



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:48 AM GMT

PDB ID : 2UUV
Title : ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE IN P1
Authors : Razeto, A.; Mattioli, F.; Carpanelli, E.; Aliverti, A.; Pandini, V.; Coda, A.;
Mattevi, A.
Deposited on : 2007-03-07
Resolution : 1.99 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 ⓘ 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 (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

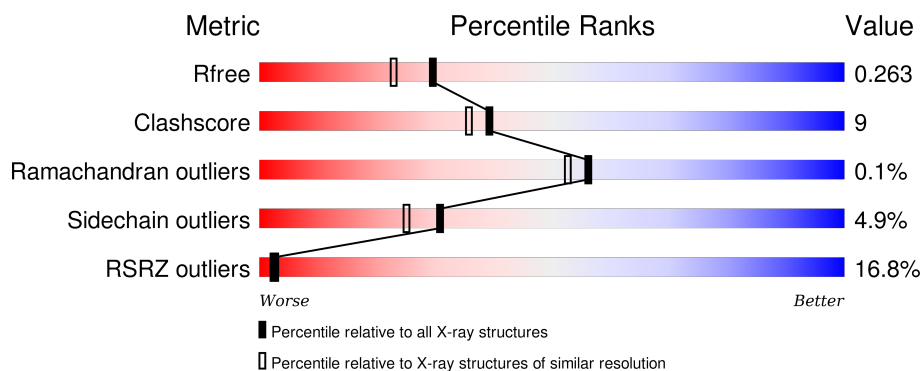
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	584	<div> <div>11%</div> <div>76%</div> <div>11%</div> <div>•</div> <div>10%</div> </div>
1	B	584	<div> <div>14%</div> <div>75%</div> <div>13%</div> <div>•</div> <div>10%</div> </div>
1	C	584	<div> <div>22%</div> <div>65%</div> <div>15%</div> <div>• •</div> <div>16%</div> </div>
1	D	584	<div> <div>11%</div> <div>74%</div> <div>15%</div> <div>•</div> <div>10%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PL3	D	1586	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17951 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 ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	1	0
			4200	2709	717	756	18			
1	B	523	Total	C	N	O	S	0	1	0
			4186	2695	718	755	18			
1	C	491	Total	C	N	O	S	0	2	0
			3947	2548	677	704	18			
1	D	528	Total	C	N	O	S	0	1	0
			4221	2722	719	762	18			

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



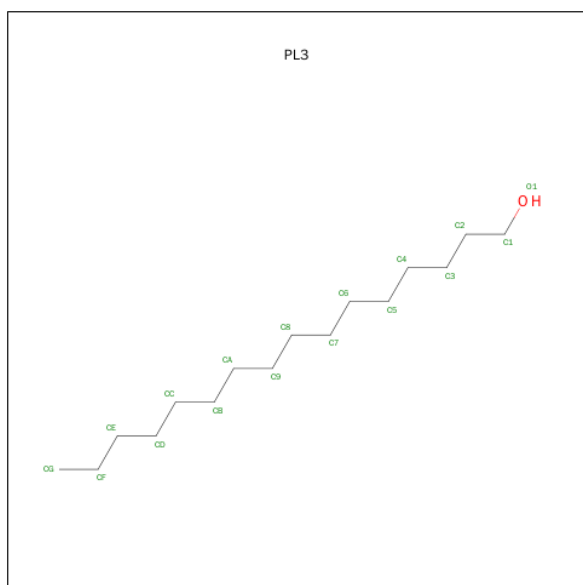
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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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 HEXADECAN-1-OL (three-letter code: PL3) (formula: C₁₆H₃₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	16	1		
3	B	1	Total	C	O	0	0
			17	16	1		
3	D	1	Total	C	O	0	0
			17	16	1		

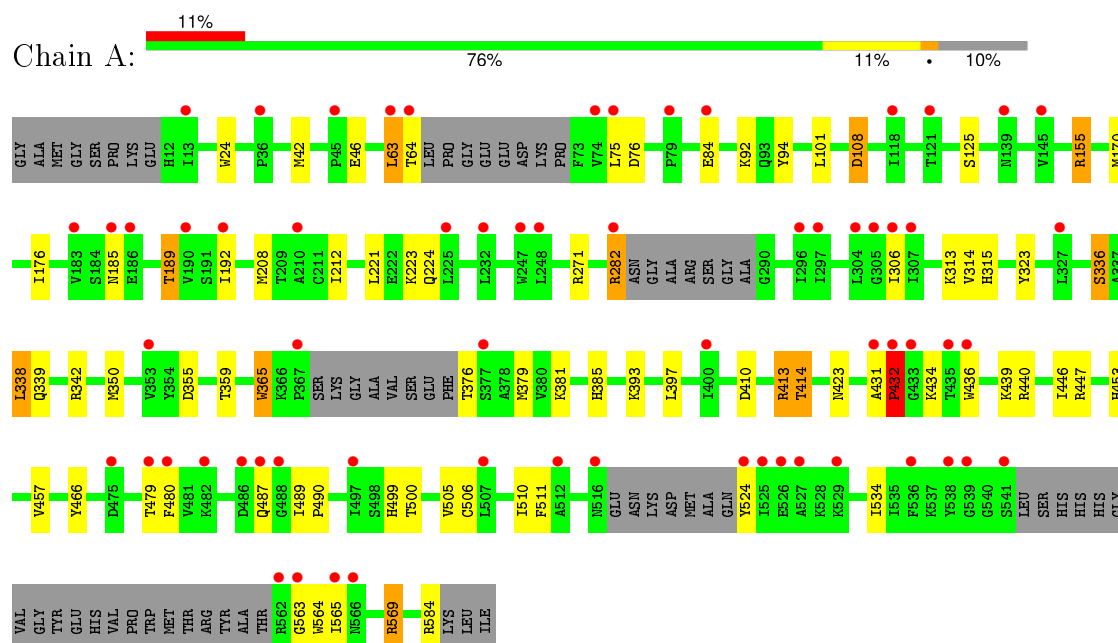
- Molecule 4 is water.

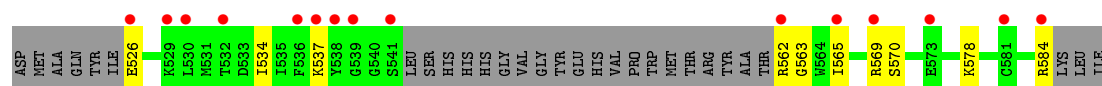
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		
4	B	265	Total	O	0	0
			265	265		
4	C	239	Total	O	0	0
			239	239		
4	D	312	Total	O	0	0
			312	312		

3 Residue-property plots [i](#)

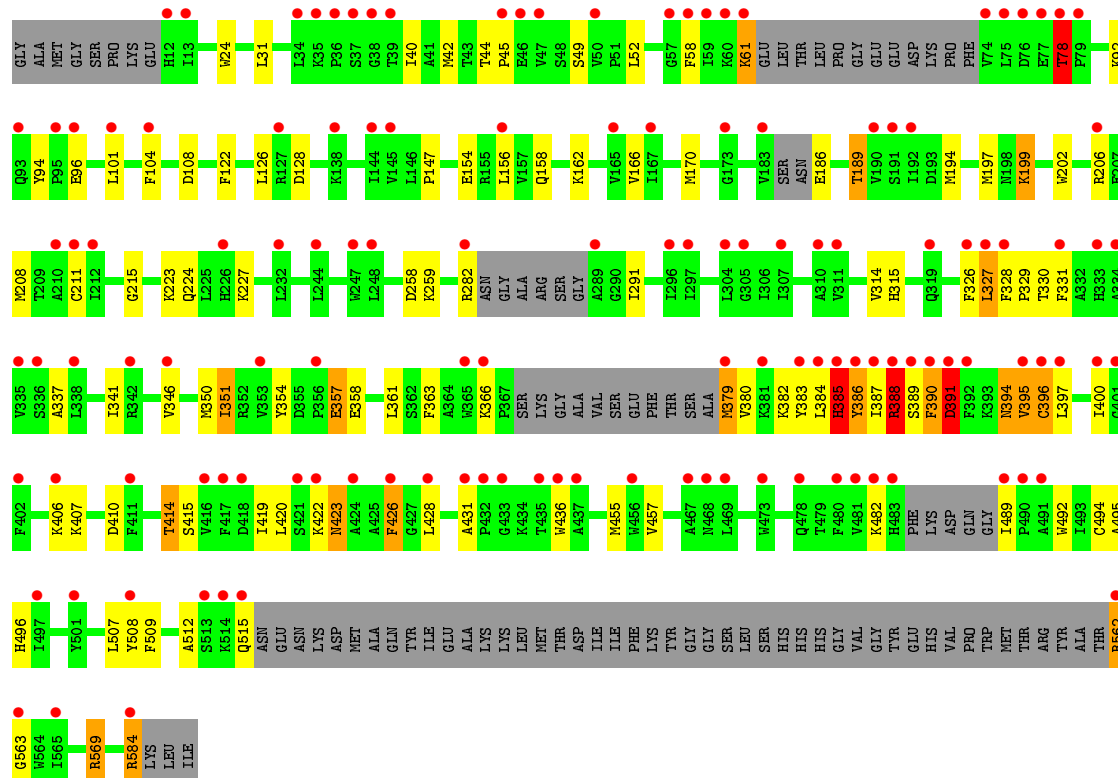
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE

