Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:25 AM GMT

PDB ID	:	2ACZ
Title	:	Complex II (Succinate Dehydrogenase) From E. Coli with Atpenin A5 inhibitor co-crystallized at the ubiquinone binding site
Authors	:	Horsefield, R.; Yankovskaya, V.; Sexton, G.; Whittingham, W.; Shiomi, K.; Omura, S.; Byrne, B.; Cecchini, G.; Iwata, S.
Deposited on	:	2005-07-19
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

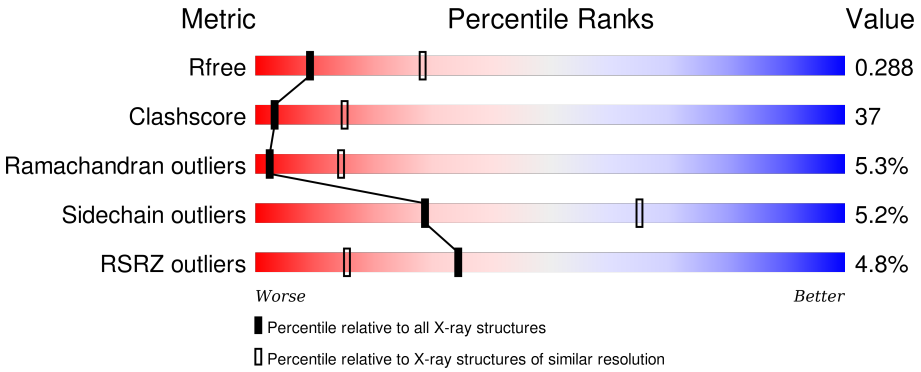
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	588	6% 40% 52% 7%
2	B	238	3% 48% 47%
3	C	129	7% 52% 44%
4	D	115	% 57% 41%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	AT5	C	131	-	-	-	X
12	CDN	C	132	X	-	-	X
5	OAA	A	589	-	-	X	X
9	F3S	B	304	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8521 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 Succinate dehydrogenase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	91	0	0
			4522	2812	821	861	28			

- Molecule 2 is a protein called Succinate dehydrogenase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1869	1172	329	348	20			

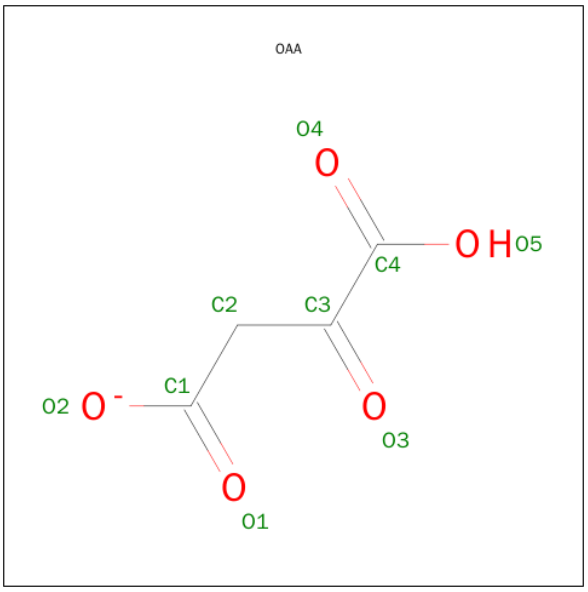
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b556 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	129	Total	C	N	O	S	0	0	0
			1008	668	166	168	6			

- Molecule 4 is a protein called Succinate dehydrogenase hydrophobic membrane anchor protein.

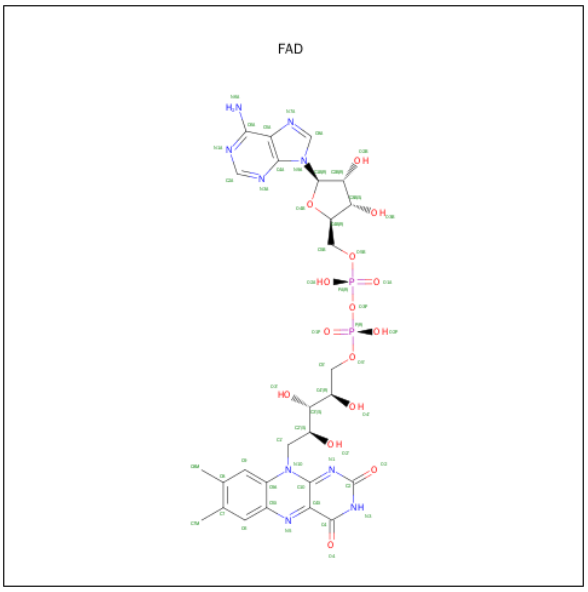
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	113	Total	C	N	O	S	0	0	0
			898	615	136	144	3			

- Molecule 5 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



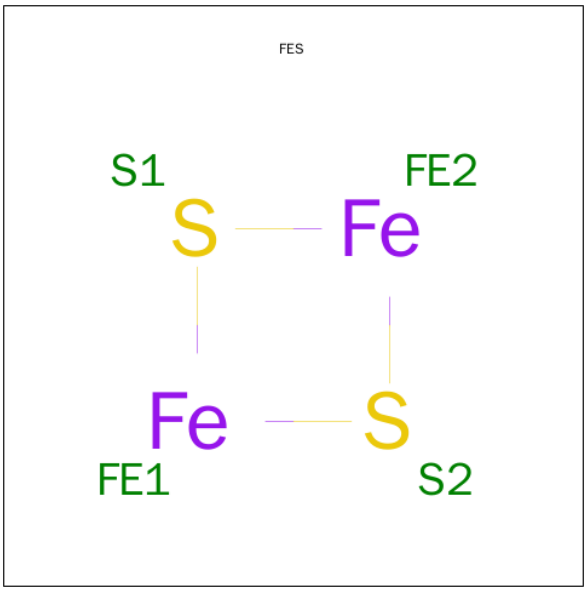
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



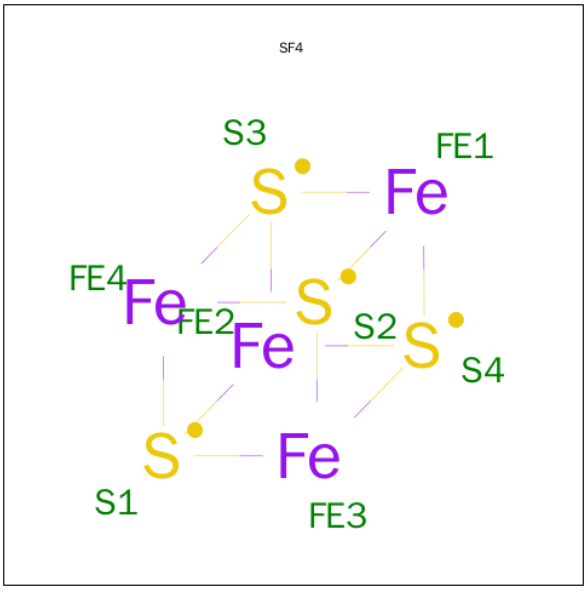
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



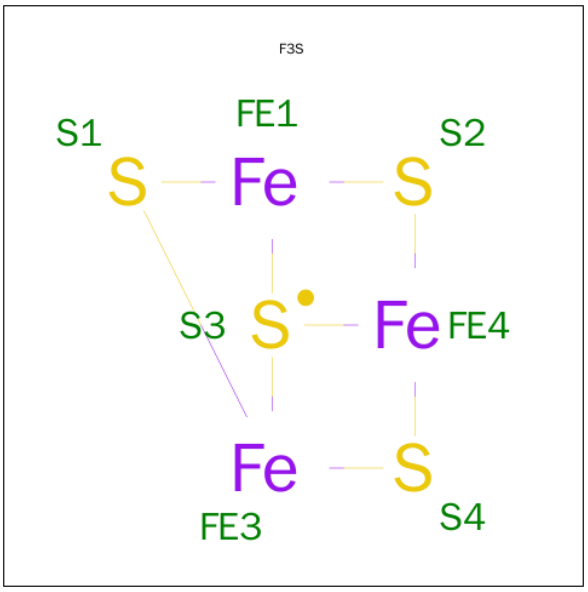
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	B	1	4	2	2	0	0

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



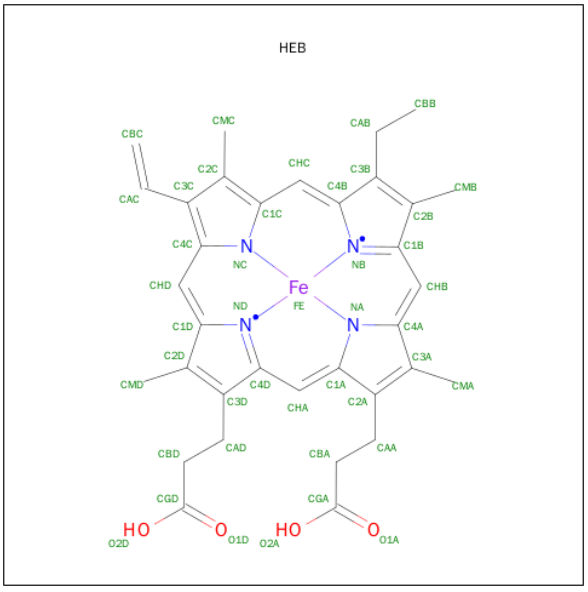
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	B	1	8	4	4	0	0

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



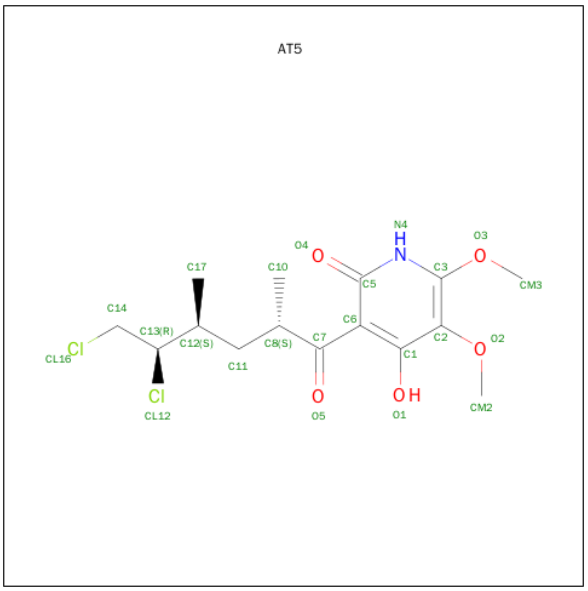
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	B	1	7	3	4	0	0

- Molecule 10 is HEME B/C (three-letter code: HEB) (formula: $C_{34}H_{34}FeN_4O_4$).



