Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:32 PM GMT

PDB ID	:	1PHH
Title	:	CRYSTAL STRUCTURE OF P-HYDROXYBENZOATE HYDROXYLASE COMPLEXED WITH ITS REACTION PRODUCT 3,4-DIHYDROXYBENZOATE
Authors	:	Schreuder, H.A.; Drenth, J.
Deposited on	:	1987-11-04
Resolution	:	2.30 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 (i)) were used in the production of this report:

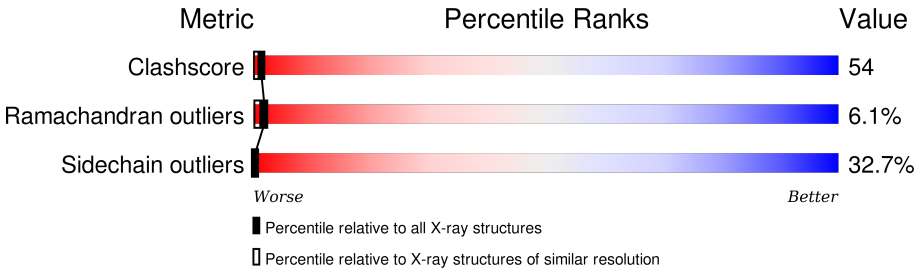
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	394	22% 39% 29% 10%

2 Entry composition

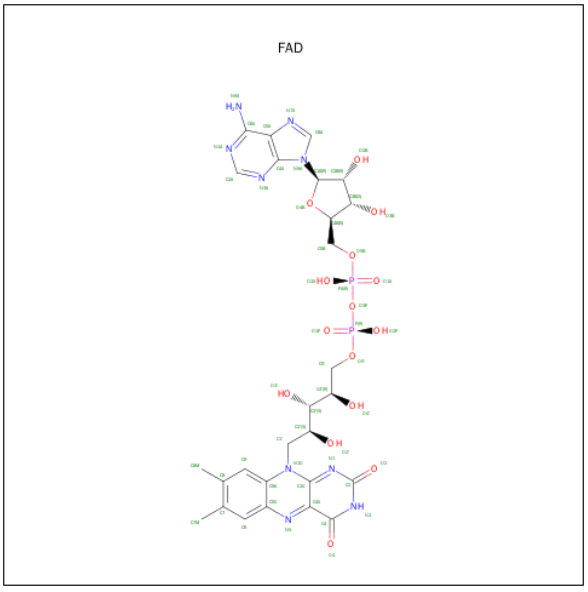
There are 4 unique types of molecules in this entry. The entry contains 3462 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P-HYDROXYBENZOATE HYDROXYLASE.

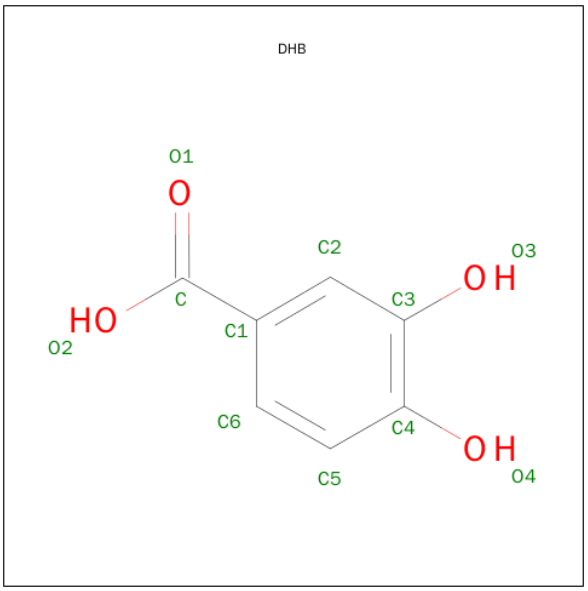
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3125	1976	563	575	11			

- 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		

- Molecule 3 is 3,4-DIHYDROXYBENZOIC ACID (three-letter code: DHB) (formula: $C_7H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 7 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	273	Total O 273 273	0	0

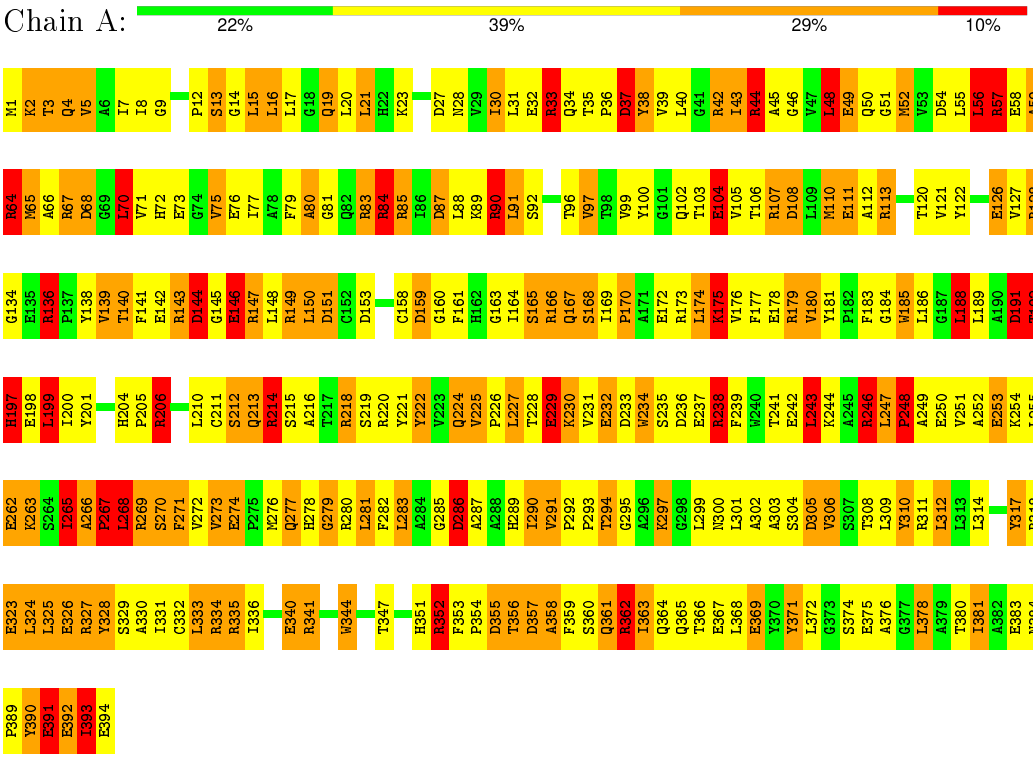
3 Residue-property plots (i)

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

Note EDS was not executed.