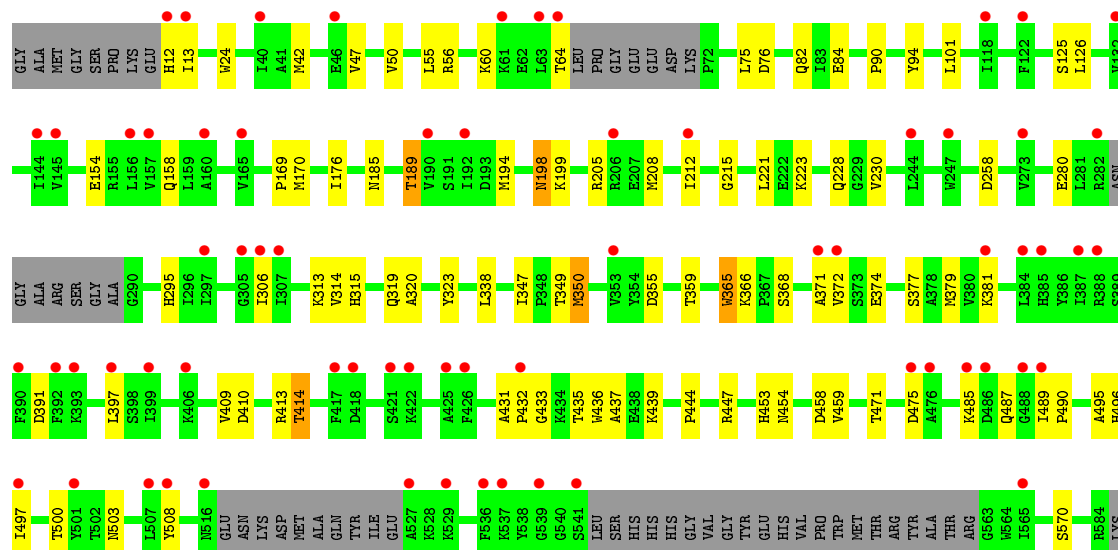
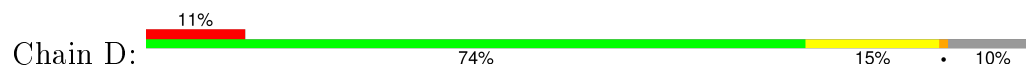




• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE



• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.80 Å 98.00 Å 107.00 Å 114.00° 93.00° 103.00°	Depositor
Resolution (Å)	19.98 – 1.99 19.98 – 1.99	Depositor EDS
% Data completeness (in resolution range)	92.7 (19.98-1.99) 80.5 (19.98-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 1.99 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.264 0.227 , 0.263	Depositor DCC
R_{free} test set	8878 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 176351 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17951	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PL3, 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	0.77	0/4308	0.76	3/5833 (0.1%)
1	B	0.75	1/4292 (0.0%)	0.77	4/5809 (0.1%)
1	C	1.33	37/4051 (0.9%)	0.96	17/5485 (0.3%)
1	D	0.75	0/4331	0.76	2/5865 (0.0%)
All	All	0.93	38/16982 (0.2%)	0.81	26/22992 (0.1%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	61	LYS	C-O	21.04	1.63	1.23
1	C	390	PHE	CG-CD1	17.50	1.65	1.38
1	C	395	VAL	CB-CG1	16.88	1.88	1.52
1	C	61	LYS	CD-CE	16.15	1.91	1.51
1	C	395	VAL	CB-CG2	14.70	1.83	1.52
1	C	384	LEU	C-N	14.51	1.67	1.34
1	C	426	PHE	C-N	13.89	1.58	1.33
1	C	327	LEU	C-O	13.23	1.48	1.23
1	C	390	PHE	CE1-CZ	12.68	1.61	1.37
1	C	388	ARG	C-O	11.48	1.45	1.23
1	C	388	ARG	CD-NE	11.26	1.65	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	THR	CB-OG1	10.98	1.65	1.43
1	C	396	CYS	C-N	9.94	1.56	1.34
1	C	391	ASP	CG-OD2	9.77	1.47	1.25
1	C	383	TYR	CG-CD2	9.48	1.51	1.39
1	C	382	LYS	C-N	8.93	1.54	1.34
1	C	391	ASP	CB-CG	8.68	1.70	1.51
1	C	389	SER	C-N	8.50	1.53	1.34
1	C	388	ARG	CZ-NH1	8.35	1.44	1.33
1	C	389	SER	CA-CB	8.20	1.65	1.52
1	C	426	PHE	C-O	8.09	1.38	1.23
1	C	390	PHE	C-O	-7.95	1.08	1.23
1	C	415	SER	CB-OG	7.75	1.52	1.42
1	C	387	ILE	CA-CB	7.63	1.72	1.54
1	C	391	ASP	N-CA	-7.48	1.31	1.46
1	C	61	LYS	CG-CD	7.12	1.76	1.52
1	C	423	ASN	CG-OD1	7.11	1.39	1.24
1	C	390	PHE	CE2-CZ	6.18	1.49	1.37
1	C	394	ASN	CG-OD1	5.99	1.37	1.24
1	C	422	LYS	C-N	5.96	1.47	1.34
1	C	390	PHE	CA-CB	5.84	1.66	1.53
1	C	383	TYR	CE1-CZ	5.82	1.46	1.38
1	C	384	LEU	C-O	5.66	1.34	1.23
1	C	389	SER	CB-OG	5.53	1.49	1.42
1	B	422	LYS	CD-CE	5.29	1.64	1.51
1	C	385	HIS	CD2-NE2	5.23	1.52	1.42
1	C	78	THR	CB-CG2	5.15	1.69	1.52
1	C	363	PHE	CG-CD2	5.11	1.46	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	389	SER	O-C-N	10.75	139.90	122.70
1	B	187	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	C	386	TYR	CB-CG-CD2	-8.38	115.97	121.00
1	C	389	SER	CA-C-N	-8.21	99.13	117.20
1	C	388	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	B	413	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	B	187	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	C	61	LYS	CG-CD-CE	-7.75	88.65	111.90
1	C	389	SER	C-N-CA	-6.86	104.56	121.70
1	C	395	VAL	CG1-CB-CG2	-6.74	100.12	110.90
1	D	413	ARG	NE-CZ-NH2	-6.39	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	396	CYS	CA-C-N	-6.33	103.27	117.20
1	C	385	HIS	CA-C-O	-6.29	106.89	120.10
1	C	387	ILE	CA-CB-CG1	6.25	122.87	111.00
1	C	61	LYS	CA-C-O	-6.23	107.01	120.10
1	C	61	LYS	CD-CE-NZ	-5.93	98.06	111.70
1	D	391	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	396	CYS	CA-C-O	5.74	132.15	120.10
1	B	413	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	432	PRO	N-CA-C	-5.70	97.28	112.10
1	A	413	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	391	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	A	63	LEU	CA-CB-CG	5.56	128.10	115.30
1	C	395	VAL	CA-CB-CG1	-5.31	102.93	110.90
1	C	390	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	C	386	TYR	CB-CG-CD1	5.15	124.09	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	431	ALA	Peptide
1	B	431	ALA	Peptide
1	C	391	ASP	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4200	0	4201	67	0
1	B	4186	0	4191	66	0
1	C	3947	0	3956	99	0
1	D	4221	0	4223	71	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	17	0	33	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	33	8	0
3	D	17	0	33	11	0
4	A	318	0	0	18	0
4	B	265	0	0	27	0
4	C	239	0	0	27	0
4	D	312	0	0	11	0
All	All	17951	0	16794	300	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 9.