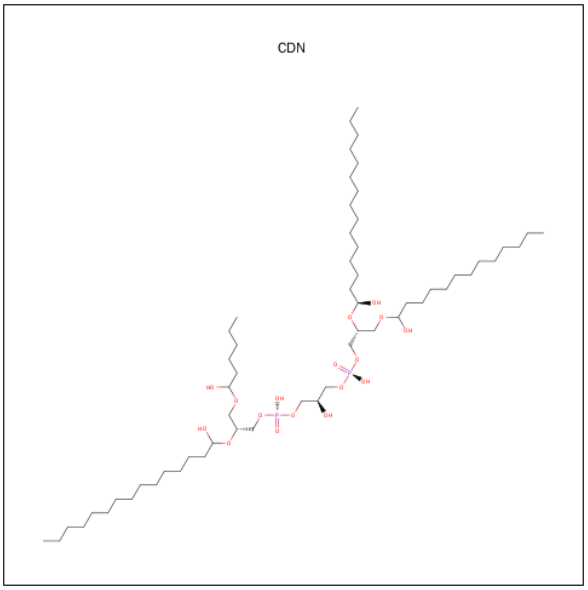
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
10	C	1	43	34	1	4	4	0	0

- Molecule 11 is 3-[(2S,4S,5R)-5,6-DICHLORO-2,4-DIMETHYL-1-OXOHEXYL]-4-HYDROXY-5,6-DIMETHOXY-2(1H)-PYRIDINONE (three-letter code: AT5) (formula: $C_{15}H_{21}Cl_2NO_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Cl	N	O	0	0
			23	15	2	1	5		

- Molecule 12 is CARDIOLIPIN (three-letter code: CDN) (formula: $C_{58}H_{120}O_{17}P_2$).



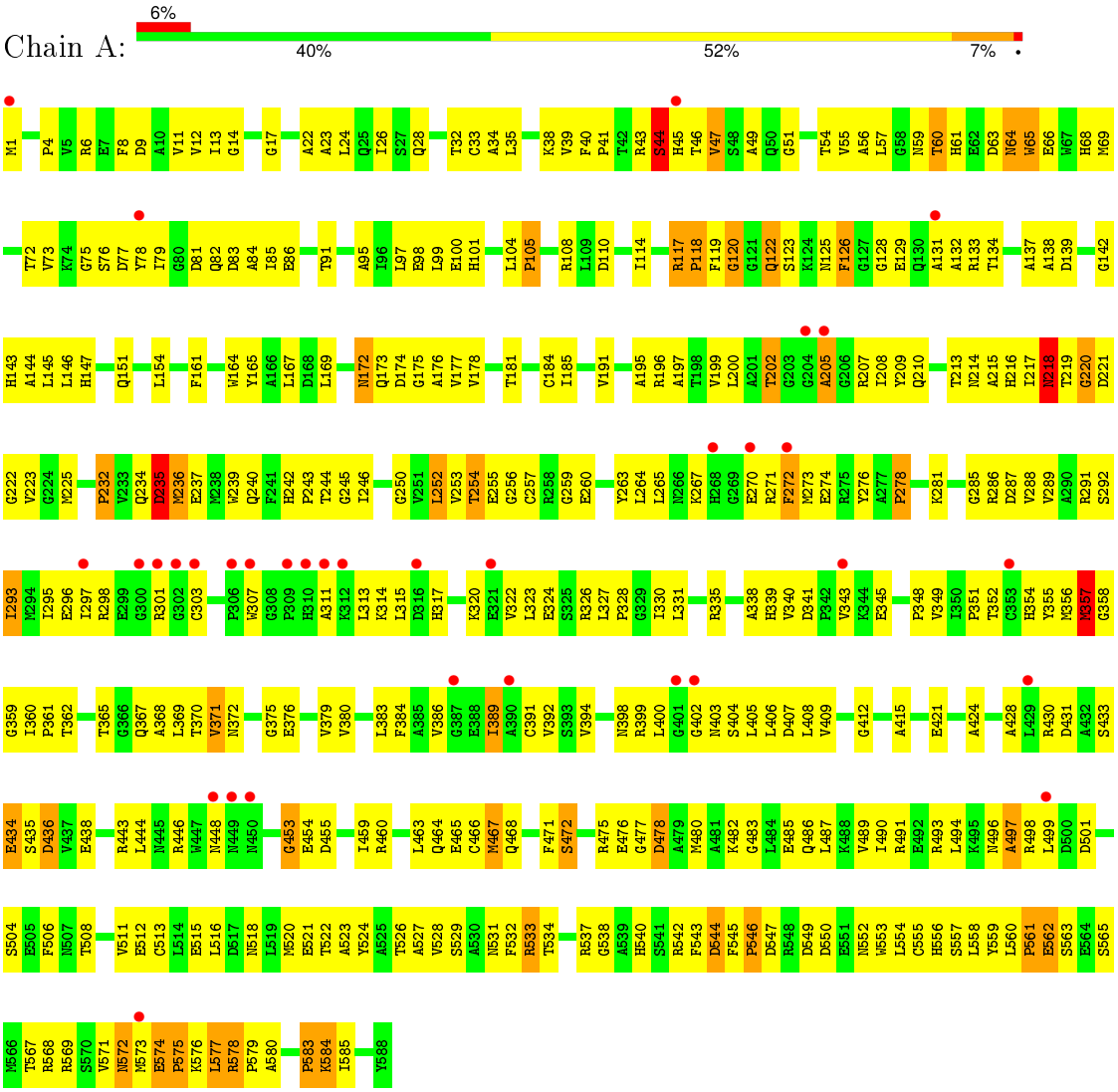
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	O	P	0	0
			77	58	17	2		

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.

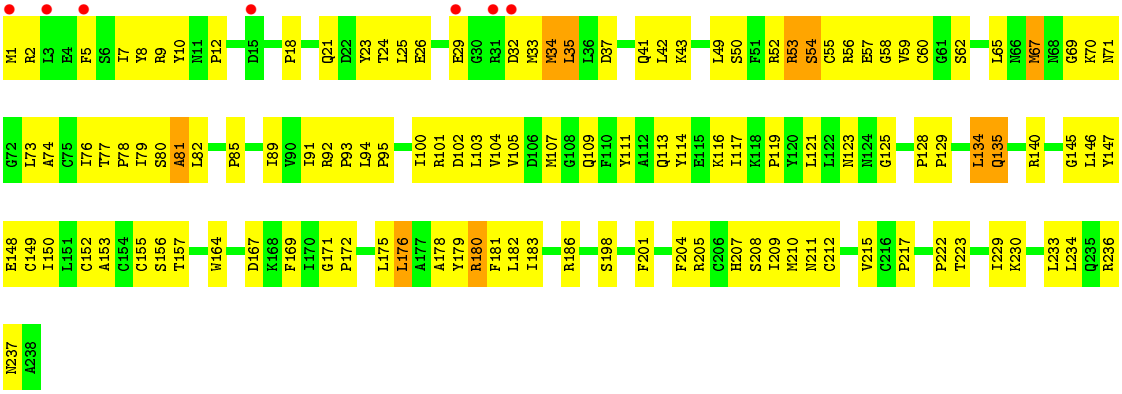
- Molecule 1: Succinate dehydrogenase flavoprotein subunit

Chain A:

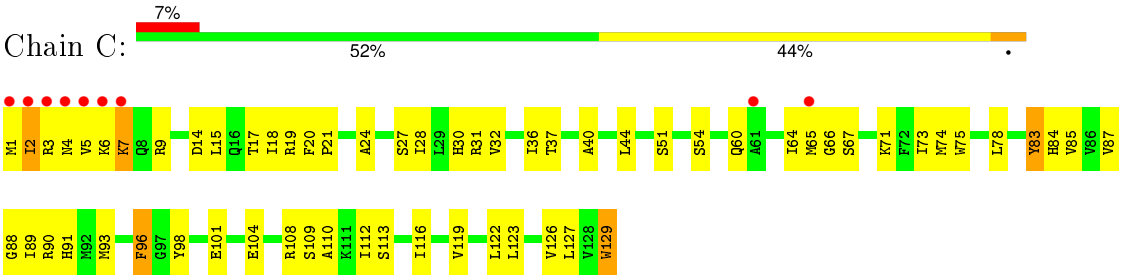


- Molecule 2: Succinate dehydrogenase iron-sulfur protein

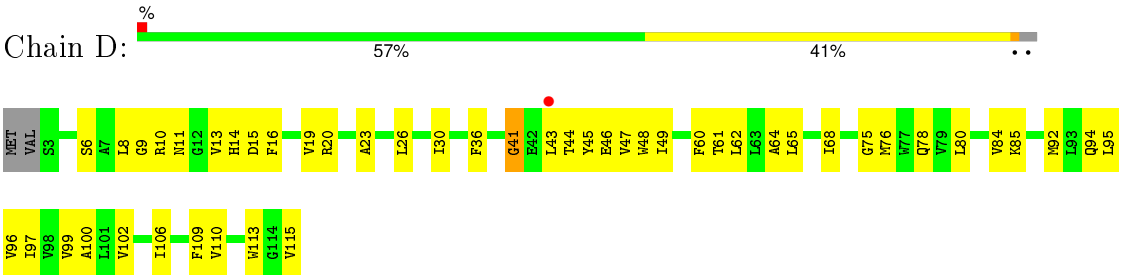
Chain B:



- Molecule 3: Succinate dehydrogenase cytochrome b556 subunit



- Molecule 4: Succinate dehydrogenase hydrophobic membrane anchor protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	138.76Å 138.76Å 521.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.10 39.40 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.10) 97.9 (39.40-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.308 0.251 , 0.288	Depositor DCC
R_{free} test set	966 reflections (2.84%)	DCC
Wilson B-factor (Å^2)	80.4	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 34954 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8521	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OAA, CDN, F3S, AT5, FES, HEB, SF4, 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	0.45	1/4611 (0.0%)	0.68	0/6237
2	B	0.46	0/1908	0.72	0/2578
3	C	0.51	0/1030	0.68	0/1394
4	D	0.56	0/923	0.65	0/1262
All	All	0.47	1/8472 (0.0%)	0.68	0/11471

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	SER	C-N	10.51	1.58	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4522	0	4426	390	0
2	B	1869	0	1850	142	0
3	C	1008	0	1066	78	0
4	D	898	0	936	45	0
5	A	9	0	2	5	0
6	A	53	0	29	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	4	0	0	1	0
8	B	8	0	0	0	0
9	B	7	0	0	4	0
10	C	43	0	32	10	0
11	C	23	0	20	4	0
12	C	77	0	112	19	0
All	All	8521	0	8473	630	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 37.

