ARG	CA-CB-CG	13.88	143.93	113.40
1	A	211	ARG	CA-CB-CG	13.79	143.75	113.40
1	B	300	ARG	NE-CZ-NH2	13.55	127.08	120.30
1	A	398	ARG	NE-CZ-NH1	13.34	126.97	120.30
1	B	183	ARG	CD-NE-CZ	12.73	141.43	123.60
1	B	183	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	B	398	ARG	NE-CZ-NH2	-10.21	115.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	297	ARG	NE-CZ-NH2	9.93	125.26	120.30
1	A	37	VAL	CA-C-N	9.82	138.82	117.20
1	A	183	ARG	CD-NE-CZ	9.58	137.01	123.60
1	B	398	ARG	CD-NE-CZ	9.52	136.93	123.60
1	B	300	ARG	NE-CZ-NH1	-9.15	115.72	120.30
1	A	398	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	A	177	LEU	CA-CB-CG	8.97	135.92	115.30
1	B	127	MET	C-N-CA	8.90	143.95	121.70
1	B	244	TYR	CB-CG-CD1	8.90	126.34	121.00
1	B	325	ARG	CD-NE-CZ	8.58	135.62	123.60
1	A	251	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	211	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	B	446	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	A	383	PHE	CB-CG-CD1	-8.04	115.17	120.80
1	B	7	PHE	N-CA-C	7.94	132.45	111.00
1	B	128	ASN	N-CA-CB	-7.83	96.52	110.60
1	A	127	MET	C-N-CA	7.75	141.07	121.70
1	B	114	ARG	NE-CZ-NH1	-7.71	116.44	120.30
1	B	536	ASP	CB-CG-OD1	7.68	125.22	118.30
1	B	128	ASN	CB-CA-C	-7.67	95.06	110.40
1	B	258	ASN	CB-CG-OD1	-7.67	106.27	121.60
1	B	526	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	A	128	ASN	CB-CA-C	-7.54	95.33	110.40
1	A	511	ASP	CB-CG-OD1	-7.50	111.55	118.30
1	B	183	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	A	128	ASN	N-CA-CB	-7.30	97.47	110.60
1	A	398	ARG	CD-NE-CZ	7.21	133.70	123.60
1	B	177	LEU	CA-CB-CG	7.21	131.88	115.30
1	B	446	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	B	114	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	B	297	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	A	526	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	A	65	ASP	N-CA-CB	6.79	122.83	110.60
1	A	65	ASP	CB-CG-OD1	6.78	124.41	118.30
1	A	487	LEU	CA-CB-CG	6.70	130.70	115.30
1	B	104	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	487	LEU	CA-CB-CG	6.68	130.67	115.30
1	A	446	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	B	244	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	B	211	ARG	CG-CD-NE	6.62	125.70	111.80
1	A	190	TYR	CB-CG-CD1	6.60	124.96	121.00
1	A	325	ARG	CD-NE-CZ	6.58	132.81	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	526	ARG	CG-CD-NE	6.38	125.19	111.80