All (300) 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:61:LYS:CD	1:C:61:LYS:CG	1.76	1.62
1:C:395:VAL:CB	1:C:395:VAL:CG2	1.83	1.56
1:C:61:LYS:CD	1:C:61:LYS:CE	1.91	1.49
1:C:395:VAL:CB	1:C:395:VAL:CG1	1.88	1.48
1:C:78:THR:OG1	1:C:78:THR:CB	1.65	1.40
1:A:506:CYS:SG	4:A:2280:HOH:O	1.91	1.26
1:B:224[B]:GLN:OE1	4:B:2129:HOH:O	1.59	1.15
1:C:390:PHE:C	1:C:391:ASP:N	2.03	1.10
1:A:365:TRP:HE1	1:A:446:ILE:CD1	1.64	1.09
1:A:365:TRP:HE1	1:A:446:ILE:HD11	1.16	1.09
1:A:365:TRP:NE1	1:A:446:ILE:HD11	1.70	1.05
1:B:224[B]:GLN:NE2	4:B:2127:HOH:O	1.87	1.05
1:D:126:LEU:H	3:D:1586:PL3:H3C2	1.17	1.03
1:C:584:ARG:HG3	1:C:584:ARG:HH11	1.24	1.01
1:C:330:THR:HB	4:C:2166:HOH:O	1.62	0.99
1:A:342:ARG:HD3	4:A:2223:HOH:O	1.62	0.99
1:D:125:SER:HB2	3:D:1586:PL3:H1C2	1.44	0.98
1:C:330:THR:HG21	4:C:2165:HOH:O	1.64	0.96
1:C:431:ALA:H	1:C:436:TRP:HE1	1.16	0.92
3:B:1586:PL3:H2C2	4:B:2244:HOH:O	1.73	0.87
1:A:410:ASP:O	1:A:414:THR:HG23	1.75	0.87
1:B:338:LEU:HG	1:B:500:THR:HG21	1.58	0.85
1:A:338:LEU:HG	1:A:500:THR:HG21	1.57	0.84
1:C:385:HIS:O	1:C:388:ARG:HB2	1.78	0.83
1:D:366:LYS:HD2	1:D:372:VAL:O	1.78	0.83
1:C:61:LYS:CE	1:C:61:LYS:CG	2.57	0.82
1:B:139:ASN:HB3	4:B:2044:HOH:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:LEU:N	3:D:1586:PL3:H3C2	1.95	0.81
1:D:126:LEU:H	3:D:1586:PL3:C3	1.92	0.80
1:B:264:GLU:HG3	4:B:2063:HOH:O	1.81	0.80
1:D:410:ASP:O	1:D:414:THR:HG23	1.81	0.80
1:C:61:LYS:CB	1:C:61:LYS:CD	2.62	0.78
1:B:563:GLY:HA2	4:B:2250:HOH:O	1.83	0.78
1:A:563:GLY:HA2	4:A:2302:HOH:O	1.84	0.77
1:A:569:ARG:HH11	1:A:569:ARG:HB3	1.46	0.77
1:C:224:GLN:HG3	4:C:2083:HOH:O	1.85	0.77
1:D:338:LEU:HG	1:D:500:THR:HG21	1.67	0.77
1:A:208:MET:HE3	1:A:314:VAL:HG23	1.65	0.76
1:D:323:TYR:CE1	1:D:433:GLY:HA2	2.21	0.76
1:A:125:SER:HA	3:A:1586:PL3:H1C1	1.67	0.76
1:C:92:LYS:HE3	4:C:2073:HOH:O	1.85	0.75
1:D:199:LYS:HG2	4:D:2081:HOH:O	1.86	0.75
1:D:189:THR:HG21	4:D:2150:HOH:O	1.85	0.75
1:A:569:ARG:CB	1:A:569:ARG:HH11	2.00	0.74
1:C:258:ASP:HB2	4:C:2117:HOH:O	1.88	0.74
1:C:410:ASP:O	1:C:414:THR:HG23	1.88	0.73
1:A:410:ASP:O	1:A:414:THR:CG2	2.37	0.72
1:D:349:THR:O	4:D:2251:HOH:O	2.05	0.72
1:D:508:TYR:HB2	4:D:2284:HOH:O	1.90	0.71
1:C:224:GLN:OE1	1:C:227:LYS:HE2	1.90	0.71
1:C:395:VAL:CG1	1:C:395:VAL:CA	2.70	0.70
1:A:84:GLU:HB2	4:A:2042:HOH:O	1.91	0.69
1:B:365:TRP:O	1:B:365:TRP:CD1	2.46	0.69
1:A:189:THR:HG21	4:A:2117:HOH:O	1.93	0.69
1:A:176:ILE:HG21	3:A:1586:PL3:H3C1	1.75	0.69
1:B:379:MET:SD	1:B:436:TRP:CZ2	2.86	0.68
1:C:351:ILE:HD12	1:C:400:ILE:HG12	1.75	0.68
1:A:393:LYS:HD2	4:A:2245:HOH:O	1.94	0.68
1:B:139:ASN:HB2	4:B:2099:HOH:O	1.95	0.67
1:D:377:SER:O	1:D:381:LYS:HG2	1.95	0.66
1:B:228:GLN:HG3	4:B:2131:HOH:O	1.94	0.66
1:B:439:LYS:HG2	4:B:2217:HOH:O	1.97	0.65
1:B:212:ILE:HD13	1:B:221:LEU:HD11	1.78	0.65
1:C:395:VAL:CA	1:C:395:VAL:CG2	2.72	0.65
1:B:365:TRP:CZ3	1:B:446:ILE:HD11	2.33	0.64
1:B:562:ARG:HD2	4:B:2251:HOH:O	1.97	0.64
1:A:208:MET:HE2	1:A:315:HIS:HA	1.78	0.64
1:C:426:PHE:N	4:C:2201:HOH:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:LYS:HG3	1:B:537:LYS:O	1.97	0.64
1:B:189:THR:HG21	4:B:2098:HOH:O	1.97	0.64
1:D:487:GLN:HE21	1:D:489:ILE:HD12	1.62	0.64
1:C:208:MET:HE2	1:C:315:HIS:HA	1.80	0.64
1:A:569:ARG:NH1	1:A:569:ARG:HB3	2.12	0.63
1:A:365:TRP:HE1	1:A:446:ILE:HD13	1.61	0.63
1:C:584:ARG:HH11	1:C:584:ARG:CG	2.08	0.63
1:D:368:SER:HB2	1:D:377:SER:HA	1.80	0.63
1:A:92:LYS:HE3	1:A:185:ASN:O	1.99	0.62
1:C:78:THR:HG1	1:C:78:THR:CB	2.08	0.62
1:B:220:GLU:HG3	1:B:224[B]:GLN:HE21	1.62	0.62
1:D:379:MET:HE1	1:D:431:ALA:HA	1.81	0.62
1:B:414:THR:HG22	4:B:2206:HOH:O	1.98	0.62
1:D:205:ARG:HH12	1:D:228:GLN:HB3	1.64	0.62
1:C:496:HIS:CE1	1:C:508:TYR:CD1	2.88	0.62
1:A:499:HIS:CE1	4:A:2163:HOH:O	2.53	0.62
1:C:328:PHE:CD1	4:C:2200:HOH:O	2.51	0.62
1:C:104:PHE:HB3	4:C:2032:HOH:O	1.99	0.61
1:A:192:ILE:HD12	1:A:306:ILE:HD11	1.81	0.61
1:D:60:LYS:O	1:D:64:THR:HG23	2.00	0.61
1:B:365:TRP:CZ3	1:B:446:ILE:CD1	2.84	0.61
1:D:50:VAL:HG11	1:D:372:VAL:HB	1.83	0.61
1:B:63:LEU:CD1	3:B:1586:PL3:HGC1	2.31	0.60
1:A:510:ILE:HG21	3:A:1586:PL3:HAC1	1.84	0.60
1:C:584:ARG:NH1	1:C:584:ARG:HG3	2.04	0.60
1:C:61:LYS:CD	1:C:61:LYS:NZ	2.65	0.60
1:B:92:LYS:HE3	1:B:185:ASN:O	2.00	0.60
1:B:463:THR:HG22	4:B:2237:HOH:O	2.01	0.60
1:C:330:THR:HG22	1:C:331:PHE:H	1.66	0.59
1:B:63:LEU:HD11	3:B:1586:PL3:CG	2.32	0.58
1:B:365:TRP:O	1:B:365:TRP:HD1	1.86	0.58