All (630) 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)
10:C:130:HEB:HBB1	12:C:132:CDN:C24	1.84	1.07
3:C:6:LYS:HE3	3:C:7:LYS:HG3	1.33	1.06
1:A:577:LEU:HD21	1:A:580:ALA:HA	1.38	1.04
2:B:180:ARG:HH11	2:B:180:ARG:HG2	1.23	1.02
1:A:578:ARG:HB3	1:A:579:PRO:HD3	1.39	1.00
1:A:577:LEU:HD23	1:A:577:LEU:H	1.23	1.00
1:A:119:PHE:HB2	2:B:135:GLN:H	1.28	0.96
1:A:119:PHE:CD2	2:B:134:LEU:HA	2.01	0.96
4:D:9:GLY:HA2	4:D:14:HIS:HD2	1.31	0.94
1:A:205:ALA:HB2	1:A:220:GLY:H	1.31	0.93
1:A:240:GLN:HB2	1:A:357:MET:HE1	1.50	0.93
1:A:362:THR:HG22	1:A:368:ALA:HA	1.49	0.92
10:C:130:HEB:HAC	4:D:23:ALA:HB1	1.51	0.92
3:C:2:ILE:HG12	3:C:5:VAL:HB	1.51	0.92
1:A:577:LEU:H	1:A:577:LEU:CD2	1.83	0.90
2:B:34:MET:HA	2:B:34:MET:HE3	1.51	0.89
1:A:128:GLY:HA3	1:A:400:LEU:HD11	1.51	0.88
2:B:94:LEU:HB3	2:B:157:THR:HG21	1.55	0.88
1:A:205:ALA:CB	1:A:220:GLY:H	1.87	0.88
12:C:132:CDN:OA3	4:D:41:GLY:O	1.91	0.87
1:A:82:GLN:HB2	1:A:577:LEU:HB3	1.57	0.85
2:B:180:ARG:NH1	2:B:180:ARG:HG2	1.89	0.83
2:B:172:PRO:HG3	9:B:304:F3S:S3	2.18	0.83
1:A:54:THR:HG22	1:A:134:THR:OG1	1.78	0.83
3:C:78:LEU:HD21	12:C:132:CDN:H162	1.61	0.83
1:A:9:ASP:H	1:A:32:THR:CG2	1.91	0.82
1:A:324:GLU:O	1:A:328:PRO:HG3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:GLU:HB2	1:A:568:ARG:HH12	1.45	0.81
1:A:234:GLN:HG3	1:A:361:PRO:HG3	1.62	0.81
1:A:117:ARG:HG3	1:A:118:PRO:HD2	1.63	0.81
1:A:257:CYS:HB3	1:A:315:LEU:HD21	1.63	0.81
2:B:9:ARG:HH12	2:B:49:LEU:HA	1.46	0.81
1:A:559:TYR:HB2	1:A:569:ARG:HH21	1.45	0.80
2:B:35:LEU:HD21	2:B:91:ILE:HD11	1.64	0.80
4:D:9:GLY:HA2	4:D:14:HIS:CD2	2.17	0.79
1:A:263:TYR:HB3	1:A:265:LEU:HD21	1.63	0.79
3:C:60:GLN:O	3:C:64:ILE:HG13	1.83	0.79
3:C:32:VAL:O	3:C:36:ILE:HD13	1.82	0.78
2:B:35:LEU:O	2:B:35:LEU:HD12	1.84	0.78
3:C:1:MET:HG3	3:C:6:LYS:HA	1.65	0.78
1:A:331:LEU:O	1:A:335:ARG:HG3	1.83	0.77
2:B:140:ARG:HD3	2:B:140:ARG:O	1.84	0.77
1:A:9:ASP:H	1:A:32:THR:HG23	1.47	0.77
4:D:62:LEU:HD23	4:D:65:LEU:HD12	1.66	0.77
1:A:263:TYR:HB2	1:A:314:LYS:HB3	1.67	0.76
3:C:93:MET:HG2	3:C:98:TYR:HB2	1.67	0.76
1:A:82:GLN:CB	1:A:577:LEU:HB3	2.14	0.76
1:A:237:GLU:OE1	1:A:529:SER:HB3	1.85	0.76
2:B:77:THR:CG2	2:B:82:LEU:HD11	2.16	0.76
1:A:559:TYR:CA	1:A:569:ARG:HH21	1.99	0.76
1:A:242:HIS:O	1:A:351:PRO:HA	1.86	0.76
3:C:119:VAL:O	3:C:123:LEU:HD12	1.86	0.75
1:A:49:ALA:HB3	1:A:142:GLY:HA3	1.67	0.75
3:C:6:LYS:HG2	3:C:7:LYS:N	2.02	0.75
1:A:560:LEU:HB3	1:A:568:ARG:HB2	1.66	0.75
10:C:130:HEB:HBB1	12:C:132:CDN:H241	1.65	0.75
2:B:43:LYS:HE2	2:B:49:LEU:O	1.87	0.75
1:A:232:PRO:HB3	1:A:558:LEU:HD11	1.68	0.74
1:A:232:PRO:CB	1:A:558:LEU:HD11	2.17	0.74
1:A:392:VAL:HG13	1:A:394:VAL:HG13	1.68	0.74
1:A:577:LEU:HD23	1:A:577:LEU:N	2.00	0.74
1:A:544:ASP:HB2	1:A:545:PHE:CE1	2.23	0.74
12:C:132:CDN:HA21	4:D:41:GLY:O	1.87	0.74
2:B:81:ALA:C	2:B:82:LEU:HD12	2.09	0.74
1:A:47:VAL:HG13	1:A:146:LEU:HD23	1.68	0.73
3:C:2:ILE:CG1	3:C:5:VAL:HB	2.18	0.73
1:A:475:ARG:O	1:A:542:ARG:HA	1.88	0.73
1:A:254:THR:HG22	1:A:330:ILE:HD11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:THR:O	1:A:568:ARG:HD2	1.88	0.73
1:A:357:MET:HE2	1:A:357:MET:N	2.02	0.73
2:B:77:THR:HG22	2:B:82:LEU:HD11	1.70	0.73
2:B:9:ARG:HH12	2:B:49:LEU:CA	2.01	0.73
3:C:28:ILE:HD11	11:C:131:AT5:H172	1.70	0.73
1:A:47:VAL:HG13	1:A:146:LEU:CD2	2.18	0.72
1:A:584:LYS:HG2	1:A:585:ILE:H	1.54	0.72
1:A:559:TYR:CB	1:A:569:ARG:HH21	2.02	0.72
1:A:117:ARG:HG3	1:A:118:PRO:CD	2.19	0.72
1:A:555:CYS:HB2	1:A:571:VAL:HG13	1.71	0.72
1:A:434:GLU:O	1:A:438:GLU:HB2	1.89	0.72
2:B:146:LEU:CD1	2:B:183:ILE:HD11	2.20	0.71
1:A:12:VAL:HB	1:A:35:LEU:HD12	1.72	0.71
4:D:92:MET:O	4:D:96:VAL:HG23	1.89	0.71
1:A:17:GLY:HA3	1:A:408:LEU:HD13	1.71	0.71
1:A:471:PHE:CE2	1:A:480:MET:HG3	2.25	0.71
1:A:82:GLN:HB3	1:A:577:LEU:HD13	1.73	0.71
1:A:108:ARG:HD2	1:A:119:PHE:O	1.91	0.71
3:C:51:SER:HB3	4:D:48:TRP:HE1	1.56	0.71
3:C:104:GLU:CD	3:C:104:GLU:H	1.94	0.70
4:D:16:PHE:O	4:D:20:ARG:HD3	1.91	0.70
1:A:256:GLY:O	1:A:260:GLU:HG2	1.91	0.70
1:A:537:ARG:HH12	1:A:554:LEU:HD12	1.56	0.70
1:A:545:PHE:N	1:A:546:PRO:HD3	2.07	0.70
1:A:568:ARG:O	1:A:569:ARG:HG2	1.92	0.69
3:C:126:VAL:HG11	12:C:132:CDN:OB9	1.92	0.69
1:A:222:GLY:HA3	1:A:389:ILE:HD12	1.74	0.69
1:A:523:ALA:O	1:A:526:THR:HB	1.93	0.69
1:A:370:THR:HG23	1:A:380:VAL:HG22	1.73	0.69
1:A:577:LEU:HG	1:A:578:ARG:N	2.08	0.69
1:A:467:MET:SD	1:A:523:ALA:HB1	2.33	0.68
1:A:578:ARG:HB3	1:A:579:PRO:CD	2.20	0.68
1:A:44:SER:O	1:A:47:VAL:HG22	1.93	0.68
1:A:218:ASN:N	1:A:218:ASN:HD22	1.91	0.68
1:A:327:LEU:N	1:A:328:PRO:HD3	2.08	0.68
1:A:355:TYR:CE2	1:A:399:ARG:HD3	2.29	0.68
2:B:92:ARG:HD3	3:C:17:THR:HG21	1.76	0.68
4:D:6:SER:HB2	4:D:94:GLN:NE2	2.08	0.68
2:B:1:MET:H1	2:B:29:GLU:HB2	1.58	0.68
1:A:234:GLN:HG3	1:A:361:PRO:CG	2.24	0.68
1:A:242:HIS:HB2	1:A:354:HIS:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ARG:NH1	2:B:49:LEU:HA	2.09	0.67
2:B:76:ILE:O	2:B:78:PRO:HD3	1.94	0.67
1:A:453:GLY:HA3	1:A:496:ASN:O	1.93	0.67
1:A:287:ASP:OD1	1:A:538:GLY:HA2	1.94	0.67
4:D:9:GLY:CA	4:D:14:HIS:HD2	2.08	0.67
1:A:75:GLY:O	1:A:398:ASN:HB3	1.93	0.67
10:C:130:HEB:HBB1	12:C:132:CDN:H243	1.76	0.67
1:A:357:MET:H	1:A:357:MET:CE	2.08	0.67
2:B:82:LEU:O	2:B:89:ILE:HG12	1.95	0.67
2:B:92:ARG:HH11	3:C:17:THR:HG21	1.58	0.67
1:A:69:MET:O	1:A:73:VAL:HG23	1.95	0.67
1:A:562:GLU:HB2	1:A:568:ARG:NH1	2.09	0.67
1:A:9:ASP:CG	1:A:32:THR:HG22	2.15	0.66
1:A:24:LEU:O	1:A:28:GLN:HG2	1.95	0.66
1:A:119:PHE:CB	2:B:135:GLN:H	2.04	0.66
1:A:61:HIS:NE2	1:A:131:ALA:HB3	2.10	0.66
1:A:46:THR:HB	1:A:146:LEU:HD13	1.78	0.66
1:A:54:THR:HA	1:A:134:THR:HA	1.78	0.66
1:A:357:MET:HE2	1:A:357:MET:H	1.58	0.66
1:A:117:ARG:CG	1:A:118:PRO:HD2	2.26	0.66
1:A:23:ALA:HB2	1:A:35:LEU:HD13	1.78	0.66
1:A:578:ARG:CB	1:A:579:PRO:HD3	2.21	0.65
2:B:34:MET:CE	2:B:34:MET:HA	2.25	0.65
3:C:90:ARG:HE	3:C:109:SER:HB2	1.61	0.65
1:A:320:LYS:HE2	1:A:324:GLU:OE1	1.96	0.65
2:B:10:TYR:CE2	2:B:12:PRO:HG3	2.30	0.65
1:A:167:LEU:HB2	1:A:181:THR:OG1	1.95	0.65
1:A:105:PRO:HD2	1:A:144:ALA:HB1	1.78	0.65
2:B:95:PRO:HD2	2:B:157:THR:CG2	2.27	0.65
2:B:230:LYS:HA	2:B:233:LEU:HD12	1.78	0.65
1:A:559:TYR:HB2	1:A:569:ARG:NH2	2.11	0.64
1:A:298:ARG:NH1	1:A:543:PHE:HZ	1.95	0.64
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.80	0.64
10:C:130:HEB:HHA	10:C:130:HEB:HBD1	1.79	0.64
1:A:240:GLN:NE2	1:A:399:ARG:HB3	2.12	0.64
1:A:291:ARG:NH2	1:A:538:GLY:O	2.31	0.64
1:A:245:GLY:O	1:A:349:VAL:HA	1.96	0.64
1:A:208:ILE:HG13	1:A:209:TYR:CD1	2.32	0.63
1:A:239:TRP:CZ3	1:A:356:MET:HB2	2.32	0.63
1:A:298:ARG:HH11	1:A:543:PHE:HZ	1.44	0.63
1:A:123:SER:HA	1:A:134:THR:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:TYR:HA	2:B:182:LEU:HD12	1.79	0.63
3:C:112:ILE:O	3:C:116:ILE:HG13	1.98	0.63
1:A:205:ALA:HB2	1:A:220:GLY:N	2.09	0.63
2:B:71:ASN:OD1	2:B:94:LEU:HD23	1.98	0.63
1:A:49:ALA:HA	6:A:601:FAD:N5	2.14	0.62
1:A:286:ARG:HH21	5:A:589:OAA:H22	1.63	0.62
2:B:211:ASN:ND2	3:C:21:PRO:HD2	2.15	0.62
1:A:583:PRO:O	1:A:584:LYS:HB2	1.98	0.62
1:A:508:THR:OG1	2:B:50:SER:HB2	1.99	0.62
1:A:125:ASN:OD1	1:A:132:ALA:HB2	1.99	0.62
1:A:9:ASP:OD2	1:A:32:THR:HG22	2.00	0.62
1:A:286:ARG:NH2	5:A:589:OAA:H22	2.14	0.62
1:A:221:ASP:O	1:A:225:MET:HG3	2.00	0.62
1:A:6:ARG:HB3	1:A:8:PHE:HE1	1.64	0.62
1:A:532:PHE:CD1	1:A:569:ARG:HD3	2.35	0.62
3:C:1:MET:HG3	3:C:6:LYS:CA	2.29	0.61
2:B:211:ASN:HD21	3:C:21:PRO:HD2	1.65	0.61
2:B:35:LEU:HD23	2:B:67:MET:CE	2.30	0.61
3:C:83:TYR:CE2	3:C:87:VAL:HG21	2.35	0.61
1:A:54:THR:HG23	1:A:402:GLY:HA3	1.81	0.61
1:A:562:GLU:CB	1:A:568:ARG:HH12	2.12	0.61
1:A:126:PHE:HE2	5:A:589:OAA:H21	1.63	0.61
2:B:35:LEU:HD21	2:B:91:ILE:CD1	2.29	0.61
1:A:370:THR:HG23	1:A:380:VAL:CG2	2.31	0.61
2:B:94:LEU:HB3	2:B:157:THR:CG2	2.27	0.61
1:A:234:GLN:O	1:A:236:MET:N	2.33	0.61
1:A:454:GLU:OE2	1:A:493:ARG:NE	2.30	0.61
2:B:223:THR:HG22	9:B:304:F3S:S1	2.41	0.60
1:A:298:ARG:NH1	1:A:543:PHE:CZ	2.69	0.60
1:A:567:THR:C	1:A:568:ARG:HD2	2.22	0.60
1:A:38:LYS:NZ	1:A:217:ILE:HG23	2.16	0.60
4:D:95:LEU:O	4:D:99:VAL:HG23	2.01	0.60
1:A:49:ALA:HA	6:A:601:FAD:C5X	2.31	0.60
1:A:177:VAL:HG21	1:A:383:LEU:HB2	1.82	0.60
1:A:104:LEU:HD12	1:A:105:PRO:HD2	1.84	0.60
1:A:571:VAL:HG12	1:A:572:ASN:N	2.17	0.59
1:A:532:PHE:HD1	1:A:569:ARG:HH11	1.49	0.59
2:B:69:GLY:O	3:C:19:ARG:HB3	2.02	0.59
1:A:199:VAL:HG22	1:A:384:PHE:HB2	1.83	0.59
1:A:119:PHE:CG	2:B:134:LEU:HA	2.36	0.59
2:B:209:ILE:HG23	3:C:24:ALA:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASP:H	1:A:398:ASN:ND2	2.01	0.59
1:A:463:LEU:HD13	1:A:520:MET:CE	2.32	0.59
3:C:6:LYS:HG2	3:C:7:LYS:H	1.67	0.59
1:A:205:ALA:HA	1:A:218:ASN:HB3	1.84	0.59
1:A:371:VAL:HA	1:A:376:GLU:O	2.03	0.59
1:A:63:ASP:OD1	1:A:64:ASN:N	2.33	0.59
1:A:164:TRP:CZ2	1:A:184:CYS:HB2	2.37	0.59
1:A:577:LEU:HG	1:A:578:ARG:H	1.67	0.59
1:A:571:VAL:CG1	1:A:572:ASN:N	2.66	0.59
2:B:201:PHE:O	2:B:205:ARG:HG2	2.03	0.59
2:B:114:TYR:O	2:B:119:PRO:HG3	2.03	0.59
1:A:72:THR:HA	1:A:400:LEU:HD22	1.84	0.58
1:A:287:ASP:H	1:A:398:ASN:HD21	1.51	0.58
1:A:219:THR:O	1:A:221:ASP:N	2.36	0.58
1:A:216:HIS:HB2	2:B:53:ARG:HE	1.69	0.58
1:A:208:ILE:HG13	1:A:209:TYR:HD1	1.67	0.58
2:B:60:CYS:SG	2:B:62:SER:HB2	2.43	0.58
1:A:59:ASN:ND2	1:A:120:GLY:HA3	2.19	0.58
3:C:2:ILE:HG13	3:C:3:ARG:N	2.19	0.58