- Molecule 1: P-HYDROXYBENZOATE HYDROXYLASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	71.90Å 146.30Å 88.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3462	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DHB, 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	0.89	0/3190	2.39	179/4317 (4.1%)

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	2

There are no bond length outliers.

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	274	GLU	CA-CB-CG	18.63	154.38	113.40
1	A	42	ARG	NE-CZ-NH1	17.27	128.93	120.30
1	A	175	LYS	CA-CB-CG	16.88	150.54	113.40
1	A	179	ARG	NE-CZ-NH1	16.79	128.69	120.30
1	A	42	ARG	NE-CZ-NH2	-16.36	112.12	120.30
1	A	33	ARG	NE-CZ-NH1	14.24	127.42	120.30
1	A	33	ARG	NE-CZ-NH2	-14.12	113.24	120.30
1	A	327	ARG	NE-CZ-NH1	13.77	127.19	120.30
1	A	63	ARG	NE-CZ-NH1	13.60	127.10	120.30
1	A	325	LEU	CA-CB-CG	13.47	146.29	115.30
1	A	111	GLU	CA-CB-CG	13.14	142.31	113.40
1	A	280	ARG	CD-NE-CZ	12.98	141.77	123.60
1	A	324	LEU	CA-CB-CG	12.09	143.10	115.30
1	A	267	PRO	CA-N-CD	-11.96	94.75	111.50
1	A	362	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	A	267	PRO	N-CA-C	11.48	141.95	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	85	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	A	214	ARG	CD-NE-CZ	10.89	138.85	123.60
1	A	266	ALA	N-CA-CB	-10.89	94.86	110.10
1	A	48	LEU	CA-CB-CG	10.18	138.71	115.30
1	A	280	ARG	NE-CZ-NH2	-10.13	115.24	120.30
1	A	371	TYR	CB-CG-CD1	10.04	127.02	121.00
1	A	83	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	A	63	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	A	87	ASP	CB-CG-OD1	9.77	127.09	118.30
1	A	341	ARG	CA-CB-CG	9.72	134.78	113.40
1	A	327	ARG	CD-NE-CZ	9.52	136.93	123.60
1	A	375	GLU	CA-CB-CG	9.43	134.15	113.40
1	A	166	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	A	113	ARG	NE-CZ-NH2	9.31	124.95	120.30
1	A	166	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	A	61	VAL	N-CA-CB	9.30	131.96	111.50
1	A	328	TYR	CB-CG-CD1	9.07	126.44	121.00
1	A	153	ASP	CB-CG-OD2	-8.93	110.26	118.30
1	A	206	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	A	145	GLY	N-CA-C	-8.74	91.26	113.10
1	A	323	GLU	N-CA-CB	8.70	126.26	110.60
1	A	140	THR	CA-CB-CG2	8.62	124.47	112.40
1	A	85	ARG	CD-NE-CZ	8.60	135.63	123.60
1	A	248	PRO	N-CA-C	8.60	134.45	112.10
1	A	196	SER	C-N-CA	8.52	142.99	121.70
1	A	85	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	A	362	ARG	CD-NE-CZ	8.35	135.30	123.60
1	A	388	LEU	CB-CA-C	8.26	125.89	110.20
1	A	364	GLN	CB-CG-CD	8.25	133.04	111.60
1	A	84	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	A	136	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	341	ARG	NE-CZ-NH2	8.09	124.35	120.30
1	A	68	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	A	199	LEU	CA-CB-CG	7.92	133.52	115.30
1	A	266	ALA	N-CA-C	7.80	132.07	111.00
1	A	197	HIS	N-CA-C	7.75	131.91	111.00
1	A	60	GLY	N-CA-C	7.74	132.45	113.10
1	A	191	ASP	CB-CG-OD1	7.72	125.24	118.30
1	A	63	ARG	CD-NE-CZ	7.69	134.37	123.60
1	A	185	TRP	CA-CB-CG	7.69	128.31	113.70
1	A	90	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	A	334	ARG	NE-CZ-NH1	7.63	124.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	352	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	87	ASP	N-CA-CB	7.51	124.12	110.60
1	A	44	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	A	234	TRP	CB-CA-C	7.40	125.19	110.40
1	A	321	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	179	ARG	CD-NE-CZ	7.39	133.95	123.60
1	A	64	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	305	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	180	VAL	CB-CA-C	7.26	125.20	111.40
1	A	280	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	214	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	375	GLU	CG-CD-OE1	7.14	132.58	118.30
1	A	146	GLU	CA-CB-CG	7.13	129.09	113.40
1	A	136	ARG	CD-NE-CZ	7.05	133.47	123.60
1	A	188	LEU	CA-CB-CG	7.01	131.43	115.30
1	A	371	TYR	CB-CG-CD2	-7.00	116.80	121.00
1	A	144	ASP	C-N-CA	6.94	136.88	122.30
1	A	107	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	391	GLU	CB-CA-C	-6.77	96.86	110.40
1	A	294	THR	CA-C-N	6.75	129.70	116.20
1	A	192	THR	N-CA-CB	6.67	122.96	110.30
1	A	179	ARG	NH1-CZ-NH2	-6.65	112.09	119.40
1	A	68	ASP	CA-C-N	6.64	129.48	116.20
1	A	139	VAL	CA-CB-CG1	6.56	120.74	110.90
1	A	60	GLY	C-N-CA	6.55	138.07	121.70
