



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:26 AM GMT

PDB ID : 3OWA
Title : Crystal Structure of Acyl-CoA Dehydrogenase complexed with FAD from Bacillus anthracis
Authors : Kim, Y.; Maltseva, N.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2010-09-17
Resolution : 1.97 Å(reported)

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

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

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

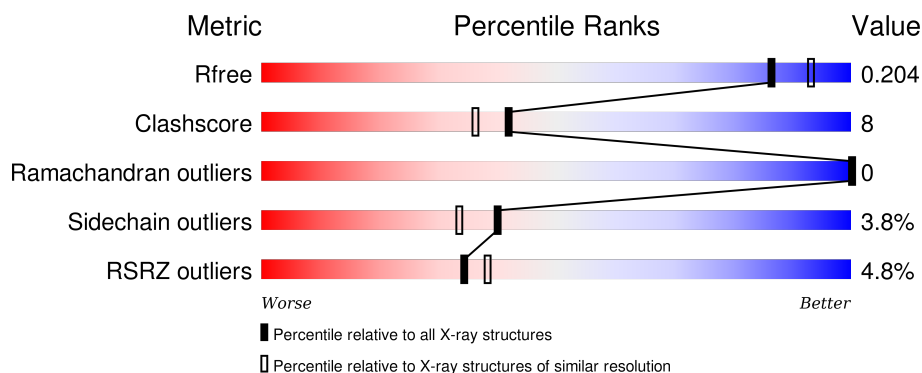
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	597	<div> <div>4%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	B	597	<div> <div>5%</div> <div>84%</div> <div>11%</div> <div>..</div> </div>
1	C	597	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	D	597	<div> <div>6%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1PE	A	602	-	-	X	X
3	1PE	B	602	-	-	X	X
3	1PE	C	602	-	-	-	X
3	1PE	D	602	-	-	X	X
5	GOL	B	606	-	-	-	X
5	GOL	B	607	-	-	-	X
6	SO4	A	606	-	-	-	X
6	SO4	B	604	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20926 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 Acyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	Se	0	13	0
			4653	2960	786	889	3	15			
1	B	572	Total	C	N	O	S	Se	0	8	0
			4508	2865	758	869	3	13			
1	C	587	Total	C	N	O	S	Se	0	14	0
			4689	2978	790	901	3	17			
1	D	582	Total	C	N	O	S	Se	0	5	0
			4567	2901	773	876	3	14			

There are 12 discrepancies between the modelled and reference sequences:

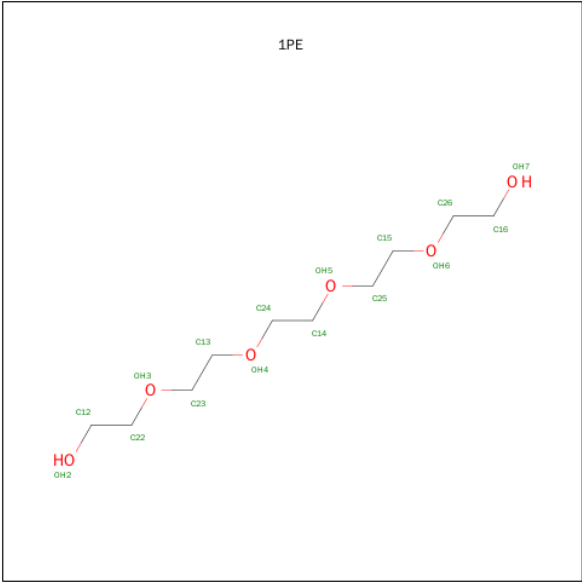
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q81XJ1
A	-1	ASN	-	EXPRESSION TAG	UNP Q81XJ1
A	0	ALA	-	EXPRESSION TAG	UNP Q81XJ1
B	-2	SER	-	EXPRESSION TAG	UNP Q81XJ1
B	-1	ASN	-	EXPRESSION TAG	UNP Q81XJ1
B	0	ALA	-	EXPRESSION TAG	UNP Q81XJ1
C	-2	SER	-	EXPRESSION TAG	UNP Q81XJ1
C	-1	ASN	-	EXPRESSION TAG	UNP Q81XJ1
C	0	ALA	-	EXPRESSION TAG	UNP Q81XJ1
D	-2	SER	-	EXPRESSION TAG	UNP Q81XJ1
D	-1	ASN	-	EXPRESSION TAG	UNP Q81XJ1
D	0	ALA	-	EXPRESSION TAG	UNP Q81XJ1

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



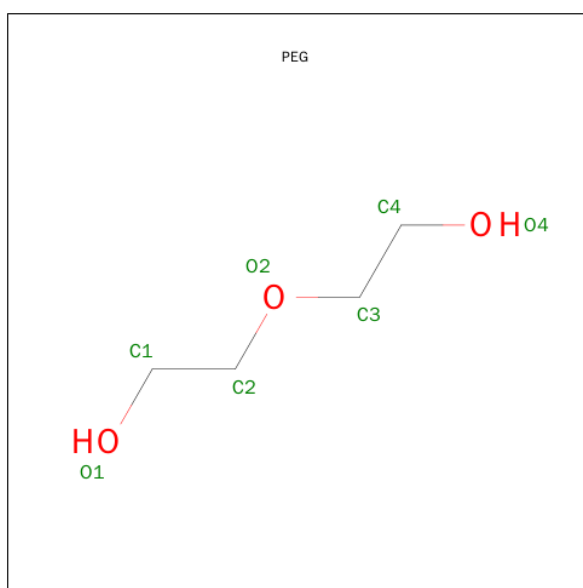
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

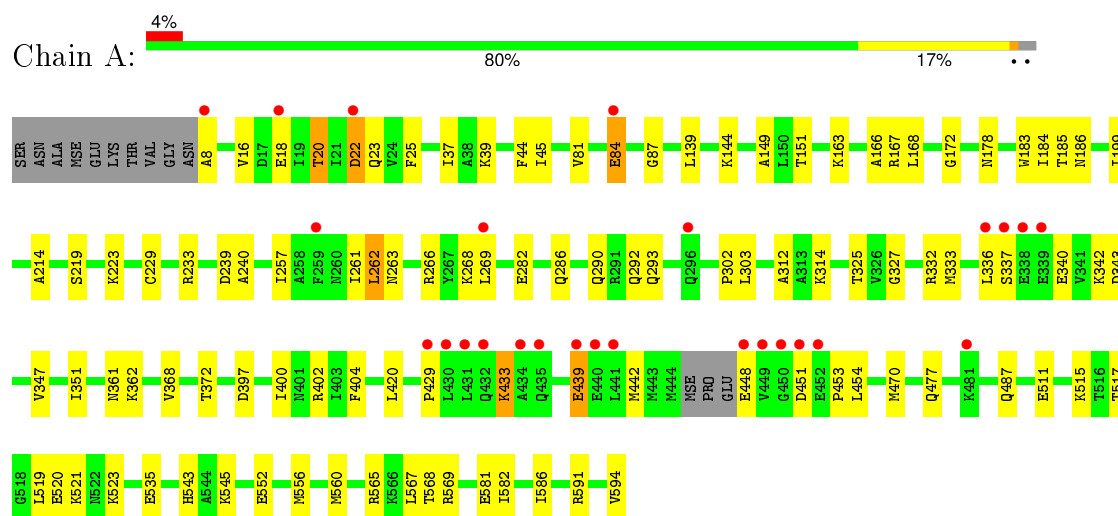
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	530	Total	O	0	0
			530	530		
7	B	517	Total	O	0	0
			517	517		
7	C	612	Total	O	0	0
			612	612		
7	D	488	Total	O	0	0
			488	488		