1	B	457	GLU	OE1-CD-OE2	6.31	130.88	123.30
1	A	211	ARG	CG-CD-NE	6.30	125.03	111.80
1	B	413	TRP	CA-CB-CG	6.29	125.66	113.70
1	A	37	VAL	CA-C-O	-6.23	107.02	120.10
1	A	37	VAL	O-C-N	-6.17	112.83	122.70
1	A	258	ASN	CB-CG-ND2	6.14	131.45	116.70
1	A	190	TYR	CB-CG-CD2	-6.11	117.34	121.00
1	B	279	TYR	CB-CG-CD1	6.07	124.64	121.00
1	A	396	ARG	CD-NE-CZ	6.06	132.08	123.60
1	A	396	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	136	GLU	CA-CB-CG	5.97	126.54	113.40
1	A	259	MET	CA-C-N	5.96	128.12	116.20
1	A	552	GLN	C-N-CA	5.95	136.57	121.70
1	A	413	TRP	CA-CB-CG	5.89	124.89	113.70
1	A	536	ASP	CB-CG-OD1	5.83	123.54	118.30
1	B	258	ASN	CB-CG-ND2	5.81	130.64	116.70
1	B	128	ASN	N-CA-C	5.79	126.63	111.00
1	B	251	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	279	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	B	65	ASP	CA-CB-CG	5.68	125.91	113.40
1	A	125	LYS	CA-CB-CG	5.58	125.67	113.40
1	B	330	ARG	N-CA-CB	-5.57	100.57	110.60
1	A	121	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	128	ASN	N-CA-C	5.54	125.96	111.00
1	A	364	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	249	TYR	C-N-CA	5.51	135.47	121.70
1	A	258	ASN	OD1-CG-ND2	-5.45	109.36	121.90
1	A	258	ASN	CA-CB-CG	5.39	125.26	113.40
1	A	249	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	A	123	MET	CA-CB-CG	5.36	122.41	113.30
1	B	426	SER	N-CA-CB	-5.35	102.48	110.50
1	A	165	TRP	CA-CB-CG	5.33	123.82	113.70
1	A	198	SER	N-CA-CB	5.33	118.49	110.50
1	A	383	PHE	N-CA-CB	-5.29	101.07	110.60
1	A	526	ARG	CG-CD-NE	5.28	122.90	111.80
1	A	536	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	440	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	A	259	MET	CA-C-O	-5.23	109.11	120.10
1	B	453	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	288	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	187	TYR	CA-C-N	5.20	128.65	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	255	SER	N-CA-CB	5.20	118.30	110.50
1	A	536	ASP	OD1-CG-OD2	-5.20	113.42	123.30
1	A	249	TYR	CB-CA-C	5.20	120.79	110.40
1	A	303	MET	CA-CB-CG	-5.17	104.50	113.30
1	A	294	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	A	373	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	214	MET	CG-SD-CE	5.09	108.34	100.20
1	A	244	TYR	CB-CG-CD1	5.08	124.05	121.00
1	B	435	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	211	ARG	N-CA-CB	5.06	119.71	110.60
1	A	68	TYR	CB-CG-CD1	5.03	124.02	121.00