1:A:161:PHE:HB3	1:A:164:TRP:CD1	2.39	0.58
3:C:71:LYS:HD3	3:C:129:TRP:CD1	2.39	0.58
2:B:94:LEU:CB	2:B:157:THR:HG21	2.32	0.57
2:B:56:ARG:O	2:B:56:ARG:HG2	2.04	0.57
1:A:556:HIS:HB2	1:A:572:ASN:HB3	1.85	0.57
1:A:244:THR:HG22	1:A:349:VAL:HG21	1.86	0.57
1:A:386:VAL:HG11	1:A:415:ALA:HB2	1.86	0.57
4:D:102:VAL:HG12	4:D:106:ILE:HD12	1.85	0.57
1:A:338:ALA:O	1:A:340:VAL:HG23	2.03	0.57
1:A:511:VAL:O	1:A:515:GLU:HG3	2.05	0.57
1:A:369:LEU:HD23	1:A:379:VAL:HA	1.86	0.57
3:C:83:TYR:CD2	3:C:83:TYR:C	2.77	0.57
3:C:85:VAL:O	3:C:89:ILE:HG13	2.05	0.57
1:A:45:HIS:CE1	1:A:214:ASN:HA	2.40	0.57
1:A:76:SER:O	1:A:79:ILE:HG22	2.04	0.57
1:A:252:LEU:HD13	1:A:354:HIS:CE1	2.40	0.57
1:A:205:ALA:CB	1:A:220:GLY:N	2.64	0.57
3:C:6:LYS:HE3	3:C:7:LYS:CG	2.22	0.56
4:D:10:ARG:H	4:D:14:HIS:CD2	2.23	0.56
1:A:126:PHE:CE2	5:A:589:OAA:H21	2.40	0.56
2:B:35:LEU:HD23	2:B:67:MET:HE1	1.86	0.56
1:A:368:ALA:O	1:A:380:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ASN:HD22	1:A:173:GLN:H	1.54	0.56
1:A:38:LYS:HE2	6:A:601:FAD:C8A	2.35	0.56
4:D:44:THR:HG22	4:D:46:GLU:HG2	1.86	0.56
3:C:1:MET:CG	3:C:6:LYS:HA	2.36	0.56
1:A:139:ASP:OD2	1:A:330:ILE:HG12	2.06	0.55
2:B:9:ARG:HH11	2:B:49:LEU:HD13	1.71	0.55
2:B:117:ILE:HD13	2:B:178:ALA:HA	1.86	0.55
3:C:71:LYS:HD3	3:C:129:TRP:HD1	1.70	0.55
3:C:88:GLY:O	3:C:91:HIS:HB2	2.07	0.55
10:C:130:HEB:CBB	12:C:132:CDN:C24	2.74	0.55
1:A:64:ASN:HD21	1:A:66:GLU:HB2	1.72	0.55
1:A:270:GLU:HG2	1:A:271:ARG:N	2.21	0.55
1:A:476:GLU:HB2	1:A:544:ASP:OD1	2.05	0.55
2:B:92:ARG:CD	3:C:17:THR:HG21	2.35	0.55
1:A:54:THR:OG1	1:A:403:ASN:ND2	2.39	0.55
2:B:117:ILE:O	2:B:117:ILE:HD12	2.06	0.55
2:B:116:LYS:NZ	2:B:167:ASP:O	2.40	0.55
1:A:216:HIS:CB	2:B:53:ARG:HE	2.20	0.55
1:A:45:HIS:HB2	1:A:218:ASN:HD21	1.72	0.54
3:C:28:ILE:HD11	11:C:131:AT5:C17	2.38	0.54
1:A:455:ASP:HB2	1:A:498:ARG:HH21	1.72	0.54
1:A:320:LYS:HG2	1:A:320:LYS:O	2.07	0.54
3:C:14:ASP:O	3:C:17:THR:HB	2.07	0.54
3:C:78:LEU:HD21	12:C:132:CDN:C16	2.35	0.54
1:A:232:PRO:HB2	1:A:558:LEU:HD11	1.89	0.54
2:B:95:PRO:HD2	2:B:157:THR:HG22	1.88	0.54
1:A:485:GLU:O	1:A:489:VAL:HG23	2.07	0.54
2:B:1:MET:N	2:B:29:GLU:HB2	2.22	0.54
2:B:95:PRO:CG	3:C:18:ILE:HD11	2.38	0.54
4:D:15:ASP:O	4:D:19:VAL:HG23	2.08	0.54
2:B:25:LEU:HD13	2:B:42:LEU:HD23	1.89	0.54
1:A:147:HIS:O	1:A:151:GLN:HG3	2.07	0.54
1:A:172:ASN:HD21	1:A:430:ARG:HG3	1.73	0.54
1:A:446:ARG:HH22	1:A:497:ALA:HB3	1.71	0.54
1:A:557:SER:HB2	1:A:569:ARG:HH12	1.73	0.54
1:A:164:TRP:CH2	1:A:184:CYS:HB2	2.43	0.54
2:B:59:VAL:O	2:B:59:VAL:HG12	2.07	0.54
2:B:229:ILE:O	2:B:233:LEU:HG	2.08	0.53
1:A:8:PHE:CE2	1:A:34:ALA:HB2	2.43	0.53
1:A:573:MET:O	1:A:574:GLU:CB	2.56	0.53
1:A:235:ASP:N	1:A:235:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:ILE:HD11	2:B:152:CYS:HB3	1.90	0.53
2:B:77:THR:HG22	2:B:82:LEU:CD1	2.37	0.53
1:A:295:ILE:C	1:A:297:ILE:H	2.09	0.53
1:A:126:PHE:O	1:A:129:GLU:HG2	2.09	0.53
1:A:528:VAL:HG12	1:A:569:ARG:HD2	1.90	0.53
2:B:9:ARG:HH12	2:B:49:LEU:CB	2.22	0.53
1:A:151:GLN:HB3	2:B:119:PRO:O	2.08	0.53
1:A:573:MET:O	1:A:574:GLU:HB2	2.08	0.53
12:C:132:CDN:OB3	4:D:41:GLY:HA2	2.08	0.53
3:C:15:LEU:HD13	11:C:131:AT5:H101	1.90	0.53
2:B:58:GLY:HA2	7:B:302:FES:S2	2.48	0.53
2:B:223:THR:CG2	9:B:304:F3S:S1	2.96	0.53
3:C:96:PHE:N	3:C:96:PHE:CD2	2.76	0.53
1:A:263:TYR:HB3	1:A:265:LEU:CD2	2.36	0.53
1:A:55:VAL:HG13	1:A:57:LEU:HG	1.89	0.53
1:A:404:SER:O	1:A:407:ASP:HB3	2.09	0.53
1:A:254:THR:HG22	1:A:330:ILE:CD1	2.38	0.53
2:B:35:LEU:HD11	2:B:91:ILE:CD1	2.39	0.53
2:B:117:ILE:HD13	2:B:178:ALA:CA	2.37	0.53
1:A:86:GLU:OE1	1:A:578:ARG:HB3	2.09	0.52
1:A:254:THR:HA	5:A:589:OAA:O5	2.09	0.52
1:A:265:LEU:HD22	1:A:271:ARG:HG2	1.90	0.52
3:C:78:LEU:HD11	12:C:132:CDN:H142	1.91	0.52
1:A:214:ASN:HD22	1:A:214:ASN:N	2.07	0.52
2:B:2:ARG:HE	2:B:24:THR:HG21	1.75	0.52
3:C:83:TYR:HD2	3:C:83:TYR:C	2.11	0.52
1:A:38:LYS:HG2	1:A:165:TYR:HD1	1.75	0.52
1:A:165:TYR:OH	1:A:221:ASP:OD1	2.24	0.52
3:C:30:HIS:CD2	3:C:84:HIS:ND1	2.77	0.52
2:B:198:SER:O	4:D:11:ASN:HB2	2.10	0.52
2:B:156:SER:OG	2:B:172:PRO:HD2	2.10	0.52
1:A:531:ASN:O	1:A:542:ARG:NH1	2.43	0.52
1:A:324:GLU:C	1:A:328:PRO:HG3	2.30	0.52
1:A:369:LEU:HD21	1:A:379:VAL:HG22	1.92	0.52
1:A:172:ASN:O	1:A:175:GLY:N	2.40	0.52
1:A:295:ILE:C	1:A:297:ILE:N	2.64	0.51
10:C:130:HEB:CAC	4:D:23:ALA:HB1	2.34	0.51
2:B:111:TYR:O	2:B:114:TYR:HB3	2.11	0.51
2:B:52:ARG:NH2	2:B:105:VAL:O	2.43	0.51
1:A:202:THR:OG1	1:A:222:GLY:HA3	2.10	0.51
1:A:14:GLY:HA2	6:A:601:FAD:C1B	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLY:HA2	6:A:601:FAD:H1B	1.90	0.51
2:B:209:ILE:HG12	3:C:27:SER:OG	2.11	0.51
2:B:67:MET:HE3	2:B:74:ALA:HA	1.92	0.51
1:A:276:TYR:CE2	1:A:292:SER:HA	2.46	0.51
4:D:26:LEU:O	4:D:30:ILE:HG13	2.11	0.51
1:A:76:SER:O	1:A:79:ILE:CG2	2.58	0.51
3:C:30:HIS:CD2	3:C:84:HIS:HD1	2.28	0.51
3:C:85:VAL:HG13	10:C:130:HEB:HBC1	1.93	0.51
3:C:108:ARG:O	3:C:112:ILE:HG13	2.11	0.51
1:A:532:PHE:CG	1:A:569:ARG:HD3	2.46	0.50
1:A:218:ASN:N	1:A:218:ASN:ND2	2.57	0.50
1:A:459:ILE:HG23	1:A:490:ILE:CG2	2.41	0.50
1:A:22:ALA:O	1:A:26:ILE:HG13	2.10	0.50
1:A:475:ARG:HE	1:A:540:HIS:HD2	1.59	0.50
1:A:556:HIS:O	1:A:571:VAL:HA	2.11	0.50
1:A:139:ASP:HB2	1:A:327:LEU:HA	1.93	0.50
1:A:459:ILE:HD13	1:A:494:LEU:HA	1.93	0.50
1:A:119:PHE:CE2	2:B:134:LEU:HA	2.47	0.50
1:A:361:PRO:HA	1:A:391:CYS:O	2.12	0.50
2:B:207:HIS:HE1	3:C:31:ARG:NH2	2.09	0.50
1:A:78:TYR:CD2	1:A:583:PRO:HA	2.46	0.50
1:A:54:THR:O	1:A:406:LEU:HD22	2.12	0.50
1:A:47:VAL:HG13	1:A:146:LEU:HD22	1.94	0.50
1:A:295:ILE:HG23	1:A:298:ARG:HH21	1.76	0.50
1:A:577:LEU:CG	1:A:578:ARG:H	2.25	0.49
1:A:82:GLN:HG2	1:A:575:PRO:HA	1.94	0.49
1:A:355:TYR:CD2	1:A:399:ARG:HD3	2.47	0.49
1:A:232:PRO:CD	1:A:370:THR:HG22	2.42	0.49
1:A:264:LEU:C	1:A:265:LEU:HD23	2.32	0.49
1:A:252:LEU:HG	1:A:253:VAL:N	2.26	0.49
1:A:463:LEU:O	1:A:467:MET:HG2	2.12	0.49
2:B:123:ASN:ND2	2:B:125:GLY:H	2.10	0.49
4:D:44:THR:HB	4:D:47:VAL:HG23	1.95	0.49
1:A:549:ASP:OD1	1:A:552:ASN:HB2	2.12	0.49
1:A:232:PRO:HD2	1:A:370:THR:HG22	1.94	0.49
2:B:212:CYS:SG	2:B:223:THR:HG23	2.52	0.49
1:A:9:ASP:N	1:A:32:THR:CG2	2.70	0.49
2:B:35:LEU:CD2	2:B:91:ILE:HD11	2.40	0.49
1:A:533:ARG:HB3	1:A:540:HIS:CE1	2.47	0.49
1:A:205:ALA:C	1:A:207:ARG:H	2.16	0.49
1:A:404:SER:HB3	6:A:601:FAD:O2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:HB2	1:A:398:ASN:HD21	1.77	0.49
4:D:44:THR:HG22	4:D:46:GLU:H	1.77	0.49
3:C:119:VAL:O	3:C:122:LEU:HB3	2.12	0.49
2:B:146:LEU:HD11	2:B:183:ILE:HD11	1.95	0.49
1:A:412:GLY:O	1:A:415:ALA:HB3	2.12	0.49
1:A:119:PHE:HB2	2:B:135:GLN:N	2.12	0.49
1:A:307:TRP:CD1	1:A:348:PRO:HG2	2.47	0.49
1:A:405:LEU:HG	6:A:601:FAD:C2	2.43	0.49
1:A:463:LEU:HD13	1:A:520:MET:HE1	1.94	0.49
3:C:89:ILE:HG22	3:C:93:MET:CE	2.43	0.48
2:B:155:CYS:SG	2:B:156:SER:N	2.85	0.48
1:A:559:TYR:HA	1:A:569:ARG:HH21	1.78	0.48
1:A:197:ALA:HB1	1:A:384:PHE:CE1	2.48	0.48
1:A:174:ASP:HB2	1:A:430:ARG:NH2	2.27	0.48
4:D:109:PHE:HB3	4:D:113:TRP:CZ3	2.47	0.48
1:A:81:ASP:HB3	1:A:83:ASP:OD1	2.13	0.48
1:A:240:GLN:CB	1:A:357:MET:HE1	2.35	0.48
1:A:128:GLY:CA	1:A:400:LEU:HD11	2.33	0.48
1:A:263:TYR:O	1:A:313:LEU:HA	2.13	0.48
1:A:40:PHE:O	1:A:43:ARG:HG2	2.14	0.48
1:A:99:LEU:HD11	1:A:409:VAL:HG21	1.94	0.48
3:C:1:MET:CB	3:C:6:LYS:HA	2.44	0.48
1:A:359:GLY:N	1:A:391:CYS:HB2	2.28	0.48
1:A:490:ILE:HA	1:A:493:ARG:HB3	1.96	0.48
2:B:201:PHE:HA	2:B:205:ARG:HD3	1.96	0.48
1:A:272:PHE:CZ	1:A:293:ILE:HG23	2.48	0.48
1:A:341:ASP:OD1	1:A:343:VAL:HG23	2.14	0.48
1:A:534:THR:HB	1:A:553:TRP:HE1	1.78	0.48
1:A:210:GLN:CD	1:A:465:GLU:HA	2.33	0.48
1:A:242:HIS:HE1	1:A:286:ARG:HH21	1.62	0.48
2:B:9:ARG:NH1	2:B:49:LEU:CD1	2.77	0.48
1:A:78:TYR:O	1:A:554:LEU:HD11	2.13	0.48
3:C:37:THR:O	3:C:40:ALA:HB3	2.13	0.48
1:A:368:ALA:CB	1:A:383:LEU:HD23	2.44	0.48
1:A:234:GLN:HB3	1:A:235:ASP:OD1	2.13	0.48
1:A:545:PHE:N	1:A:546:PRO:CD	2.76	0.48
1:A:143:HIS:HE1	2:B:147:TYR:O	1.97	0.48
1:A:267:LYS:HZ1	1:A:301:ARG:HD3	1.78	0.48
12:C:132:CDN:HA21	4:D:41:GLY:C	2.35	0.47
2:B:95:PRO:HB3	3:C:18:ILE:HD11	1.96	0.47
3:C:20:PHE:N	3:C:20:PHE:CD1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ASN:HD22	1:A:173:GLN:N	2.11	0.47
1:A:172:ASN:HB3	1:A:176:ALA:H	1.78	0.47
2:B:150:ILE:CD1	2:B:152:CYS:HB3	2.43	0.47
1:A:125:ASN:O	1:A:259:GLY:HA3	2.15	0.47
1:A:307:TRP:HD1	1:A:348:PRO:HG2	1.79	0.47
2:B:95:PRO:CB	3:C:18:ILE:HD11	2.45	0.47
1:A:444:LEU:HG	1:A:448:ASN:ND2	2.29	0.47
1:A:9:ASP:CB	1:A:32:THR:HG22	2.44	0.47
1:A:323:LEU:HB3	1:A:331:LEU:HD21	1.96	0.47
1:A:459:ILE:HG21	1:A:494:LEU:HD13	1.97	0.47
1:A:240:GLN:HE22	1:A:399:ARG:HB3	1.78	0.47
1:A:252:LEU:HG	1:A:253:VAL:H	1.78	0.47
2:B:150:ILE:HG13	2:B:152:CYS:HB3	1.97	0.47
3:C:110:ALA:O	3:C:113:SER:HB2	2.14	0.47
2:B:215:VAL:O	2:B:217:PRO:HD3	2.14	0.47
1:A:11:VAL:HG23	1:A:195:ALA:CB	2.43	0.47
1:A:240:GLN:NE2	1:A:399:ARG:O	2.47	0.47
1:A:215:ALA:C	1:A:217:ILE:H	2.15	0.47
1:A:292:SER:O	1:A:296:GLU:HG2	2.14	0.47
2:B:55:CYS:O	2:B:56:ARG:HB3	2.13	0.47
1:A:65:TRP:O	1:A:68:HIS:HB3	2.15	0.47
1:A:537:ARG:NH1	1:A:554:LEU:HD12	2.25	0.47
1:A:137:ALA:O	1:A:138:ALA:HB3	2.15	0.47
1:A:421:GLU:O	1:A:424:ALA:HB3	2.15	0.47
1:A:322:VAL:O	1:A:326:ARG:HB2	2.15	0.47
1:A:549:ASP:HB3	1:A:553:TRP:HB2	1.96	0.47
1:A:1:MET:O	1:A:1:MET:HG3	2.15	0.47