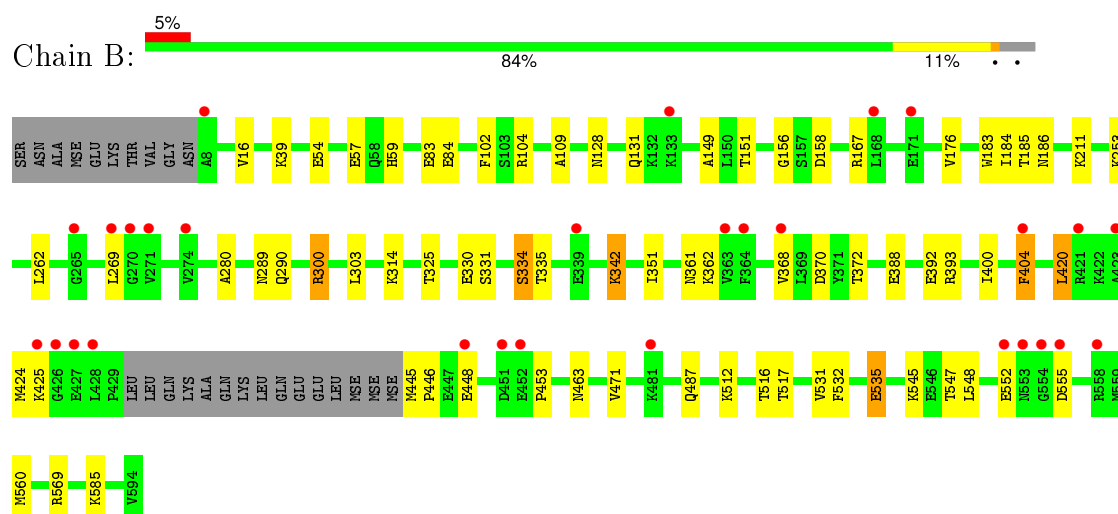
3 Residue-property plots [i](#)

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.

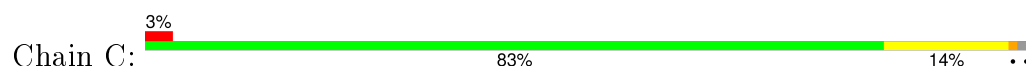
• Molecule 1: Acyl-CoA dehydrogenase

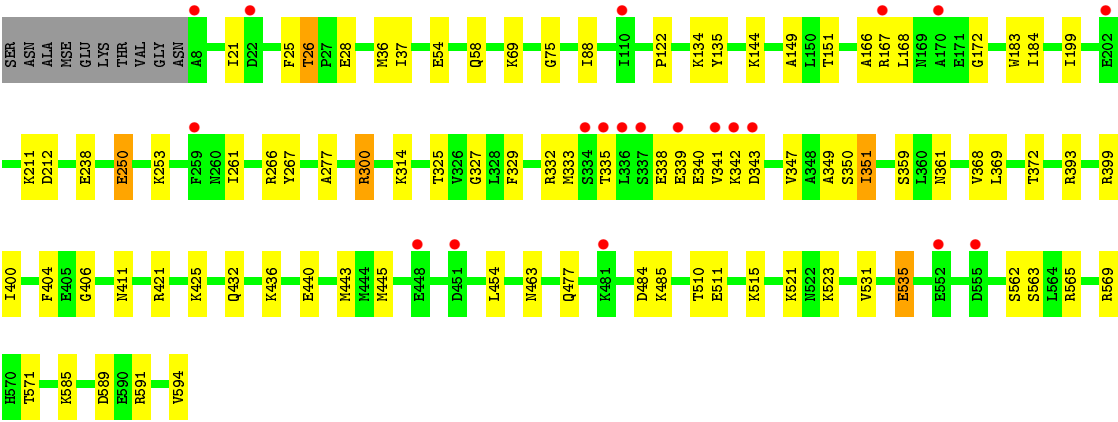


• Molecule 1: Acyl-CoA dehydrogenase

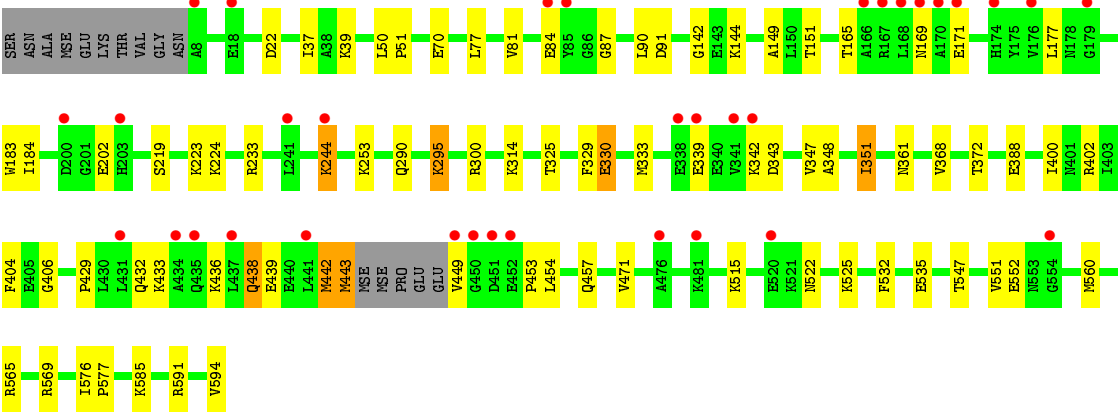
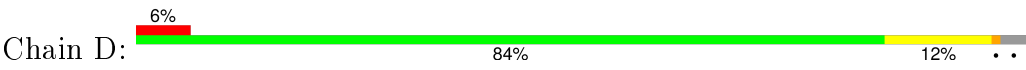


• Molecule 1: Acyl-CoA dehydrogenase





● Molecule 1: Acyl-CoA dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.61Å 98.03Å 107.74Å 92.80° 106.63° 105.30°	Depositor
Resolution (Å)	50.00 – 1.97 42.17 – 1.97	Depositor EDS
% Data completeness (in resolution range)	96.9 (50.00-1.97) 92.8 (42.17-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.162 , 0.201 0.166 , 0.204	Depositor DCC
R_{free} test set	9833 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 195012 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20926	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, SO4, FAD, 1PE