1:B:410:ASP:O	1:B:414:THR:HG23	2.03	0.58
1:B:63:LEU:HD11	3:B:1586:PL3:HGC1	1.85	0.58
1:D:447:ARG:NH1	3:D:1586:PL3:H5C2	2.19	0.58
1:B:63:LEU:CD1	3:B:1586:PL3:CG	2.81	0.58
1:A:212:ILE:HD13	1:A:221:LEU:HD11	1.86	0.57
1:D:24:TRP:CZ3	2:D:1585:FAD:HM83	2.39	0.57
1:C:208:MET:HE3	1:C:314:VAL:HG23	1.86	0.57
1:A:192:ILE:HD12	1:A:306:ILE:CD1	2.34	0.57
1:A:365:TRP:NE1	1:A:446:ILE:CD1	2.42	0.57
1:C:431:ALA:N	1:C:436:TRP:HE1	1.95	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:LEU:HD21	1:C:428:LEU:HD11	1.87	0.56
1:D:82:GLN:HB3	1:D:84:GLU:OE2	2.05	0.56
1:B:351:ILE:HD12	1:B:400:ILE:HG12	1.88	0.56
1:C:96:GLU:N	1:C:96:GLU:OE1	2.33	0.56
1:B:466:TYR:OH	4:B:2231:HOH:O	2.18	0.56
1:C:126:LEU:HB2	4:C:2209:HOH:O	2.06	0.56
1:B:198:ASN:H	1:B:198:ASN:HD22	1.54	0.55
1:C:391:ASP:O	1:C:395:VAL:HG23	2.05	0.55
1:D:439:LYS:HD2	4:D:2261:HOH:O	2.07	0.55
1:C:395:VAL:CG1	1:C:395:VAL:CG2	2.85	0.55
1:A:208:MET:O	1:A:313:LYS:HE2	2.07	0.54
1:D:458:ASP:OD2	3:D:1586:PL3:H2C1	2.07	0.54
1:B:562:ARG:HG2	4:B:2254:HOH:O	2.06	0.54
1:D:12:HIS:CE1	4:D:2001:HOH:O	2.61	0.54
1:B:220:GLU:HG3	1:B:224[B]:GLN:NE2	2.23	0.53
1:B:350:MET:HE3	4:B:2146:HOH:O	2.07	0.53
1:B:82:GLN:HG2	4:B:2041:HOH:O	2.09	0.53
1:B:562:ARG:HB2	4:B:2249:HOH:O	2.08	0.53
1:D:56:ARG:HB2	4:D:2051:HOH:O	2.09	0.53
1:D:379:MET:CE	1:D:431:ALA:HA	2.39	0.53
1:C:419:ILE:O	1:C:423:ASN:ND2	2.42	0.53
1:C:58:PHE:HZ	4:C:2177:HOH:O	1.90	0.52
1:D:350:MET:HB3	1:D:436:TRP:CH2	2.44	0.52
1:D:198:ASN:H	1:D:198:ASN:HD22	1.55	0.52
1:C:330:THR:HG23	1:C:394:ASN:HB3	1.92	0.52
1:A:155:ARG:O	1:A:155:ARG:HD3	2.10	0.52
1:B:450:LEU:HD11	3:B:1586:PL3:HCC1	1.91	0.52
1:D:319:GLN:HA	1:D:319:GLN:OE1	2.08	0.52
1:C:259:LYS:N	4:C:2117:HOH:O	2.43	0.52
1:C:166:VAL:HB	1:C:189:THR:HB	1.91	0.51
1:D:176:ILE:HG21	3:D:1586:PL3:H5C1	1.92	0.51
1:D:208:MET:HE2	1:D:315:HIS:HA	1.92	0.51
1:C:329:PRO:HD3	4:C:2200:HOH:O	2.10	0.51
1:A:479:THR:HG21	1:A:534:ILE:HD11	1.92	0.51
1:B:496:HIS:CE1	1:B:508:TYR:CD1	2.99	0.51
1:B:271:ARG:HD2	4:B:2178:HOH:O	2.10	0.50
1:A:76:ASP:O	1:A:453:HIS:HA	2.11	0.50
1:C:224:GLN:HG3	4:C:2099:HOH:O	2.11	0.50
1:C:223:LYS:HE3	1:C:224:GLN:NE2	2.26	0.50
1:C:327:LEU:HB3	1:C:395:VAL:CG1	2.42	0.50
1:A:42:MET:CE	1:A:365:TRP:HH2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:PHE:HB3	4:C:2201:HOH:O	2.10	0.50
1:D:379:MET:HE1	1:D:432:PRO:HD2	1.94	0.50
1:A:385:HIS:HE1	4:C:2159:HOH:O	1.94	0.50
1:B:410:ASP:OD1	1:B:413:ARG:NH2	2.45	0.50
1:C:563:GLY:HA2	4:C:2224:HOH:O	2.12	0.49
1:B:379:MET:SD	1:B:436:TRP:HZ2	2.35	0.49
1:B:146:LEU:HD23	4:B:2107:HOH:O	2.11	0.49
1:B:537:LYS:CG	1:B:537:LYS:O	2.60	0.49
1:C:455:MET:N	1:C:515:GLN:HE21	2.09	0.49
1:C:328:PHE:HA	4:C:2200:HOH:O	2.11	0.49
1:A:223:LYS:NZ	1:A:224[B]:GLN:NE2	2.61	0.49
1:C:457:VAL:HG23	1:C:512:ALA:HB2	1.94	0.48
1:C:52:LEU:O	4:C:2015:HOH:O	2.20	0.48
1:C:354:TYR:HD1	1:C:358:GLU:HG2	1.77	0.48
1:C:108:ASP:HA	4:C:2037:HOH:O	2.13	0.48
1:D:55:LEU:HD13	1:D:365:TRP:HB2	1.95	0.48
1:B:562:ARG:CG	4:B:2254:HOH:O	2.60	0.48
1:C:357:GLU:HB2	1:C:494:CYS:HB3	1.95	0.48
1:A:24:TRP:CZ3	2:A:1585:FAD:HM83	2.48	0.48
1:A:499:HIS:HB2	1:A:506:CYS:HB3	1.96	0.48
1:B:506:CYS:HB2	4:B:2237:HOH:O	2.12	0.48
1:B:154:GLU:HA	1:B:273:VAL:HG11	1.96	0.48
1:D:350:MET:HB3	1:D:436:TRP:CZ2	2.49	0.48
1:B:111:LYS:NZ	4:B:2056:HOH:O	2.44	0.47
1:C:194:MET:HE3	1:C:197[B]:MET:HE3	1.96	0.47
1:D:359:THR:HG23	1:D:397:LEU:HB2	1.96	0.47
1:A:379:MET:HE1	4:A:2262:HOH:O	2.13	0.47
1:C:337:ALA:O	1:C:341:ILE:HG13	2.15	0.47
1:C:361:LEU:HB2	4:C:2177:HOH:O	2.14	0.47
1:C:354:TYR:CD1	1:C:358:GLU:HG2	2.50	0.47
1:A:379:MET:SD	1:A:436:TRP:CZ2	3.07	0.47
1:D:320:ALA:HB3	1:D:409:VAL:HG21	1.97	0.47
1:B:228:GLN:CG	4:B:2131:HOH:O	2.60	0.47
1:D:212:ILE:HD13	1:D:221:LEU:HD11	1.96	0.47
1:B:12:HIS:N	4:B:2001:HOH:O	2.48	0.47
1:D:323:TYR:HE2	1:D:350:MET:SD	2.38	0.47
1:D:154:GLU:O	1:D:158:GLN:HG3	2.15	0.47
1:C:330:THR:HG22	1:C:331:PHE:N	2.28	0.47
1:C:386:TYR:HE2	4:C:2063:HOH:O	1.98	0.46
1:C:101:LEU:HD11	1:C:156:LEU:HD13	1.98	0.46
1:B:328:PHE:CE1	1:B:425:ALA:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:MET:HE2	1:C:436:TRP:CZ3	2.49	0.46
1:C:31:LEU:HG	1:C:42:MET:CE	2.46	0.46
1:A:92:LYS:CE	1:A:185:ASN:O	2.63	0.46
1:B:76:ASP:O	1:B:453:HIS:HA	2.15	0.46
1:D:374:GLU:OE2	1:D:439:LYS:HA	2.15	0.46
1:D:208:MET:HE3	1:D:314:VAL:HG23	1.98	0.46
1:C:366:LYS:HD3	1:C:380:VAL:HG11	1.97	0.46
1:A:155:ARG:C	1:A:155:ARG:HD3	2.36	0.46