1	A	362	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	110	MET	CG-SD-CE	6.52	110.64	100.20
1	A	107	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	128	ARG	O-C-N	6.46	133.03	122.70
1	A	58	GLU	CA-CB-CG	6.37	127.41	113.40
1	A	128	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	A	49	GLU	CB-CG-CD	6.35	131.34	114.20
1	A	49	GLU	OE1-CD-OE2	-6.32	115.72	123.30
1	A	143	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	38	TYR	CB-CG-CD2	-6.29	117.23	121.00
1	A	234	TRP	CA-CB-CG	-6.25	101.83	113.70
1	A	261	LEU	N-CA-C	-6.21	94.22	111.00
1	A	328	TYR	CB-CG-CD2	-6.16	117.30	121.00
1	A	37	ASP	N-CA-CB	6.14	121.66	110.60
1	A	159	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	A	212	SER	C-N-CA	6.12	136.99	121.70
1	A	5	VAL	O-C-N	6.11	132.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	290	ILE	CA-CB-CG2	6.09	123.08	110.90
1	A	49	GLU	CA-CB-CG	6.08	126.77	113.40
1	A	144	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	A	38	TYR	CB-CG-CD1	6.02	124.61	121.00
1	A	33	ARG	CA-CB-CG	5.99	126.58	113.40
1	A	104	GLU	CA-CB-CG	5.96	126.50	113.40
1	A	200	ILE	O-C-N	5.95	132.23	122.70
1	A	57	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	265	ILE	C-N-CA	5.94	136.55	121.70
1	A	327	ARG	CA-CB-CG	5.93	126.44	113.40
1	A	269	ARG	N-CA-CB	-5.90	99.98	110.60
1	A	49	GLU	CG-CD-OE1	5.83	129.96	118.30
1	A	144	ASP	CA-C-O	5.83	132.33	120.10
1	A	319	GLU	CB-CA-C	5.83	122.05	110.40
1	A	75	VAL	N-CA-CB	5.82	124.31	111.50
1	A	133	GLN	N-CA-C	-5.80	95.35	111.00
1	A	200	ILE	N-CA-CB	5.79	124.13	110.80
1	A	198	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	A	268	LEU	CA-C-O	5.78	132.24	120.10
1	A	113	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	A	305	ASP	CB-CA-C	5.76	121.91	110.40
1	A	188	LEU	CB-CA-C	5.72	121.07	110.20
1	A	266	ALA	C-N-CA	5.70	145.95	122.00
1	A	97	VAL	CA-CB-CG1	5.70	119.45	110.90
1	A	158	CYS	CA-C-O	5.70	132.06	120.10
1	A	229	GLU	N-CA-C	-5.69	95.64	111.00
1	A	333	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	276	MET	C-N-CA	5.67	135.88	121.70
1	A	44	ARG	CD-NE-CZ	-5.60	115.76	123.60
1	A	213	GLN	CB-CG-CD	-5.58	97.10	111.60
1	A	277	GLN	CB-CA-C	-5.56	99.28	110.40
1	A	249	ALA	CA-C-O	5.55	131.75	120.10
1	A	369	GLU	OE1-CD-OE2	5.53	129.94	123.30
1	A	326	GLU	CA-CB-CG	5.53	125.57	113.40
1	A	325	LEU	CB-CA-C	5.51	120.68	110.20
1	A	56	LEU	CB-CA-C	5.49	120.64	110.20
1	A	56	LEU	CB-CG-CD1	5.49	120.33	111.00
1	A	357	ASP	N-CA-C	-5.49	96.19	111.00
1	A	196	SER	CB-CA-C	5.48	120.51	110.10
1	A	145	GLY	CA-C-N	-5.47	105.16	117.20
1	A	37	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	142	GLU	CG-CD-OE1	5.45	129.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	256	VAL	CA-CB-CG1	5.44	119.07	110.90
1	A	353	PHE	O-C-N	5.44	131.44	121.10
1	A	70	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	341	ARG	CB-CG-CD	5.42	125.68	111.60
1	A	243	LEU	CB-CA-C	5.41	120.49	110.20
1	A	197	HIS	CB-CA-C	-5.41	99.59	110.40
1	A	37	ASP	CA-CB-CG	5.40	125.28	113.40
1	A	68	ASP	N-CA-C	5.40	125.57	111.00
1	A	335	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	67	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	108	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	238	ARG	CD-NE-CZ	-5.28	116.21	123.60
1	A	376	ALA	N-CA-CB	5.27	117.47	110.10
1	A	326	GLU	CG-CD-OE1	5.25	128.80	118.30
1	A	333	LEU	CB-CA-C	5.24	120.15	110.20
1	A	326	GLU	OE1-CD-OE2	-5.23	117.03	123.30
1	A	294	THR	N-CA-C	5.19	125.01	111.00
1	A	61	VAL	CA-CB-CG1	5.18	118.67	110.90
1	A	352	ARG	CA-C-O	5.18	130.98	120.10
1	A	192	THR	N-CA-C	-5.18	97.01	111.00
1	A	236	ASP	CB-CA-C	5.17	120.75	110.40
1	A	286	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	153	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	196	SER	N-CA-C	-5.12	97.16	111.00
1	A	128	ARG	CD-NE-CZ	-5.09	116.48	123.60
1	A	340	GLU	CA-CB-CG	5.07	124.55	113.40
1	A	351	HIS	CA-CB-CG	-5.06	105.00	113.60
1	A	16	LEU	CB-CA-C	5.06	119.81	110.20
1	A	310	TYR	CB-CG-CD1	5.06	124.03	121.00
1	A	198	GLU	CG-CD-OE1	5.05	128.41	118.30
1	A	326	GLU	CB-CG-CD	5.05	127.83	114.20
1	A	104	GLU	CG-CD-OE2	-5.04	108.22	118.30
1	A	383	GLU	CA-CB-CG	5.03	124.47	113.40
1	A	222	TYR	O-C-N	5.03	130.74	122.70
1	A	3	THR	N-CA-CB	5.02	119.84	110.30
1	A	134	GLY	N-CA-C	-5.02	100.55	113.10
1	A	246	ARG	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	ARG	Sidechain
1	A	33	ARG	Sidechain