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	0.74	1/4706 (0.0%)	0.67	1/6304 (0.0%)
1	B	0.72	1/4566 (0.0%)	0.67	0/6131
1	C	0.77	0/4744	0.70	3/6358 (0.0%)
1	D	0.74	1/4620 (0.0%)	0.67	0/6194
All	All	0.74	3/18636 (0.0%)	0.68	4/24987 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	171	GLU	CG-CD	7.51	1.63	1.51
1	A	229	CYS	CB-SG	-5.76	1.72	1.81
1	B	392	GLU	CB-CG	5.04	1.61	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	393[A]	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	C	393[B]	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	397	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	399	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4653	0	4733	79	0
1	B	4508	0	4554	78	0
1	C	4689	0	4739	79	0
1	D	4567	0	4638	68	0
2	A	53	0	30	7	0
2	B	53	0	31	10	0
2	C	53	0	31	7	0
2	D	53	0	31	5	0
3	A	16	0	22	9	0
3	B	16	0	22	13	0
3	C	16	0	22	4	0
3	D	16	0	22	14	0
4	A	7	0	10	0	0
4	B	7	0	10	0	0
4	C	7	0	10	0	0
4	D	7	0	10	1	0
5	A	6	0	8	1	0
5	B	24	0	32	6	0
5	C	18	0	24	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	530	0	0	23	0
7	B	517	0	0	24	0
7	C	612	0	0	27	0
7	D	488	0	0	21	0
All	All	20926	0	18979	319	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 8.