1	B	136	GLU	CA-CB-CG	5.02	124.44	113.40
1	B	383	PHE	N-CA-CB	-5.01	101.58	110.60
1	B	121	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	VAL	Mainchain

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	4287	0	4166	103	2
1	B	4269	0	4136	104	1
2	A	53	0	29	3	0
2	B	53	0	29	1	0
3	B	11	0	5	0	0
4	A	42	0	0	1	0
4	B	38	0	0	2	0
All	All	8753	0	8365	195	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (195) 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:B:297:ARG:HB3	1:B:298:PRO:HD3	1.56	0.86
1:A:349:GLY:H	1:A:352:ASN:HD21	1.27	0.83
1:A:550:PRO:HB2	1:A:552:GLN:NE2	1.94	0.82
1:B:397:VAL:HG13	1:B:407:THR:HG21	1.66	0.78
1:A:57:THR:HG22	1:A:74:ILE:HD11	1.64	0.77
1:B:349:GLY:H	1:B:352:ASN:HD21	1.35	0.75
1:B:550:PRO:HB2	1:B:552:GLN:NE2	2.02	0.74
1:B:309:PRO:HG2	1:B:460:VAL:HB	1.69	0.73
1:A:309:PRO:HG2	1:A:460:VAL:HB	1.71	0.73
1:A:365:ARG:HD2	4:A:2032:HOH:O	1.88	0.73
1:A:513:ILE:O	1:A:516:THR:HB	1.89	0.73
1:B:131:LEU:HD12	1:B:141:VAL:HG12	1.70	0.72
1:A:79:ASN:ND2	1:A:82:ASP:H	1.88	0.72
1:B:513:ILE:O	1:B:516:THR:HB	1.89	0.72
1:A:142:VAL:HG22	1:A:146:VAL:HG21	1.73	0.70
1:A:253:LEU:HD21	1:B:253:LEU:HD11	1.73	0.70
1:B:389:THR:HB	1:B:390:PRO:HD2	1.74	0.70
1:B:57:THR:HG22	1:B:74:ILE:HD11	1.75	0.69
1:B:310:THR:HG22	1:B:459:THR:HG22	1.74	0.69
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.74	0.68
1:A:550:PRO:HB2	1:A:552:GLN:HE21	1.57	0.67
1:B:312:ARG:HG2	1:B:316:LEU:HD23	1.75	0.67
1:B:505:THR:HG22	1:B:506:HIS:H	1.61	0.65
1:B:361:GLU:HB3	1:B:362:PRO:HD3	1.78	0.65
1:A:131:LEU:HD12	1:A:141:VAL:HG12	1.76	0.65
1:A:282:THR:HG22	1:A:352:ASN:HD22	1.62	0.65
1:A:397:VAL:HG13	1:A:407:THR:HG21	1.79	0.64
1:A:189:PRO:HG2	1:A:270:MET:CE	2.28	0.64
1:A:282:THR:HG22	1:A:352:ASN:ND2	2.14	0.62
1:B:342:ILE:HA	1:B:345:GLN:HG3	1.80	0.62
1:B:282:THR:HG22	1:B:352:ASN:HD22	1.64	0.62
1:B:387:GLU:HA	1:B:396:ARG:NH2	2.15	0.61
1:B:182:GLU:O	1:B:183:ARG:HB2	2.00	0.61
1:A:310:THR:HG22	1:A:459:THR:HG22	1.82	0.61
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.31	0.60
1:A:361:GLU:HB3	1:A:362:PRO:HD3	1.82	0.60
1:A:244:TYR:CD2	1:B:183:ARG:HD2	2.37	0.60
1:B:79:ASN:ND2	1:B:82:ASP:H	1.99	0.59
1:B:407:THR:HG22	1:B:409:ASP:OD1	2.03	0.59
1:A:492:ILE:HG12	1:A:513:ILE:HG13	1.84	0.58
1:B:552:GLN:NE2	1:B:552:GLN:H	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:THR:HG21	1:A:469:VAL:HG21	1.85	0.58
1:B:142:VAL:HG22	1:B:146:VAL:HG21	1.85	0.58