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	3125	0	3121	340	4
2	A	53	0	31	1	0
3	A	11	0	3	1	0
4	A	273	0	0	43	0
All	All	3462	0	3155	340	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 54.

All (340) 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:A:322:GLY:HA2	1:A:324:LEU:HD12	1.25	1.19
1:A:266:ALA:HB1	1:A:267:PRO:HD2	1.40	1.02
1:A:195:VAL:HG21	1:A:213:GLN:HE21	1.25	1.01
1:A:268:LEU:HD13	1:A:293:PRO:HD2	1.45	0.96
1:A:56:LEU:HG	1:A:61:VAL:HG12	1.49	0.95
1:A:314:LEU:HD22	1:A:318:ARG:HH11	1.32	0.92
1:A:192:THR:N	1:A:193:PRO:HD2	1.88	0.88
1:A:192:THR:N	1:A:193:PRO:CD	2.33	0.88
1:A:266:ALA:HB1	1:A:267:PRO:CD	2.03	0.88
1:A:332:CYS:O	1:A:336:ILE:HG12	1.74	0.87
1:A:39:VAL:HB	1:A:42:ARG:NH2	1.91	0.84
1:A:34:GLN:HA	4:A:486:HOH:O	1.78	0.82
1:A:63:ARG:HH22	1:A:67:ARG:NH1	1.78	0.81
1:A:253:GLU:HA	4:A:530:HOH:O	1.79	0.81
1:A:204:HIS:HD2	1:A:206:ARG:H	1.27	0.79
1:A:355:ASP:HA	4:A:491:HOH:O	1.82	0.79
1:A:192:THR:H	1:A:193:PRO:HD2	1.47	0.78
1:A:55:LEU:HD11	4:A:447:HOH:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:NH2	1:A:261:LEU:HG	1.99	0.78
1:A:17:LEU:HG	1:A:21:LEU:HD22	1.66	0.76
1:A:48:LEU:HD21	1:A:100:TYR:HB3	1.66	0.76
1:A:204:HIS:CD2	1:A:206:ARG:H	2.03	0.76
1:A:147:ARG:HH12	1:A:149:ARG:HB2	1.49	0.76
1:A:195:VAL:HG21	1:A:213:GLN:NE2	1.99	0.75
1:A:159:ASP:HB3	1:A:163:GLY:HA3	1.69	0.75
1:A:192:THR:H	1:A:193:PRO:CD	1.95	0.75
1:A:64:ARG:NH1	1:A:67:ARG:HH21	1.84	0.74
1:A:225:VAL:HG11	4:A:650:HOH:O	1.87	0.74
1:A:266:ALA:CB	1:A:267:PRO:HD2	2.09	0.74
1:A:230:LYS:O	1:A:233:ASP:HB2	1.88	0.74
1:A:356:THR:HB	1:A:361:GLN:HG2	1.68	0.74
1:A:218:ARG:HH21	1:A:261:LEU:HG	1.54	0.73
1:A:261:LEU:O	1:A:263:LYS:N	2.21	0.73
1:A:356:THR:CB	1:A:361:GLN:HG2	2.18	0.73
1:A:70:LEU:H	1:A:70:LEU:HD22	1.53	0.72
1:A:108:ASP:HA	1:A:111:GLU:HG2	1.70	0.72
1:A:242:GLU:OE1	1:A:246:ARG:NH1	2.22	0.72
1:A:331:ILE:HG12	1:A:392:GLU:OE2	1.90	0.72
1:A:64:ARG:NH1	1:A:67:ARG:NH2	2.38	0.71
1:A:5:VAL:O	1:A:28:ASN:HA	1.90	0.71
1:A:191:ASP:HB3	1:A:261:LEU:HD23	1.71	0.71
1:A:371:TYR:O	1:A:378:LEU:HD13	1.89	0.71
1:A:30:ILE:HG22	1:A:120:THR:HG23	1.72	0.71
1:A:392:GLU:HG3	1:A:393:ILE:H	1.56	0.71
1:A:194:PRO:HD2	1:A:256:VAL:HG12	1.73	0.71
1:A:99:VAL:HG23	4:A:543:HOH:O	1.91	0.71
1:A:308:THR:HG22	1:A:328:TYR:HD1	1.56	0.70
1:A:194:PRO:HD2	1:A:256:VAL:CG1	2.22	0.70
1:A:33:ARG:HD3	1:A:34:GLN:OE1	1.92	0.70
1:A:235:SER:HB2	1:A:238:ARG:HB2	1.73	0.69
1:A:314:LEU:HD22	1:A:318:ARG:NH1	2.06	0.69
1:A:40:LEU:HD13	1:A:110:MET:HE3	1.73	0.69
1:A:312:LEU:HD23	1:A:328:TYR:HB2	1.71	0.69
1:A:4:GLN:HG2	1:A:317:TYR:CE1	2.27	0.69
1:A:323:GLU:HA	4:A:635:HOH:O	1.91	0.69
1:A:304:SER:CB	1:A:335:ARG:HE	2.05	0.69
1:A:204:HIS:NE2	4:A:465:HOH:O	2.25	0.68
1:A:4:GLN:HG2	1:A:317:TYR:CZ	2.28	0.68
1:A:252:ALA:HB3	1:A:253:GLU:OE2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASP:HB2	1:A:146:GLU:HG2	1.75	0.68
1:A:144:ASP:HB2	1:A:146:GLU:CG	2.24	0.67
1:A:256:VAL:HB	4:A:516:HOH:O	1.94	0.67
1:A:206:ARG:HD2	4:A:465:HOH:O	1.95	0.67
1:A:247:LEU:HB2	1:A:251:VAL:HB	1.77	0.66
1:A:181:TYR:HE2	1:A:292:PRO:HG3	1.60	0.66
1:A:170:PRO:HB2	1:A:173:ARG:HD3	1.77	0.66
1:A:164:ILE:O	1:A:168:SER:OG	2.12	0.66
1:A:329:SER:O	1:A:333:LEU:HB2	1.94	0.66
1:A:230:LYS:HB2	1:A:233:ASP:OD2	1.96	0.65
1:A:218:ARG:HH21	1:A:261:LEU:CG	2.08	0.65
1:A:167:GLN:HA	4:A:463:HOH:O	1.95	0.65
1:A:181:TYR:CE2	1:A:292:PRO:HG3	2.32	0.65
1:A:211:CYS:HA	1:A:221:TYR:CD1	2.32	0.64
1:A:211:CYS:HA	1:A:221:TYR:HD1	1.62	0.64
1:A:214:ARG:HB2	4:A:533:HOH:O	1.96	0.64
1:A:311:ARG:HH12	1:A:391:GLU:HG3	1.63	0.63
1:A:70:LEU:HD23	1:A:99:VAL:HG22	1.80	0.63
1:A:73:GLU:HB3	1:A:89:LYS:HG2	1.79	0.63
1:A:8:ILE:HD13	1:A:129:LEU:HD21	1.81	0.63
1:A:371:TYR:HB3	1:A:381:ILE:HD11	1.79	0.63
1:A:319:GLU:HB3	1:A:321:ARG:HH12	1.64	0.63