All (319) 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)
2:B:601:FAD:C4'	2:B:601:FAD:C5'	1.79	1.58
1:D:439:GLU:O	1:D:442:MSE:HG3	1.61	1.01
1:C:329[A]:PHE:CE1	1:C:351:ILE:HD12	1.97	0.99
1:B:300[B]:ARG:CG	1:B:300[B]:ARG:HH11	1.77	0.97
1:B:314:LYS:HZ3	3:B:602:1PE:H251	1.31	0.94
1:B:300[B]:ARG:HG3	1:B:300[B]:ARG:HH11	1.31	0.94
1:C:400:ILE:HD11	2:C:601:FAD:HM83	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:1PE:H232	7:B:1369:HOH:O	1.70	0.90
1:D:400:ILE:HD11	2:D:601:FAD:HM83	1.54	0.89
1:D:532:PHE:HE1	3:D:602:1PE:H231	1.35	0.88
1:D:532:PHE:CE1	3:D:602:1PE:H231	2.10	0.85
1:D:330:GLU:HG2	7:D:1227:HOH:O	1.75	0.85
3:C:602:1PE:H142	7:C:1925:HOH:O	1.76	0.85
5:A:604:GOL:H31	7:A:2071:HOH:O	1.77	0.84
1:C:75:GLY:HA3	1:C:88:ILE:HD11	1.60	0.83
1:C:75:GLY:CA	1:C:88:ILE:HD11	2.09	0.83
1:D:551:VAL:HG12	1:D:552:GLU:HG3	1.61	0.83
1:A:314:LYS:HZ1	3:A:602:1PE:H141	1.45	0.82
1:C:591:ARG:HD3	7:C:2027:HOH:O	1.80	0.81
1:B:84:GLU:HG2	1:B:342:LYS:HE3	1.61	0.81
2:B:601:FAD:C3'	2:B:601:FAD:C5'	2.59	0.80
1:D:400:ILE:CD1	2:D:601:FAD:HM83	2.13	0.78
2:B:601:FAD:H9	2:B:601:FAD:H2'	1.63	0.78
1:C:400:ILE:CD1	2:C:601:FAD:HM83	2.13	0.78
1:B:531:VAL:O	1:B:535:GLU:HG2	1.84	0.77
1:D:565:ARG:O	1:D:569:ARG:HG3	1.84	0.77
1:D:535:GLU:HB2	3:D:602:1PE:H222	1.67	0.77
1:B:314:LYS:NZ	3:B:602:1PE:H251	1.99	0.76
1:D:471:VAL:HG13	1:D:547:THR:HG21	1.68	0.75
1:C:562[B]:SER:O	1:C:565[B]:ARG:HG3	1.85	0.75
1:B:314:LYS:NZ	3:B:602:1PE:H162	2.02	0.74
1:B:535:GLU:HB3	7:B:1945:HOH:O	1.85	0.74
1:D:224:LYS:NZ	7:D:1982:HOH:O	2.22	0.73
1:C:329[A]:PHE:CE1	1:C:351:ILE:CD1	2.71	0.73
1:D:522:ASN:OD1	1:D:525:LYS:HE3	1.87	0.73
1:C:368:VAL:O	1:C:372[A]:THR:HG23	1.87	0.73
1:D:439:GLU:O	1:D:442:MSE:CG	2.36	0.73
1:C:300:ARG:NH1	7:C:1172:HOH:O	2.22	0.72
1:C:443:MSE:SE	1:C:445:MSE:HE2	2.39	0.72
1:D:429:PRO:O	1:D:433:LYS:HG2	1.89	0.72
1:A:314:LYS:NZ	3:A:602:1PE:H131	2.04	0.72
1:A:163:LYS:HE2	7:A:1763:HOH:O	1.90	0.71
2:B:601:FAD:C9	2:B:601:FAD:H2'	2.21	0.70
1:C:523:LYS:HG3	7:C:1843:HOH:O	1.90	0.69
1:A:183:TRP:O	2:A:601:FAD:N5	2.25	0.69
1:B:453:PRO:HA	7:B:1219:HOH:O	1.92	0.69
1:A:400:ILE:HD11	2:A:601:FAD:HM83	1.75	0.69
1:A:565:ARG:O	1:A:569:ARG:HG3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:619:HOH:O	5:B:607:GOL:H12	1.93	0.68
1:A:84:GLU:OE1	1:A:342:LYS:HG3	1.95	0.67
1:A:581:GLU:HG3	7:A:795:HOH:O	1.95	0.66
1:A:556:MSE:HE3	7:A:2011:HOH:O	1.95	0.66
1:A:523:LYS:HG3	7:A:1915:HOH:O	1.94	0.66
1:C:349:ALA:HA	7:C:1337:HOH:O	1.97	0.65
1:D:388:GLU:HG3	7:D:2137:HOH:O	1.96	0.65
1:C:343:ASP:HB3	7:C:1341:HOH:O	1.95	0.65
1:A:293:GLN:HE22	1:B:156:GLY:H	1.42	0.65
1:B:300[B]:ARG:HG3	1:B:300[B]:ARG:NH1	2.05	0.65
1:B:149:ALA:HA	1:B:184:ILE:HD12	1.79	0.65
1:A:16:VAL:HG13	1:A:433:LYS:HG2	1.78	0.64
1:D:368:VAL:O	1:D:372:THR:HG23	1.98	0.63
1:D:314:LYS:HZ1	3:D:602:1PE:H261	1.64	0.63
1:C:406:GLY:CA	7:C:1927:HOH:O	2.46	0.63
1:B:331:SER:HB2	7:B:1713:HOH:O	1.98	0.63
1:B:54:GLU:HG2	7:B:1385:HOH:O	1.99	0.62
1:C:75:GLY:HA3	1:C:88:ILE:CD1	2.30	0.62
1:C:329[B]:PHE:O	1:C:329[B]:PHE:HD2	1.82	0.61
1:A:314:LYS:HZ2	3:A:602:1PE:H131	1.63	0.61
1:A:556:MSE:HB3	7:A:2011:HOH:O	2.00	0.61
1:A:470:MSE:CE	1:A:567:LEU:HD12	2.30	0.61
1:D:576:ILE:HB	1:D:577:PRO:HD3	1.82	0.61
1:C:440:GLU:HG3	1:C:445:MSE:HE3	1.82	0.61
1:B:300[B]:ARG:NH1	7:B:1957:HOH:O	2.33	0.61
1:B:167:ARG:HH11	1:B:176:VAL:HG21	1.65	0.60
1:A:269[B]:LEU:HD22	1:A:362:LYS:HG2	1.83	0.60
1:C:211:LYS:HE3	7:C:1246:HOH:O	2.01	0.60
1:B:400:ILE:HD11	2:B:601:FAD:HM83	1.84	0.59
1:C:21:ILE:HD13	1:C:515:LYS:HD2	1.84	0.59
1:C:212:ASP:HB2	7:C:1515:HOH:O	2.00	0.59
1:A:314:LYS:NZ	3:A:602:1PE:H141	2.15	0.59
1:C:406:GLY:HA2	7:C:1927:HOH:O	2.03	0.59
1:D:333:MSE:SE	1:D:347:VAL:HG13	2.53	0.59
1:C:421[A]:ARG:HE	1:C:425:LYS:HZ2	1.51	0.59
1:D:406:GLY:CA	7:D:1657:HOH:O	2.52	0.58
1:D:432:GLN:O	1:D:436:LYS:HG3	2.03	0.58
1:A:293:GLN:NE2	1:B:156:GLY:H	2.01	0.58
1:A:552:GLU:OE1	1:A:560:MSE:HG3	2.04	0.58
1:C:144:LYS:HE2	7:C:1771:HOH:O	2.03	0.58
1:C:406:GLY:N	7:C:1927:HOH:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASN:ND2	7:A:1542:HOH:O	2.37	0.58
1:D:438:GLN:HG3	7:D:2076:HOH:O	2.04	0.58
1:A:582:ILE:HG12	7:A:1571:HOH:O	2.04	0.57
5:C:604:GOL:H2	7:C:1644:HOH:O	2.05	0.57
1:B:532:PHE:HE1	3:B:602:1PE:H252	1.68	0.57
1:A:470:MSE:HE1	1:A:567:LEU:HD12	1.87	0.57
1:C:421[A]:ARG:HH11	1:C:425:LYS:HZ1	1.53	0.57
1:B:552:GLU:HB2	1:B:560:MSE:CE	2.35	0.57
1:A:149:ALA:HA	1:A:184:ILE:HD12	1.87	0.57
1:C:369:LEU:HA	1:C:372[B]:THR:HG22	1.85	0.56
1:B:446:PRO:HG2	1:B:569:ARG:NH1	2.19	0.56
1:B:585:LYS:HE3	7:B:1781:HOH:O	2.05	0.56
1:A:511:GLU:O	1:A:515:LYS:HG3	2.04	0.56
1:C:338:GLU:HA	1:C:341:VAL:HG12	1.87	0.56
1:A:400:ILE:CD1	2:A:601:FAD:HM83	2.35	0.56
1:A:543:HIS:HD2	7:A:2009:HOH:O	1.89	0.56
1:C:515:LYS:HE3	7:C:1330:HOH:O	2.04	0.56
1:D:348:ALA:O	1:D:351:ILE:HD12	2.06	0.56
1:A:333:MSE:SE	1:A:347:VAL:HG13	2.55	0.56
1:B:128:ASN:H	1:B:131:GLN:NE2	2.03	0.56