3:C:127:LEU:HB2	12:C:132:CDN:H512	1.97	0.47
4:D:64:ALA:O	4:D:68:ILE:HG13	2.14	0.47
1:A:567:THR:O	1:A:568:ARG:CD	2.61	0.46
1:A:263:TYR:CD1	1:A:314:LYS:HD3	2.50	0.46
1:A:436:ASP:N	1:A:436:ASP:OD2	2.48	0.46
2:B:164:TRP:O	4:D:85:LYS:NZ	2.46	0.46
1:A:4:PRO:HB2	1:A:191:VAL:HG22	1.96	0.46
2:B:70:LYS:HB2	3:C:19:ARG:HD3	1.98	0.46
1:A:365:THR:OG1	1:A:367:GLN:HG3	2.15	0.46
1:A:242:HIS:CE1	1:A:286:ARG:HH21	2.34	0.46
1:A:532:PHE:HD1	1:A:569:ARG:NH1	2.12	0.46
4:D:43:LEU:HD21	4:D:48:TRP:CE3	2.50	0.46
4:D:75:GLY:O	4:D:78:GLN:HB2	2.15	0.46
1:A:104:LEU:HD12	1:A:105:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:GLN:NE2	2:B:23:TYR:OH	2.48	0.46
1:A:327:LEU:N	1:A:328:PRO:CD	2.76	0.46
1:A:520:MET:O	1:A:522:THR:N	2.48	0.46
1:A:468:GLN:O	1:A:472:SER:HB2	2.16	0.46
2:B:79:ILE:O	2:B:80:SER:C	2.54	0.46
2:B:128:PRO:HA	2:B:129:PRO:HD3	1.80	0.46
3:C:2:ILE:HG13	3:C:3:ARG:H	1.81	0.46
1:A:69:MET:HG2	1:A:85:ILE:HG22	1.97	0.46
3:C:18:ILE:HG22	3:C:20:PHE:CE1	2.51	0.46
1:A:255:GLU:CD	1:A:286:ARG:HH12	2.19	0.46
1:A:276:TYR:CE2	1:A:295:ILE:HD12	2.51	0.46
2:B:208:SER:HA	9:B:304:F3S:S1	2.56	0.45
1:A:242:HIS:CE1	1:A:286:ARG:NH2	2.85	0.45
2:B:157:THR:O	2:B:157:THR:CG2	2.63	0.45
1:A:81:ASP:N	1:A:81:ASP:OD2	2.49	0.45
1:A:499:LEU:HG	1:A:501:ASP:O	2.15	0.45
1:A:399:ARG:CZ	1:A:404:SER:HB2	2.46	0.45
1:A:200:LEU:HD12	1:A:360:ILE:CD1	2.46	0.45
3:C:44:LEU:HB3	12:C:132:CDN:H381	1.98	0.45
1:A:38:LYS:HZ2	1:A:217:ILE:HG23	1.79	0.45
2:B:157:THR:HG22	2:B:157:THR:O	2.16	0.45
1:A:314:LYS:NZ	1:A:317:HIS:HB3	2.32	0.45
1:A:145:LEU:HD23	1:A:145:LEU:C	2.36	0.45
2:B:34:MET:CA	2:B:34:MET:HE3	2.36	0.45
2:B:209:ILE:HD11	11:C:131:AT5:N4	2.32	0.45
1:A:276:TYR:CZ	1:A:292:SER:HA	2.52	0.45
2:B:89:ILE:HG22	2:B:89:ILE:O	2.15	0.45
2:B:94:LEU:HD22	2:B:157:THR:HG21	1.98	0.45
1:A:471:PHE:CE2	1:A:527:ALA:HA	2.52	0.45
1:A:486:GLN:O	1:A:490:ILE:HG13	2.16	0.45
1:A:491:ARG:NH1	1:A:524:TYR:HE1	2.15	0.45
1:A:165:TYR:CE1	6:A:601:FAD:N6A	2.85	0.45
1:A:307:TRP:HA	1:A:307:TRP:HE3	1.82	0.45
4:D:45:TYR:O	4:D:49:ILE:HG22	2.17	0.45
1:A:513:CYS:O	1:A:516:LEU:HB3	2.16	0.45
2:B:180:ARG:HD3	2:B:181:PHE:CE1	2.52	0.45
4:D:110:VAL:HA	4:D:113:TRP:CE2	2.52	0.45
1:A:579:PRO:O	1:A:580:ALA:HB3	2.17	0.45
1:A:82:GLN:HB3	1:A:577:LEU:HB3	1.96	0.44
1:A:215:ALA:C	1:A:217:ILE:N	2.71	0.44
2:B:121:LEU:HD11	2:B:186:ARG:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ILE:HB	2:B:104:VAL:O	2.17	0.44
2:B:148:GLU:O	2:B:149:CYS:C	2.53	0.44
1:A:307:TRP:CE3	1:A:307:TRP:HA	2.52	0.44
1:A:100:GLU:OE2	1:A:101:HIS:HD2	1.99	0.44
2:B:234:LEU:HD23	4:D:13:VAL:HG13	1.99	0.44
1:A:220:GLY:O	1:A:223:VAL:N	2.51	0.44
1:A:359:GLY:HA3	1:A:389:ILE:O	2.17	0.44
1:A:104:LEU:HA	1:A:105:PRO:HD3	1.80	0.44
1:A:125:ASN:CG	1:A:132:ALA:HB2	2.37	0.44
2:B:176:LEU:HD12	2:B:222:PRO:HA	1.99	0.44
1:A:254:THR:C	1:A:256:GLY:N	2.70	0.44
1:A:545:PHE:O	1:A:547:ASP:N	2.49	0.44
1:A:571:VAL:CG1	1:A:572:ASN:H	2.30	0.44
4:D:6:SER:HB2	4:D:94:GLN:HE22	1.82	0.44
2:B:53:ARG:HH11	2:B:53:ARG:CG	2.31	0.44
1:A:172:ASN:ND2	1:A:430:ARG:HG3	2.32	0.44
2:B:23:TYR:CD2	2:B:42:LEU:HD13	2.52	0.44
2:B:109:GLN:O	2:B:113:GLN:HG2	2.18	0.44
1:A:357:MET:N	1:A:357:MET:CE	2.72	0.44
1:A:151:GLN:O	1:A:154:LEU:HB2	2.17	0.44
2:B:37:ASP:O	2:B:41:GLN:HG2	2.16	0.44
1:A:169:LEU:N	1:A:169:LEU:HD23	2.33	0.44
1:A:274:GLU:O	1:A:278:PRO:HA	2.17	0.44
2:B:60:CYS:SG	2:B:62:SER:CB	3.06	0.44
1:A:213:THR:HG21	1:A:252:LEU:HD12	2.00	0.44
1:A:559:TYR:CA	1:A:569:ARG:NH2	2.75	0.44
2:B:9:ARG:HH12	2:B:49:LEU:HB2	1.83	0.44
1:A:81:ASP:O	1:A:85:ILE:HG13	2.18	0.44
1:A:272:PHE:CE1	1:A:273:MET:HE1	2.53	0.44
1:A:13:ILE:HD12	1:A:200:LEU:HD23	2.00	0.44
3:C:93:MET:HG2	3:C:98:TYR:CB	2.45	0.44
2:B:236:ARG:HH11	2:B:236:ARG:HG3	1.83	0.44
1:A:326:ARG:O	1:A:327:LEU:HD23	2.18	0.43
2:B:65:LEU:CD1	2:B:74:ALA:HB2	2.48	0.43
2:B:7:ILE:HG12	2:B:91:ILE:HB	2.00	0.43
1:A:43:ARG:O	1:A:44:SER:C	2.57	0.43
1:A:43:ARG:O	1:A:44:SER:O	2.36	0.43
1:A:529:SER:HA	1:A:569:ARG:NH1	2.34	0.43
1:A:84:ALA:CB	1:A:394:VAL:HG12	2.49	0.43
3:C:89:ILE:HG22	3:C:93:MET:HE1	2.01	0.43
1:A:243:PRO:HD3	1:A:286:ARG:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:MET:CE	1:A:236:MET:HA	2.48	0.43
1:A:84:ALA:HB1	1:A:394:VAL:HG12	2.00	0.43
1:A:298:ARG:HB2	1:A:298:ARG:HE	1.63	0.43
3:C:96:PHE:N	3:C:96:PHE:HD2	2.16	0.43
4:D:80:LEU:CD2	4:D:84:VAL:HG21	2.48	0.43
1:A:559:TYR:N	1:A:569:ARG:NH2	2.67	0.43
2:B:207:HIS:CE1	3:C:31:ARG:NH2	2.86	0.43
1:A:433:SER:O	1:A:435:SER:N	2.51	0.43
1:A:482:LYS:HD3	1:A:482:LYS:HA	1.85	0.43
10:C:130:HEB:CBB	12:C:132:CDN:H241	2.42	0.43
1:A:205:ALA:HB1	1:A:220:GLY:H	1.75	0.43
1:A:287:ASP:OD2	1:A:288:VAL:N	2.50	0.43
1:A:270:GLU:HG2	1:A:271:ARG:H	1.83	0.43
2:B:169:PHE:CD1	2:B:205:ARG:HB2	2.54	0.43
4:D:44:THR:CG2	4:D:46:GLU:HG2	2.49	0.43
1:A:253:VAL:HG13	1:A:330:ILE:HD12	2.00	0.43
1:A:61:HIS:NE2	1:A:131:ALA:CB	2.80	0.43
2:B:100:ILE:HG12	3:C:9:ARG:NH2	2.34	0.43
3:C:123:LEU:HB3	12:C:132:CDN:H521	2.01	0.43
2:B:211:ASN:O	2:B:215:VAL:HG22	2.19	0.43
1:A:320:LYS:HG3	1:A:343:VAL:HG11	1.99	0.43
1:A:560:LEU:HD12	1:A:561:PRO:CD	2.48	0.43
1:A:293:ILE:HG22	1:A:311:ALA:HB2	2.00	0.43
2:B:236:ARG:C	2:B:237:ASN:HD22	2.23	0.43
2:B:171:GLY:O	2:B:175:LEU:HG	2.19	0.43
1:A:254:THR:C	1:A:256:GLY:H	2.23	0.42
1:A:255:GLU:CB	1:A:286:ARG:HH22	2.32	0.42
2:B:33:MET:O	2:B:79:ILE:HG12	2.19	0.42
3:C:73:ILE:O	3:C:75:TRP:N	2.52	0.42
2:B:209:ILE:O	2:B:210:MET:HB2	2.20	0.42
3:C:122:LEU:O	3:C:126:VAL:HG23	2.18	0.42
2:B:67:MET:CE	2:B:74:ALA:HA	2.49	0.42
1:A:39:VAL:CG2	1:A:43:ARG:HB2	2.49	0.42
2:B:54:SER:O	2:B:55:CYS:C	2.56	0.42
4:D:76:MET:HB3	4:D:97:ILE:HD13	1.99	0.42
1:A:242:HIS:CD2	1:A:252:LEU:HD11	2.54	0.42
1:A:285:GLY:O	1:A:289:VAL:HG23	2.19	0.42
4:D:115:VAL:OXT	4:D:115:VAL:HG12	2.20	0.42
2:B:35:LEU:HD11	2:B:91:ILE:HD11	2.02	0.42
2:B:65:LEU:HD22	2:B:103:LEU:HD13	2.02	0.42
1:A:39:VAL:HG21	1:A:43:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:CYS:O	2:B:57:GLU:HG2	2.20	0.42
1:A:242:HIS:CG	1:A:252:LEU:HD11	2.55	0.42
1:A:324:GLU:HG2	1:A:331:LEU:CD1	2.49	0.42
4:D:62:LEU:HD23	4:D:65:LEU:CD1	2.45	0.42
1:A:220:GLY:O	1:A:221:ASP:C	2.56	0.42
1:A:60:THR:HG21	1:A:123:SER:O	2.18	0.42
1:A:129:GLU:HG3	1:A:131:ALA:O	2.20	0.42
1:A:222:GLY:HA3	1:A:389:ILE:CD1	2.45	0.42
1:A:508:THR:HG22	1:A:512:GLU:OE2	2.20	0.42
1:A:6:ARG:HD2	1:A:191:VAL:HG11	2.02	0.42
10:C:130:HEB:HBB1	12:C:132:CDN:H242	1.89	0.42
1:A:174:ASP:HB2	1:A:430:ARG:CZ	2.50	0.42
2:B:150:ILE:CG1	2:B:152:CYS:HB3	2.50	0.42
1:A:178:VAL:O	1:A:178:VAL:HG23	2.20	0.42
1:A:108:ARG:CD	1:A:119:PHE:O	2.65	0.41
2:B:211:ASN:HD21	3:C:24:ALA:HB2	1.86	0.41
4:D:6:SER:CB	4:D:94:GLN:HE22	2.33	0.41
2:B:5:PHE:HB2	2:B:23:TYR:HB2	2.02	0.41
6:A:601:FAD:H1'1	6:A:601:FAD:H9	1.80	0.41
3:C:20:PHE:HA	3:C:21:PRO:HD3	1.93	0.41
1:A:577:LEU:N	1:A:577:LEU:CD2	2.61	0.41
1:A:255:GLU:CD	1:A:286:ARG:HH22	2.24	0.41
4:D:61:THR:O	4:D:64:ALA:HB3	2.21	0.41
1:A:576:LYS:O	1:A:576:LYS:HG3	2.20	0.41
3:C:2:ILE:HD11	3:C:5:VAL:HG21	2.01	0.41
4:D:49:ILE:HG12	4:D:49:ILE:O	2.21	0.41
4:D:97:ILE:O	4:D:100:ALA:HB3	2.20	0.41
1:A:460:ARG:HG2	1:A:464:GLN:OE1	2.19	0.41
1:A:119:PHE:CD2	2:B:134:LEU:CA	2.90	0.41
4:D:13:VAL:H	4:D:13:VAL:HG23	1.64	0.41
1:A:108:ARG:HG3	2:B:135:GLN:HG2	2.03	0.41
1:A:207:ARG:C	1:A:209:TYR:H	2.23	0.41
1:A:276:TYR:HE2	1:A:295:ILE:HD12	1.86	0.41
1:A:79:ILE:HG12	1:A:79:ILE:O	2.19	0.41
4:D:36:PHE:CE2	4:D:48:TRP:HZ3	2.39	0.41
1:A:122:GLN:HE21	1:A:122:GLN:HB3	1.58	0.41
3:C:123:LEU:CB	12:C:132:CDN:H521	2.50	0.41
1:A:242:HIS:HB2	1:A:354:HIS:CB	2.46	0.41
1:A:554:LEU:HD12	1:A:554:LEU:HA	1.95	0.41
1:A:556:HIS:N	1:A:572:ASN:O	2.39	0.41
2:B:145:GLY:O	2:B:146:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:TYR:OH	1:A:295:ILE:HB	2.21	0.41
1:A:246:ILE:HD13	1:A:338:ALA:HB2	2.03	0.41
4:D:113:TRP:C	4:D:113:TRP:CD1	2.94	0.41
1:A:267:LYS:HZ1	1:A:301:ARG:HH11	1.69	0.41
4:D:80:LEU:HD23	4:D:84:VAL:HG21	2.03	0.41
1:A:483:GLY:O	1:A:487:LEU:HD13	2.21	0.41
1:A:97:LEU:HA	1:A:97:LEU:HD23	1.94	0.41
1:A:91:THR:O	1:A:91:THR:HG22	2.21	0.41
1:A:443:ARG:HH22	1:A:518:ASN:HD21	1.69	0.41
1:A:8:PHE:O	1:A:195:ALA:HA	2.21	0.41
2:B:8:TYR:CG	2:B:93:PRO:HD3	2.56	0.41
1:A:185:ILE:HG13	1:A:185:ILE:H	1.62	0.41
3:C:44:LEU:HD23	3:C:44:LEU:HA	1.88	0.40
3:C:65:MET:HG2	12:C:132:CDN:HA51	2.03	0.40
1:A:405:LEU:HA	1:A:408:LEU:HG	2.03	0.40
2:B:73:LEU:HG	2:B:217:PRO:CG	2.51	0.40
1:A:95:ALA:O	1:A:98:GLU:HB3	2.22	0.40
3:C:66:GLY:O	3:C:67:SER:C	2.58	0.40
3:C:30:HIS:NE2	3:C:84:HIS:CE1	2.89	0.40
1:A:208:ILE:HG13	1:A:209:TYR:CE1	2.57	0.40
2:B:179:TYR:CE2	2:B:183:ILE:HD13	2.56	0.40
3:C:73:ILE:C	3:C:75:TRP:N	2.74	0.40
1:A:213:THR:HA	1:A:250:GLY:O	2.21	0.40
1:A:340:VAL:HG13	1:A:345:GLU:OE1	2.22	0.40
2:B:2:ARG:NE	2:B:24:THR:HG21	2.36	0.40
1:A:405:LEU:O	1:A:408:LEU:HB2	2.21	0.40
1:A:476:GLU:HG3	1:A:478:ASP:OD2	2.21	0.40
1:A:372:ASN:O	1:A:375:GLY:N	2.53	0.40
2:B:107:MET:CE	2:B:153:ALA:HB2	2.51	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	586/588 (100%)	461 (79%)	81 (14%)	44 (8%)	1 7
2	B	236/238 (99%)	205 (87%)	25 (11%)	6 (2%)	7 32
3	C	127/129 (98%)	111 (87%)	11 (9%)	5 (4%)	4 22
4	D	111/115 (96%)	100 (90%)	10 (9%)	1 (1%)	21 61
All	All	1060/1070 (99%)	877 (83%)	127 (12%)	56 (5%)	2 14