1:A:218:ARG:HH21	1:A:261:LEU:CD2	2.12	0.62
1:A:356:THR:HG21	4:A:623:HOH:O	1.99	0.62
1:A:166:ARG:HD3	1:A:273:VAL:HG21	1.81	0.62
1:A:72:HIS:O	1:A:96:THR:HB	1.99	0.62
1:A:164:ILE:HD11	4:A:591:HOH:O	2.00	0.61
1:A:39:VAL:O	1:A:42:ARG:HB2	2.01	0.61
1:A:363:ILE:HG22	4:A:421:HOH:O	2.00	0.60
1:A:175:LYS:HD3	1:A:274:GLU:HG2	1.83	0.60
1:A:246:ARG:C	1:A:247:LEU:HD23	2.22	0.60
1:A:392:GLU:CG	1:A:393:ILE:H	2.13	0.60
1:A:311:ARG:NH1	1:A:391:GLU:OE2	2.35	0.60
1:A:75:VAL:HG12	1:A:199:LEU:HB2	1.84	0.59
1:A:308:THR:CG2	1:A:312:LEU:HD22	2.32	0.59
1:A:67:ARG:HD3	4:A:404:HOH:O	2.02	0.59
1:A:174:LEU:HD12	1:A:273:VAL:HB	1.85	0.59
1:A:165:SER:HB3	1:A:281:LEU:HD21	1.83	0.59
1:A:390:TYR:HB3	1:A:391:GLU:HG2	1.83	0.59
1:A:8:ILE:HG22	1:A:159:ASP:OD1	2.02	0.59
1:A:144:ASP:HB2	1:A:146:GLU:CB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:O	1:A:222:TYR:HA	2.02	0.58
1:A:64:ARG:HH11	1:A:67:ARG:HH21	1.46	0.58
1:A:368:LEU:O	1:A:372:LEU:HB2	2.03	0.58
1:A:271:PHE:HB3	1:A:290:ILE:HB	1.84	0.58
1:A:57:ARG:HD3	1:A:62:ASP:OD2	2.03	0.58
1:A:46:GLY:O	1:A:99:VAL:HA	2.03	0.58
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.67	0.58
1:A:57:ARG:NH1	1:A:66:ALA:HB2	2.19	0.58
1:A:7:ILE:HB	1:A:30:ILE:HG13	1.85	0.58
1:A:308:THR:HG23	1:A:312:LEU:HD22	1.86	0.58
1:A:322:GLY:CA	1:A:324:LEU:HD12	2.17	0.58
1:A:184:GLY:HA3	1:A:267:PRO:HD3	1.85	0.57
1:A:356:THR:OG1	1:A:361:GLN:HG2	2.04	0.57
1:A:173:ARG:NH2	4:A:456:HOH:O	2.37	0.57
1:A:321:ARG:NH1	1:A:321:ARG:HG2	2.18	0.57
1:A:354:PRO:O	1:A:355:ASP:HB2	2.04	0.57
1:A:295:GLY:O	1:A:297:LYS:HD2	2.04	0.57
1:A:63:ARG:HH22	1:A:67:ARG:HH12	1.52	0.57
1:A:88:LEU:O	1:A:92:SER:OG	2.20	0.57
1:A:129:LEU:N	1:A:129:LEU:HD23	2.20	0.56
1:A:161:PHE:HA	1:A:286:ASP:O	2.04	0.56
1:A:161:PHE:CD1	1:A:290:ILE:HG13	2.40	0.56
1:A:215:SER:OG	1:A:216:ALA:N	2.38	0.56
1:A:87:ASP:O	1:A:91:LEU:HB2	2.05	0.56
1:A:107:ARG:HD3	4:A:455:HOH:O	2.06	0.56
1:A:186:LEU:HD11	1:A:231:VAL:HG23	1.87	0.56
1:A:336:ILE:HG13	4:A:548:HOH:O	2.05	0.56
1:A:244:LYS:O	1:A:251:VAL:HG21	2.06	0.56
1:A:77:ILE:HD13	1:A:201:TYR:HB2	1.86	0.56
1:A:108:ASP:HA	1:A:111:GLU:CG	2.36	0.56
1:A:378:LEU:HA	1:A:381:ILE:HG13	1.88	0.56
1:A:2:LYS:HE3	4:A:513:HOH:O	2.05	0.56
1:A:57:ARG:NE	1:A:62:ASP:OD2	2.40	0.55
1:A:372:LEU:HA	1:A:378:LEU:CD1	2.36	0.55
1:A:146:GLU:O	1:A:148:LEU:HG	2.07	0.55
1:A:237:GLU:HG2	4:A:632:HOH:O	2.06	0.55
1:A:128:ARG:C	1:A:129:LEU:HD23	2.26	0.55
1:A:220:ARG:HB2	4:A:533:HOH:O	2.04	0.55
1:A:322:GLY:O	1:A:325:LEU:HB3	2.07	0.55
1:A:191:ASP:OD1	1:A:191:ASP:O	2.23	0.55
1:A:17:LEU:HG	1:A:21:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:NE	1:A:287:ALA:O	2.24	0.55
1:A:289:HIS:C	1:A:290:ILE:HG12	2.28	0.54
1:A:188:LEU:HG	1:A:239:PHE:CD2	2.42	0.54
1:A:262:GLU:OE1	1:A:262:GLU:HA	2.07	0.54
1:A:7:ILE:CG2	1:A:30:ILE:HG13	2.37	0.54
1:A:54:ASP:HA	1:A:57:ARG:HB2	1.89	0.54
1:A:40:LEU:HD11	1:A:107:ARG:HB2	1.90	0.54
1:A:144:ASP:HB2	1:A:146:GLU:HB3	1.90	0.53
1:A:17:LEU:O	1:A:21:LEU:HB2	2.07	0.53
1:A:268:LEU:HD12	1:A:292:PRO:HB3	1.90	0.53
1:A:282:PHE:HA	4:A:416:HOH:O	2.08	0.53
1:A:49:GLU:OE1	1:A:297:LYS:HE3	2.08	0.53
1:A:294:THR:CG2	1:A:347:THR:OG1	2.57	0.53
1:A:374:SER:O	1:A:378:LEU:HD22	2.09	0.53
1:A:227:LEU:C	1:A:229:GLU:H	2.11	0.53
1:A:319:GLU:HB3	1:A:321:ARG:NH1	2.23	0.53
1:A:128:ARG:NE	4:A:608:HOH:O	2.42	0.52
1:A:390:TYR:O	1:A:391:GLU:HB3	2.09	0.52
1:A:334:ARG:HD2	4:A:595:HOH:O	2.10	0.52
1:A:234:TRP:CE3	1:A:238:ARG:HD2	2.43	0.52
1:A:48:LEU:CD2	1:A:100:TYR:HB3	2.36	0.52
1:A:251:VAL:CG2	1:A:251:VAL:O	2.57	0.52
1:A:164:ILE:O	1:A:164:ILE:HG13	2.08	0.52
1:A:246:ARG:O	1:A:247:LEU:HD23	2.09	0.52
1:A:314:LEU:HD13	1:A:318:ARG:HH12	1.75	0.52
1:A:45:ALA:HB3	1:A:102:GLN:HB2	1.90	0.52
1:A:330:ALA:O	1:A:334:ARG:HG3	2.10	0.52