1:B:400:ILE:CD1	2:B:601:FAD:HM83	2.36	0.56
1:D:552:GLU:OE1	1:D:560:MSE:HG3	2.06	0.56
2:A:601:FAD:H2'	2:A:601:FAD:H9	1.87	0.55
1:D:454:LEU:HA	1:D:457:GLN:HE21	1.69	0.55
1:C:26:THR:CG2	1:C:28:GLU:H	2.18	0.55
1:B:300[B]:ARG:HH11	1:B:300[B]:ARG:HG2	1.69	0.55
1:A:303:LEU:HG	1:B:487:GLN:HB3	1.88	0.55
1:A:20:THR:HG22	1:A:23:GLN:HG3	1.88	0.55
1:B:300[A]:ARG:NH1	7:B:630:HOH:O	2.39	0.55
1:B:368:VAL:O	1:B:372[A]:THR:HG23	2.07	0.55
1:D:314:LYS:HZ2	3:D:602:1PE:H232	1.71	0.54
1:B:552:GLU:HB2	1:B:560:MSE:HE1	1.89	0.54
1:B:183:TRP:O	2:B:601:FAD:N5	2.41	0.54
1:B:128:ASN:H	1:B:131:GLN:HE21	1.56	0.54
1:C:333:MSE:HE1	7:C:932:HOH:O	2.07	0.54
1:C:342:LYS:HA	7:C:1794:HOH:O	2.07	0.54
1:D:314:LYS:HZ3	3:D:602:1PE:H122	1.73	0.53
1:D:342:LYS:N	1:D:342:LYS:HD3	2.23	0.53
1:B:289:ASN:HB3	5:B:608:GOL:H2	1.91	0.53
1:A:290[A]:GLN:HG2	7:A:1115:HOH:O	2.06	0.53
1:B:314:LYS:HZ1	3:B:602:1PE:H162	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLY:HA2	1:C:88:ILE:HD11	1.90	0.53
1:C:329[A]:PHE:CZ	1:C:351:ILE:CD1	2.92	0.53
1:A:292:GLN:HB2	7:B:1846:HOH:O	2.08	0.53
1:A:343:ASP:OD1	1:A:343:ASP:C	2.47	0.53
1:B:314:LYS:HZ3	3:B:602:1PE:H162	1.72	0.52
1:C:26:THR:HG23	1:C:28:GLU:H	1.73	0.52
1:A:487:GLN:HB3	1:B:303:LEU:HG	1.91	0.52
1:C:58:GLN:HG2	7:C:937:HOH:O	2.08	0.52
1:A:535:GLU:HG3	7:A:1987:HOH:O	2.10	0.52
1:D:84:GLU:OE2	1:D:342:LYS:HG3	2.10	0.52
1:B:57:GLU:HG3	7:B:1707:HOH:O	2.10	0.52
1:A:183:TRP:O	2:A:601:FAD:C4X	2.58	0.52
5:B:607:GOL:H11	7:B:673:HOH:O	2.10	0.51
1:D:406:GLY:HA2	7:D:1657:HOH:O	2.09	0.51
1:B:185:THR:O	1:B:186:ASN:HB2	2.10	0.51
1:D:165:THR:O	1:D:177:LEU:HA	2.09	0.51
1:A:185:THR:O	1:A:186:ASN:HB2	2.09	0.51
1:B:314:LYS:HZ1	3:B:602:1PE:H222	1.75	0.51
1:C:144:LYS:NZ	7:C:806:HOH:O	2.44	0.51
1:D:314:LYS:HE3	3:D:602:1PE:H252	1.93	0.51
1:A:8:ALA:HB3	1:A:332:ARG:HH11	1.76	0.51
1:B:516:THR:HG22	1:B:517:THR:HG23	1.91	0.51
1:D:183:TRP:O	2:D:601:FAD:N5	2.44	0.51
1:B:290[A]:GLN:HG2	7:B:718:HOH:O	2.10	0.51
1:C:134:LYS:HE3	1:C:135:TYR:CZ	2.45	0.51
1:D:591:ARG:HD3	7:D:1998:HOH:O	2.10	0.51
3:D:602:1PE:H151	7:D:1484:HOH:O	2.11	0.51
1:C:314:LYS:HZ3	3:C:602:1PE:H122	1.76	0.51
1:C:421[A]:ARG:HH11	1:C:425:LYS:NZ	2.09	0.51
1:A:144[B]:LYS:NZ	7:A:2112:HOH:O	2.43	0.51
1:B:314:LYS:HD3	3:B:602:1PE:H141	1.92	0.50
1:C:339:GLU:HG2	1:C:340:GLU:N	2.26	0.50
1:A:262:LEU:HD22	1:A:266:ARG:HD3	1.93	0.50
1:C:183:TRP:O	2:C:601:FAD:N5	2.45	0.50
1:C:134:LYS:HE2	7:C:677:HOH:O	2.11	0.50
1:A:20:THR:HG23	1:A:22:ASP:H	1.77	0.50
1:C:314:LYS:NZ	3:C:602:1PE:H122	2.26	0.50
1:D:453:PRO:HA	7:D:1475:HOH:O	2.12	0.50
1:D:169:ASN:HA	7:D:1230:HOH:O	2.11	0.50
1:B:388[B]:GLU:CD	1:B:388[B]:GLU:H	2.15	0.49
1:A:453:PRO:O	1:A:454:LEU:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ASP:HB3	7:D:1251:HOH:O	2.12	0.49
1:B:269:LEU:HD23	1:B:269:LEU:C	2.33	0.49
1:A:545:LYS:HD3	7:B:1536:HOH:O	2.11	0.49
1:D:454:LEU:HA	1:D:457:GLN:NE2	2.27	0.49
1:B:471:VAL:HG13	1:B:547:THR:HG21	1.94	0.49
1:D:290[B]:GLN:HG2	7:D:635:HOH:O	2.12	0.49
1:A:84:GLU:CD	1:A:342:LYS:HG3	2.33	0.49
1:B:548:LEU:HD22	1:B:560:MSE:HE3	1.94	0.49
1:C:369:LEU:O	1:C:372[B]:THR:HG22	2.12	0.49
1:B:335:THR:HG21	7:B:633:HOH:O	2.11	0.49
1:D:314:LYS:NZ	3:D:602:1PE:H122	2.27	0.49
1:A:39:LYS:HE2	7:A:1926:HOH:O	2.12	0.49
1:C:300:ARG:NH2	7:C:689:HOH:O	2.40	0.49
1:A:25:PHE:HB3	1:A:327:GLY:HA3	1.94	0.49
1:D:300[A]:ARG:NH1	7:D:1273:HOH:O	2.32	0.48
1:C:183:TRP:O	2:C:601:FAD:C4X	2.61	0.48
1:D:400:ILE:HD11	2:D:601:FAD:C8M	2.34	0.48
1:C:122:PRO:HG3	1:C:261:ILE:HG13	1.96	0.48
1:A:337:SER:OG	1:A:340:GLU:HG3	2.12	0.48
1:D:351:ILE:HD13	7:D:1249:HOH:O	2.12	0.48
1:C:400:ILE:HD11	2:C:601:FAD:C8M	2.33	0.48
1:C:266:ARG:NE	1:C:411:ASN:OD1	2.47	0.48
1:C:325:THR:CB	1:C:361:ASN:HD21	2.27	0.48
1:B:370:ASP:OD2	5:B:607:GOL:H11	2.14	0.48
1:A:178:ASN:ND2	1:A:239:ASP:H	2.11	0.48
1:B:104:ARG:HG3	1:B:104:ARG:O	2.14	0.47
3:A:602:1PE:H261	7:A:1389:HOH:O	2.13	0.47
2:B:601:FAD:C2'	2:B:601:FAD:H9	2.34	0.47
1:C:26:THR:HG21	7:C:702:HOH:O	2.14	0.47
1:C:329[B]:PHE:O	1:C:329[B]:PHE:CD2	2.66	0.47
1:A:314:LYS:HZ2	3:A:602:1PE:C13	2.27	0.47
1:D:219:SER:O	1:D:233:ARG:HD3	2.14	0.47
1:D:314:LYS:NZ	3:D:602:1PE:H261	2.27	0.47
1:A:368:VAL:O	1:A:372:THR:HG23	2.14	0.47
1:C:69:LYS:CE	7:C:624:HOH:O	2.61	0.47
1:C:531:VAL:O	1:C:535:GLU:HG2	2.15	0.47
1:B:300[B]:ARG:CG	1:B:300[B]:ARG:NH1	2.50	0.47
1:A:44:PHE:HD1	1:A:45:ILE:HD12	1.80	0.47
1:D:314:LYS:HZ1	3:D:602:1PE:H252	1.80	0.46
1:C:332:ARG:NH1	7:C:1653:HOH:O	2.44	0.46
1:A:219:SER:O	1:A:233:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:1PE:C23	7:B:1369:HOH:O	2.47	0.46
1:D:151:THR:OG1	2:D:601:FAD:H1'1	2.16	0.46
1:C:168[A]:LEU:HG	1:C:172:GLY:HA2	1.97	0.46
1:D:149:ALA:HA	1:D:184:ILE:HD12	1.97	0.46
1:A:535:GLU:HB2	3:A:602:1PE:H162	1.98	0.46
1:D:81:VAL:HB	1:D:87:GLY:HA3	1.98	0.46
1:A:151:THR:OG1	2:A:601:FAD:H1'1	2.16	0.45
1:D:325:THR:CB	1:D:361:ASN:HD21	2.29	0.45