1:A:342:ILE:HA	1:A:345:GLN:HG3	1.84	0.58
1:A:414:ILE:HD11	2:A:600:FAD:HM71	1.85	0.58
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.86	0.58
1:B:550:PRO:HB2	1:B:552:GLN:HE21	1.70	0.57
1:B:282:THR:HG22	1:B:352:ASN:ND2	2.20	0.57
1:A:292:ALA:O	1:A:296:ILE:HG13	2.05	0.57
1:A:79:ASN:HD22	1:A:82:ASP:H	1.52	0.56
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.87	0.56
1:A:519:TRP:CE3	1:B:211:ARG:HG2	2.40	0.56
1:B:106:SER:HB2	1:B:422:HIS:HE1	1.68	0.56
1:A:253:LEU:HD11	1:B:253:LEU:HD21	1.88	0.56
1:A:106:SER:HB2	1:A:422:HIS:HE1	1.72	0.55
1:A:552:GLN:H	1:A:552:GLN:NE2	2.04	0.55
1:B:307:ASN:HB3	1:B:358:TYR:HE2	1.72	0.55
1:A:387:GLU:HA	1:A:396:ARG:NH2	2.22	0.54
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.37	0.54
1:A:312:ARG:HG2	1:A:316:LEU:HD23	1.90	0.54
1:B:187:TYR:O	1:B:307:ASN:HB2	2.09	0.53
1:B:505:THR:HG23	4:B:2025:HOH:O	2.07	0.53
1:B:389:THR:HB	1:B:390:PRO:CD	2.38	0.53
1:A:419:ASN:HB2	1:A:474:ASN:OD1	2.09	0.53
1:B:188:THR:HB	1:B:189:PRO:CD	2.38	0.53
1:A:289:LEU:HD22	1:A:351:TRP:CZ2	2.44	0.53
1:A:505:THR:HG22	1:A:506:HIS:H	1.72	0.53
1:A:407:THR:HG22	1:A:409:ASP:OD1	2.10	0.52
1:A:200:MET:HE3	1:A:265:ILE:HD12	1.89	0.52
1:A:307:ASN:HB3	1:A:358:TYR:HE2	1.75	0.52
1:B:289:LEU:HD22	1:B:351:TRP:CZ2	2.45	0.52
1:B:337:GLU:H	1:B:337:GLU:CD	2.13	0.51
1:B:492:ILE:HG12	1:B:513:ILE:HG13	1.91	0.51
1:A:324:LYS:HB2	1:A:416:TRP:CE2	2.46	0.51
1:A:502:GLU:OE1	1:A:513:ILE:HG12	2.11	0.51
1:A:389:THR:HB	1:A:390:PRO:HD2	1.92	0.51
1:A:445:LYS:O	1:A:449:GLU:HG3	2.11	0.50
1:A:182:GLU:O	1:A:183:ARG:HB2	2.11	0.50
2:A:600:FAD:H8A	2:A:600:FAD:O5B	2.12	0.49
1:B:505:THR:HG21	1:B:513:ILE:CD1	2.42	0.49
1:B:431:VAL:HG22	1:B:465:MET:HG3	1.94	0.49
1:A:505:THR:HG21	1:A:513:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG13	1:A:558:TRP:CH2	2.47	0.49
1:B:177:LEU:HB2	1:B:265:ILE:CG2	2.43	0.49
1:B:181:VAL:O	1:B:255:SER:HB2	2.13	0.49
1:A:519:TRP:CZ3	1:B:211:ARG:HG2	2.48	0.48
1:A:177:LEU:HB2	1:A:265:ILE:HG22	1.94	0.48
1:B:419:ASN:HB2	1:B:474:ASN:OD1	2.12	0.48
1:B:80:VAL:HG11	1:B:231:GLU:HB3	1.95	0.48
1:A:142:VAL:HG22	1:A:146:VAL:CG2	2.41	0.48
1:B:79:ASN:HD22	1:B:82:ASP:H	1.60	0.48
1:A:452:LEU:HD12	1:A:487:LEU:CD2	2.44	0.48
1:A:197:HIS:HE1	1:A:251:ASP:OD2	1.96	0.48
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.48	0.48
1:B:452:LEU:HD12	1:B:487:LEU:CD2	2.44	0.47
1:B:307:ASN:HB3	1:B:358:TYR:CE2	2.49	0.47
1:B:398:ARG:HA	1:B:401:THR:HB	1.95	0.47