1:C:569:ARG:HA	4:C:2228:HOH:O	2.16	0.46
1:A:359:THR:HG23	1:A:397:LEU:HB2	1.98	0.46
1:A:271:ARG:HD2	4:A:2198:HOH:O	2.17	0.45
1:C:154:GLU:O	1:C:158:GLN:HG3	2.16	0.45
1:C:354:TYR:O	1:C:396:CYS:HB3	2.16	0.45
1:D:444:PRO:HA	3:D:1586:PL3:HAC1	1.98	0.45
1:B:143:LEU:C	1:B:144:ILE:HD12	2.37	0.45
1:B:480:PHE:CZ	1:B:511:PHE:HB2	2.52	0.45
1:D:169:PRO:HG3	1:D:306:ILE:HD12	1.99	0.45
1:C:202:TRP:CE2	1:C:211:CYS:HB2	2.52	0.45
1:D:12:HIS:HE1	4:D:2001:HOH:O	1.99	0.45
1:A:339:GLN:HG3	1:A:466:TYR:CZ	2.51	0.44
1:A:499:HIS:HE1	4:A:2163:HOH:O	1.95	0.44
1:B:231:SER:HB3	1:B:315:HIS:CE1	2.52	0.44
1:D:76:ASP:HB2	1:D:454:ASN:HB2	2.00	0.44
1:D:459:VAL:CG2	3:D:1586:PL3:H6C1	2.48	0.44
1:B:63:LEU:CD1	3:B:1586:PL3:HGC2	2.47	0.44
1:D:84:GLU:H	1:D:84:GLU:CD	2.21	0.44
1:C:194:MET:O	1:C:215:GLY:HA3	2.17	0.44
1:A:564:TRP:CH2	1:B:279:LEU:HD13	2.53	0.44
1:C:492:TRP:HZ2	4:C:2177:HOH:O	2.01	0.44
1:D:258:ASP:HB2	4:D:2251:HOH:O	2.17	0.44
1:C:327:LEU:HB3	1:C:395:VAL:HG12	2.00	0.43
1:C:326:PHE:HD2	1:C:400:ILE:HD12	1.83	0.43
1:D:496:HIS:CE1	1:D:508:TYR:CD1	3.06	0.43
1:C:24:TRP:CZ3	2:C:1585:FAD:HM83	2.52	0.43
1:A:439:LYS:HE3	4:A:2268:HOH:O	2.19	0.43
1:C:31:LEU:CD2	1:C:42:MET:HE2	2.48	0.43
1:B:212:ILE:HD13	1:B:221:LEU:CD1	2.48	0.43
1:D:205:ARG:NH1	1:D:228:GLN:HB3	2.30	0.43
1:A:480:PHE:CZ	1:A:511:PHE:HB2	2.53	0.43
1:A:223:LYS:HZ2	1:A:224[B]:GLN:NE2	2.16	0.43
1:C:122:PHE:HB3	1:C:128:ASP:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:THR:HB	1:C:45:PRO:HD2	2.01	0.43
1:A:223:LYS:NZ	1:A:224[B]:GLN:HE21	2.16	0.43
1:A:315:HIS:HB3	4:A:2204:HOH:O	2.19	0.43
1:D:435:THR:O	1:D:439:LYS:HD3	2.19	0.43
1:A:108:ASP:HB2	4:A:2126:HOH:O	2.18	0.43
1:C:562:ARG:N	1:D:280:GLU:H	2.16	0.43
1:C:379:MET:HB2	1:C:428:LEU:HB3	2.00	0.43
1:D:447:ARG:HH12	3:D:1586:PL3:H5C2	1.83	0.42
1:B:63:LEU:HD12	3:B:1586:PL3:HGC2	2.01	0.42
1:D:323:TYR:CD1	1:D:433:GLY:HA2	2.54	0.42
1:B:198:ASN:N	1:B:198:ASN:HD22	2.15	0.42
1:A:432:PRO:O	1:A:432:PRO:CD	2.66	0.42
1:D:350:MET:HG2	1:D:436:TRP:CE2	2.53	0.42
1:D:208:MET:HE1	1:D:230:VAL:HG12	2.01	0.42
1:C:147:PRO:HG2	1:C:197[B]:MET:HE1	1.99	0.42
1:C:194:MET:CE	1:C:197[B]:MET:HE3	2.49	0.42
1:C:31:LEU:HG	1:C:42:MET:HE2	2.01	0.42
1:C:199:LYS:HD2	4:C:2081:HOH:O	2.20	0.42
1:B:24:TRP:CZ3	2:B:1585:FAD:HM83	2.54	0.42
1:A:489:ILE:HB	4:A:2288:HOH:O	2.19	0.42
1:A:432:PRO:O	1:A:432:PRO:HD2	2.18	0.42
1:A:500:THR:HG22	1:A:505:VAL:HG12	2.01	0.42
4:A:2242:HOH:O	1:C:282:ARG:HD2	2.20	0.42
1:B:13:ILE:HG22	1:B:18:GLN:HG3	2.02	0.42
1:A:42:MET:HE2	1:A:365:TRP:HH2	1.85	0.42
1:C:495:ALA:HA	1:C:508:TYR:O	2.20	0.42
1:B:208:MET:HE2	1:B:315:HIS:HA	2.01	0.42
1:B:186:GLU:OE1	1:B:187:ARG:HD2	2.19	0.42
1:C:291[A]:ILE:HG23	1:D:295:HIS:O	2.20	0.42
1:D:205:ARG:NH1	1:D:228:GLN:O	2.51	0.41
1:A:379:MET:CE	4:A:2262:HOH:O	2.67	0.41
1:A:376:THR:HG21	4:A:2037:HOH:O	2.20	0.41
1:C:78:THR:OG1	1:C:78:THR:CG2	2.60	0.41
1:C:326:PHE:CD2	1:C:400:ILE:HD12	2.54	0.41
1:C:326:PHE:CE2	1:C:420:LEU:HD13	2.55	0.41
1:C:326:PHE:O	1:C:397:LEU:HD12	2.20	0.41
1:D:489:ILE:HA	1:D:490:PRO:HD3	1.94	0.41
1:D:76:ASP:O	1:D:453:HIS:HA	2.20	0.41
1:A:489:ILE:HD12	4:A:2288:HOH:O	2.20	0.41
1:B:365:TRP:CZ3	1:B:446:ILE:HG12	2.56	0.41
1:C:194:MET:CE	1:C:197[B]:MET:CE	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:MET:SD	1:A:436:TRP:HZ2	2.43	0.41
1:D:47:VAL:HG21	1:D:371:ALA:CB	2.50	0.41
1:A:323:TYR:CE1	1:A:434:LYS:HG2	2.56	0.41
1:C:507:LEU:HD21	1:C:509:PHE:CZ	2.55	0.41
1:D:223:LYS:HD3	4:D:2171:HOH:O	2.20	0.41
1:A:410:ASP:OD1	1:A:413:ARG:NH2	2.51	0.41
1:D:495:ALA:HA	1:D:508:TYR:O	2.20	0.41
1:B:495:ALA:HA	1:B:508:TYR:O	2.20	0.41
1:A:379:MET:CE	1:A:379:MET:HA	2.50	0.41
1:A:282:ARG:HD2	4:B:2252:HOH:O	2.20	0.41
1:D:125:SER:HA	3:D:1586:PL3:H3C1	2.02	0.41
1:C:407:LYS:HG3	4:C:2164:HOH:O	2.19	0.41
1:D:471:THR:O	1:D:475:ASP:HB2	2.19	0.41
1:C:208:MET:CE	1:C:315:HIS:CA	2.99	0.41
1:C:40:ILE:HG22	1:C:52:LEU:HD12	2.02	0.41
1:C:282:ARG:C	4:C:2143:HOH:O	2.59	0.41
1:D:487:GLN:NE2	1:D:489:ILE:HD12	2.32	0.41
1:B:187:ARG:NH2	1:B:578:LYS:O	2.54	0.40
1:B:304:LEU:HA	4:B:2176:HOH:O	2.20	0.40
1:D:194:MET:O	1:D:215:GLY:HA3	2.21	0.40
1:D:338:LEU:HD21	1:D:497:ILE:HG21	2.02	0.40
1:C:206:ARG:O	1:D:503:ASN:HB2	2.21	0.40
1:D:185:ASN:ND2	4:D:2153:HOH:O	2.51	0.40
1:A:336:SER:HB3	1:A:423:ASN:OD1	2.21	0.40
1:A:447:ARG:HG3	1:A:457:VAL:CG1	2.51	0.40
1:A:63:LEU:HA	1:A:490:PRO:HB3	2.02	0.40
1:C:162:LYS:NZ	4:C:2031:HOH:O	2.54	0.40