1:B:393:ARG:HD3	5:B:606:GOL:O3	2.16	0.45
3:C:602:1PE:H252	3:C:602:1PE:H262	1.77	0.45
1:A:336:LEU:HA	1:A:340:GLU:OE1	2.16	0.45
1:B:420[B]:LEU:C	1:B:420[B]:LEU:HD13	2.37	0.45
1:C:484:ASP:OD1	1:C:485:LYS:HD3	2.17	0.45
1:D:295:LYS:NZ	7:D:1758:HOH:O	2.50	0.45
1:D:84:GLU:OE1	1:D:342:LYS:HE2	2.17	0.45
1:B:532:PHE:CE1	3:B:602:1PE:H252	2.50	0.45
3:A:602:1PE:H161	3:A:602:1PE:H151	1.72	0.45
1:B:290[A]:GLN:OE1	5:B:608:GOL:H11	2.17	0.45
1:B:330:GLU:HG2	7:B:1907:HOH:O	2.17	0.45
1:C:149:ALA:HA	1:C:184:ILE:HD12	1.99	0.45
1:C:69:LYS:HE3	7:C:624:HOH:O	2.17	0.45
1:D:402:ARG:NH2	7:D:1424:HOH:O	2.49	0.45
1:A:214:ALA:O	1:A:240:ALA:HA	2.16	0.45
1:B:535:GLU:HG2	1:B:535:GLU:H	1.58	0.44
1:C:421[A]:ARG:HD3	7:C:1586:HOH:O	2.17	0.44
1:D:329:PHE:CE1	1:D:351:ILE:HG13	2.52	0.44
1:C:454:LEU:HD11	1:C:510:THR:HG22	1.99	0.44
1:A:257:ILE:O	1:A:261:ILE:HG12	2.18	0.44
1:A:325:THR:CB	1:A:361:ASN:HD21	2.29	0.44
1:B:300[B]:ARG:HD3	1:B:300[B]:ARG:N	2.33	0.44
1:B:269:LEU:HD22	1:B:362:LYS:HG2	1.99	0.44
1:A:293:GLN:NE2	1:B:158:ASP:H	2.15	0.44
1:A:293:GLN:HE21	1:B:158:ASP:H	1.66	0.44
1:B:445:MSE:HG3	1:B:446:PRO:HD2	1.99	0.44
1:C:585:LYS:HE2	1:C:589:ASP:OD2	2.18	0.44
1:B:325:THR:CB	1:B:361:ASN:HD21	2.30	0.44
1:C:571:THR:HB	7:C:1944:HOH:O	2.18	0.44
1:A:439:GLU:O	1:A:442:MSE:HG3	2.17	0.44
1:B:362:LYS:HE3	1:B:404[B]:PHE:O	2.19	0.43
1:A:429:PRO:O	1:A:433:LYS:HB2	2.18	0.43
2:C:601:FAD:H62A	4:D:603:PEG:H22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:1PE:C15	7:B:1747:HOH:O	2.66	0.43
1:C:277:ALA:HA	1:C:372[B]:THR:HG21	2.00	0.43
1:A:591[B]:ARG:NH2	7:A:1769:HOH:O	2.50	0.43
2:A:601:FAD:H2'	2:A:601:FAD:C9	2.48	0.43
1:A:8:ALA:HB1	7:A:1641:HOH:O	2.19	0.42
1:C:166:ALA:O	1:C:199:ILE:HA	2.18	0.42
1:D:532:PHE:CD1	3:D:602:1PE:H121	2.54	0.42
1:B:545[A]:LYS:NZ	7:B:1137:HOH:O	2.46	0.42
1:A:81:VAL:O	1:A:87:GLY:HA3	2.19	0.42
1:A:168[A]:LEU:HG	1:A:172:GLY:HA2	2.00	0.42
1:C:75:GLY:CA	1:C:88:ILE:CD1	2.92	0.42
1:A:282:GLU:O	1:A:286:GLN:HG3	2.19	0.42
1:D:70:GLU:HG2	7:D:2040:HOH:O	2.18	0.42
1:D:453:PRO:O	1:D:454:LEU:HB2	2.19	0.42
1:D:339:GLU:HG3	7:D:1606:HOH:O	2.19	0.42
1:D:442:MSE:HG2	1:D:442:MSE:H	1.53	0.42
1:B:253:LYS:HG2	7:B:779:HOH:O	2.18	0.42
1:B:151:THR:OG1	2:B:601:FAD:H1'1	2.20	0.42
1:C:26:THR:HG22	1:C:28:GLU:N	2.35	0.42
1:B:59:HIS:HE1	7:B:873:HOH:O	2.02	0.42
1:A:312:ALA:CB	1:A:586:ILE:HD11	2.49	0.42
1:A:223[B]:LYS:HE2	7:A:836:HOH:O	2.20	0.42
1:D:585:LYS:HE3	7:D:662:HOH:O	2.18	0.42
1:A:351:ILE:HG23	7:A:798:HOH:O	2.20	0.42
1:C:511:GLU:OE2	1:C:515:LYS:NZ	2.38	0.42
1:B:183:TRP:O	2:B:601:FAD:C4X	2.68	0.42
1:B:585:LYS:HE2	7:B:1444:HOH:O	2.20	0.42
1:C:36[B]:MSE:HB3	1:C:36[B]:MSE:HE2	1.89	0.42
1:A:517:THR:HG22	1:A:521:LYS:HD2	2.02	0.42
1:A:470:MSE:CE	1:A:567:LEU:CD1	2.98	0.41
1:A:263:ASN:ND2	7:A:1384:HOH:O	2.52	0.41
1:D:443:MSE:H	1:D:443:MSE:HG2	1.72	0.41
1:A:453:PRO:HA	7:A:1529:HOH:O	2.19	0.41
1:A:517:THR:HG22	1:A:517:THR:O	2.20	0.41
1:D:244:LYS:H	1:D:244:LYS:HG3	1.64	0.41
1:C:25:PHE:HB3	1:C:327:GLY:HA3	2.01	0.41
1:C:151:THR:OG1	2:C:601:FAD:H1'1	2.21	0.41
1:C:421[A]:ARG:HE	1:C:425:LYS:NZ	2.17	0.41
1:C:69:LYS:HE2	7:C:624:HOH:O	2.20	0.41
7:A:1705:HOH:O	1:C:238:GLU:CD	2.58	0.41
3:D:602:1PE:H232	3:D:602:1PE:H122	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ILE:HG23	7:B:1026:HOH:O	2.21	0.41
1:B:16:VAL:O	1:B:16:VAL:HG12	2.20	0.41
1:C:535:GLU:H	1:C:535:GLU:HG2	1.68	0.41
1:D:532:PHE:HD1	3:D:602:1PE:H121	1.85	0.41
1:A:314:LYS:HZ1	3:A:602:1PE:C14	2.25	0.41
1:B:331:SER:O	1:B:334:SER:HB2	2.21	0.41
1:B:280:ALA:HB3	1:B:372[B]:THR:HG22	2.03	0.41
1:B:211:LYS:HD3	7:B:1203:HOH:O	2.21	0.41
3:B:602:1PE:H242	3:B:602:1PE:H232	1.85	0.41
1:A:302:PRO:HB2	1:B:487:GLN:HB2	2.02	0.41
1:A:166:ALA:O	1:A:199:ILE:HA	2.22	0.40
1:D:50:LEU:N	1:D:51:PRO:CD	2.84	0.40
1:D:37:ILE:HD13	1:D:90:LEU:HD13	2.02	0.40
1:C:250:GLU:HB3	1:C:253:LYS:HD2	2.03	0.40
1:B:102:PHE:O	1:B:109:ALA:HB2	2.20	0.40
1:B:400:ILE:O	1:B:400:ILE:HG13	2.20	0.40
1:A:139:LEU:HD23	1:A:144[B]:LYS:O	2.21	0.40
1:B:425:LYS:HA	7:B:1602:HOH:O	2.20	0.40
1:D:406:GLY:N	7:D:1657:HOH:O	2.54	0.40
1:B:388[B]:GLU:CD	1:B:388[B]:GLU:N	2.74	0.40
1:A:402:ARG:NH2	7:A:1971:HOH:O	2.54	0.40
1:C:347:VAL:O	1:C:351:ILE:HG22	2.21	0.40
1:D:565:ARG:NH1	7:D:2030:HOH:O	2.52	0.40
1:C:300:ARG:HA	1:C:300:ARG:NH1	2.36	0.40
1:D:77:LEU:HD12	1:D:142:GLY:HA3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	593/597 (99%)	588 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	576/597 (96%)	566 (98%)	10 (2%)	0	100	100
1	C	599/597 (100%)	594 (99%)	5 (1%)	0	100	100
1	D	583/597 (98%)	575 (99%)	8 (1%)	0	100	100
All	All	2351/2388 (98%)	2323 (99%)	28 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/474 (104%)	473 (96%)	20 (4%)	37	30
1	B	477/474 (101%)	460 (96%)	17 (4%)	42	36
1	C	497/474 (105%)	474 (95%)	23 (5%)	33	25
1	D	483/474 (102%)	465 (96%)	18 (4%)	41	35
All	All	1950/1896 (103%)	1872 (96%)	78 (4%)	40	31