1:B:275:GLY:HA3	1:B:359:GLY:O	2.14	0.47
1:A:211:ARG:HG2	1:B:519:TRP:CE3	2.49	0.47
1:A:309:PRO:HG2	1:A:460:VAL:CB	2.44	0.47
1:B:14:PRO:HG3	1:B:558:TRP:CZ2	2.50	0.47
1:B:309:PRO:O	1:B:460:VAL:HG23	2.14	0.47
1:A:188:THR:HB	1:A:189:PRO:CD	2.45	0.46
1:B:177:LEU:HB2	1:B:265:ILE:HG22	1.96	0.46
1:B:142:VAL:HG22	1:B:146:VAL:CG2	2.45	0.46
1:A:177:LEU:HB2	1:A:265:ILE:CG2	2.45	0.46
1:B:445:LYS:O	1:B:449:GLU:HG3	2.16	0.46
1:B:189:PRO:HG2	1:B:270:MET:CE	2.46	0.46
1:B:197:HIS:HE1	1:B:251:ASP:OD2	1.99	0.46
1:A:124:GLY:O	1:A:125:LYS:C	2.54	0.46
1:B:283:LEU:HA	1:B:284:PRO:HD3	1.70	0.46
1:B:346:LEU:O	1:B:347:ASN:HB2	2.16	0.46
1:A:555:HIS:HB3	1:A:559:LYS:HE3	1.98	0.46
1:A:387:GLU:H	1:A:387:GLU:CD	2.20	0.45
1:A:194:TRP:O	1:A:197:HIS:HD2	1.99	0.45
1:B:510:MET:HE2	4:B:2035:HOH:O	2.16	0.45
1:A:189:PRO:HG2	1:A:270:MET:HE3	1.97	0.45
1:B:31:ILE:HD13	1:B:85:SER:HB3	1.98	0.45
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.98	0.45
1:A:16:LEU:HD11	1:A:20:ASP:HB3	1.98	0.45
1:B:16:LEU:HD11	1:B:20:ASP:HB3	1.99	0.45
1:A:283:LEU:HA	1:A:284:PRO:HD3	1.81	0.45
1:B:188:THR:CB	1:B:189:PRO:CD	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:TYR:O	1:A:307:ASN:HB2	2.16	0.44
1:A:527:PHE:CE2	1:A:531:LEU:HD11	2.52	0.44
1:B:24:PHE:O	1:B:28:ILE:HG12	2.17	0.44
1:B:57:THR:HG22	1:B:74:ILE:CD1	2.45	0.44
1:A:280:LEU:HB3	1:A:384:TYR:HB2	1.98	0.44
1:B:429:ALA:HB2	1:B:439:GLN:NE2	2.33	0.44
1:B:13:PRO:HG3	1:B:95:PHE:CE1	2.52	0.44
1:A:13:PRO:HG3	1:A:95:PHE:CE1	2.52	0.44
1:B:521:ASN:O	1:B:522:SER:HB2	2.17	0.44
1:A:309:PRO:O	1:A:460:VAL:HG23	2.18	0.44
1:A:309:PRO:HB2	1:A:353:PHE:CE1	2.53	0.44
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.98	0.44
1:B:79:ASN:HD22	1:B:79:ASN:C	2.21	0.44
1:B:309:PRO:HB2	1:B:353:PHE:CE1	2.53	0.43
1:A:79:ASN:HD22	1:A:79:ASN:C	2.20	0.43
1:B:488:MET:O	1:B:492:ILE:HD12	2.17	0.43
1:A:307:ASN:HB3	1:A:358:TYR:CE2	2.53	0.43
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.53	0.43
1:A:488:MET:O	1:A:492:ILE:HD12	2.17	0.43
1:A:443:THR:HA	1:A:491:LEU:HD21	2.00	0.43
1:B:188:THR:HB	1:B:189:PRO:HD3	2.01	0.43
2:B:600:FAD:H8A	2:B:600:FAD:O5B	2.18	0.43
1:A:37:VAL:HG12	1:A:37:VAL:O	2.19	0.43
1:A:136:GLU:O	1:B:297:ARG:NH1	2.51	0.43
1:B:457:GLU:HG2	1:B:458:PHE:N	2.31	0.43
1:A:190:TYR:CE1	1:A:270:MET:HG3	2.53	0.43
1:A:112:ALA:HA	1:A:113:PRO:HD3	1.79	0.43
1:B:427:PRO:HD2	1:B:467:HIS:O	2.19	0.43
1:A:440:TYR:CE2	1:A:444:LYS:HE2	2.53	0.43
1:A:198:SER:O	1:A:240:HIS:HA	2.19	0.43