There are no symmetry-related clashes.

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	512/584 (88%)	503 (98%)	8 (2%)	1 (0%)	52	48
1	B	512/584 (88%)	502 (98%)	9 (2%)	1 (0%)	52	48
1	C	477/584 (82%)	462 (97%)	15 (3%)	0	100	100
1	D	519/584 (89%)	511 (98%)	7 (1%)	1 (0%)	52	48
All	All	2020/2336 (86%)	1978 (98%)	39 (2%)	3 (0%)	56	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	437	ALA
1	A	432	PRO
1	B	432	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	460/507 (91%)	437 (95%)	23 (5%)	30	24
1	B	458/507 (90%)	431 (94%)	27 (6%)	24	18
1	C	433/507 (85%)	412 (95%)	21 (5%)	31	26
1	D	463/507 (91%)	446 (96%)	17 (4%)	41	38
All	All	1814/2028 (89%)	1726 (95%)	88 (5%)	31	25

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	64	THR
1	A	75	LEU
1	A	94	TYR
1	A	101	LEU
1	A	108	ASP
1	A	155	ARG
1	A	170	MET

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Mol	Chain	Res	Type
1	A	189	THR
1	A	282	ARG
1	A	336	SER
1	A	338	LEU
1	A	350	MET
1	A	355	ASP
1	A	365	TRP
1	A	381	LYS
1	A	414	THR
1	A	440	ARG
1	A	487	GLN
1	A	524	TYR
1	A	565	ILE
1	A	569	ARG
1	A	584	ARG
1	B	75	LEU
1	B	94	TYR
1	B	101	LEU
1	B	170	MET
1	B	186	GLU
1	B	189	THR
1	B	198	ASN
1	B	217	MET
1	B	291	ILE
1	B	319	GLN
1	B	336	SER
1	B	338	LEU
1	B	346	VAL
1	B	350	MET
1	B	355	ASP
1	B	366	LYS
1	B	377	SER
1	B	389	SER
1	B	435	THR
1	B	436	TRP
1	B	440	ARG
1	B	526	GLU
1	B	534	ILE
1	B	565	ILE
1	B	569	ARG
1	B	570	SER
1	B	584	ARG

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Mol	Chain	Res	Type
1	C	49	SER
1	C	78	THR
1	C	94	TYR
1	C	170	MET
1	C	186	GLU
1	C	189	THR
1	C	199	LYS
1	C	346	VAL
1	C	350	MET
1	C	351	ILE
1	C	357	GLU
1	C	379	MET
1	C	385	HIS
1	C	388	ARG
1	C	406	LYS
1	C	414	THR
1	C	482	LYS
1	C	489	ILE
1	C	562	ARG
1	C	569	ARG
1	C	584	ARG
1	D	13	ILE
1	D	42	MET
1	D	75	LEU
1	D	90	PRO
1	D	94	TYR
1	D	101	LEU
1	D	170	MET
1	D	189	THR
1	D	198	ASN
1	D	313	LYS
1	D	347	ILE
1	D	350	MET
1	D	355	ASP
1	D	365	TRP
1	D	414	THR
1	D	485	LYS
1	D	570	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	136	GLN
1	A	139	ASN
1	A	185	ASN
1	A	256	GLN
1	A	412	HIS
1	B	198	ASN
1	B	315	HIS
1	B	453	HIS
1	C	82	GLN
1	C	85	ASN
1	C	93	GLN
1	C	255	HIS
1	C	315	HIS
1	C	340	GLN
1	C	423	ASN
1	C	499	HIS
1	C	515	GLN
1	D	82	GLN
1	D	198	ASN
1	D	256	GLN
1	D	315	HIS
1	D	412	HIS
1	D	468	ASN
1	D	487	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](#)

7 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	1585	-	48,58,58	1.44	6 (12%)	54,89,89	2.05	11 (20%)
3	PL3	A	1586	-	16,16,16	0.83	1 (6%)	15,15,15	0.84	1 (6%)
2	FAD	B	1585	-	48,58,58	1.29	7 (14%)	54,89,89	2.34	10 (18%)
3	PL3	B	1586	-	16,16,16	0.89	1 (6%)	15,15,15	0.70	0
2	FAD	C	1585	-	48,58,58	1.14	3 (6%)	54,89,89	2.28	10 (18%)
2	FAD	D	1585	-	48,58,58	1.30	5 (10%)	54,89,89	2.49	12 (22%)
3	PL3	D	1586	-	16,16,16	0.94	1 (6%)	15,15,15	0.74	1 (6%)

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	1585	-	-	0/30/50/50	0/6/6/6
3	PL3	A	1586	-	-	0/14/14/14	0/0/0/0
2	FAD	B	1585	-	-	0/30/50/50	0/6/6/6
3	PL3	B	1586	-	-	0/14/14/14	0/0/0/0
2	FAD	C	1585	-	-	0/30/50/50	0/6/6/6
2	FAD	D	1585	-	-	0/30/50/50	0/6/6/6
3	PL3	D	1586	-	-	0/14/14/14	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1586	PL3	O1-C1	-3.39	1.23	1.42
3	D	1586	PL3	O1-C1	-3.35	1.23	1.42
3	A	1586	PL3	O1-C1	-3.09	1.25	1.42
2	A	1585	FAD	C6-C5X	-2.38	1.38	1.41
2	B	1585	FAD	C5X-N5	2.01	1.38	1.35
2	B	1585	FAD	C5'-C4'	2.01	1.54	1.51
2	C	1585	FAD	C1'-N10	2.10	1.50	1.48
2	D	1585	FAD	C4X-N5	2.16	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1585	FAD	C2A-N1A	2.16	1.38	1.33
2	B	1585	FAD	C4-N3	2.21	1.37	1.33
2	A	1585	FAD	C2A-N3A	2.31	1.36	1.32
2	A	1585	FAD	C4-N3	2.49	1.37	1.33
2	B	1585	FAD	C2A-N3A	2.56	1.36	1.32
2	D	1585	FAD	C5X-N5	2.65	1.39	1.35
2	A	1585	FAD	C5X-N5	2.75	1.39	1.35
2	D	1585	FAD	C4-N3	2.83	1.38	1.33
2	C	1585	FAD	C2A-N3A	2.96	1.37	1.32
2	A	1585	FAD	C4X-N5	3.35	1.38	1.33
2	B	1585	FAD	C4X-N5	3.36	1.38	1.33
2	C	1585	FAD	C4X-N5	3.47	1.38	1.33
2	B	1585	FAD	C1'-N10	3.62	1.52	1.48
2	D	1585	FAD	C1'-N10	3.62	1.52	1.48
2	D	1585	FAD	C2A-N3A	4.20	1.39	1.32
2	A	1585	FAD	C1'-N10	5.24	1.53	1.48