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	20	THR
1	A	22	ASP
1	A	37	ILE
1	A	84	GLU
1	A	167	ARG
1	A	262	LEU
1	A	268	LYS
1	A	404[A]	PHE
1	A	404[B]	PHE
1	A	420	LEU
1	A	433	LYS
1	A	439	GLU

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Mol	Chain	Res	Type
1	A	448	GLU
1	A	451	ASP
1	A	477	GLN
1	A	519	LEU
1	A	520	GLU
1	A	568	THR
1	A	594	VAL
1	B	39	LYS
1	B	83	GLU
1	B	262	LEU
1	B	300[A]	ARG
1	B	300[B]	ARG
1	B	334	SER
1	B	342	LYS
1	B	404[A]	PHE
1	B	404[B]	PHE
1	B	420[A]	LEU
1	B	420[B]	LEU
1	B	424	MSE
1	B	448	GLU
1	B	463	ASN
1	B	512	LYS
1	B	535	GLU
1	B	555	ASP
1	C	26	THR
1	C	37	ILE
1	C	54[A]	GLU
1	C	54[B]	GLU
1	C	167	ARG
1	C	250	GLU
1	C	267	TYR
1	C	300	ARG
1	C	335	THR
1	C	350	SER
1	C	351	ILE
1	C	359	SER
1	C	404	PHE
1	C	432[A]	GLN
1	C	432[B]	GLN
1	C	436	LYS
1	C	463	ASN
1	C	477	GLN

