Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 02:29 PM EDT

PDB ID	:	8T8A
Title	:	Structure of arginine oxidase from Pseudomonas sp. TRU 7192
Authors	:	Takahashi, K.; Yamaguchi, H.; Tatsumi, M.; Sugiki, M.
Deposited on	:	2023-06-22
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

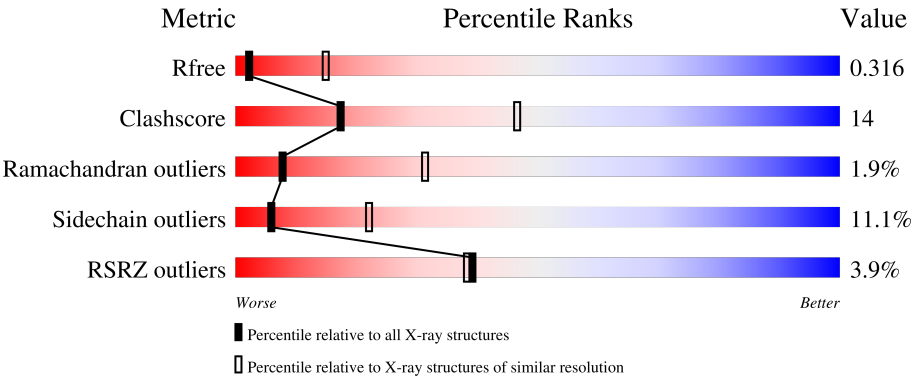
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	596	4% 69% 26%
1	B	596	2% 69% 26%
1	C	596	7% 70% 23%
1	D	596	2% 66% 30%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17774 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 Amine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4269	2719	728	806	16			
1	B	581	Total	C	N	O	S	0	0	0
			4429	2836	751	825	17			
1	C	581	Total	C	N	O	S	0	0	0
			4267	2702	735	813	17			
1	D	583	Total	C	N	O	S	0	0	0
			4482	2859	763	844	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A0A177SH44
A	2	HIS	-	expression tag	UNP A0A177SH44
A	3	HIS	-	expression tag	UNP A0A177SH44
A	4	HIS	-	expression tag	UNP A0A177SH44
A	5	HIS	-	expression tag	UNP A0A177SH44
A	6	HIS	-	expression tag	UNP A0A177SH44
A	7	HIS	-	expression tag	UNP A0A177SH44
A	237	VAL	ILE	conflict	UNP A0A177SH44
A	254	LYS	GLN	conflict	UNP A0A177SH44
A	313	ILE	VAL	conflict	UNP A0A177SH44
B	1	MET	-	expression tag	UNP A0A177SH44
B	2	HIS	-	expression tag	UNP A0A177SH44
B	3	HIS	-	expression tag	UNP A0A177SH44
B	4	HIS	-	expression tag	UNP A0A177SH44
B	5	HIS	-	expression tag	UNP A0A177SH44
B	6	HIS	-	expression tag	UNP A0A177SH44
B	7	HIS	-	expression tag	UNP A0A177SH44
B	237	VAL	ILE	conflict	UNP A0A177SH44
B	254	LYS	GLN	conflict	UNP A0A177SH44
B	313	ILE	VAL	conflict	UNP A0A177SH44
C	1	MET	-	expression tag	UNP A0A177SH44

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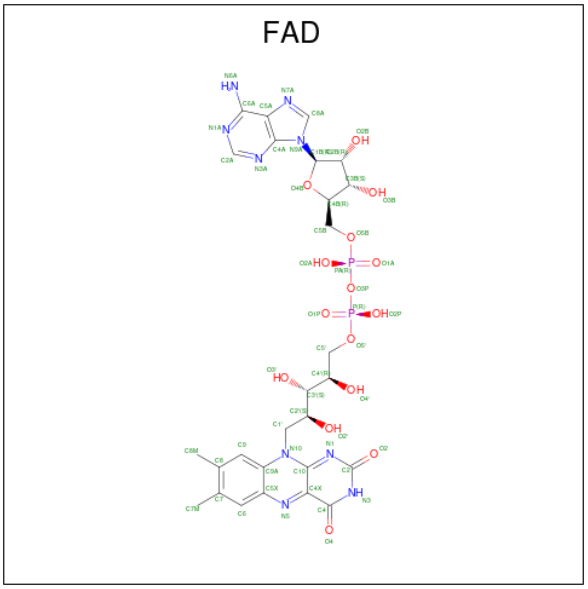
Chain	Residue	Modelled	Actual	Comment	Reference
C	2	HIS	-	expression tag	UNP A0A177SH44
C	3	HIS	-	expression tag	UNP A0A177SH44
C	4	HIS	-	expression tag	UNP A0A177SH44
C	5	HIS	-	expression tag	UNP A0A177SH44
C	6	HIS	-	expression tag	UNP A0A177SH44
C	7	HIS	-	expression tag	UNP A0A177SH44
C	237	VAL	ILE	conflict	UNP A0A177SH44
C	254	LYS	GLN	conflict	UNP A0A177SH44
C	313	ILE	VAL	conflict	UNP A0A177SH44
D	1	MET	-	expression tag	UNP A0A177SH44
D	2	HIS	-	expression tag	UNP A0A177SH44
D	3	HIS	-	expression tag	UNP A0A177SH44
D	4	HIS	-	expression tag	UNP A0A177SH44
D	5	HIS	-	expression tag	UNP A0A177SH44
D	6	HIS	-	expression tag	UNP A0A177SH44
D	7	HIS	-	expression tag	UNP A0A177SH44
D	237	VAL	ILE	conflict	UNP A0A177SH44
D	254	LYS	GLN	conflict	UNP A0A177SH44
D	313	ILE	VAL	conflict	UNP A0A177SH44

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 3 is water.

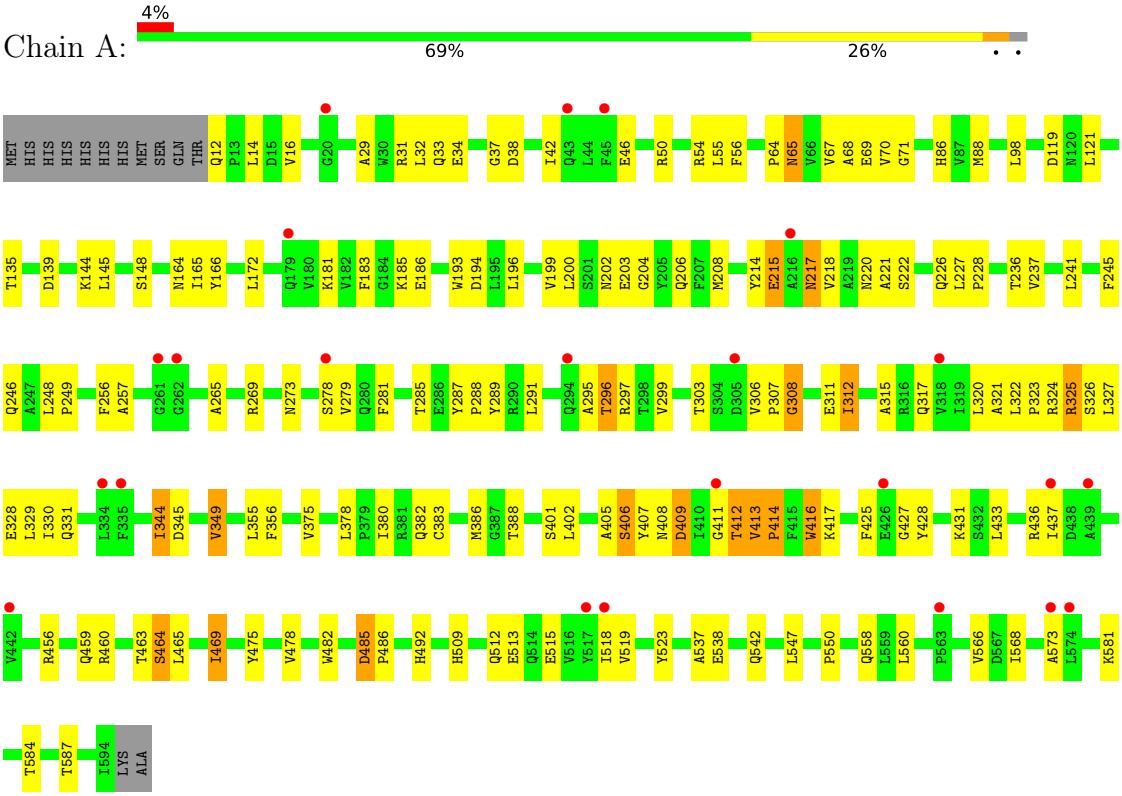
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	26	Total	O	0	0
			26	26		
3	C	26	Total	O	0	0
			26	26		
3	D	29	Total	O	0	0
			29	29		

3 Residue-property plots (i)

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

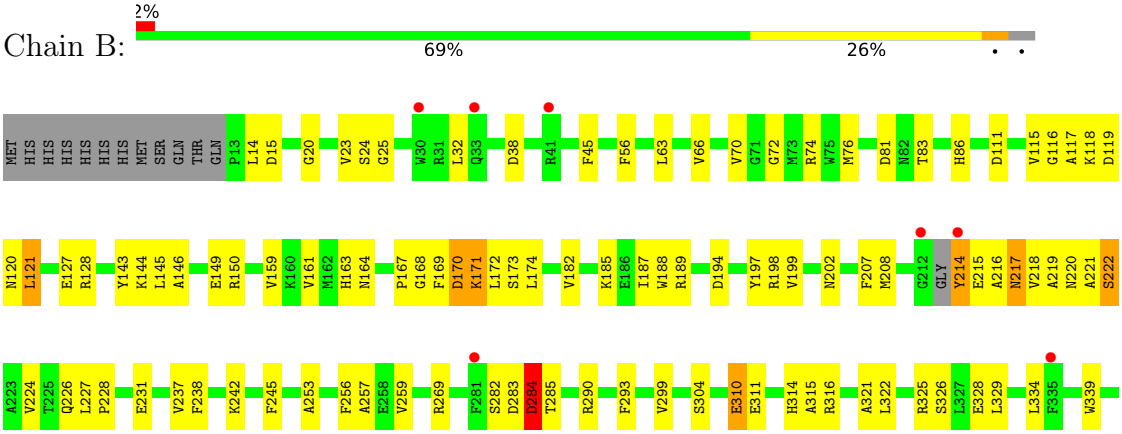
• Molecule 1: Amine oxidoreductase

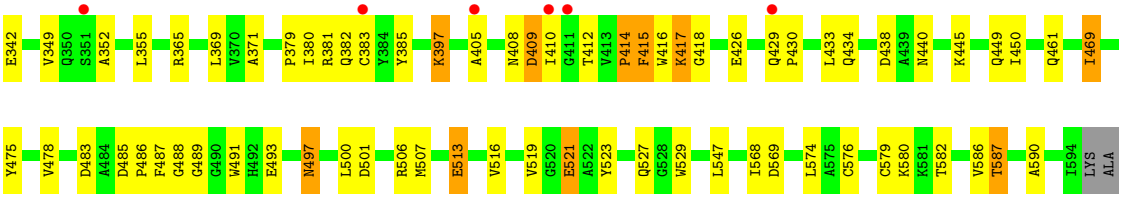
Chain A:



• Molecule 1: Amine oxidoreductase

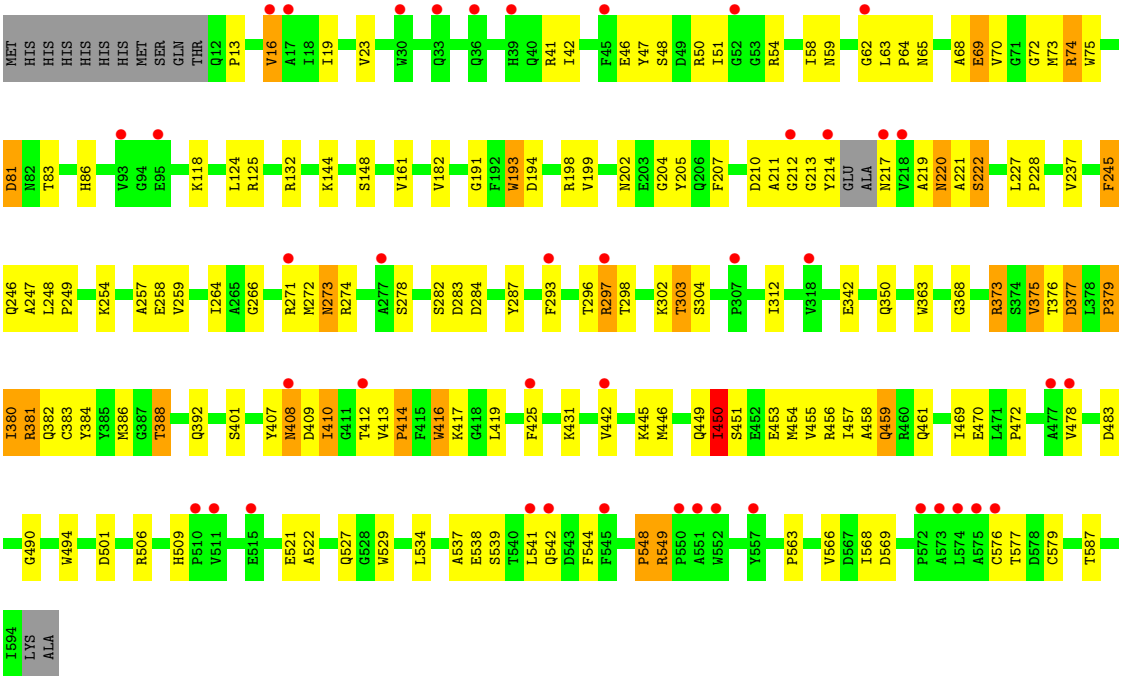
Chain B:





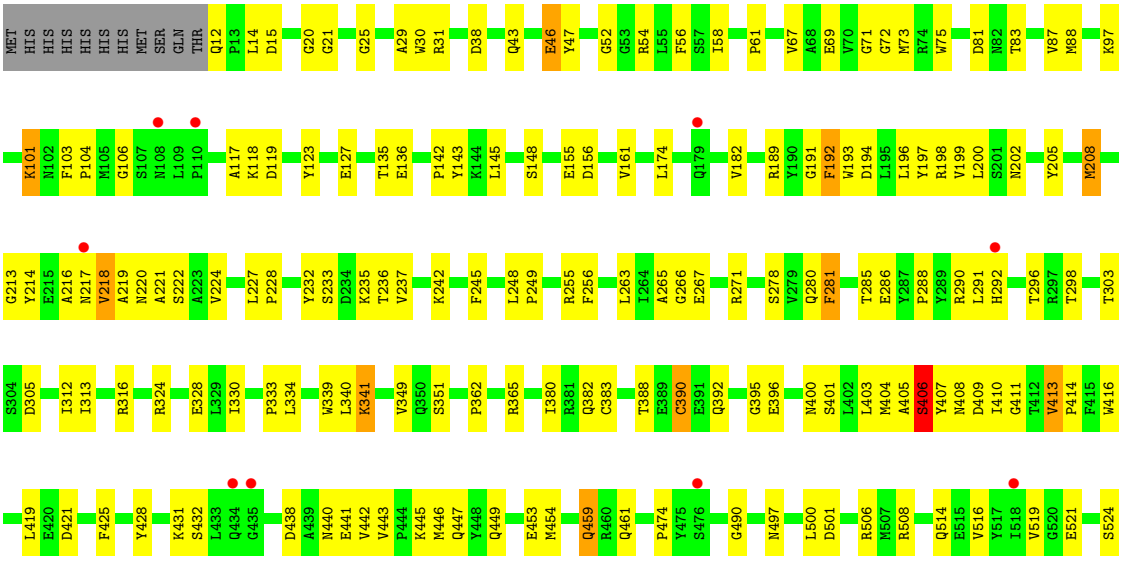
• Molecule 1: Amine oxidoreductase

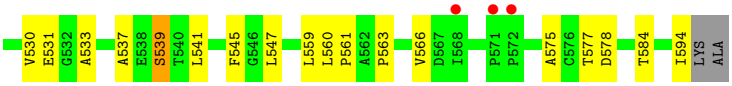
Chain C:



• Molecule 1: Amine oxidoreductase

Chain D:




V530
E531
G532
A533
A537
E538
S539
T540
L541
F545
G546
L547
L559
L560
P561
A562
P563
V566
D567
I568
P571
P572
A575
C576
T577
D578
T584
I594
LYS
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	168.27Å 200.22Å 168.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 3.40 48.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.04-3.40) 100.0 (48.99-3.40)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.212 , 0.313 0.235 , 0.316	Depositor DCC
R_{free} test set	1970 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	85.5	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 96.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17774	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.67	0/4384	0.77	0/6003
1	B	0.65	0/4550	0.78	0/6210
1	C	0.68	0/4385	0.78	0/6002
1	D	0.67	0/4603	0.77	0/6281
All	All	0.67	0/17922	0.78	0/24496

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
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	485	ASP	Peptide
1	B	485	ASP	Peptide

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	4269	0	3792	104	0
1	B	4429	0	4115	121	1
1	C	4267	0	3724	116	0
1	D	4482	0	4188	132	1
2	A	53	0	31	1	0
2	B	53	0	31	4	0
2	C	53	0	31	1	0
2	D	53	0	31	4	0
3	A	34	0	0	4	0
3	B	26	0	0	0	0
3	C	26	0	0	2	0
3	D	29	0	0	1	0
All	All	17774	0	15943	465	1

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 14.