1:B:96:PRO:HG3	1:B:553:TYR:OH	2.19	0.42
1:A:96:PRO:HG3	1:A:553:TYR:OH	2.19	0.42
1:A:471:ILE:HG21	1:A:484:VAL:HG13	2.01	0.42
1:A:80:VAL:HG11	1:A:231:GLU:HB3	2.01	0.42
1:B:93:PHE:O	1:B:94:SER:HB2	2.19	0.42
1:B:51:TYR:CD2	1:B:411:LEU:HD11	2.54	0.42
1:B:505:THR:OG1	1:B:513:ILE:HD13	2.20	0.42
1:A:229:LYS:HD2	1:A:231:GLU:OE2	2.19	0.42
1:B:491:LEU:O	1:B:492:ILE:C	2.57	0.42
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.50	0.42
1:B:90:ALA:HB1	1:B:95:PHE:O	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:HD13	1:A:85:SER:HB3	2.01	0.42
1:A:12:LEU:HB3	1:A:13:PRO:HD2	2.00	0.42
1:B:12:LEU:HB3	1:B:13:PRO:HD2	2.01	0.42
1:A:51:TYR:CD2	1:A:411:LEU:HD11	2.54	0.42
1:A:219:ASP:HA	1:A:220:PRO:HD3	1.67	0.42
1:B:90:ALA:HB2	1:B:97:LEU:HD21	2.01	0.42
1:B:555:HIS:HB3	1:B:559:LYS:HE3	2.01	0.42
1:B:224:GLU:H	1:B:224:GLU:CD	2.24	0.41
1:B:225:THR:HG21	1:B:234:PRO:HG3	2.02	0.41
1:A:25:ILE:HA	1:A:25:ILE:HD13	1.86	0.41
1:A:337:GLU:CD	1:A:337:GLU:H	2.24	0.41
1:A:253:LEU:HD21	1:B:253:LEU:CD1	2.45	0.41
1:B:361:GLU:N	1:B:362:PRO:CD	2.83	0.41
1:B:520:ASN:HD22	1:B:520:ASN:HA	1.63	0.41
1:A:188:THR:CB	1:A:189:PRO:CD	2.98	0.41
1:A:244:TYR:CE2	1:B:183:ARG:HD2	2.55	0.41
1:B:324:LYS:HB2	1:B:416:TRP:CE2	2.55	0.41
1:A:516:THR:HG23	1:B:217:LEU:CD2	2.50	0.41
1:B:502:GLU:OE1	1:B:513:ILE:HG12	2.20	0.41
1:A:211:ARG:HG2	1:B:519:TRP:CZ3	2.56	0.41
1:A:13:PRO:HA	1:A:14:PRO:HD3	1.88	0.41
1:A:195:MET:SD	1:B:195:MET:SD	3.19	0.41
1:B:552:GLN:HE21	1:B:552:GLN:H	1.69	0.41
1:A:83:VAL:HG21	1:A:123:MET:CE	2.51	0.41
1:B:471:ILE:HG21	1:B:484:VAL:HG13	2.03	0.41
1:A:101:SER:O	1:A:124:GLY:HA3	2.21	0.40
1:A:414:ILE:CD1	2:A:600:FAD:HM71	2.51	0.40
1:A:518:ASN:O	1:A:519:TRP:C	2.58	0.40
1:A:389:THR:HB	1:A:390:PRO:CD	2.51	0.40
1:B:219:ASP:HA	1:B:220:PRO:HD3	1.91	0.40
1:B:272:ASN:HA	1:B:273:PRO:HD3	1.96	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LYS:NZ	1:A:489:ARG:CD[4_565]	1.98	0.22
1:A:37:VAL:O	1:B:391:GLU:OE2[6_655]	2.00	0.20

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	546/560 (98%)	512 (94%)	33 (6%)	1 (0%)	52 83
1	B	546/560 (98%)	512 (94%)	32 (6%)	2 (0%)	39 72
All	All	1092/1120 (98%)	1024 (94%)	65 (6%)	3 (0%)	46 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	PRO
1	B	418	PRO
1	B	371	ILE

5.3.2 Protein sidechains (i)

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	455/481 (95%)	420 (92%)	35 (8%)	16 38
1	B	452/481 (94%)	419 (93%)	33 (7%)	17 41