1:A:31:LEU:HD21	1:A:141:PHE:CD2	2.45	0.52
1:A:128:ARG:HG3	4:A:399:HOH:O	2.10	0.51
1:A:393:ILE:O	1:A:394:GLU:HB2	2.10	0.51
1:A:327:ARG:O	1:A:331:ILE:HG13	2.11	0.51
1:A:334:ARG:HB3	4:A:511:HOH:O	2.11	0.51
1:A:285:GLY:O	1:A:287:ALA:N	2.44	0.51
1:A:244:LYS:HA	1:A:251:VAL:HG23	1.92	0.51
1:A:368:LEU:O	1:A:372:LEU:HD23	2.10	0.51
1:A:366:THR:HA	1:A:369:GLU:HG3	1.92	0.51
1:A:56:LEU:HG	1:A:61:VAL:CG1	2.32	0.51
1:A:372:LEU:HA	1:A:378:LEU:HD13	1.93	0.51
1:A:44:ARG:NH2	4:A:661:HOH:O	2.34	0.51
1:A:89:LYS:HD2	4:A:657:HOH:O	2.11	0.50
1:A:352:ARG:HG3	1:A:352:ARG:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:CD1	1:A:310:TYR:HD1	2.24	0.50
1:A:195:VAL:HG13	1:A:219:SER:OG	2.11	0.50
1:A:308:THR:O	1:A:312:LEU:HB2	2.10	0.50
1:A:283:LEU:O	1:A:328:TYR:OH	2.28	0.50
1:A:214:ARG:HA	1:A:214:ARG:HE	1.76	0.50
1:A:212:SER:N	1:A:220:ARG:O	2.44	0.50
1:A:229:GLU:OE2	1:A:234:TRP:NE1	2.35	0.50
1:A:231:VAL:C	1:A:233:ASP:H	2.14	0.50
1:A:161:PHE:O	1:A:166:ARG:NH2	2.45	0.50
1:A:108:ASP:O	1:A:111:GLU:HB2	2.11	0.49
1:A:9:GLY:O	1:A:14:GLY:HA3	2.12	0.49
1:A:277:GLN:HG2	4:A:416:HOH:O	2.12	0.49
1:A:97:VAL:HG21	4:A:472:HOH:O	2.11	0.49
1:A:304:SER:HB2	1:A:335:ARG:HE	1.75	0.49
1:A:189:LEU:HD11	1:A:218:ARG:NE	2.26	0.49
1:A:169:ILE:HG23	1:A:278:HIS:CG	2.48	0.49
1:A:220:ARG:HH22	1:A:263:LYS:HE2	1.78	0.49
1:A:169:ILE:HD11	1:A:281:LEU:HD13	1.95	0.49
1:A:204:HIS:CD2	1:A:205:PRO:HD2	2.48	0.49
1:A:4:GLN:HB2	1:A:27:ASP:O	2.13	0.48
1:A:357:ASP:C	1:A:359:PHE:H	2.15	0.48
1:A:323:GLU:C	1:A:325:LEU:N	2.65	0.48
1:A:81:GLY:HA3	4:A:546:HOH:O	2.13	0.48
1:A:57:ARG:CD	1:A:62:ASP:OD2	2.61	0.48
1:A:294:THR:HG21	1:A:347:THR:HA	1.95	0.48
1:A:51:GLY:O	1:A:55:LEU:HB2	2.14	0.48
1:A:271:PHE:C	1:A:271:PHE:CD1	2.87	0.48
1:A:100:TYR:CZ	1:A:104:GLU:HB3	2.49	0.48
1:A:214:ARG:HE	1:A:214:ARG:CA	2.27	0.47
1:A:191:ASP:CA	1:A:193:PRO:HD2	2.43	0.47
1:A:213:GLN:HG3	1:A:215:SER:O	2.14	0.47
1:A:70:LEU:CD2	1:A:70:LEU:H	2.23	0.47
1:A:188:LEU:HD22	1:A:260:SER:HB3	1.96	0.47
1:A:39:VAL:HB	1:A:42:ARG:HH21	1.71	0.47
1:A:356:THR:HB	1:A:361:GLN:CG	2.40	0.47
1:A:243:LEU:HD22	1:A:247:LEU:HD21	1.96	0.47
1:A:12:PRO:CG	1:A:299:LEU:HD11	2.45	0.47
1:A:193:PRO:HA	1:A:194:PRO:HD3	1.67	0.47
1:A:185:TRP:O	1:A:266:ALA:HA	2.15	0.47
1:A:49:GLU:HG2	1:A:300:ASN:CG	2.34	0.47
1:A:90:ARG:NH2	4:A:411:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ALA:O	1:A:362:ARG:HB2	2.15	0.47
1:A:43:ILE:HB	1:A:263:LYS:HD2	1.96	0.47
1:A:243:LEU:O	1:A:244:LYS:C	2.52	0.47
1:A:304:SER:HB3	1:A:335:ARG:HH21	1.79	0.47
1:A:238:ARG:HG3	1:A:238:ARG:HH11	1.80	0.47
1:A:31:LEU:HD12	1:A:121:VAL:HB	1.96	0.47
1:A:231:VAL:C	1:A:233:ASP:N	2.68	0.46
1:A:238:ARG:HA	1:A:241:THR:HG22	1.97	0.46
1:A:144:ASP:N	1:A:146:GLU:HG2	2.31	0.46
1:A:191:ASP:HB3	1:A:218:ARG:NE	2.30	0.46
1:A:3:THR:OG1	1:A:4:GLN:N	2.49	0.46
1:A:285:GLY:C	1:A:287:ALA:H	2.16	0.46
1:A:355:ASP:O	1:A:356:THR:C	2.54	0.46
1:A:265:ILE:HB	1:A:266:ALA:H	1.52	0.46
1:A:147:ARG:NH2	4:A:518:HOH:O	2.41	0.46
1:A:149:ARG:NE	4:A:518:HOH:O	2.36	0.46
1:A:160:GLY:HA2	1:A:286:ASP:HB2	1.98	0.46
1:A:362:ARG:HA	1:A:362:ARG:HD3	1.64	0.46
1:A:224:GLN:HG2	1:A:225:VAL:N	2.29	0.46
1:A:30:ILE:CG2	1:A:120:THR:HG23	2.44	0.46
1:A:235:SER:HB2	1:A:238:ARG:CB	2.45	0.46
1:A:63:ARG:HG2	4:A:619:HOH:O	2.16	0.45
1:A:33:ARG:NH1	1:A:34:GLN:OE1	2.48	0.45
1:A:356:THR:HG22	1:A:360:SER:OG	2.16	0.45
1:A:111:GLU:HB2	1:A:112:ALA:H	1.64	0.45
1:A:251:VAL:HG22	1:A:251:VAL:O	2.16	0.45
1:A:84:ARG:NH1	4:A:527:HOH:O	2.48	0.45
1:A:291:VAL:HG13	1:A:340:GLU:OE2	2.17	0.45
1:A:191:ASP:HB3	1:A:261:LEU:CD2	2.44	0.45
1:A:37:ASP:O	1:A:40:LEU:N	2.50	0.45
1:A:384:ASN:HA	1:A:388:LEU:HD13	1.98	0.45
1:A:144:ASP:CB	1:A:146:GLU:H	2.29	0.44
1:A:357:ASP:O	1:A:359:PHE:N	2.51	0.44
1:A:49:GLU:HB3	1:A:386:VAL:O	2.17	0.44
1:A:61:VAL:HG13	1:A:65:MET:HE2	1.98	0.44