All (465) 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:355:LEU:HD11	1:B:450:ILE:HD11	1.26	1.16
1:B:355:LEU:CD1	1:B:450:ILE:HD11	1.94	0.96
1:D:541:LEU:HB3	1:D:547:LEU:HD12	1.49	0.95
1:A:388:THR:HG23	1:A:401:SER:OG	1.68	0.94
1:B:445:LYS:HA	1:B:449:GLN:HE22	1.33	0.93
1:D:446:MET:H	1:D:449:GLN:HE22	1.21	0.88
1:C:46:GLU:HG3	1:C:48:SER:H	1.37	0.88
1:B:145:LEU:HD12	1:B:146:ALA:O	1.74	0.86
1:B:379:PRO:HD2	1:B:461:GLN:HE22	1.40	0.85
1:C:446:MET:H	1:C:449:GLN:HE22	1.24	0.85
1:B:63:LEU:HD22	1:B:66:VAL:HG21	1.58	0.85
1:D:197:TYR:CE1	1:D:198:ARG:HG3	2.12	0.83
1:B:380:ILE:HA	1:B:416:TRP:HZ2	1.44	0.82
1:B:355:LEU:CD1	1:B:450:ILE:CD1	2.58	0.81
1:B:355:LEU:HD11	1:B:450:ILE:CD1	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:PRO:HD2	1:D:316:ARG:HA	1.64	0.80
1:D:419:LEU:HB2	1:D:454:MET:HG2	1.63	0.80
1:B:339:TRP:CE2	1:B:506:ARG:HD3	2.17	0.79
1:D:339:TRP:CE2	1:D:506:ARG:HD3	2.17	0.79
1:B:369:LEU:HD13	1:B:385:TYR:OH	1.83	0.78
1:C:271:ARG:NH2	1:C:274:ARG:NH2	2.31	0.78
1:D:54:ARG:HD3	1:D:490:GLY:O	1.85	0.77
1:D:500:LEU:HD12	1:D:501:ASP:N	2.00	0.76
1:C:413:VAL:N	1:C:414:PRO:HD2	2.01	0.75
1:D:56:PHE:CE1	1:D:58:ILE:HD11	2.20	0.75
1:D:419:LEU:O	1:D:454:MET:HG3	1.85	0.75
1:B:63:LEU:HD22	1:B:66:VAL:CG2	2.17	0.75
1:D:446:MET:H	1:D:449:GLN:NE2	1.85	0.74
1:C:382:GLN:HG2	1:C:383:CYS:H	1.52	0.73
1:D:117:ALA:O	1:D:119:ASP:N	2.23	0.72
1:B:76:MET:CE	1:B:231:GLU:OE1	2.38	0.72
1:B:253:ALA:O	1:B:256:PHE:HB3	1.90	0.72
1:D:248:LEU:HB3	1:D:249:PRO:HD3	1.72	0.72
1:C:350:GLN:CB	1:C:410:ILE:HD11	2.21	0.71
1:D:81:ASP:OD1	1:D:83:THR:HG23	1.91	0.70
1:D:193:TRP:HE1	1:D:219:ALA:H	1.39	0.70
1:A:380:ILE:HA	1:A:416:TRP:HZ2	1.56	0.70
1:B:76:MET:HE1	1:B:231:GLU:OE1	1.91	0.70
1:B:169:PHE:HA	1:B:172:LEU:HD12	1.74	0.69
1:C:50:ARG:HH11	1:C:246:GLN:HE21	1.38	0.69
1:A:469:ILE:HD12	1:A:469:ILE:H	1.57	0.69
1:D:219:ALA:O	1:D:220:ASN:C	2.31	0.68
1:B:334:LEU:HD22	1:B:516:VAL:HG21	1.76	0.68
1:D:73:MET:SD	1:D:103:PHE:CZ	2.87	0.68
1:A:317:GLN:CB	3:A:725:HOH:O	2.42	0.67
1:B:145:LEU:CD1	1:B:146:ALA:O	2.42	0.67
1:C:382:GLN:HG2	1:C:383:CYS:N	2.09	0.67
1:B:414:PRO:HD2	1:B:417:LYS:HB2	1.76	0.67
1:D:56:PHE:CZ	1:D:58:ILE:HD11	2.29	0.67
1:B:339:TRP:CZ2	1:B:506:ARG:HD3	2.30	0.67
1:D:446:MET:N	1:D:449:GLN:HE22	1.92	0.67
1:D:81:ASP:CG	1:D:83:THR:HG23	2.15	0.66
1:B:120:ASN:HA	1:B:369:LEU:CD2	2.26	0.66
1:C:494:TRP:CD1	1:C:527:GLN:OE1	2.49	0.66
1:D:383:CYS:SG	1:D:403:LEU:HD11	2.36	0.66
1:B:74:ARG:HD2	1:B:238:PHE:CG	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:HD11	1:B:150:ARG:CA	2.27	0.65
1:D:219:ALA:HB1	1:D:221:ALA:HB2	1.79	0.65
1:D:197:TYR:CE1	1:D:198:ARG:CG	2.80	0.65
1:B:145:LEU:HD13	1:B:149:GLU:HB2	1.78	0.65
1:A:121:LEU:HD21	1:A:465:LEU:O	1.96	0.64
1:A:388:THR:HG23	1:A:401:SER:HG	1.61	0.64
1:A:416:TRP:HA	1:A:416:TRP:CE3	2.31	0.64
1:D:214:TYR:HA	1:D:407:TYR:HE2	1.61	0.64
1:C:451:SER:HB2	1:C:453:GLU:HG2	1.81	0.63
3:A:727:HOH:O	1:B:144:LYS:CB	2.46	0.63
1:D:411:GLY:N	3:D:701:HOH:O	2.25	0.63
1:B:500:LEU:HD12	1:B:501:ASP:N	2.14	0.62
1:C:191:GLY:HA3	1:C:220:ASN:ND2	2.14	0.62
1:A:145:LEU:CD2	1:A:204:GLY:HA2	2.29	0.62
1:A:221:ALA:HB3	1:A:226:GLN:HG3	1.82	0.62
1:B:349:VAL:HG13	1:B:489:GLY:N	2.15	0.62
1:C:271:ARG:HH21	1:C:274:ARG:NH2	1.97	0.62
1:D:197:TYR:CD1	1:D:198:ARG:HG3	2.35	0.61
1:B:380:ILE:HA	1:B:416:TRP:CZ2	2.32	0.61
1:C:459:GLN:HE21	1:C:459:GLN:HA	1.65	0.61
1:B:86:HIS:HE1	1:B:529:TRP:CE3	2.18	0.61
1:D:445:LYS:HA	1:D:449:GLN:HE22	1.66	0.61
1:D:29:ALA:HB1	1:D:256:PHE:CD1	2.35	0.60
1:A:54:ARG:O	1:A:71:GLY:HA3	2.00	0.60
1:D:196:LEU:HA	1:D:199:VAL:HG22	1.83	0.60
1:B:167:PRO:HB3	1:B:586:VAL:HG21	1.84	0.60
1:D:54:ARG:O	1:D:71:GLY:HA3	2.01	0.60
1:D:508:ARG:NH1	1:D:539:SER:OG	2.35	0.60
1:C:382:GLN:CG	1:C:383:CYS:H	2.15	0.59
1:D:54:ARG:CD	1:D:490:GLY:O	2.50	0.58
1:D:219:ALA:C	1:D:221:ALA:N	2.53	0.58
1:C:417:LYS:NZ	1:C:483:ASP:OD2	2.35	0.58
1:B:74:ARG:HD2	1:B:238:PHE:CD1	2.38	0.58
1:A:416:TRP:HA	1:A:416:TRP:HE3	1.65	0.58
1:A:33:GLN:HA	1:A:37:GLY:HA3	1.86	0.57
1:D:194:ASP:HA	1:D:197:TYR:CE2	2.39	0.57
1:B:168:GLY:HA2	1:B:171:LYS:HD2	1.85	0.57
1:D:388:THR:HG23	1:D:401:SER:HB3	1.85	0.57
1:B:483:ASP:HA	1:B:488:GLY:O	2.05	0.57
1:C:50:ARG:HD2	1:C:246:GLN:NE2	2.20	0.57
1:A:378:LEU:HD23	1:B:202:ASN:OD1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:PHE:CD1	1:C:455:VAL:HG21	2.40	0.57
1:D:278:SER:HB3	1:D:292:HIS:HB2	1.87	0.57
1:C:212:GLY:HA2	1:C:373:ARG:HH12	1.69	0.56
1:B:326:SER:HA	1:B:329:LEU:HD12	1.86	0.56
1:C:210:ASP:HA	1:C:381:ARG:HH22	1.70	0.56
1:C:350:GLN:CB	1:C:410:ILE:CD1	2.82	0.56
1:D:193:TRP:HE1	1:D:218:VAL:HA	1.69	0.56
1:D:267:GLU:CD	1:D:267:GLU:H	2.06	0.56
1:C:68:ALA:O	1:C:69:GLU:C	2.43	0.56
1:B:216:ALA:O	1:B:218:VAL:N	2.38	0.56
1:C:23:VAL:HG22	1:C:534:LEU:HD21	1.86	0.56
1:C:219:ALA:O	1:C:221:ALA:N	2.39	0.56
1:B:143:TYR:CE2	1:B:207:PHE:HA	2.40	0.56
1:C:214:TYR:O	1:C:382:GLN:OE1	2.23	0.56
1:A:324:ARG:HD2	1:A:344:ILE:O	2.06	0.56
1:A:181:LYS:HA	1:A:185:LYS:O	2.05	0.56
1:C:446:MET:H	1:C:449:GLN:NE2	1.99	0.56
1:C:382:GLN:NE2	1:C:384:TYR:CE1	2.74	0.55
1:D:73:MET:SD	1:D:103:PHE:HZ	2.29	0.55
1:A:349:VAL:HA	3:A:703:HOH:O	2.07	0.55
1:D:81:ASP:CG	1:D:83:THR:CG2	2.75	0.55
1:A:145:LEU:HD21	1:A:204:GLY:HA2	1.88	0.55
1:B:194:ASP:O	1:B:198:ARG:HD2	2.07	0.55
1:D:227:LEU:HB3	1:D:228:PRO:HD3	1.87	0.55
1:A:144:LYS:HB2	1:A:203:GLU:HG3	1.88	0.55
1:A:414:PRO:HD2	1:A:417:LYS:HB2	1.88	0.55
1:A:509:HIS:CE1	1:A:512:GLN:HA	2.42	0.55
1:C:204:GLY:O	1:C:207:PHE:HB3	2.07	0.55
1:C:73:MET:CG	1:C:74:ARG:N	2.70	0.55
1:C:283:ASP:O	1:C:284:ASP:C	2.44	0.55
1:D:217:ASN:O	1:D:218:VAL:C	2.45	0.55
1:B:259:VAL:HB	1:B:269:ARG:NH1	2.22	0.55
1:B:145:LEU:HD11	1:B:150:ARG:HA	1.88	0.54
1:C:446:MET:N	1:C:449:GLN:HE22	1.98	0.54
1:B:72:GLY:HA2	2:B:601:FAD:C4X	2.37	0.54
1:C:13:PRO:HB3	1:C:287:TYR:CZ	2.42	0.54
1:C:537:ALA:O	1:C:541:LEU:HD13	2.07	0.54
1:C:382:GLN:CG	1:C:383:CYS:N	2.71	0.54
1:C:416:TRP:HA	1:C:416:TRP:CE3	2.42	0.54
1:D:334:LEU:HD12	1:D:514:GLN:HG3	1.89	0.54
1:B:214:TYR:O	1:B:215:GLU:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:GLY:O	1:C:214:TYR:C	2.46	0.54
1:C:254:LYS:CB	3:C:712:HOH:O	2.56	0.54
1:B:14:LEU:O	1:B:315:ALA:HA	2.08	0.54
1:C:50:ARG:HG2	1:C:51:ILE:H	1.73	0.54
1:B:145:LEU:CD1	1:B:150:ARG:N	2.71	0.53
1:C:193:TRP:HA	1:C:193:TRP:CE3	2.43	0.53
1:B:493:GLU:HA	1:B:527:GLN:OE1	2.07	0.53
1:D:29:ALA:O	1:D:30:TRP:C	2.43	0.53
1:B:168:GLY:O	1:B:169:PHE:C	2.44	0.53
1:D:334:LEU:HD13	1:D:516:VAL:HG21	1.90	0.53
1:D:81:ASP:OD1	1:D:81:ASP:O	2.26	0.53
1:A:54:ARG:HB2	2:A:601:FAD:O4'	2.08	0.53
1:C:296:THR:HB	1:C:303:THR:HG22	1.90	0.53
1:C:73:MET:HG3	1:C:74:ARG:N	2.24	0.53
1:D:380:ILE:HD12	1:D:461:GLN:HB3	1.90	0.53
1:A:325:ARG:O	1:A:329:LEU:HG	2.08	0.53
1:B:369:LEU:HD13	1:B:385:TYR:CZ	2.42	0.53
1:C:210:ASP:HA	1:C:381:ARG:NH2	2.24	0.53
1:B:293:PHE:HB2	1:B:311:GLU:HG2	1.91	0.53
1:D:193:TRP:NE1	1:D:218:VAL:HA	2.24	0.53
1:B:416:TRP:HA	1:B:416:TRP:CE3	2.43	0.52
1:C:449:GLN:O	1:C:450:ILE:C	2.47	0.52
1:B:120:ASN:HA	1:B:369:LEU:HD21	1.91	0.52
1:D:380:ILE:HG13	1:D:461:GLN:OE1	2.08	0.52
1:B:187:ILE:HG23	1:B:224:VAL:HG22	1.91	0.52
1:A:215:GLU:C	1:A:217:ASN:N	2.61	0.52
1:D:72:GLY:HA2	2:D:601:FAD:C4X	2.39	0.52
1:C:576:CYS:SG	1:C:579:CYS:HA	2.50	0.52
1:A:65:ASN:N	1:A:65:ASN:HD22	2.08	0.52
1:A:248:LEU:HB3	1:A:249:PRO:HD3	1.92	0.52
1:D:459:GLN:HE22	1:D:474:PRO:HD3	1.74	0.52
1:A:12:GLN:N	3:A:704:HOH:O	2.43	0.51
1:B:20:GLY:HA3	1:B:321:ALA:HB3	1.92	0.51
1:C:350:GLN:HA	1:C:410:ILE:HD13	1.92	0.51
1:B:352:ALA:HA	1:B:409:ASP:HB3	1.93	0.51
1:B:469:ILE:H	1:B:469:ILE:HD12	1.75	0.51
1:D:214:TYR:HA	1:D:407:TYR:CE2	2.43	0.51
1:B:257:ALA:HA	1:B:269:ARG:HD2	1.92	0.51
1:C:419:LEU:O	1:C:454:MET:HG3	2.11	0.51
1:D:431:LYS:O	1:D:432:SER:C	2.49	0.51
1:B:76:MET:HE3	1:B:231:GLU:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:TRP:HA	1:D:416:TRP:CE3	2.46	0.51
1:C:350:GLN:HA	1:C:410:ILE:CD1	2.40	0.51
1:B:397:LYS:O	1:B:397:LYS:NZ	2.36	0.51
1:A:50:ARG:HD2	1:A:246:GLN:HE22	1.76	0.50
1:A:215:GLU:C	1:A:217:ASN:H	2.12	0.50
1:A:248:LEU:HB3	1:A:249:PRO:CD	2.41	0.50
1:B:445:LYS:CA	1:B:449:GLN:HE22	2.14	0.50
1:C:72:GLY:HA2	2:C:601:FAD:C4X	2.41	0.50
1:D:447:GLN:HG2	1:D:447:GLN:O	2.11	0.50
1:B:121:LEU:HD12	1:B:369:LEU:HD11	1.92	0.50
1:D:46:GLU:OE2	2:D:601:FAD:H1B	2.12	0.50
1:A:469:ILE:HD13	1:D:199:VAL:HA	1.94	0.50
1:A:217:ASN:O	1:A:218:VAL:C	2.47	0.50
1:B:115:VAL:O	1:B:116:GLY:C	2.49	0.50
1:D:216:ALA:C	1:D:218:VAL:N	2.65	0.50
1:D:445:LYS:HA	1:D:449:GLN:NE2	2.26	0.50
1:B:189:ARG:HA	1:B:497:ASN:HD22	1.76	0.50
1:B:408:ASN:HD22	1:B:416:TRP:HD1	1.60	0.50
1:C:451:SER:CB	1:C:453:GLU:HG2	2.42	0.50
1:B:334:LEU:CD2	1:B:516:VAL:HG11	2.41	0.50
1:C:382:GLN:NE2	1:C:384:TYR:HE1	2.09	0.50
1:C:407:TYR:O	1:C:408:ASN:C	2.48	0.50
1:D:81:ASP:C	1:D:83:THR:H	2.13	0.50
1:A:538:GLU:OE1	1:A:542:GLN:NE2	2.45	0.50
1:A:542:GLN:HA	1:A:547:LEU:O	2.11	0.49
1:A:16:VAL:HA	1:A:317:GLN:O	2.12	0.49
1:C:161:VAL:HG13	1:C:199:VAL:HG21	1.94	0.49
1:D:155:GLU:O	1:D:156:ASP:C	2.50	0.49
1:D:405:ALA:O	1:D:406:SER:C	2.50	0.49
1:B:429:GLN:OE1	1:B:434:GLN:HA	2.12	0.49
1:A:54:ARG:HH21	1:A:323:PRO:HG3	1.77	0.49
1:C:350:GLN:O	1:C:490:GLY:N	2.41	0.49
1:C:538:GLU:OE1	1:C:542:GLN:NE2	2.45	0.49
1:D:81:ASP:C	1:D:83:THR:N	2.64	0.49
1:D:221:ALA:O	1:D:222:SER:C	2.49	0.49
1:A:297:ARG:O	1:A:303:THR:HA	2.13	0.49
1:A:321:ALA:HA	1:A:519:VAL:O	2.12	0.49
1:B:145:LEU:HD11	1:B:150:ARG:N	2.27	0.49
1:C:576:CYS:HG	1:C:579:CYS:HA	1.78	0.49
1:B:349:VAL:CG1	1:B:489:GLY:N	2.76	0.49
1:D:419:LEU:CB	1:D:454:MET:HG2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:ILE:HG23	1:C:461:GLN:HE21	1.77	0.49
1:B:24:SER:HB3	2:B:601:FAD:O1P	2.13	0.48
1:C:211:ALA:O	1:C:375:VAL:HG11	2.13	0.48
1:A:50:ARG:HH11	1:A:246:GLN:NE2	2.10	0.48
1:A:405:ALA:C	1:A:407:TYR:N	2.66	0.48
1:A:427:GLY:HA3	1:A:475:TYR:O	2.13	0.48
1:B:349:VAL:HG13	1:B:489:GLY:HA3	1.95	0.48
1:B:379:PRO:HD2	1:B:461:GLN:NE2	2.18	0.48
1:D:174:LEU:HD21	1:D:500:LEU:HD11	1.95	0.48
1:A:16:VAL:HG23	1:A:42:ILE:HA	1.96	0.48
1:A:538:GLU:HA	1:A:538:GLU:OE2	2.14	0.48