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	118	PRO
1	A	220	GLY
1	A	235	ASP
1	A	546	PRO
1	A	562	GLU
1	A	563	SER
1	A	575	PRO
3	C	2	ILE
1	A	51	GLY
1	A	120	GLY
1	A	205	ALA
1	A	218	ASN
1	A	236	MET
1	A	339	HIS
1	A	357	MET
1	A	358	GLY
1	A	453	GLY
1	A	472	SER
1	A	521	GLU
1	A	574	GLU
2	B	54	SER
2	B	204	PHE
3	C	96	PHE
1	A	44	SER
1	A	272	PHE
1	A	434	GLU
1	A	467	MET
1	A	497	ALA
1	A	578	ARG
1	A	584	LYS
1	A	41	PRO
1	A	77	ASP

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Mol	Chain	Res	Type
1	A	281	LYS
1	A	428	ALA
1	A	431	ASP
1	A	466	CYS
2	B	18	PRO
2	B	81	ALA
2	B	102	ASP
3	C	54	SER
3	C	74	MET
1	A	56	ALA
1	A	254	THR
1	A	303	CYS
1	A	477	GLY
2	B	85	PRO
3	C	7	LYS
4	D	41	GLY
1	A	105	PRO
1	A	565	SER
1	A	232	PRO
1	A	278	PRO
1	A	561	PRO
1	A	583	PRO
1	A	114	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	473/473 (100%)	444 (94%)	29 (6%)	23	59
2	B	208/208 (100%)	197 (95%)	11 (5%)	28	64
3	C	109/109 (100%)	105 (96%)	4 (4%)	41	76
4	D	94/96 (98%)	92 (98%)	2 (2%)	61	86
All	All	884/886 (100%)	838 (95%)	46 (5%)	29	65