All	All	907/962 (94%)	839 (92%)	68 (8%)	17 40

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	19	SER
1	A	79	ASN

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Mol	Chain	Res	Type
1	A	94	SER
1	A	95	PHE
1	A	106	SER
1	A	125	LYS
1	A	128	ASN
1	A	142	VAL
1	A	175	SER
1	A	177	LEU
1	A	200	MET
1	A	211	ARG
1	A	237	LYS
1	A	251	ASP
1	A	310	THR
1	A	329	SER
1	A	331	THR
1	A	345	GLN
1	A	381	VAL
1	A	391	GLU
1	A	396	ARG
1	A	407	THR
1	A	409	ASP
1	A	418	PRO
1	A	422	HIS
1	A	432	SER
1	A	457	GLU
1	A	467	HIS
1	A	480	GLN
1	A	503	TYR
1	A	505	THR
1	A	516	THR
1	A	552	GLN
1	A	554	SER
1	B	19	SER
1	B	79	ASN
1	B	94	SER
1	B	95	PHE
1	B	106	SER
1	B	125	LYS
1	B	128	ASN
1	B	142	VAL
1	B	175	SER
1	B	177	LEU

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Mol	Chain	Res	Type
1	B	200	MET
1	B	211	ARG
1	B	237	LYS
1	B	251	ASP
1	B	310	THR
1	B	329	SER
1	B	331	THR
1	B	345	GLN
1	B	381	VAL
1	B	391	GLU
1	B	396	ARG
1	B	407	THR
1	B	409	ASP
1	B	418	PRO
1	B	422	HIS
1	B	432	SER
1	B	457	GLU
1	B	503	TYR
1	B	505	THR
1	B	516	THR
1	B	520	ASN
1	B	523	SER
1	B	552	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	467	HIS
1	A	520	ASN
1	A	552	GLN
1	B	79	ASN
1	B	128	ASN
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	439	GLN
1	B	467	HIS
1	B	485	GLN

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Mol	Chain	Res	Type
1	B	520	ASN
1	B	552	GLN

5.3.3 RNA (i)

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)

3 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	600	1	48,58,58	1.55	7 (14%)	54,89,89	2.45	12 (22%)
2	FAD	B	600	1	48,58,58	1.53	7 (14%)	54,89,89	2.22	11 (20%)
3	FCR	B	601	-	11,11,11	0.95	0	16,16,16	1.58	3 (18%)

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	600	1	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	600	1	-	0/30/50/50	0/6/6/6
3	FCR	B	601	-	-	0/6/6/6	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	PA-O2A	-4.59	1.35	1.54
2	B	600	FAD	C10-N10	-4.55	1.33	1.39
2	B	600	FAD	PA-O2A	-4.44	1.36	1.54
2	A	600	FAD	C10-N10	-4.03	1.34	1.39
2	A	600	FAD	P-O2P	-3.12	1.41	1.54
2	B	600	FAD	P-O2P	-3.08	1.41	1.54
2	A	600	FAD	C4-N3	2.21	1.37	1.33
2	B	600	FAD	C4-N3	2.28	1.37	1.33
2	B	600	FAD	C4X-C10	2.51	1.45	1.41
2	A	600	FAD	C4X-C10	2.53	1.45	1.41
2	A	600	FAD	O5'-C5'	3.06	1.57	1.44
2	B	600	FAD	O5'-C5'	3.08	1.57	1.44
2	B	600	FAD	O4B-C1B	3.24	1.45	1.41
2	A	600	FAD	O4B-C1B	4.14	1.46	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	FAD	C4X-C4-N3	-5.43	116.16	123.59