1:D:174:LEU:HD21	1:D:500:LEU:CD1	2.43	0.48
1:D:404:MET:HG2	1:D:405:ALA:N	2.29	0.48
1:B:487:PHE:O	1:B:489:GLY:N	2.46	0.48
1:D:453:GLU:O	1:D:454:MET:C	2.51	0.48
1:B:283:ASP:O	1:B:284:ASP:C	2.51	0.48
1:B:72:GLY:HA2	2:B:601:FAD:N5	2.29	0.48
1:B:383:CYS:HA	1:B:405:ALA:HA	1.94	0.48
1:C:62:GLY:C	1:C:64:PRO:HD3	2.33	0.48
1:D:43:GLN:HE22	1:D:271:ARG:HD3	1.79	0.48
1:D:324:ARG:NE	1:D:328:GLU:OE2	2.44	0.48
1:D:541:LEU:HA	1:D:545:PHE:HB2	1.95	0.48
1:C:73:MET:CG	1:C:74:ARG:H	2.27	0.48
1:D:52:GLY:HA2	1:D:249:PRO:HG2	1.94	0.48
1:D:281:PHE:CZ	1:D:333:PRO:HG2	2.49	0.48
1:A:14:LEU:O	1:A:315:ALA:HA	2.14	0.47
1:D:127:GLU:HG3	1:D:142:PRO:HB3	1.95	0.47
1:C:65:ASN:N	1:C:65:ASN:HD22	2.12	0.47
1:C:453:GLU:O	1:C:454:MET:C	2.52	0.47
1:D:208:MET:HE2	1:D:208:MET:HB3	1.77	0.47
1:A:433:LEU:HA	1:A:436:ARG:HD3	1.97	0.47
1:B:259:VAL:HB	1:B:269:ARG:HH12	1.78	0.47
1:C:379:PRO:C	1:C:381:ARG:N	2.67	0.47
1:A:327:LEU:O	1:A:329:LEU:N	2.47	0.47
1:B:173:SER:O	1:B:174:LEU:C	2.51	0.47
1:B:349:VAL:HG13	1:B:489:GLY:CA	2.44	0.47
1:D:380:ILE:HG22	1:D:382:GLN:O	2.14	0.47
1:A:380:ILE:O	1:A:382:GLN:N	2.38	0.47
1:B:227:LEU:HB3	1:B:228:PRO:HD3	1.97	0.47
1:C:388:THR:HG23	1:C:401:SER:HB3	1.96	0.47
1:A:145:LEU:CD2	1:A:204:GLY:CA	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:O	1:A:312:ILE:HA	2.15	0.47
1:C:538:GLU:O	1:C:541:LEU:N	2.48	0.47
1:D:400:ASN:HD21	1:D:432:SER:CB	2.27	0.47
1:C:521:GLU:O	1:C:522:ALA:C	2.53	0.47
1:B:325:ARG:O	1:B:328:GLU:HB2	2.15	0.47
1:C:445:LYS:HA	1:C:449:GLN:HE22	1.80	0.47
1:A:412:THR:O	1:A:413:VAL:C	2.53	0.47
1:D:38:ASP:O	1:D:263:LEU:HG	2.15	0.46
1:D:67:VAL:HG12	1:D:69:GLU:HG2	1.97	0.46
1:A:324:ARG:HG3	1:A:523:TYR:OH	2.15	0.46
1:C:118:LYS:HB3	1:C:132:ARG:HD3	1.97	0.46
1:D:191:GLY:O	1:D:192:PHE:C	2.54	0.46
1:D:194:ASP:HA	1:D:197:TYR:CD2	2.50	0.46
1:A:519:VAL:HG11	1:A:537:ALA:HA	1.97	0.46
1:B:32:LEU:HD23	1:B:547:LEU:HD11	1.96	0.46
1:B:430:PRO:HG3	1:B:475:TYR:CD1	2.51	0.46
1:C:494:TRP:CG	1:C:527:GLN:OE1	2.69	0.46
1:D:54:ARG:NE	1:D:490:GLY:O	2.48	0.46
1:C:194:ASP:OD2	1:C:220:ASN:ND2	2.48	0.46
1:C:383:CYS:SG	1:C:384:TYR:N	2.89	0.46
1:A:221:ALA:O	1:A:222:SER:C	2.54	0.46
1:D:202:ASN:O	1:D:205:TYR:HB3	2.15	0.46
1:B:117:ALA:O	1:B:118:LYS:C	2.53	0.46
1:B:310:GLU:O	1:B:311:GLU:HB3	2.16	0.46
1:B:417:LYS:HA	1:B:417:LYS:HD3	1.51	0.46
1:C:456:ARG:O	1:C:457:ILE:C	2.52	0.46
1:A:307:PRO:O	1:A:308:GLY:C	2.54	0.46
1:A:388:THR:CG2	1:A:401:SER:OG	2.52	0.46
1:A:573:ALA:HB2	1:C:431:LYS:CB	2.46	0.46
1:B:416:TRP:HA	1:B:416:TRP:HE3	1.81	0.46
1:D:339:TRP:CH2	1:D:506:ARG:HB3	2.50	0.46
1:D:405:ALA:O	1:D:407:TYR:N	2.48	0.46
1:A:279:VAL:HG23	1:A:330:ILE:HG21	1.97	0.46
1:A:428:TYR:O	1:A:475:TYR:HB2	2.15	0.46
1:C:63:LEU:N	1:C:64:PRO:HD3	2.31	0.46
1:C:413:VAL:N	1:C:414:PRO:CD	2.77	0.46
1:D:192:PHE:CE2	1:D:196:LEU:HD11	2.51	0.46
1:A:202:ASN:O	1:A:206:GLN:HG2	2.15	0.45
1:A:380:ILE:HA	1:A:416:TRP:CZ2	2.44	0.45
1:B:290:ARG:HD2	1:B:314:HIS:CD2	2.51	0.45
1:B:414:PRO:HD2	1:B:417:LYS:CB	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:O	1:B:219:ALA:C	2.52	0.45
1:C:221:ALA:O	1:C:222:SER:C	2.54	0.45
1:C:227:LEU:HB3	1:C:228:PRO:HD3	1.98	0.45
1:D:340:LEU:O	1:D:341:LYS:C	2.52	0.45
1:C:248:LEU:CB	1:C:249:PRO:HD3	2.47	0.45
1:A:464:SER:O	1:A:465:LEU:C	2.54	0.45
1:B:174:LEU:HD21	1:B:500:LEU:CD1	2.47	0.45
1:B:355:LEU:CD1	1:B:450:ILE:HD12	2.42	0.45
1:B:380:ILE:O	1:B:382:GLN:N	2.50	0.45
1:C:86:HIS:HE1	1:C:529:TRP:CE3	2.35	0.45
1:B:576:CYS:SG	1:B:579:CYS:HB3	2.57	0.45
1:C:380:ILE:HG23	1:C:461:GLN:NE2	2.32	0.45
1:B:20:GLY:O	1:B:25:GLY:HA3	2.16	0.45
1:C:272:MET:O	1:C:273:ASN:C	2.55	0.45
1:C:376:THR:OG1	1:C:377:ASP:N	2.49	0.45
1:D:233:SER:HG	1:D:236:THR:H	1.65	0.45
1:A:587:THR:HG23	1:C:368:GLY:HA2	1.98	0.44
1:C:245:PHE:C	1:C:247:ALA:N	2.70	0.44
1:C:380:ILE:O	1:C:382:GLN:N	2.50	0.44
1:D:54:ARG:NH1	2:D:601:FAD:O1A	2.50	0.44
1:A:68:ALA:HB1	1:A:356:PHE:CD2	2.53	0.44
1:B:507:MET:HG2	1:B:523:TYR:CG	2.52	0.44
1:C:380:ILE:HG12	1:C:461:GLN:NE2	2.32	0.44
1:D:193:TRP:HB3	1:D:205:TYR:OH	2.17	0.44
1:C:13:PRO:HB3	1:C:287:TYR:CE2	2.53	0.44
1:D:46:GLU:OE2	1:D:47:TYR:N	2.49	0.44
1:D:390:CYS:HA	1:D:396:GLU:O	2.17	0.44
1:A:181:LYS:CA	1:A:185:LYS:O	2.64	0.44
1:B:412:THR:O	1:B:414:PRO:HD3	2.17	0.44
1:C:68:ALA:O	1:C:70:VAL:N	2.51	0.44
1:A:29:ALA:HB1	1:A:256:PHE:CE1	2.52	0.44
1:A:31:ARG:NH2	1:A:550:PRO:HG3	2.32	0.44
1:A:322:LEU:HB3	1:A:326:SER:HB2	1.98	0.44
1:C:297:ARG:O	1:C:303:THR:HA	2.18	0.44
1:B:587:THR:O	1:B:590:ALA:N	2.51	0.44
1:A:16:VAL:CG2	1:A:42:ILE:HA	2.48	0.44
1:B:161:VAL:HG13	1:B:199:VAL:HG21	2.00	0.44
1:C:454:MET:O	1:C:455:VAL:C	2.53	0.44
1:D:500:LEU:HD12	1:D:500:LEU:C	2.37	0.44
1:D:575:ALA:O	1:D:577:THR:N	2.51	0.44
1:D:30:TRP:CD1	1:D:255:ARG:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ALA:O	1:B:222:SER:C	2.55	0.44
1:C:501:ASP:HB2	1:C:563:PRO:HA	1.98	0.44
1:A:54:ARG:HA	1:A:482:TRP:CH2	2.53	0.43
1:A:183:PHE:CG	1:C:470:GLU:OE1	2.71	0.43
1:B:430:PRO:HD2	1:B:433:LEU:HB2	1.99	0.43
1:A:287:TYR:C	1:A:289:TYR:H	2.21	0.43
1:B:221:ALA:HB3	1:B:226:GLN:HG3	2.00	0.43
1:C:210:ASP:CA	1:C:381:ARG:HH22	2.32	0.43
1:D:101:LYS:HE2	1:D:101:LYS:HB2	1.79	0.43
1:A:382:GLN:NE2	1:A:407:TYR:O	2.51	0.43
1:B:322:LEU:HB3	1:B:326:SER:HB2	2.00	0.43
1:C:69:GLU:HB3	1:C:72:GLY:O	2.18	0.43
1:C:274:ARG:HA	1:C:274:ARG:HD3	1.60	0.43
1:D:161:VAL:HG21	1:D:200:LEU:HD11	1.99	0.43
1:D:21:GLY:N	1:D:46:GLU:HG2	2.33	0.43
1:B:170:ASP:OD1	1:B:170:ASP:N	2.51	0.43
1:D:577:THR:OG1	1:D:578:ASP:N	2.52	0.43
1:B:214:TYR:O	1:B:217:ASN:N	2.51	0.43
1:B:414:PRO:HB2	1:B:415:PHE:H	1.66	0.43
1:D:265:ALA:O	1:D:266:GLY:C	2.57	0.43
1:D:291:LEU:O	1:D:312:ILE:HA	2.18	0.43
1:A:227:LEU:N	1:A:228:PRO:HD2	2.33	0.43
1:A:320:LEU:O	1:A:518:ILE:HA	2.19	0.43
1:D:392:GLN:O	1:D:395:GLY:N	2.52	0.43
1:B:500:LEU:HD12	1:B:500:LEU:C	2.39	0.43
1:D:104:PRO:C	1:D:106:GLY:H	2.21	0.43
1:B:290:ARG:NH1	1:B:314:HIS:CG	2.88	0.42
1:C:202:ASN:O	1:C:205:TYR:N	2.52	0.42
1:B:215:GLU:O	1:B:216:ALA:C	2.57	0.42
1:A:193:TRP:O	1:A:194:ASP:C	2.55	0.42
1:A:194:ASP:HA	1:B:415:PHE:CZ	2.55	0.42
1:A:265:ALA:O	1:A:269:ARG:HG3	2.20	0.42
1:A:356:PHE:HB3	1:A:402:LEU:HD11	2.01	0.42
1:C:16:VAL:O	1:C:42:ILE:HA	2.19	0.42
1:D:135:THR:OG1	1:D:136:GLU:N	2.52	0.42
1:B:187:ILE:HG23	1:B:224:VAL:CG2	2.49	0.42
1:B:207:PHE:O	1:B:208:MET:C	2.55	0.42
1:C:81:ASP:OD1	1:C:81:ASP:N	2.42	0.42
1:C:506:ARG:CB	3:C:708:HOH:O	2.67	0.42
1:A:68:ALA:HB1	1:A:356:PHE:CE2	2.54	0.42
1:A:181:LYS:CB	1:A:185:LYS:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ALA:HA	1:A:519:VAL:HG23	2.01	0.42
1:C:202:ASN:O	1:C:205:TYR:HB3	2.19	0.42
1:C:274:ARG:HB3	1:C:293:PHE:CD1	2.55	0.42
1:D:143:TYR:HB3	1:D:145:LEU:CD1	2.50	0.42
1:D:362:PRO:HB2	1:D:365:ARG:HG2	2.01	0.42
1:A:281:PHE:HA	1:A:288:PRO:O	2.18	0.42
1:C:509:HIS:HB2	1:C:544:PHE:CE2	2.55	0.42
1:D:298:THR:HA	1:D:303:THR:HA	2.01	0.42
1:D:419:LEU:HB2	1:D:454:MET:CG	2.41	0.42
1:C:272:MET:HB3	1:C:273:ASN:H	1.72	0.42
1:C:59:ASN:HB3	1:C:64:PRO:HA	2.01	0.42
1:D:419:LEU:O	1:D:454:MET:CG	2.61	0.42
1:B:163:HIS:O	1:B:164:ASN:C	2.58	0.42
1:B:521:GLU:HG2	2:B:601:FAD:O3'	2.20	0.42
1:C:258:GLU:O	1:C:259:VAL:C	2.59	0.42
1:C:453:GLU:CD	1:C:453:GLU:N	2.74	0.42
1:D:339:TRP:CZ2	1:D:506:ARG:HB3	2.54	0.42
1:A:98:LEU:HB3	1:A:241:LEU:HD22	2.02	0.41
1:A:405:ALA:O	1:A:407:TYR:N	2.53	0.41
1:B:45:PHE:CD2	1:B:293:PHE:CE1	3.08	0.41
1:D:72:GLY:HA2	2:D:601:FAD:N5	2.35	0.41
1:D:560:LEU:HA	1:D:561:PRO:HD3	1.93	0.41
1:A:119:ASP:OD1	1:D:594:ILE:HG21	2.21	0.41
1:A:166:TYR:CD2	1:A:172:LEU:HD11	2.56	0.41
1:A:323:PRO:HB3	1:A:492:HIS:CE1	2.55	0.41
1:C:81:ASP:OD2	1:C:83:THR:OG1	2.39	0.41
1:D:87:VAL:N	1:D:531:GLU:OE1	2.53	0.41
1:D:519:VAL:HG11	1:D:537:ALA:HA	2.01	0.41
1:A:196:LEU:HB3	1:A:200:LEU:HD12	2.01	0.41
1:A:257:ALA:HA	1:A:269:ARG:HD2	2.02	0.41
1:A:408:ASN:O	1:A:409:ASP:CG	2.59	0.41
1:B:219:ALA:O	1:B:220:ASN:HB2	2.21	0.41
1:D:81:ASP:O	1:D:83:THR:HG23	2.20	0.41
1:D:281:PHE:CD1	1:D:281:PHE:N	2.87	0.41
1:D:339:TRP:O	1:D:340:LEU:C	2.58	0.41
1:A:355:LEU:O	1:A:405:ALA:N	2.52	0.41
1:D:530:VAL:O	1:D:533:ALA:N	2.53	0.41
1:C:373:ARG:HA	1:C:383:CYS:O	2.21	0.41
1:D:61:PRO:HG2	1:D:442:VAL:O	2.21	0.41
1:D:219:ALA:O	1:D:221:ALA:N	2.53	0.41
1:A:55:LEU:O	1:A:246:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASP:HA	1:B:415:PHE:CE1	2.56	0.41
1:C:363:TRP:CD1	1:C:472:PRO:HD2	2.54	0.41
1:C:469:ILE:HD12	1:C:469:ILE:N	2.36	0.41
1:C:548:PRO:O	1:C:549:ARG:CB	2.69	0.41
1:D:459:GLN:NE2	1:D:474:PRO:HD3	2.35	0.41
1:D:501:ASP:HB2	1:D:563:PRO:HA	2.02	0.41
1:A:273:ASN:HB3	1:A:296:THR:O	2.21	0.41
1:A:278:SER:HA	1:A:331:GLN:O	2.20	0.41
1:A:295:ALA:HB3	1:A:306:VAL:HB	2.03	0.41
1:B:188:TRP:HB3	1:B:224:VAL:HG21	2.03	0.41
1:C:193:TRP:HA	1:C:193:TRP:HE3	1.84	0.41
1:D:20:GLY:O	1:D:25:GLY:HA3	2.20	0.41
1:D:413:VAL:O	1:D:413:VAL:HG22	2.20	0.41
1:A:31:ARG:O	1:A:34:GLU:HB2	2.20	0.41
1:A:32:LEU:O	1:A:33:GLN:C	2.59	0.41
1:C:50:ARG:HH11	1:C:246:GLN:NE2	2.14	0.41
1:D:14:LEU:HD13	1:D:43:GLN:HB2	2.03	0.41
1:D:425:PHE:O	1:D:443:VAL:HG11	2.20	0.41
1:A:425:PHE:CZ	1:A:427:GLY:HA2	2.56	0.40
1:B:188:TRP:HB3	1:B:224:VAL:CG2	2.51	0.40
1:D:52:GLY:HA2	1:D:249:PRO:CG	2.51	0.40
1:B:513:GLU:H	1:B:513:GLU:HG3	1.35	0.40
1:C:124:LEU:O	1:C:125:ARG:C	2.58	0.40
1:C:458:ALA:O	1:C:459:GLN:C	2.58	0.40
1:D:296:THR:HG22	1:D:305:ASP:HA	2.02	0.40
1:A:355:LEU:N	1:A:406:SER:HB3	2.36	0.40
1:A:64:PRO:HG2	1:A:65:ASN:HD22	1.87	0.40
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.95	0.40
1:A:558:GLN:NE2	1:A:560:LEU:O	2.55	0.40
1:A:581:LYS:O	1:A:584:THR:HB	2.20	0.40
1:B:168:GLY:O	1:B:171:LYS:N	2.51	0.40
1:C:217:ASN:HA	1:C:409:ASP:OD1	2.22	0.40
1:C:257:ALA:O	1:C:266:GLY:HA3	2.22	0.40
1:D:123:TYR:O	1:D:123:TYR:CG	2.75	0.40
1:A:65:ASN:N	1:A:65:ASN:ND2	2.70	0.40
1:B:81:ASP:OD2	1:B:83:THR:OG1	2.38	0.40
1:B:145:LEU:HD12	1:B:145:LEU:C	2.42	0.40
1:B:371:ALA:HA	1:B:385:TYR:HB2	2.04	0.40
1:C:451:SER:C	1:C:453:GLU:N	2.75	0.40
1:D:52:GLY:HA2	1:D:249:PRO:CB	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:CYS:SG	1:D:390:CYS:SG[4_565]	1.16	1.04