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1585	FAD	N3A-C2A-N1A	-13.31	118.70	128.89
2	B	1585	FAD	N3A-C2A-N1A	-12.52	119.31	128.89
2	C	1585	FAD	N3A-C2A-N1A	-12.50	119.32	128.89
2	A	1585	FAD	N3A-C2A-N1A	-9.32	121.76	128.89
2	D	1585	FAD	C4X-C4-N3	-4.61	117.29	123.59
2	C	1585	FAD	C4X-C4-N3	-3.44	118.88	123.59
2	B	1585	FAD	C4X-C4-N3	-3.42	118.91	123.59
2	A	1585	FAD	C4X-C4-N3	-3.40	118.94	123.59
2	D	1585	FAD	C4A-C5A-N7A	-3.38	106.37	109.48
2	D	1585	FAD	C1B-N9A-C4A	-3.28	121.99	126.94
2	C	1585	FAD	C1B-N9A-C4A	-3.18	122.14	126.94
2	A	1585	FAD	P-O3P-PA	-3.12	123.97	132.73
2	B	1585	FAD	C1B-N9A-C4A	-3.01	122.40	126.94
2	D	1585	FAD	P-O3P-PA	-2.67	125.23	132.73
2	A	1585	FAD	O3P-P-O5'	-2.44	96.45	102.94
2	C	1585	FAD	O3P-PA-O5B	-2.29	96.86	102.94
2	A	1585	FAD	O3B-C3B-C2B	-2.14	104.86	111.83
2	D	1585	FAD	O3B-C3B-C2B	-2.11	104.97	111.83
2	C	1585	FAD	O4'-C4'-C5'	-2.06	105.71	110.19
2	C	1585	FAD	O2P-P-O3P	2.00	114.18	105.09
2	C	1585	FAD	C2A-N1A-C6A	2.03	122.40	118.77
2	C	1585	FAD	C1'-N10-C9A	2.04	121.15	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1585	FAD	O4B-C1B-N9A	2.07	112.44	108.10
3	D	1586	PL3	O1-C1-C2	2.11	125.40	111.62
3	A	1586	PL3	O1-C1-C2	2.14	125.61	111.62
2	A	1585	FAD	O4B-C1B-N9A	2.21	112.72	108.10
2	D	1585	FAD	C4-C4X-C10	2.22	121.36	119.94
2	A	1585	FAD	C4X-N5-C5X	2.25	119.35	116.76
2	D	1585	FAD	C4X-C10-N10	2.35	121.90	120.52
2	A	1585	FAD	O2'-C2'-C1'	2.40	115.83	109.94
2	B	1585	FAD	C1'-N10-C9A	2.47	121.63	118.86
2	D	1585	FAD	C1'-N10-C9A	2.64	121.82	118.86
2	B	1585	FAD	C4X-C10-N10	2.77	122.15	120.52
2	A	1585	FAD	C4-C4X-N5	2.82	122.14	118.72
2	B	1585	FAD	C2A-N1A-C6A	3.07	124.25	118.77
2	D	1585	FAD	C2A-N1A-C6A	3.30	124.66	118.77
2	B	1585	FAD	C4X-N5-C5X	3.41	120.68	116.76
2	B	1585	FAD	C4-C4X-N5	3.52	123.00	118.72
2	C	1585	FAD	C4X-N5-C5X	3.69	121.00	116.76
2	D	1585	FAD	C4X-N5-C5X	3.71	121.03	116.76
2	A	1585	FAD	C4X-C10-N10	3.87	122.80	120.52
2	D	1585	FAD	C4-N3-C2	4.98	119.55	115.25
2	B	1585	FAD	C4-N3-C2	5.67	120.15	115.25
2	A	1585	FAD	C4-N3-C2	5.70	120.18	115.25
2	C	1585	FAD	C4-N3-C2	5.81	120.27	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1585	FAD	1	0
3	A	1586	PL3	3	0
2	B	1585	FAD	1	0
3	B	1586	PL3	8	0
2	C	1585	FAD	1	0
2	D	1585	FAD	1	0
3	D	1586	PL3	11	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	523/584 (89%)	0.85	64 (12%) 5 6	11, 25, 53, 86	0
1	B	523/584 (89%)	0.96	84 (16%) 3 3	11, 26, 56, 85	0
1	C	491/584 (84%)	1.41	131 (26%) 1 1	17, 33, 58, 79	0
1	D	528/584 (90%)	0.84	67 (12%) 5 5	9, 25, 51, 68	0
All	All	2065/2336 (88%)	1.01	346 (16%) 2 3	9, 26, 55, 86	0