2	A	600	FAD	C4X-C4-N3	-4.55	117.37	123.59
2	B	600	FAD	O3P-P-O5'	-4.45	91.13	102.94
2	A	600	FAD	O3P-P-O5'	-4.25	91.66	102.94
2	A	600	FAD	N3A-C2A-N1A	-4.23	125.65	128.89
2	A	600	FAD	O4B-C1B-N9A	-3.95	99.83	108.10
2	A	600	FAD	O5B-PA-O1A	-3.78	94.93	109.62
2	B	600	FAD	O5B-PA-O1A	-3.67	95.38	109.62
2	B	600	FAD	C4X-C10-N10	-2.53	119.03	120.52
2	A	600	FAD	C4X-C10-N10	-2.36	119.13	120.52
2	B	600	FAD	N3A-C2A-N1A	-2.33	127.11	128.89
2	B	600	FAD	C1B-N9A-C4A	-2.29	123.48	126.94
3	B	601	FCR	F3-C7-C1	-2.19	108.27	112.95
3	B	601	FCR	C6-C1-C7	2.03	123.03	119.99
2	A	600	FAD	O3B-C3B-C4B	2.27	117.85	111.05
2	A	600	FAD	C4X-N5-C5X	2.49	119.63	116.76
2	A	600	FAD	C2A-N1A-C6A	2.55	123.32	118.77
2	B	600	FAD	O3P-PA-O5B	2.64	109.93	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	FAD	C2A-N1A-C6A	2.67	123.55	118.77
2	B	600	FAD	O2P-P-O3P	3.24	119.81	105.09
3	B	601	FCR	F1-C7-C1	4.13	121.78	112.95
2	A	600	FAD	O3P-PA-O5B	5.13	116.56	102.94
2	B	600	FAD	C4-N3-C2	5.82	120.28	115.25
2	A	600	FAD	C4-N3-C2	6.51	120.87	115.25
2	B	600	FAD	P-O3P-PA	9.62	159.75	132.73
2	A	600	FAD	P-O3P-PA	10.35	161.79	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	3	0
2	B	600	FAD	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	550/560 (98%)	0.02	13 (2%)	62	56	32, 49, 73, 88	1 (0%)
1	B	550/560 (98%)	0.08	21 (3%)	44	37	33, 49, 73, 86	0
All	All	1100/1120 (98%)	0.05	34 (3%)	52	46	32, 49, 73, 88	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	ARG	3.5
1	B	62	HIS	3.5
1	B	7	PHE	3.3
1	A	325	ARG	3.3
1	B	57	THR	3.2
1	B	51	TYR	3.1
1	A	7	PHE	3.1
1	A	365	ARG	3.0
1	B	345	GLN	2.8
1	B	50	SER	2.7
1	B	377	ALA	2.7
1	B	65	ASP	2.6
1	A	97	LEU	2.4
1	A	471	ILE	2.4
1	B	119	VAL	2.4
1	B	97	LEU	2.4
1	A	8	ARG	2.4
1	B	471	ILE	2.4
1	B	157	ALA	2.3
1	B	66	GLN	2.3
1	B	6	GLU	2.3
1	B	156	GLU	2.2
1	B	347	ASN	2.2
1	A	126	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	260	GLY	2.2
1	B	67	ASP	2.2
1	A	78	ARG	2.2
1	B	40	ILE	2.2
1	A	32	VAL	2.2
1	B	121	LEU	2.1
1	A	50	SER	2.1
1	A	387	GLU	2.0
1	B	19	SER	2.0
1	B	455	ILE	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^{th} 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^2)	Q<0.9
3	FCR	B	601	11/11	0.72	0.34	4.44	72,74,78,78	0
2	FAD	A	600	53/53	0.94	0.15	-0.57	46,49,53,54	0
2	FAD	B	600	53/53	0.95	0.14	-0.89	46,49,53,54	0

6.5 Other polymers (i)

There are no such residues in this entry.