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	581/596 (98%)	481 (83%)	86 (15%)	14 (2%)	6 28
1	B	577/596 (97%)	490 (85%)	79 (14%)	8 (1%)	11 37
1	C	577/596 (97%)	473 (82%)	93 (16%)	11 (2%)	8 31
1	D	581/596 (98%)	485 (84%)	85 (15%)	11 (2%)	8 31
All	All	2316/2384 (97%)	1929 (83%)	343 (15%)	44 (2%)	8 31

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ILE
1	A	217	ASN
1	C	414	PRO
1	C	548	PRO
1	C	549	ARG
1	D	118	LYS
1	D	218	VAL
1	D	406	SER
1	D	410	ILE
1	D	414	PRO
1	A	308	GLY
1	A	328	GLU
1	A	414	PRO
1	B	217	ASN
1	B	284	ASP
1	B	414	PRO

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Mol	Chain	Res	Type
1	B	580	LYS
1	C	410	ILE
1	C	450	ILE
1	D	559	LEU
1	A	86	HIS
1	A	411	GLY
1	B	310	GLU
1	B	381	ARG
1	C	69	GLU
1	C	381	ARG
1	D	232	TYR
1	A	214	TYR
1	A	215	GLU
1	A	220	ASN
1	A	406	SER
1	A	409	ASP
1	C	222	SER
1	C	577	THR
1	D	31	ARG
1	D	341	LYS
1	A	486	PRO
1	A	513	GLU
1	C	220	ASN
1	C	273	ASN
1	D	192	PHE
1	B	418	GLY
1	B	486	PRO
1	D	213	GLY

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	387/500 (77%)	341 (88%)	46 (12%)	5 19
1	B	432/500 (86%)	383 (89%)	49 (11%)	6 21
1	C	385/500 (77%)	339 (88%)	46 (12%)	5 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	445/500 (89%)	403 (91%)	42 (9%)	8 30
All	All	1649/2000 (82%)	1466 (89%)	183 (11%)	6 22

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	46	GLU
1	A	56	PHE
1	A	65	ASN
1	A	67	VAL
1	A	69	GLU
1	A	70	VAL
1	A	88	MET
1	A	135	THR
1	A	139	ASP
1	A	148	SER
1	A	164	ASN
1	A	186	GLU
1	A	199	VAL
1	A	208	MET
1	A	236	THR
1	A	237	VAL
1	A	245	PHE
1	A	285	THR
1	A	296	THR
1	A	299	VAL
1	A	311	GLU
1	A	312	ILE
1	A	325	ARG
1	A	344	ILE
1	A	345	ASP
1	A	349	VAL
1	A	375	VAL
1	A	383	CYS
1	A	386	MET
1	A	412	THR
1	A	413	VAL
1	A	416	TRP
1	A	431	LYS
1	A	437	ILE
1	A	456	ARG

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Mol	Chain	Res	Type
1	A	459	GLN
1	A	460	ARG
1	A	463	THR
1	A	464	SER
1	A	469	ILE
1	A	478	VAL
1	A	485	ASP
1	A	515	GLU
1	A	566	VAL
1	A	568	ILE
1	B	15	ASP
1	B	23	VAL
1	B	38	ASP
1	B	56	PHE
1	B	70	VAL
1	B	111	ASP
1	B	119	ASP
1	B	121	LEU
1	B	127	GLU
1	B	128	ARG
1	B	159	VAL
1	B	170	ASP
1	B	171	LYS
1	B	182	VAL
1	B	185	LYS
1	B	197	TYR
1	B	214	TYR
1	B	222	SER
1	B	237	VAL
1	B	242	LYS
1	B	245	PHE
1	B	282	SER
1	B	284	ASP
1	B	285	THR
1	B	299	VAL
1	B	304	SER
1	B	316	ARG
1	B	342	GLU
1	B	365	ARG
1	B	397	LYS
1	B	409	ASP
1	B	410	ILE

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Mol	Chain	Res	Type
1	B	415	PHE
1	B	417	LYS
1	B	426	GLU
1	B	438	ASP
1	B	440	ASN
1	B	469	ILE
1	B	478	VAL
1	B	491	TRP
1	B	497	ASN
1	B	513	GLU
1	B	519	VAL
1	B	521	GLU
1	B	568	ILE
1	B	569	ASP
1	B	574	LEU
1	B	582	THR
1	B	587	THR
1	C	16	VAL
1	C	19	ILE
1	C	41	ARG
1	C	47	TYR
1	C	54	ARG
1	C	58	ILE
1	C	74	ARG
1	C	75	TRP
1	C	81	ASP
1	C	144	LYS
1	C	148	SER
1	C	182	VAL
1	C	193	TRP
1	C	198	ARG
1	C	237	VAL
1	C	245	PHE
1	C	264	ILE
1	C	278	SER
1	C	282	SER
1	C	297	ARG
1	C	298	THR
1	C	302	LYS
1	C	303	THR
1	C	304	SER
1	C	312	ILE