1:A:301:LEU:HG	1:A:336:ILE:HD12	2.00	0.44
1:A:363:ILE:HA	1:A:363:ILE:HD13	1.69	0.44
1:A:181:TYR:OH	1:A:344:TRP:HB2	2.18	0.44
1:A:174:LEU:CD1	1:A:273:VAL:HB	2.47	0.44
1:A:19:GLN:NE2	1:A:19:GLN:CA	2.81	0.44
1:A:52:MET:HB2	1:A:303:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:MET:CA	1:A:52:MET:HE2	2.48	0.44
1:A:191:ASP:CB	1:A:218:ARG:NE	2.81	0.44
1:A:126:GLU:O	1:A:127:VAL:C	2.56	0.44
1:A:106:THR:O	1:A:110:MET:HG3	2.18	0.43
1:A:49:GLU:CB	1:A:386:VAL:O	2.65	0.43
1:A:211:CYS:HB3	1:A:221:TYR:HE1	1.82	0.43
1:A:57:ARG:NH1	1:A:62:ASP:HB3	2.34	0.43
1:A:143:ARG:C	1:A:146:GLU:HG2	2.38	0.43
1:A:170:PRO:O	1:A:173:ARG:N	2.41	0.43
1:A:392:GLU:HG3	1:A:393:ILE:N	2.30	0.43
1:A:189:LEU:N	1:A:220:ARG:HH11	2.16	0.43
1:A:13:SER:OG	1:A:302:ALA:HB1	2.19	0.43
1:A:220:ARG:HA	1:A:220:ARG:HD2	1.89	0.43
1:A:175:LYS:HD3	1:A:274:GLU:CG	2.48	0.43
1:A:380:THR:O	1:A:384:ASN:ND2	2.45	0.43
1:A:79:PHE:O	1:A:80:ALA:C	2.58	0.43
1:A:15:LEU:O	1:A:19:GLN:HB2	2.19	0.43
1:A:16:LEU:HD13	1:A:56:LEU:HD12	2.00	0.42
1:A:17:LEU:HD11	1:A:309:LEU:HG	2.01	0.42
1:A:312:LEU:CD2	1:A:328:TYR:HB2	2.44	0.42
1:A:52:MET:HA	1:A:52:MET:HE2	2.01	0.42
1:A:302:ALA:O	1:A:306:VAL:HB	2.19	0.42
1:A:17:LEU:O	1:A:21:LEU:HD22	2.20	0.42
1:A:269:ARG:HG2	1:A:270:SER:N	2.34	0.42
1:A:324:LEU:O	1:A:327:ARG:HG2	2.19	0.42
1:A:293:PRO:O	3:A:396:DHB:O3	2.37	0.42
1:A:204:HIS:HD2	1:A:206:ARG:HB2	1.84	0.42
1:A:309:LEU:HD12	1:A:309:LEU:O	2.18	0.42
1:A:244:LYS:HD3	1:A:251:VAL:O	2.19	0.42
1:A:7:ILE:HG21	1:A:30:ILE:HG13	2.01	0.42
1:A:39:VAL:HG22	1:A:110:MET:HE2	2.00	0.42
1:A:204:HIS:HD2	1:A:206:ARG:N	2.06	0.42
1:A:299:LEU:HA	1:A:299:LEU:HD12	1.86	0.42
1:A:136:ARG:HB3	4:A:495:HOH:O	2.19	0.42
1:A:113:ARG:HH11	1:A:113:ARG:HG3	1.84	0.42
1:A:57:ARG:HG3	4:A:494:HOH:O	2.18	0.42
1:A:71:VAL:HB	4:A:562:HOH:O	2.20	0.42
1:A:389:PRO:HD3	4:A:481:HOH:O	2.19	0.42
1:A:186:LEU:HA	1:A:265:ILE:O	2.20	0.42
1:A:233:ASP:O	1:A:238:ARG:NH1	2.52	0.42
1:A:218:ARG:HH21	1:A:261:LEU:HD23	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HD13	1:A:261:LEU:HA	1.61	0.42
1:A:247:LEU:HA	1:A:248:PRO:HD3	1.80	0.42
1:A:278:HIS:O	1:A:279:GLY:C	2.56	0.41
1:A:225:VAL:HA	1:A:226:PRO:HD3	1.90	0.41
1:A:214:ARG:CZ	4:A:533:HOH:O	2.69	0.41
1:A:28:ASN:OD1	1:A:113:ARG:NH2	2.49	0.41
1:A:357:ASP:C	1:A:359:PHE:N	2.74	0.41
1:A:77:ILE:HD13	1:A:201:TYR:CB	2.49	0.41
1:A:132:LEU:HD12	1:A:132:LEU:HA	1.81	0.41
1:A:232:GLU:HG3	1:A:233:ASP:N	2.34	0.41
1:A:175:LYS:N	1:A:274:GLU:O	2.53	0.41
1:A:32:GLU:HG2	1:A:122:TYR:CE1	2.55	0.41
1:A:314:LEU:HA	1:A:314:LEU:HD23	1.90	0.41
1:A:128:ARG:HD2	1:A:128:ARG:HH11	1.56	0.41
1:A:133:GLN:NE2	1:A:278:HIS:CE1	2.88	0.41
1:A:149:ARG:NH1	1:A:151:ASP:OD1	2.44	0.41
1:A:210:LEU:O	1:A:221:TYR:HA	2.21	0.41
1:A:289:HIS:O	1:A:290:ILE:HG12	2.20	0.41
1:A:84:ARG:HG3	1:A:84:ARG:NH1	2.36	0.41
1:A:79:PHE:O	1:A:79:PHE:CD1	2.74	0.41
1:A:76:GLU:OE1	1:A:83:ARG:HB3	2.21	0.41
1:A:42:ARG:NH2	2:A:395:FAD:O3B	2.54	0.41
1:A:57:ARG:C	1:A:59:ALA:H	2.25	0.41
1:A:141:PHE:CD2	1:A:141:PHE:N	2.89	0.41
1:A:204:HIS:CD2	1:A:206:ARG:HB2	2.55	0.40
1:A:111:GLU:HA	4:A:615:HOH:O	2.21	0.40
1:A:359:PHE:O	1:A:363:ILE:N	2.48	0.40
1:A:21:LEU:HA	1:A:21:LEU:HD12	1.93	0.40
1:A:251:VAL:H	1:A:251:VAL:HG12	1.43	0.40
1:A:285:GLY:C	1:A:287:ALA:N	2.75	0.40
1:A:1:MET:HB2	1:A:150:LEU:HD12	2.03	0.40
1:A:263:LYS:HE2	1:A:265:ILE:CG1	2.51	0.40
1:A:52:MET:HB2	1:A:52:MET:HE2	1.92	0.40
1:A:328:TYR:C	1:A:330:ALA:N	2.75	0.40
1:A:328:TYR:C	1:A:330:ALA:H	2.25	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)
1:A:1:MET:CE	1:A:192:THR:O[6_565]	1.96	0.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:O	1:A:57:ARG:NH2[3_556]	2.01	0.19
1:A:138:TYR:OH	1:A:228:THR:OG1[3_656]	2.08	0.12
1:A:1:MET:SD	1:A:192:THR:O[6_565]	2.09	0.11