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	CYS
1	A	47	VAL
1	A	60	THR
1	A	64	ASN
1	A	65	TRP
1	A	117	ARG
1	A	122	GLN
1	A	126	PHE
1	A	133	ARG
1	A	172	ASN
1	A	196	ARG
1	A	202	THR
1	A	218	ASN
1	A	235	ASP
1	A	252	LEU
1	A	293	ILE
1	A	352	THR
1	A	357	MET
1	A	371	VAL
1	A	389	ILE
1	A	436	ASP
1	A	478	ASP
1	A	504	SER
1	A	506	PHE
1	A	533	ARG
1	A	544	ASP
1	A	550	ASP
1	A	572	ASN
1	A	577	LEU
2	B	26	GLU
2	B	32	ASP
2	B	34	MET
2	B	35	LEU
2	B	53	ARG
2	B	67	MET
2	B	101	ARG
2	B	134	LEU
2	B	135	GLN
2	B	176	LEU
2	B	180	ARG
3	C	4	ASN
3	C	83	TYR
3	C	101	GLU

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Mol	Chain	Res	Type
3	C	129	TRP
4	D	8	LEU
4	D	60	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	82	GLN
1	A	101	HIS
1	A	122	GLN
1	A	143	HIS
1	A	147	HIS
1	A	153	ASN
1	A	172	ASN
1	A	218	ASN
1	A	240	GLN
1	A	242	HIS
1	A	367	GLN
1	A	398	ASN
1	A	403	ASN
1	A	420	GLN
1	A	448	ASN
1	A	470	ASN
1	A	540	HIS
1	A	572	ASN
2	B	21	GLN
2	B	84	GLN
2	B	123	ASN
2	B	211	ASN
2	B	237	ASN
3	C	4	ASN
3	C	30	HIS
4	D	14	HIS
4	D	78	GLN
4	D	94	GLN