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Mol	Chain	Res	Type
1	C	342	GLU
1	C	373	ARG
1	C	375	VAL
1	C	377	ASP
1	C	379	PRO
1	C	380	ILE
1	C	386	MET
1	C	388	THR
1	C	392	GLN
1	C	408	ASN
1	C	412	THR
1	C	416	TRP
1	C	442	VAL
1	C	450	ILE
1	C	459	GLN
1	C	478	VAL
1	C	539	SER
1	C	566	VAL
1	C	568	ILE
1	C	569	ASP
1	C	587	THR
1	D	12	GLN
1	D	15	ASP
1	D	46	GLU
1	D	75	TRP
1	D	88	MET
1	D	97	LYS
1	D	101	LYS
1	D	148	SER
1	D	182	VAL
1	D	189	ARG
1	D	208	MET
1	D	224	VAL
1	D	235	LYS
1	D	237	VAL
1	D	242	LYS
1	D	245	PHE
1	D	280	GLN
1	D	281	PHE
1	D	285	THR
1	D	286	GLU
1	D	290	ARG

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Mol	Chain	Res	Type
1	D	313	ILE
1	D	330	ILE
1	D	349	VAL
1	D	351	SER
1	D	390	CYS
1	D	406	SER
1	D	408	ASN
1	D	409	ASP
1	D	413	VAL
1	D	421	ASP
1	D	428	TYR
1	D	438	ASP
1	D	440	ASN
1	D	441	GLU
1	D	459	GLN
1	D	497	ASN
1	D	521	GLU
1	D	524	SER
1	D	539	SER
1	D	566	VAL
1	D	584	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	65	ASN
1	A	86	HIS
1	A	202	ASN
1	A	226	GLN
1	A	246	GLN
1	A	343	ASN
1	A	459	GLN
1	A	558	GLN
1	B	59	ASN
1	B	65	ASN
1	B	86	HIS
1	B	163	HIS
1	B	177	GLN
1	B	273	ASN
1	B	292	HIS
1	B	314	HIS

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Mol	Chain	Res	Type
1	B	382	GLN
1	B	392	GLN
1	B	408	ASN
1	B	449	GLN
1	B	459	GLN
1	B	497	ASN
1	B	558	GLN
1	C	59	ASN
1	C	65	ASN
1	C	86	HIS
1	C	246	GLN
1	C	273	ASN
1	C	382	GLN
1	C	447	GLN
1	C	449	GLN
1	C	459	GLN
1	C	468	GLN
1	C	527	GLN
1	D	40	GLN
1	D	177	GLN
1	D	314	HIS
1	D	408	ASN
1	D	449	GLN
1	D	459	GLN
1	D	468	GLN
1	D	527	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	601	-	53,58,58	0.61	0	68,89,89	0.81	2 (2%)
2	FAD	D	601	-	53,58,58	0.62	0	68,89,89	0.86	2 (2%)
2	FAD	B	601	-	53,58,58	0.67	0	68,89,89	0.76	1 (1%)
2	FAD	C	601	-	53,58,58	0.60	0	68,89,89	0.82	1 (1%)

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	601	-	-	11/30/50/50	0/6/6/6
2	FAD	D	601	-	-	7/30/50/50	0/6/6/6
2	FAD	B	601	-	-	9/30/50/50	0/6/6/6
2	FAD	C	601	-	-	12/30/50/50	0/6/6/6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FAD	C5A-C6A-N6A	2.32	123.88	120.35
2	B	601	FAD	C5A-C6A-N6A	2.30	123.84	120.35
2	A	601	FAD	C4'-C3'-C2'	2.29	118.12	113.36
2	D	601	FAD	C4'-C3'-C2'	2.28	118.10	113.36
2	C	601	FAD	C5A-C6A-N6A	2.26	123.78	120.35
2	D	601	FAD	C5A-C6A-N6A	2.05	123.46	120.35

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C1'-C2'-C3'-O3'
2	B	601	FAD	C1'-C2'-C3'-C4'
2	C	601	FAD	C5B-O5B-PA-O1A
2	C	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	PA-O3P-P-O5'
2	D	601	FAD	C5B-O5B-PA-O1A
2	D	601	FAD	O4'-C4'-C5'-O5'
2	D	601	FAD	PA-O3P-P-O5'
2	C	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	O4'-C4'-C5'-O5'
2	B	601	FAD	O2'-C2'-C3'-O3'
2	C	601	FAD	C2'-C3'-C4'-O4'
2	C	601	FAD	C3'-C4'-C5'-O5'
2	C	601	FAD	C2'-C3'-C4'-C5'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	A	601	FAD	PA-O3P-P-O5'
2	A	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C5B-O5B-PA-O3P
2	D	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	P-O3P-PA-O2A
2	B	601	FAD	C5B-O5B-PA-O2A
2	C	601	FAD	O4'-C4'-C5'-O5'
2	C	601	FAD	O3'-C3'-C4'-C5'
2	C	601	FAD	O3'-C3'-C4'-O4'
2	D	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	P-O3P-PA-O1A
2	C	601	FAD	C5B-O5B-PA-O2A
2	D	601	FAD	C5B-O5B-PA-O2A

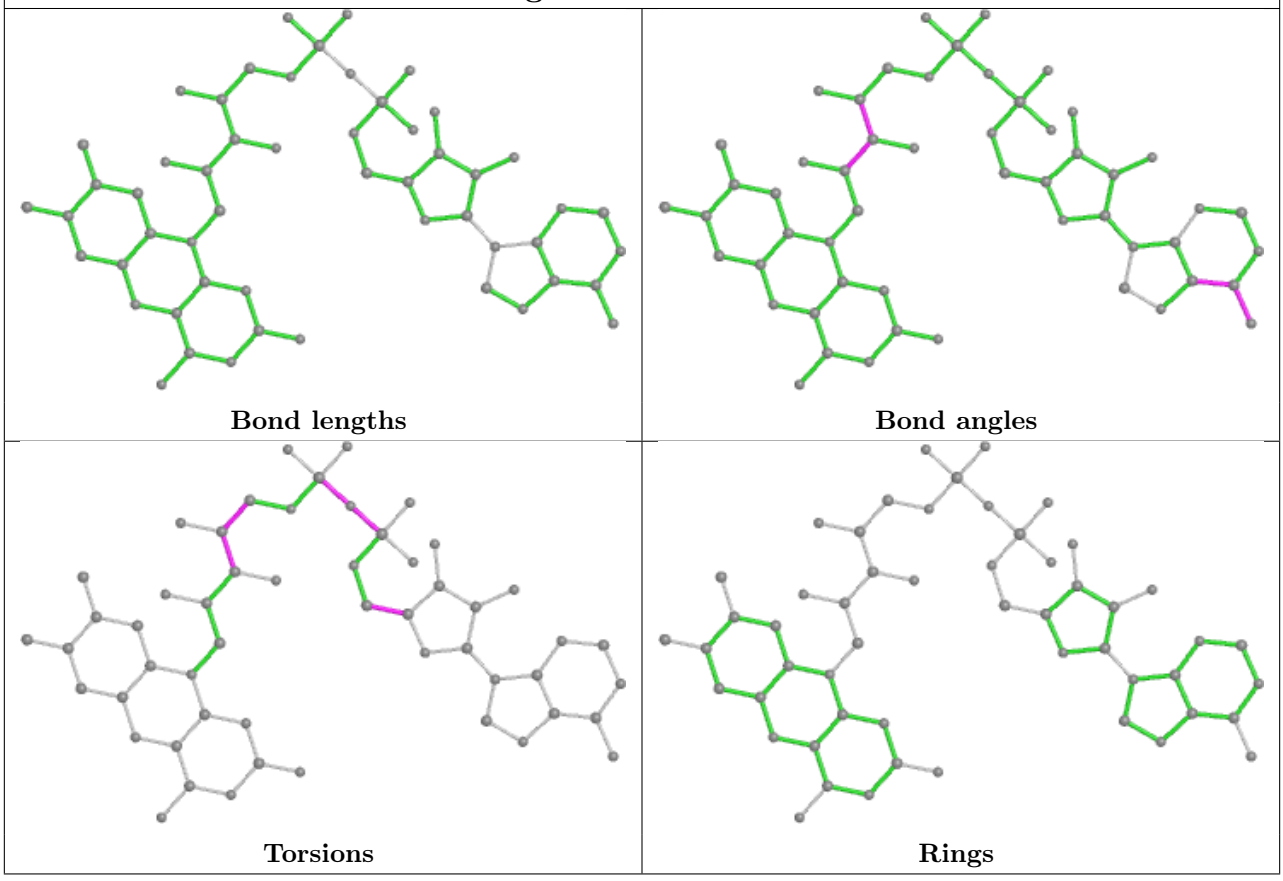
There are no ring outliers.

4 monomers are involved in 10 short contacts:

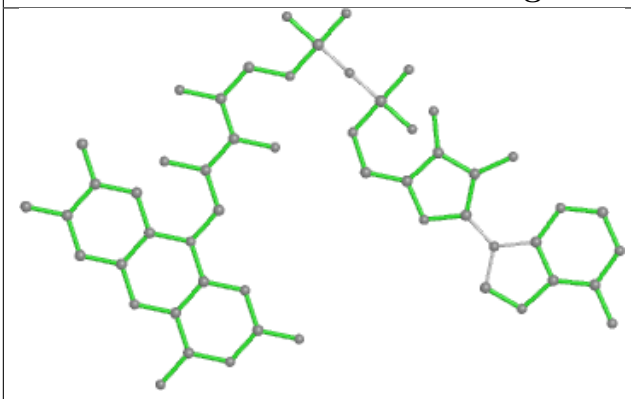
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	1	0
2	D	601	FAD	4	0
2	B	601	FAD	4	0
2	C	601	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