All (346) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	VAL	8.8
1	C	35	LYS	7.1
1	D	282	ARG	6.8
1	C	501	TYR	6.6
1	C	183	VAL	6.5
1	A	63	LEU	6.4
1	C	432	PRO	6.4
1	C	489	ILE	6.3
1	B	536	PHE	6.1
1	B	432	PRO	5.9
1	C	436	TRP	5.8
1	D	536	PHE	5.7
1	C	38	GLY	5.5
1	C	36	PRO	5.5
1	A	525	ILE	5.4
1	B	562	ARG	5.3
1	A	432	PRO	5.3
1	D	388	ARG	5.2
1	C	76	ASP	5.2
1	B	282	ARG	5.2
1	A	431	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	379	MET	5.1
1	C	282	ARG	5.1
1	C	562	ARG	5.1
1	B	12	HIS	5.0
1	A	541	SER	5.0
1	C	46	GLU	4.8
1	B	289	ALA	4.8
1	D	501	TYR	4.8
1	A	297	ILE	4.6
1	A	565	ILE	4.6
1	A	524	TYR	4.6
1	B	103	ALA	4.6
1	C	397	LEU	4.5
1	D	384	LEU	4.5
1	C	39	THR	4.5
1	D	12	HIS	4.4
1	B	185	ASN	4.4
1	C	366	LYS	4.4
1	B	99	ARG	4.4
1	C	478	GLN	4.4
1	A	64	THR	4.4
1	C	400	ILE	4.3
1	C	514	LYS	4.3
1	C	327	LEU	4.3
1	C	390	PHE	4.3
1	C	60	LYS	4.3
1	D	488	GLY	4.2
1	C	388	ARG	4.2
1	B	377	SER	4.2
1	C	387	ILE	4.2
1	C	482	LYS	4.2
1	C	12	HIS	4.1
1	D	165	VAL	4.1
1	B	532	THR	4.1
1	C	13	ILE	4.1
1	D	13	ILE	4.1
1	C	58	PHE	4.1
1	D	421	SER	4.0
1	B	516	ASN	4.0
1	D	63	LEU	4.0
1	C	456	TRP	4.0
1	B	565	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	365	TRP	4.0
1	C	75	LEU	3.9
1	C	356	PRO	3.9
1	C	426	PHE	3.9
1	D	190	VAL	3.9
1	B	497	ILE	3.9
1	C	336	SER	3.8
1	A	536	PHE	3.8
1	B	13	ILE	3.8
1	A	185	ASN	3.8
1	B	435	THR	3.8
1	D	486	ASP	3.7
1	D	353	VAL	3.7
1	B	87	HIS	3.7
1	C	326	PHE	3.7
1	C	392	PHE	3.7
1	C	389	SER	3.6
1	C	490	PRO	3.6
1	B	486	ASP	3.6
1	C	480	PHE	3.6
1	C	418	ASP	3.6
1	C	383	TYR	3.6
1	C	334	ALA	3.6
1	C	145	VAL	3.6
1	C	565	ILE	3.6
1	D	118	ILE	3.6
1	D	432	PRO	3.5
1	C	93	GLN	3.5
1	C	384	LEU	3.5
1	B	488	GLY	3.5
1	C	61	LYS	3.5
1	C	386	TYR	3.5
1	B	145	VAL	3.5
1	A	13	ILE	3.5
1	A	232	LEU	3.5
1	C	508	TYR	3.4
1	A	527	ALA	3.4
1	A	538	TYR	3.4
1	B	381	LYS	3.4
1	C	331	PHE	3.4
1	A	282	ARG	3.4
1	C	78	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	289	ALA	3.4
1	B	186	GLU	3.4
1	B	482	LYS	3.3
1	B	232	LEU	3.3
1	C	431	ALA	3.3
1	D	539	GLY	3.3
1	A	145	VAL	3.3
1	C	584	ARG	3.3
1	B	433	GLY	3.2
1	A	562	ARG	3.2
1	C	353	VAL	3.2
1	C	206	ARG	3.2
1	C	385	HIS	3.2
1	C	47	VAL	3.2
1	C	497	ILE	3.2
1	A	304	LEU	3.2
1	C	396	CYS	3.2
1	B	183	VAL	3.1
1	D	422	LYS	3.1
1	D	527	ALA	3.1
1	D	497	ILE	3.1
1	B	40	ILE	3.1
1	B	526	GLU	3.1
1	C	190	VAL	3.1
1	D	244	LEU	3.1
1	A	488	GLY	3.1
1	A	529	LYS	3.1
1	D	537	LYS	3.1
1	C	156	LEU	3.0
1	C	296	ILE	3.0
1	D	381	LYS	3.0
1	A	74	VAL	3.0
1	B	537	LYS	3.0
1	C	307	ILE	3.0
1	C	435	THR	3.0
1	A	247	TRP	3.0
1	C	192	ILE	3.0
1	D	393	LYS	3.0
1	C	416	VAL	3.0
1	B	205	ARG	3.0
1	B	244	LEU	3.0
1	C	167	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	212	ILE	3.0
1	D	508	TYR	2.9
1	D	156	LEU	2.9
1	B	507	LEU	2.9
1	A	435	THR	2.9
1	D	385	HIS	2.9
1	A	190	VAL	2.9
1	D	392	PHE	2.9
1	C	45	PRO	2.9
1	C	406	LYS	2.9
1	A	516	ASN	2.9
1	A	486	ASP	2.9
1	C	417	PHE	2.8
1	D	61	LYS	2.8
1	B	41	ALA	2.8
1	D	160	ALA	2.8
1	C	395	VAL	2.8
1	D	426	PHE	2.8
1	C	191	SER	2.8
1	B	569	ARG	2.8
1	C	57	GLY	2.8
1	D	507	LEU	2.8
1	D	144	ILE	2.8
1	D	212	ILE	2.8
1	B	541	SER	2.8
1	A	305	GLY	2.8
1	B	539	GLY	2.8
1	A	75	LEU	2.8
1	D	387	ILE	2.8
1	A	183	VAL	2.8
1	C	247	TRP	2.8
1	D	40	ILE	2.7
1	B	158	GLN	2.7
1	C	138	LYS	2.7
1	B	247	TRP	2.7
1	A	248	LEU	2.7
1	C	515	GLN	2.7
1	B	368	SER	2.7
1	B	93	GLN	2.7
1	B	529	LYS	2.7
1	C	310	ALA	2.7
1	C	424	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	248	LEU	2.7
1	D	307	ILE	2.7
1	C	563	GLY	2.7
1	B	60	LYS	2.7
1	C	381	LYS	2.7
1	B	431	ALA	2.7
1	C	319	GLN	2.7
1	B	365	TRP	2.7
1	C	144	ILE	2.6
1	C	437	ALA	2.6
1	C	305	GLY	2.6
1	C	433	GLY	2.6
1	C	468	ASN	2.6
1	D	418	ASP	2.6
1	B	64	THR	2.6
1	A	497	ILE	2.6
1	B	297	ILE	2.6
1	D	46	GLU	2.6
1	C	244	LEU	2.6
1	D	541	SER	2.6
1	B	74	VAL	2.6
1	C	95	PRO	2.6
1	B	82	GLN	2.6
1	C	328	PHE	2.6
1	D	397	LEU	2.6
1	D	157	VAL	2.6
1	D	372	VAL	2.6
1	A	436	TRP	2.6
1	A	377	SER	2.6
1	D	64	THR	2.6
1	B	139	ASN	2.6
1	D	122	PHE	2.6
1	B	573	GLU	2.6
1	B	388	ARG	2.6
1	D	132	VAL	2.6
1	B	501	TYR	2.6
1	B	538	TYR	2.6
1	D	476	ALA	2.5
1	C	467	ALA	2.5
1	C	513	SER	2.5
1	C	127	ARG	2.5
1	A	353	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	210	ALA	2.5
1	B	49	SER	2.5
1	A	539	GLY	2.5
1	B	47	VAL	2.5
1	D	273	VAL	2.5
1	B	155	ARG	2.5
1	B	584	ARG	2.5
1	B	192	ILE	2.5
1	C	421	SER	2.5
1	B	210	ALA	2.5
1	B	75	LEU	2.5
1	D	529	LYS	2.4
1	D	425	ALA	2.4
1	B	31	LEU	2.4
1	B	495	ALA	2.4
1	C	79	PRO	2.4
1	C	104	PHE	2.4
1	A	296	ILE	2.4
1	A	475	ASP	2.4
1	D	516	ASN	2.4
1	C	211	CYS	2.4
1	D	306	ILE	2.4
1	A	139	ASN	2.4
1	A	507	LEU	2.4
1	C	469	LEU	2.4
1	C	411	PHE	2.4
1	C	37	SER	2.4
1	C	335	VAL	2.3
1	A	433	GLY	2.3
1	A	225	LEU	2.3
1	C	232	LEU	2.3
1	D	485	LYS	2.3
1	B	122	PHE	2.3
1	C	402	PHE	2.3
1	B	296	ILE	2.3
1	B	48	SER	2.3
1	B	63	LEU	2.3
1	C	96	GLU	2.3
1	A	121	THR	2.3
1	C	338	LEU	2.3
1	C	422	LYS	2.3
1	B	50	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	306	ILE	2.3
1	A	482	LYS	2.3
1	C	401	GLY	2.3
1	D	406	LYS	2.3
1	B	290	GLY	2.2
1	D	390	PHE	2.2
1	A	566	ASN	2.2
1	B	96	GLU	2.2
1	B	212	ILE	2.2
1	D	399	ILE	2.2
1	B	508	TYR	2.2
1	B	52	LEU	2.2
1	A	563	GLY	2.2
1	B	353	VAL	2.2
1	B	121	THR	2.2
1	A	512	ALA	2.2
1	D	371	ALA	2.2
1	A	367	PRO	2.2
1	B	530	LEU	2.2
1	D	305	GLY	2.2
1	C	50	VAL	2.2
1	C	333	HIS	2.2
1	A	45	PRO	2.2
1	A	79	PRO	2.2
1	A	118	ILE	2.2
1	B	291	ILE	2.2
1	A	327	LEU	2.2
1	C	491	ALA	2.1
1	C	226	HIS	2.1
1	C	473	TRP	2.1
1	D	297	ILE	2.1
1	C	165	VAL	2.1
1	C	346	VAL	2.1
1	C	77	GLU	2.1
1	A	480	PHE	2.1
1	D	417	PHE	2.1
1	D	489	ILE	2.1
1	C	391	ASP	2.1
1	C	34	LEU	2.1
1	B	512	ALA	2.1
1	C	311	VAL	2.1
1	A	307	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	400	ILE	2.1
1	D	247	TRP	2.1
1	A	526	GLU	2.1
1	B	581	CYS	2.1
1	C	304	LEU	2.1
1	A	487	GLN	2.1
1	C	342	ARG	2.1
1	B	104	PHE	2.1
1	B	59	ILE	2.1
1	C	297	ILE	2.1
1	B	94	TYR	2.1
1	B	221	LEU	2.1
1	C	428	LEU	2.1
1	C	173	GLY	2.1
1	D	475	ASP	2.1
1	D	206	ARG	2.0
1	A	479	THR	2.0
1	A	186	GLU	2.0
1	A	192	ILE	2.0
1	C	59	ILE	2.0
1	A	84	GLU	2.0
1	C	101	LEU	2.0
1	C	483	HIS	2.0
1	A	36	PRO	2.0
1	B	367	PRO	2.0
1	C	481	VAL	2.0
1	D	145	VAL	2.0
1	A	210	ALA	2.0
1	B	341	ILE	2.0
1	D	192	ILE	2.0
1	D	565	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	PL3	D	1586	17/17	0.69	0.21	1.76	24,32,34,35	0
3	PL3	A	1586	17/17	0.69	0.24	1.42	35,39,44,45	0
3	PL3	B	1586	17/17	0.83	0.19	1.42	31,33,45,47	0
2	FAD	C	1585	53/53	0.97	0.08	-1.36	7,15,19,19	0
2	FAD	B	1585	53/53	0.96	0.08	-1.67	5,11,13,16	0
2	FAD	A	1585	53/53	0.97	0.07	-1.83	2,9,12,12	0
2	FAD	D	1585	53/53	0.97	0.07	-1.93	3,9,12,12	0

6.5 Other polymers

There are no such residues in this entry.