5.3.3 RNA

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)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	OAA	A	589	-	2,8,8	2.86	2 (100%)	2,10,10	3.74	2 (100%)
6	FAD	A	601	1	48,58,58	2.70	13 (27%)	54,89,89	3.18	13 (24%)
7	FES	B	302	2	0,4,4	0.00	-	0,4,4	0.00	-
8	SF4	B	303	2	0,12,12	0.00	-	0,24,24	0.00	-
9	F3S	B	304	2	0,9,9	0.00	-	0,15,15	0.00	-
10	HEB	C	130	3,4	24,50,50	0.85	1 (4%)	20,82,82	1.83	5 (25%)
11	AT5	C	131	-	19,23,23	2.38	8 (42%)	16,32,32	2.56	7 (43%)
12	CDN	C	132	-	76,76,76	2.44	10 (13%)	66,88,88	2.24	9 (13%)

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
5	OAA	A	589	-	-	0/2/8/8	0/0/0/0
6	FAD	A	601	1	-	0/30/50/50	0/6/6/6
7	FES	B	302	2	-	0/0/4/4	0/1/1/1
8	SF4	B	303	2	-	0/0/48/48	0/6/5/5
9	F3S	B	304	2	-	0/0/24/24	0/0/3/3
10	HEB	C	130	3,4	-	0/8/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	AT5	C	131	-	-	0/22/22/22	0/1/1/1
12	CDN	C	132	-	3/3/9/9	0/83/87/87	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	132	CDN	OB7-CB5	-7.90	1.21	1.39
12	C	132	CDN	OA9-CA7	-7.75	1.22	1.39
12	C	132	CDN	OB9-CB7	-7.62	1.22	1.39
12	C	132	CDN	OA6-CA5	-7.31	1.21	1.41
6	A	601	FAD	C1'-N10	-5.66	1.42	1.48
6	A	601	FAD	C5'-C4'	-4.23	1.45	1.51
6	A	601	FAD	C5A-C4A	-3.81	1.31	1.40
6	A	601	FAD	C2B-C3B	-2.57	1.46	1.53
11	C	131	AT5	C11-C12	-2.56	1.49	1.54
12	C	132	CDN	OB6-CB4	-2.48	1.41	1.44
12	C	132	CDN	OA6-CA4	-2.33	1.41	1.44
6	A	601	FAD	C2'-C3'	-2.06	1.49	1.53
11	C	131	AT5	C17-C12	2.03	1.58	1.53
6	A	601	FAD	C10-N1	2.14	1.39	1.35
6	A	601	FAD	C6-C7	2.34	1.44	1.37
11	C	131	AT5	O3-C3	2.53	1.39	1.35
10	C	130	HEB	C3C-CAC	2.59	1.53	1.47
5	A	589	OAA	C2-C3	2.75	1.54	1.51
11	C	131	AT5	C6-C7	2.80	1.56	1.49
5	A	589	OAA	O3-C3	2.97	1.27	1.22
11	C	131	AT5	C2-C3	3.07	1.49	1.40
6	A	601	FAD	C2A-N3A	3.97	1.39	1.32
12	C	132	CDN	OB6-CB5	4.14	1.52	1.41
11	C	131	AT5	C3-N4	4.25	1.38	1.32
11	C	131	AT5	O4-C5	4.29	1.35	1.24
6	A	601	FAD	C4-N3	4.47	1.41	1.33
11	C	131	AT5	C5-N4	4.63	1.41	1.33
6	A	601	FAD	C4A-N3A	5.28	1.43	1.35
6	A	601	FAD	C5X-N5	5.35	1.43	1.35
12	C	132	CDN	OB8-CB7	6.76	1.52	1.40
12	C	132	CDN	OA8-CA7	7.22	1.53	1.40
12	C	132	CDN	OA7-CA5	7.48	1.56	1.39
6	A	601	FAD	C9A-N10	7.60	1.49	1.38
6	A	601	FAD	C4X-N5	8.71	1.47	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	601	FAD	O2A-PA-O5B	-8.72	64.50	108.46
6	A	601	FAD	N3A-C2A-N1A	-7.02	123.52	128.89
6	A	601	FAD	C4X-C4-N3	-6.34	114.92	123.59
6	A	601	FAD	O3P-PA-O5B	-6.22	86.43	102.94
6	A	601	FAD	C1'-N10-C9A	-5.03	113.22	118.86
5	A	589	OAA	C1-C2-C3	-4.78	106.81	115.52
6	A	601	FAD	O2A-PA-O1A	-4.18	89.85	112.53
12	C	132	CDN	C19-C18-C17	-3.77	95.04	114.53
11	C	131	AT5	O5-C7-C6	-3.75	115.30	119.87
12	C	132	CDN	C15-C14-C13	-3.56	96.13	114.53
10	C	130	HEB	CAA-C2A-C1A	-3.23	123.50	127.01
6	A	601	FAD	C4X-C10-N10	-2.82	118.86	120.52
6	A	601	FAD	C5X-C9A-N10	-2.78	115.50	117.62
12	C	132	CDN	C21-C20-C19	-2.45	101.86	114.53
10	C	130	HEB	C3C-CAC-CBC	-2.42	121.37	126.32
12	C	132	CDN	C22-C21-C20	-2.36	102.37	114.53
6	A	601	FAD	C6-C5X-C9A	-2.30	115.96	118.98
12	C	132	CDN	C16-C15-C14	-2.09	103.73	114.53
10	C	130	HEB	CMC-C2C-C1C	-2.02	125.02	128.36
11	C	131	AT5	O3-C3-N4	2.19	122.10	118.99
5	A	589	OAA	O3-C3-C2	2.25	124.85	120.74
11	C	131	AT5	C6-C7-C8	2.27	127.31	123.14
10	C	130	HEB	CMC-C2C-C3C	2.57	130.12	125.09
6	A	601	FAD	C1'-C2'-C3'	2.69	117.51	109.82
11	C	131	AT5	CM3-O3-C3	2.98	120.27	117.31
11	C	131	AT5	C1-C2-C3	3.03	124.75	119.88
10	C	130	HEB	CBD-CAD-C3D	3.82	119.38	112.53
12	C	132	CDN	OA7-CA5-C11	3.86	116.03	109.05
11	C	131	AT5	C5-N4-C3	4.41	123.39	117.79
11	C	131	AT5	C17-C12-C11	5.59	119.44	110.76
6	A	601	FAD	O2A-PA-O3P	6.08	132.69	105.09
6	A	601	FAD	O5B-PA-O1A	6.60	135.24	109.62
12	C	132	CDN	OB7-CB5-C51	8.72	124.79	109.05
12	C	132	CDN	OA9-CA7-C31	8.72	124.80	109.05
12	C	132	CDN	OB9-CB7-C71	8.97	125.23	109.05
6	A	601	FAD	C4-N3-C2	12.07	125.68	115.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	C	132	CDN	CB5
12	C	132	CDN	CB7
12	C	132	CDN	CA7

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	589	OAA	5	0
6	A	601	FAD	9	0
7	B	302	FES	1	0
9	B	304	F3S	4	0
10	C	130	HEB	10	0
11	C	131	AT5	4	0
12	C	132	CDN	19	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, 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	577/588 (98%)	0.33	34 (5%) 26 11	41, 86, 112, 123	1 (0%)
2	B	238/238 (100%)	-0.05	7 (2%) 55 31	37, 57, 99, 118	0
3	C	129/129 (100%)	-0.06	9 (6%) 19 7	32, 60, 100, 132	0
4	D	113/115 (98%)	-0.18	1 (0%) 85 72	28, 44, 91, 100	0
All	All	1057/1070 (98%)	0.14	51 (4%) 34 15	28, 72, 109, 132	1 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	4	ASN	8.7
2	B	1	MET	4.7
3	C	5	VAL	4.6
1	A	306	PRO	4.4
3	C	1	MET	4.4
3	C	3	ARG	4.2
3	C	2	ILE	4.1
1	A	300	GLY	3.9
1	A	1	MET	3.8
1	A	303	CYS	3.5
1	A	402	GLY	3.2
1	A	390	ALA	3.2
1	A	272	PHE	3.1
1	A	387	GLY	3.1
1	A	307	TRP	3.0
2	B	32	ASP	3.0
1	A	297	ILE	2.9
1	A	448	ASN	2.8
1	A	131	ALA	2.8
2	B	31	ARG	2.7
1	A	78	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	302	GLY	2.6
4	D	43	LEU	2.6
1	A	316	ASP	2.6
1	A	312	LYS	2.6
1	A	401	GLY	2.5
2	B	29	GLU	2.5
1	A	353	CYS	2.4
2	B	15	ASP	2.4
1	A	310	HIS	2.4
1	A	499	LEU	2.4
1	A	309	PRO	2.3
1	A	449	ASN	2.3
2	B	3	LEU	2.3
3	C	6	LYS	2.3
1	A	268	HIS	2.3
1	A	301	ARG	2.2
1	A	343	VAL	2.2
1	A	321	GLU	2.2
1	A	270	GLU	2.1
1	A	204	GLY	2.1
1	A	45	HIS	2.1
1	A	573	MET	2.1
1	A	450	ASN	2.1
3	C	7	LYS	2.1
1	A	205	ALA	2.1
3	C	61	ALA	2.0
3	C	65	MET	2.0
1	A	429	LEU	2.0
1	A	311	ALA	2.0
2	B	5	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	AT5	C	131	23/23	0.83	0.32	3.83	74,78,84,85	0
12	CDN	C	132	77/77	0.77	0.61	3.66	32,55,88,91	0
5	OAA	A	589	9/9	0.87	0.49	1.85	94,95,96,96	0
10	HEB	C	130	43/43	0.97	0.21	1.49	22,28,42,46	0
6	FAD	A	601	53/53	0.89	0.38	1.02	65,79,83,86	0
8	SF4	B	303	8/8	0.99	0.20	-0.38	42,46,49,49	0
7	FES	B	302	4/4	0.99	0.20	-0.78	53,57,58,60	0
9	F3S	B	304	7/7	0.99	0.16	-1.71	33,39,41,42	0

6.5 Other polymers

There are no such residues in this entry.