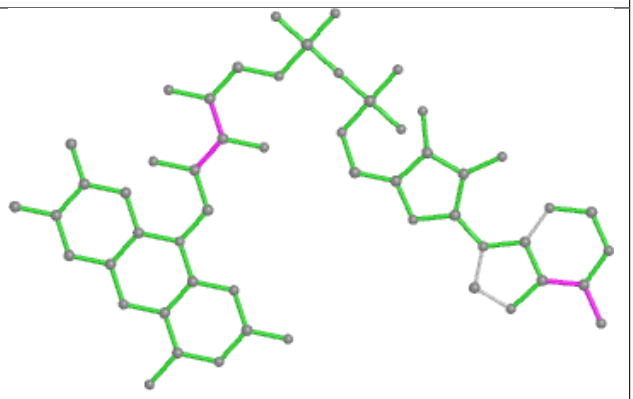
Ligand FAD A 601



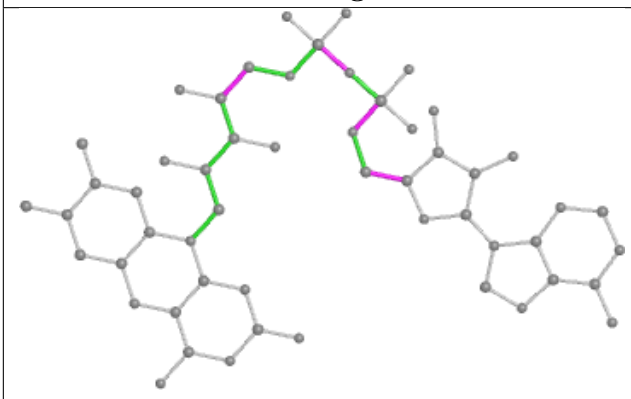
Ligand FAD D 601



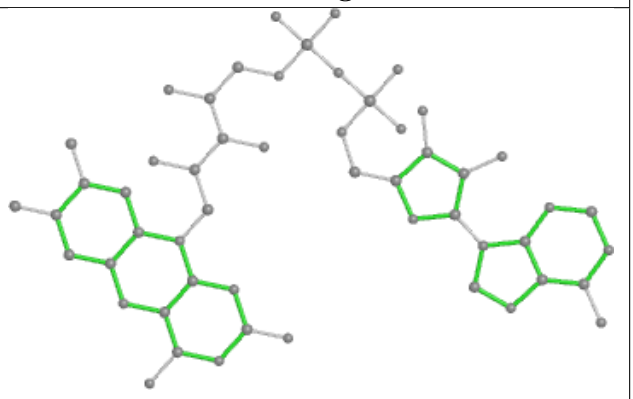
Bond lengths



Bond angles

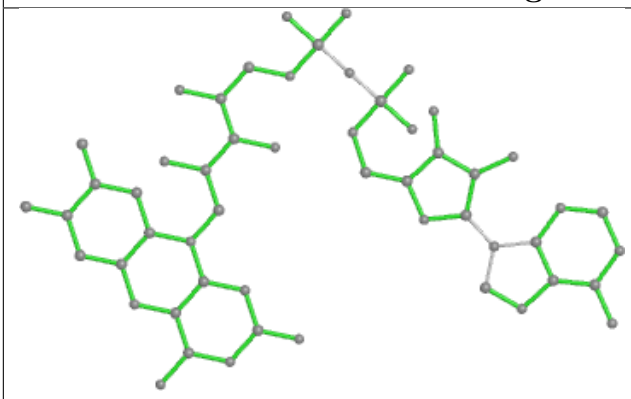


Torsions

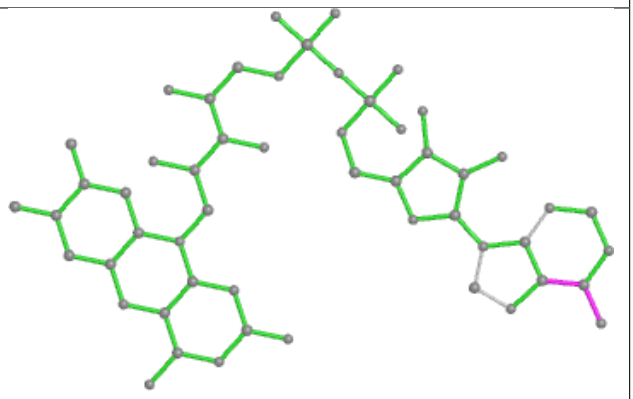


Rings

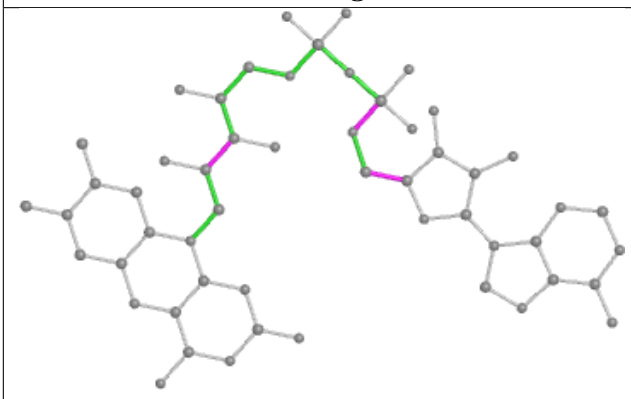
Ligand FAD B 601



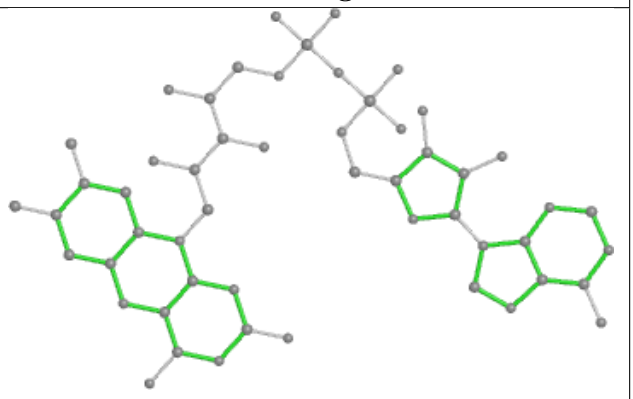
Bond lengths



Bond angles

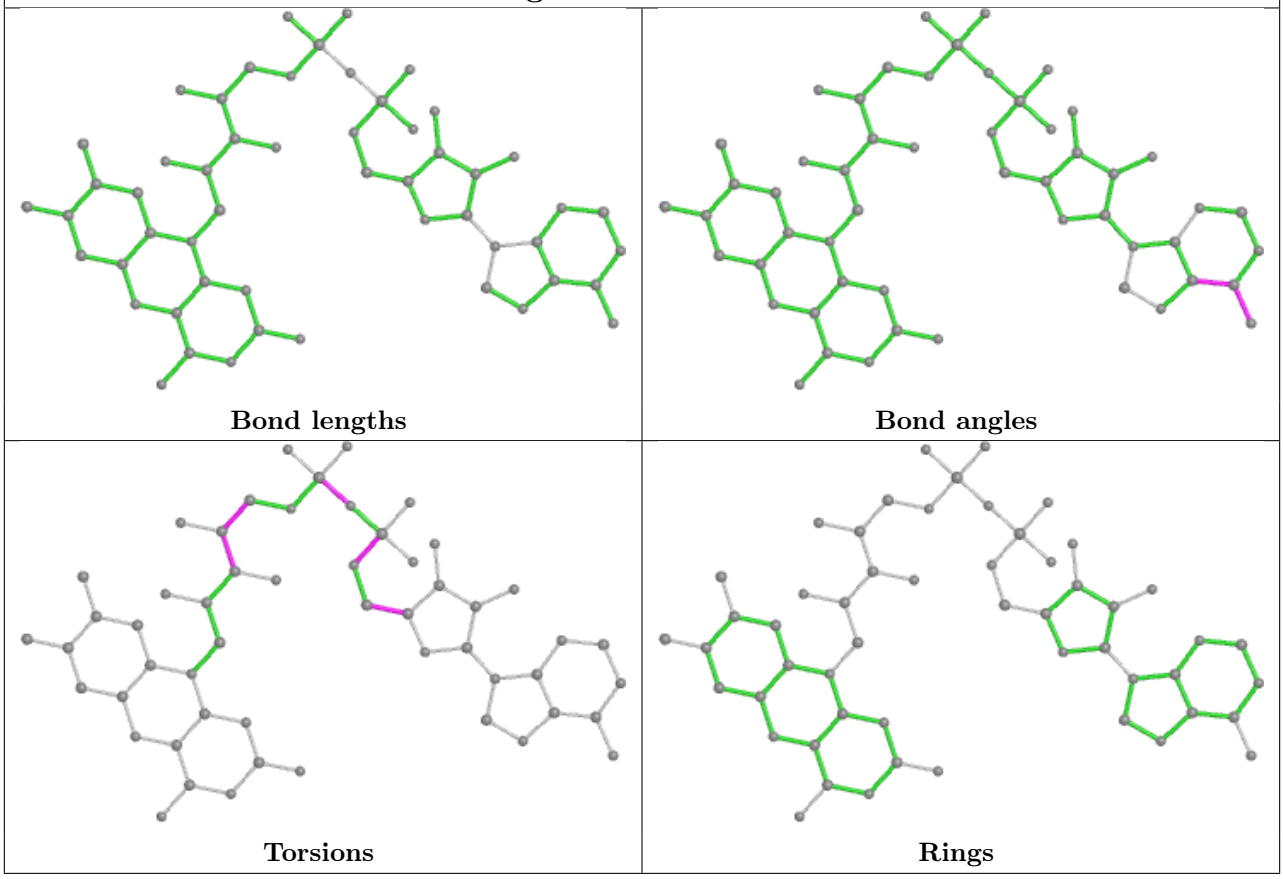


Torsions



Rings

Ligand FAD C 601



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	583/596 (97%)	0.31	23 (3%)	39	38	60, 100, 135, 184	0
1	B	581/596 (97%)	0.22	13 (2%)	62	60	59, 91, 118, 148	0
1	C	581/596 (97%)	0.43	42 (7%)	15	17	66, 99, 129, 164	0
1	D	583/596 (97%)	0.09	12 (2%)	63	62	53, 76, 112, 156	0
All	All	2328/2384 (97%)	0.26	90 (3%)	39	38	53, 92, 126, 184	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	ASN	7.9
1	A	261	GLY	7.1
1	C	442	VAL	4.5
1	B	212	GLY	4.3
1	A	179	GLN	4.1
1	A	574	LEU	3.8
1	A	45	PHE	3.8
1	A	573	ALA	3.7
1	C	412	THR	3.7
1	B	281	PHE	3.7
1	C	318	VAL	3.7
1	B	410	ILE	3.6
1	C	550	PRO	3.5
1	B	214	TYR	3.5
1	C	62	GLY	3.5
1	C	477	ALA	3.5
1	C	271	ARG	3.4
1	C	510	PRO	3.4
1	C	542	GLN	3.3
1	A	216	ALA	3.3
1	C	214	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	30	TRP	3.2
1	C	218	VAL	3.1
1	C	45	PHE	3.1
1	D	217	ASN	3.1
1	C	575	ALA	3.1
1	C	293	PHE	3.1
1	C	552	TRP	3.0
1	C	307	PRO	3.0
1	D	179	GLN	3.0
1	A	294	GLN	2.9
1	A	442	VAL	2.9
1	B	411	GLY	2.8
1	C	572	PRO	2.8
1	B	429	GLN	2.8
1	A	335	PHE	2.8
1	D	571	PRO	2.8
1	C	551	ALA	2.7
1	A	262	GLY	2.7
1	A	437	ILE	2.7
1	A	43	GLN	2.7
1	A	518	ILE	2.6
1	C	16	VAL	2.6
1	A	278	SER	2.6
1	D	572	PRO	2.6
1	C	30	TRP	2.5
1	A	426	GLU	2.5
1	C	52	GLY	2.5
1	C	212	GLY	2.5
1	C	541	LEU	2.4
1	C	95	GLU	2.4
1	C	511	VAL	2.4
1	A	439	ALA	2.4
1	C	36	GLN	2.4
1	C	545	PHE	2.3
1	D	435	GLY	2.3
1	D	568	ILE	2.3
1	C	39	HIS	2.3
1	A	517	TYR	2.3
1	D	110	PRO	2.3
1	B	351	SER	2.3
1	D	476	SER	2.3
1	C	93	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	576	CYS	2.2
1	C	478	VAL	2.2
1	C	557	TYR	2.2
1	A	334	LEU	2.2
1	C	297	ARG	2.2
1	D	292	HIS	2.2
1	B	33	GLN	2.2
1	A	20	GLY	2.2
1	B	405	ALA	2.2
1	A	305	ASP	2.1
1	B	383	CYS	2.1
1	D	434	GLN	2.1
1	A	563	PRO	2.1
1	C	425	PHE	2.1
1	C	408	ASN	2.1
1	D	518	ILE	2.1
1	D	108	ASN	2.1
1	C	574	LEU	2.1
1	A	411	GLY	2.0
1	A	318	VAL	2.0
1	C	573	ALA	2.0
1	B	335	PHE	2.0
1	C	515	GLU	2.0
1	C	277	ALA	2.0
1	C	17	ALA	2.0
1	C	33	GLN	2.0
1	B	41	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