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	392/394 (100%)	309 (79%)	59 (15%)	24 (6%)	2 1

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	VAL
1	A	146	GLU
1	A	192	THR
1	A	197	HIS
1	A	262	GLU
1	A	267	PRO
1	A	392	GLU
1	A	393	ILE
1	A	59	ALA
1	A	63	ARG
1	A	80	ALA
1	A	265	ILE
1	A	286	ASP
1	A	355	ASP
1	A	356	THR
1	A	358	ALA
1	A	170	PRO
1	A	248	PRO
1	A	391	GLU
1	A	144	ASP

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Mol	Chain	Res	Type
1	A	19	GLN
1	A	317	TYR
1	A	279	GLY
1	A	322	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	324/324 (100%)	218 (67%)	106 (33%)	0 0

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	4	GLN
1	A	13	SER
1	A	15	LEU
1	A	20	LEU
1	A	21	LEU
1	A	30	ILE
1	A	33	ARG
1	A	35	THR
1	A	36	PRO
1	A	37	ASP
1	A	38	TYR
1	A	43	ILE
1	A	44	ARG
1	A	48	LEU
1	A	50	GLN
1	A	52	MET
1	A	56	LEU
1	A	57	ARG
1	A	63	ARG
1	A	64	ARG
1	A	65	MET

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Mol	Chain	Res	Type
1	A	68	ASP
1	A	70	LEU
1	A	84	ARG
1	A	85	ARG
1	A	90	ARG
1	A	91	LEU
1	A	103	THR
1	A	104	GLU
1	A	105	VAL
1	A	126	GLU
1	A	129	LEU
1	A	132	LEU
1	A	136	ARG
1	A	139	VAL
1	A	140	THR
1	A	144	ASP
1	A	147	ARG
1	A	149	ARG
1	A	150	LEU
1	A	151	ASP
1	A	165	SER
1	A	167	GLN
1	A	168	SER
1	A	172	GLU
1	A	174	LEU
1	A	175	LYS
1	A	176	VAL
1	A	177	PHE
1	A	178	GLU
1	A	179	ARG
1	A	180	VAL
1	A	183	PHE
1	A	188	LEU
1	A	191	ASP
1	A	192	THR
1	A	195	VAL
1	A	197	HIS
1	A	199	LEU
1	A	214	ARG
1	A	218	ARG
1	A	224	GLN
1	A	225	VAL

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Mol	Chain	Res	Type
1	A	227	LEU
1	A	229	GLU
1	A	230	LYS
1	A	232	GLU
1	A	238	ARG
1	A	243	LEU
1	A	246	ARG
1	A	247	LEU
1	A	250	GLU
1	A	253	GLU
1	A	254	LYS
1	A	255	LEU
1	A	256	VAL
1	A	261	LEU
1	A	263	LYS
1	A	265	ILE
1	A	267	PRO
1	A	268	LEU
1	A	270	SER
1	A	271	PHE
1	A	272	VAL
1	A	273	VAL
1	A	281	LEU
1	A	283	LEU
1	A	291	VAL
1	A	297	LYS
1	A	305	ASP
1	A	306	VAL
1	A	312	LEU
1	A	326	GLU
1	A	341	ARG
1	A	344	TRP
1	A	352	ARG
1	A	361	GLN
1	A	362	ARG
1	A	363	ILE
1	A	365	GLN
1	A	367	GLU
1	A	378	LEU
1	A	381	ILE
1	A	390	TYR
1	A	393	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN

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

2 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	395	-	48,58,58	1.65	8 (16%)	54,89,89	2.32	13 (24%)
3	DHB	A	396	-	8,11,11	0.49	0	11,15,15	0.98	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	395	-	-	0/30/50/50	0/6/6/6
3	DHB	A	396	-	-	0/0/4/4	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	FAD	C4X-N5	-3.08	1.28	1.33
2	A	395	FAD	P-O2P	-2.66	1.43	1.54
2	A	395	FAD	C9A-N10	2.16	1.41	1.38
2	A	395	FAD	C2A-N1A	3.19	1.40	1.33
2	A	395	FAD	C5'-C4'	3.33	1.56	1.51
2	A	395	FAD	C1'-N10	3.59	1.52	1.48
2	A	395	FAD	C4-N3	4.21	1.40	1.33
2	A	395	FAD	C4-C4X	4.24	1.49	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	395	FAD	C4X-C4-N3	-6.25	115.05	123.59
2	A	395	FAD	N3A-C2A-N1A	-5.77	124.47	128.89
2	A	395	FAD	C6-C5X-N5	-2.87	115.27	118.96
2	A	395	FAD	O3P-PA-O5B	-2.74	95.66	102.94
2	A	395	FAD	C9-C9A-C5X	-2.51	115.16	119.62
2	A	395	FAD	O4'-C4'-C5'	-2.17	105.46	110.19
2	A	395	FAD	C4X-N5-C5X	2.48	119.61	116.76
2	A	395	FAD	O2P-P-O5'	2.54	121.26	108.46
2	A	395	FAD	C6-C5X-C9A	2.65	122.46	118.98
2	A	395	FAD	O3P-P-O5'	2.65	109.97	102.94
2	A	395	FAD	P-O3P-PA	2.80	140.58	132.73
2	A	395	FAD	C1'-C2'-C3'	2.86	117.99	109.82
2	A	395	FAD	C4-N3-C2	9.93	123.83	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	395	FAD	1	0
3	A	396	DHB	1	0

5.7 Other polymers (i)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.