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

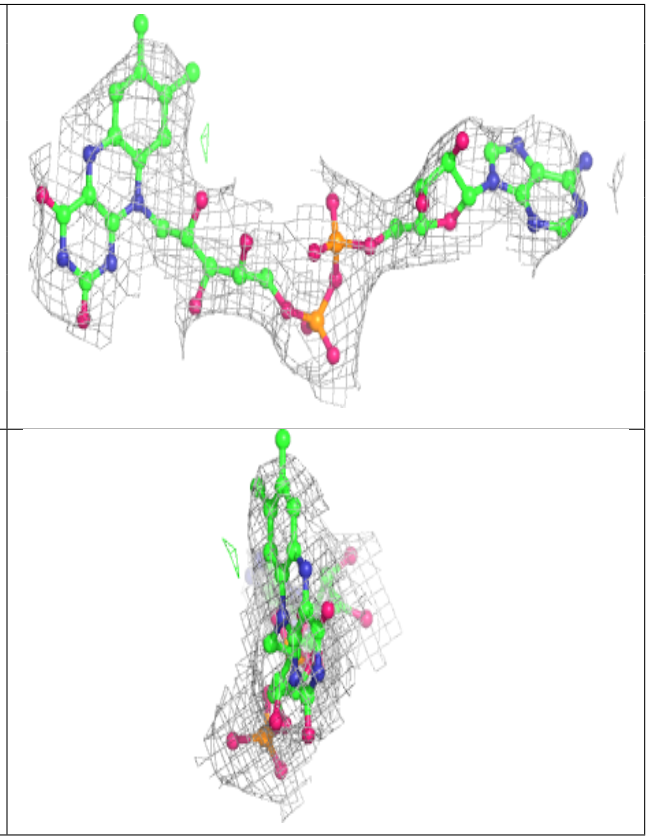
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

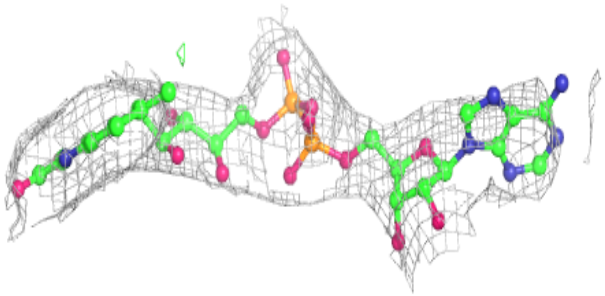
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	A	601	53/53	0.92	0.20	86,98,141,152	0
2	FAD	B	601	53/53	0.92	0.24	76,91,101,106	0
2	FAD	C	601	53/53	0.93	0.22	81,100,124,138	0
2	FAD	D	601	53/53	0.95	0.20	61,67,89,102	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD A 601:

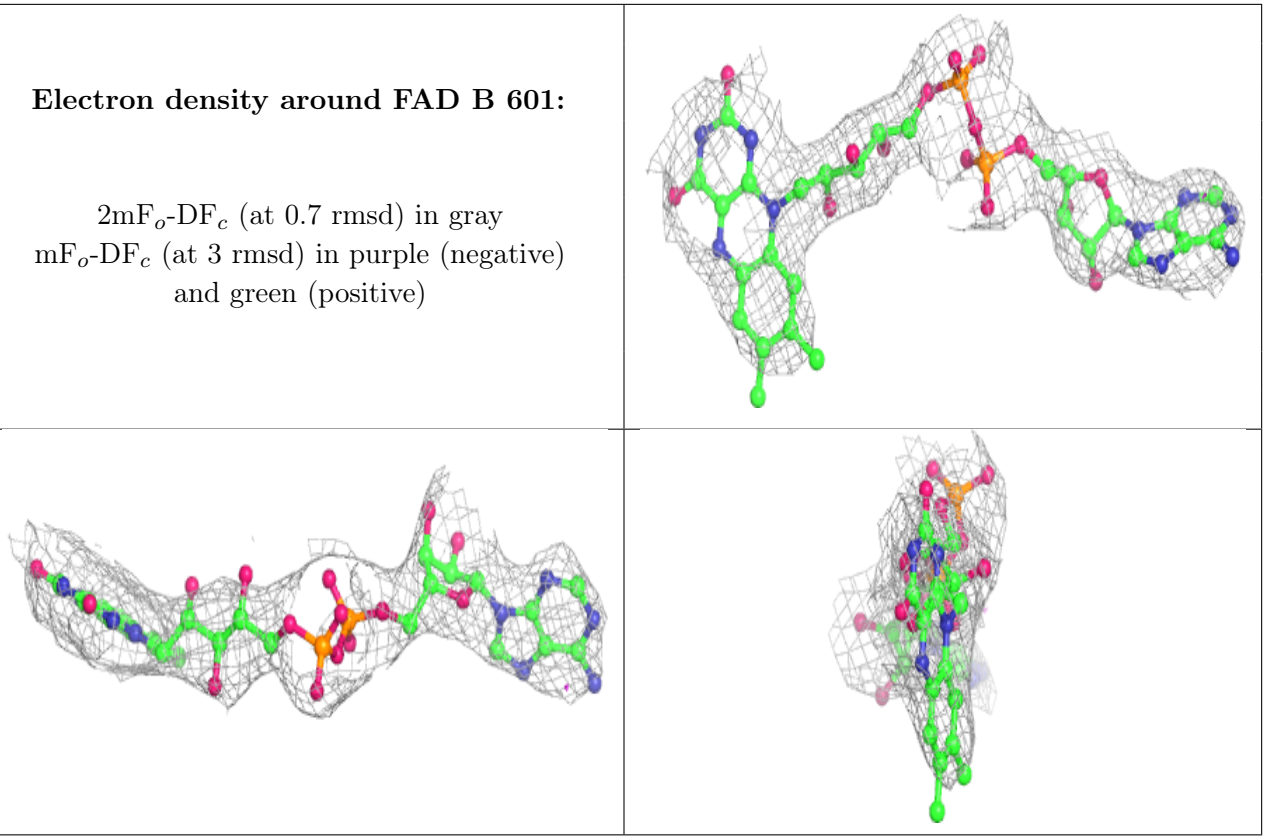
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





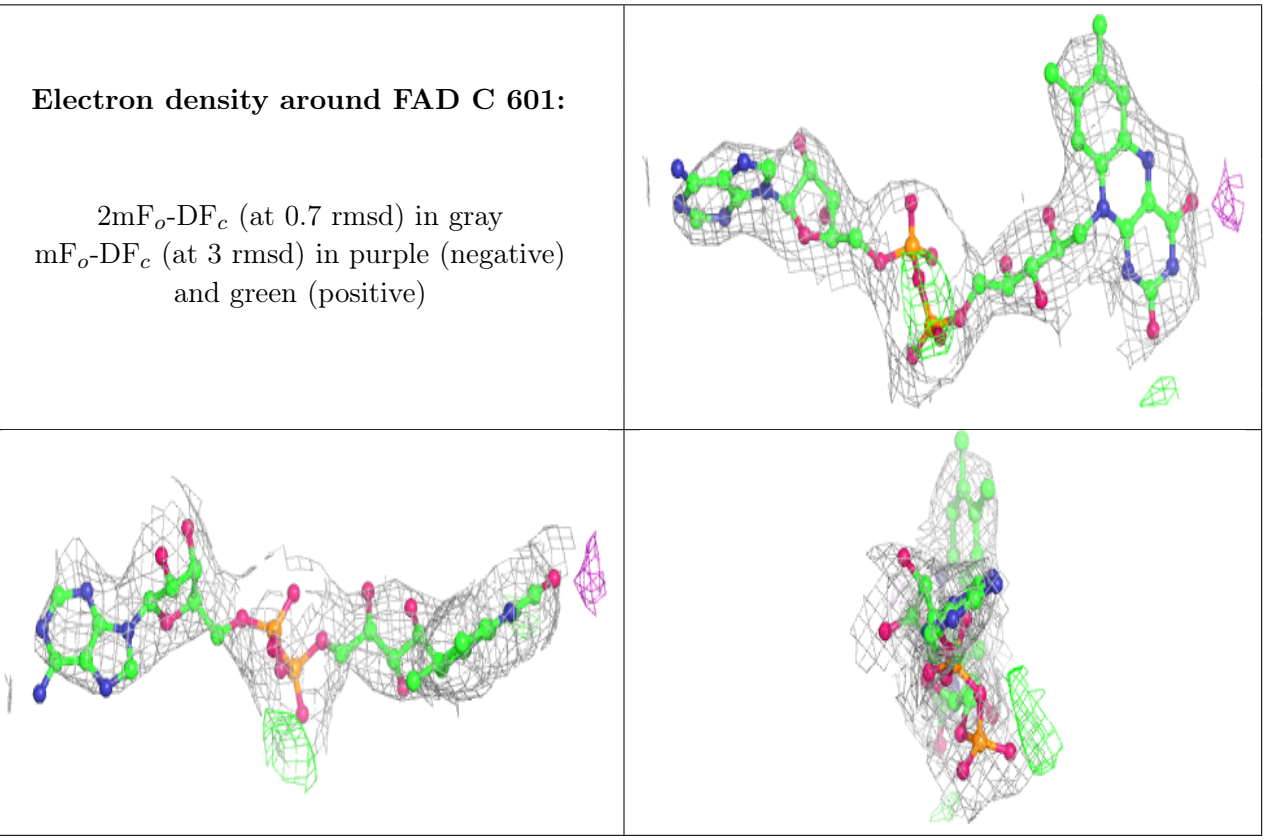
Electron density around FAD B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



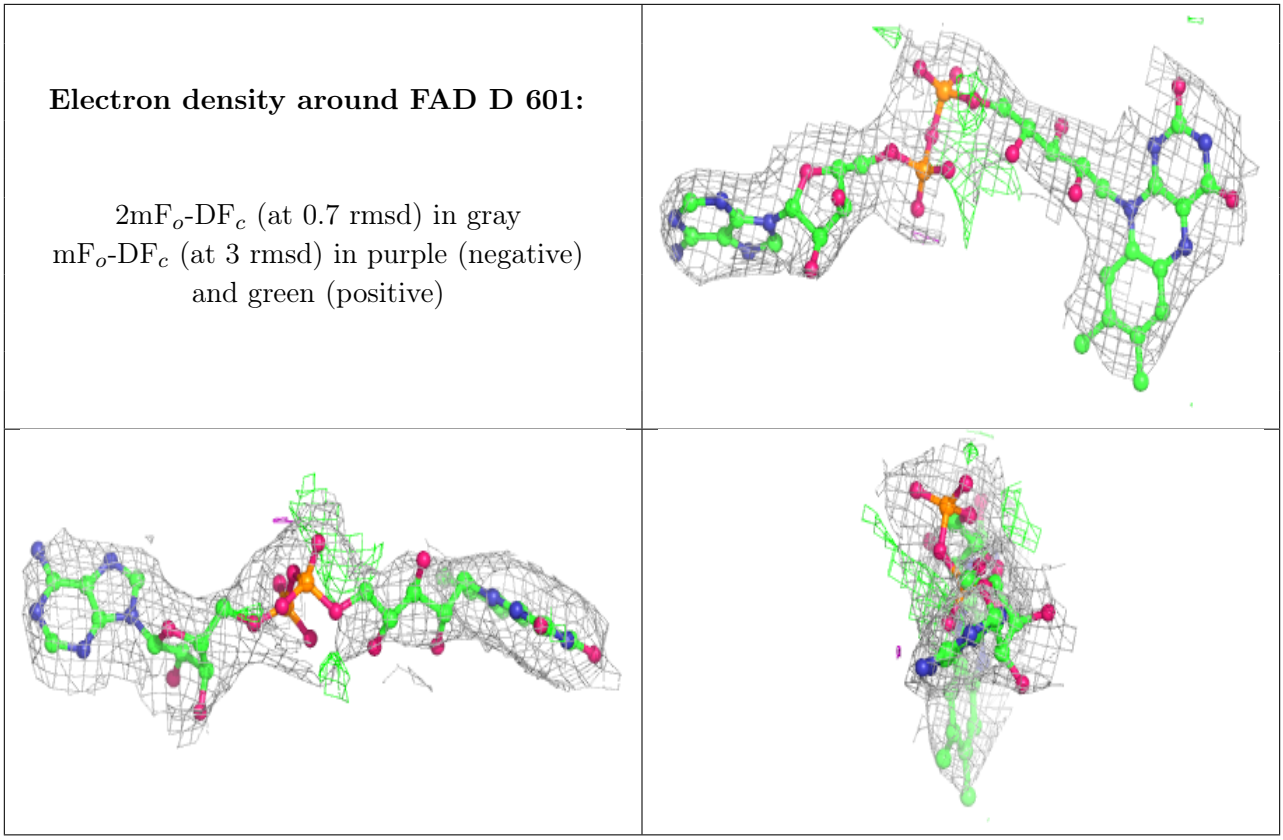
Electron density around FAD C 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FAD D 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.