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Mol	Chain	Res	Type
1	C	521	LYS
1	C	535	GLU
1	C	563	SER
1	C	569	ARG
1	C	594	VAL
1	D	22	ASP
1	D	39	LYS
1	D	91	ASP
1	D	144	LYS
1	D	202	GLU
1	D	223	LYS
1	D	244	LYS
1	D	253	LYS
1	D	295	LYS
1	D	330	GLU
1	D	351	ILE
1	D	404	PHE
1	D	438	GLN
1	D	442	MSE
1	D	443	MSE
1	D	449	VAL
1	D	515	LYS
1	D	594	VAL

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

Mol	Chain	Res	Type
1	A	178	ASN
1	A	263	ASN
1	A	289	ASN
1	A	293	GLN
1	A	361	ASN
1	A	411	ASN
1	A	463	ASN
1	B	131	GLN
1	B	289	ASN
1	B	361	ASN
1	B	463	ASN
1	C	361	ASN
1	C	463	ASN
1	C	477	GLN
1	D	361	ASN

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Mol	Chain	Res	Type
1	D	457	GLN
1	D	538	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

22 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	-	48,58,58	2.21	7 (14%)	54,89,89	2.40	14 (25%)
3	1PE	A	602	-	15,15,15	0.75	0	14,14,14	0.73	0
4	PEG	A	603	-	6,6,6	0.46	0	5,5,5	0.32	0
5	GOL	A	604	-	5,5,5	0.33	0	5,5,5	0.69	0
6	SO4	A	606	-	4,4,4	0.12	0	6,6,6	0.10	0
2	FAD	B	601	-	48,58,58	2.91	6 (12%)	54,89,89	2.55	11 (20%)
3	1PE	B	602	-	15,15,15	0.79	0	14,14,14	0.78	1 (7%)
4	PEG	B	603	-	6,6,6	0.53	0	5,5,5	0.25	0
6	SO4	B	604	-	4,4,4	0.19	0	6,6,6	0.19	0
5	GOL	B	605	-	5,5,5	0.41	0	5,5,5	0.37	0
5	GOL	B	606	-	5,5,5	0.35	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	607	-	5,5,5	0.30	0	5,5,5	0.59	0
5	GOL	B	608	-	5,5,5	0.36	0	5,5,5	0.54	0
2	FAD	C	601	-	48,58,58	1.35	5 (10%)	54,89,89	2.35	13 (24%)
3	1PE	C	602	-	15,15,15	0.64	0	14,14,14	0.79	0
4	PEG	C	603	-	6,6,6	0.53	0	5,5,5	0.22	0
5	GOL	C	604	-	5,5,5	0.36	0	5,5,5	0.35	0
5	GOL	C	605	-	5,5,5	0.34	0	5,5,5	0.25	0
5	GOL	C	606	-	5,5,5	0.40	0	5,5,5	0.48	0
2	FAD	D	601	-	48,58,58	1.24	6 (12%)	54,89,89	2.24	6 (11%)
3	1PE	D	602	-	15,15,15	0.69	0	14,14,14	0.58	0
4	PEG	D	603	-	6,6,6	0.63	0	5,5,5	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	601	-	-	0/30/50/50	0/6/6/6
3	1PE	A	602	-	-	0/13/13/13	0/0/0/0
4	PEG	A	603	-	-	0/4/4/4	0/0/0/0
5	GOL	A	604	-	-	0/4/4/4	0/0/0/0
6	SO4	A	606	-	-	0/0/0/0	0/0/0/0
2	FAD	B	601	-	-	0/30/50/50	0/6/6/6
3	1PE	B	602	-	-	0/13/13/13	0/0/0/0
4	PEG	B	603	-	-	0/4/4/4	0/0/0/0
6	SO4	B	604	-	-	0/0/0/0	0/0/0/0
5	GOL	B	605	-	-	0/4/4/4	0/0/0/0
5	GOL	B	606	-	-	0/4/4/4	0/0/0/0
5	GOL	B	607	-	-	0/4/4/4	0/0/0/0
5	GOL	B	608	-	-	0/4/4/4	0/0/0/0
2	FAD	C	601	-	-	0/30/50/50	0/6/6/6
3	1PE	C	602	-	-	0/13/13/13	0/0/0/0
4	PEG	C	603	-	-	0/4/4/4	0/0/0/0
5	GOL	C	604	-	-	0/4/4/4	0/0/0/0
5	GOL	C	605	-	-	0/4/4/4	0/0/0/0
5	GOL	C	606	-	-	0/4/4/4	0/0/0/0
2	FAD	D	601	-	-	0/30/50/50	0/6/6/6
3	1PE	D	602	-	-	0/13/13/13	0/0/0/0
4	PEG	D	603	-	-	0/4/4/4	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4'-C3'	-10.20	1.32	1.53
2	C	601	FAD	C5X-N5	2.03	1.38	1.35
2	D	601	FAD	C2A-N1A	2.17	1.38	1.33
2	D	601	FAD	C5X-N5	2.30	1.39	1.35
2	B	601	FAD	C1'-N10	2.34	1.50	1.48
2	A	601	FAD	C5X-N5	2.41	1.39	1.35
2	B	601	FAD	C2A-N1A	2.55	1.38	1.33
2	B	601	FAD	C4-N3	2.61	1.37	1.33
2	C	601	FAD	C4-N3	2.73	1.38	1.33
2	D	601	FAD	C1'-N10	2.74	1.51	1.48
2	A	601	FAD	C2A-N1A	2.76	1.39	1.33
2	C	601	FAD	C4X-N5	3.08	1.38	1.33
2	C	601	FAD	C2A-N3A	3.08	1.37	1.32
2	D	601	FAD	C2A-N3A	3.13	1.37	1.32
2	D	601	FAD	C4X-N5	3.18	1.38	1.33
2	A	601	FAD	C4X-N5	3.30	1.38	1.33
2	D	601	FAD	C4-N3	3.38	1.39	1.33
2	B	601	FAD	C2A-N3A	3.51	1.38	1.32
2	B	601	FAD	C4X-N5	3.61	1.39	1.33
2	A	601	FAD	C1'-N10	4.13	1.52	1.48
2	A	601	FAD	C2A-N3A	4.20	1.39	1.32
2	C	601	FAD	C1'-N10	4.79	1.53	1.48
2	A	601	FAD	C2'-C3'	6.93	1.67	1.53
2	B	601	FAD	C5'-C4'	18.21	1.79	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	N3A-C2A-N1A	-12.34	119.44	128.89
2	D	601	FAD	N3A-C2A-N1A	-12.06	119.66	128.89
2	C	601	FAD	N3A-C2A-N1A	-11.34	120.21	128.89
2	A	601	FAD	N3A-C2A-N1A	-10.51	120.85	128.89
2	A	601	FAD	C4X-C4-N3	-4.24	117.79	123.59
2	B	601	FAD	C4X-C4-N3	-4.08	118.01	123.59
2	C	601	FAD	C4X-C4-N3	-3.92	118.22	123.59
2	D	601	FAD	P-O3P-PA	-3.77	122.15	132.73
2	D	601	FAD	C4X-C4-N3	-3.61	118.66	123.59
2	A	601	FAD	P-O3P-PA	-3.49	122.93	132.73
2	C	601	FAD	P-O3P-PA	-3.28	123.53	132.73
2	C	601	FAD	C2B-C1B-N9A	-3.07	109.61	114.29
2	A	601	FAD	O3'-C3'-C2'	-2.73	101.88	108.75
2	B	601	FAD	P-O3P-PA	-2.42	125.92	132.73
2	A	601	FAD	C2B-C1B-N9A	-2.28	110.82	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C9A-C5X-N5	-2.27	119.00	122.36
2	C	601	FAD	C9A-C5X-N5	-2.14	119.19	122.36
2	A	601	FAD	C4A-C5A-N7A	-2.11	107.54	109.48
2	C	601	FAD	C2A-N1A-C6A	2.09	122.50	118.77
3	B	602	1PE	OH4-C13-C23	2.13	119.85	110.36
2	A	601	FAD	C6-C5X-C9A	2.15	121.80	118.98
2	A	601	FAD	C4-C4X-C10	2.20	121.35	119.94
2	C	601	FAD	O2A-PA-O3P	2.24	115.24	105.09
2	A	601	FAD	C1'-N10-C9A	2.26	121.40	118.86
2	C	601	FAD	O2P-P-O3P	2.29	115.48	105.09
2	B	601	FAD	O2'-C2'-C3'	2.50	115.30	109.02
2	B	601	FAD	C1'-N10-C9A	2.51	121.68	118.86
2	C	601	FAD	C4-C4X-C10	2.69	121.66	119.94
2	A	601	FAD	O2'-C2'-C1'	2.75	116.71	109.94
2	A	601	FAD	C4X-N5-C5X	2.82	120.01	116.76
2	D	601	FAD	C5X-C9A-N10	2.84	119.78	117.62
2	B	601	FAD	O2'-C2'-C1'	2.84	116.93	109.94
2	C	601	FAD	O2'-C2'-C1'	3.00	117.33	109.94
2	B	601	FAD	C4X-N5-C5X	3.03	120.24	116.76
2	D	601	FAD	C4X-N5-C5X	3.74	121.07	116.76
2	C	601	FAD	C4X-N5-C5X	4.01	121.38	116.76
2	A	601	FAD	O2'-C2'-C3'	4.39	120.06	109.02
2	A	601	FAD	C5X-C9A-N10	4.47	121.02	117.62
2	B	601	FAD	C5X-C9A-N10	4.54	121.07	117.62
2	C	601	FAD	C5X-C9A-N10	4.88	121.33	117.62
2	D	601	FAD	C4-N3-C2	5.38	119.89	115.25
2	C	601	FAD	C4-N3-C2	5.39	119.91	115.25
2	B	601	FAD	O4'-C4'-C5'	5.67	122.54	110.19
2	A	601	FAD	C4-N3-C2	6.70	121.03	115.25
2	B	601	FAD	C4-N3-C2	7.10	121.38	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	7	0
3	A	602	1PE	9	0
5	A	604	GOL	1	0
2	B	601	FAD	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	1PE	13	0
5	B	606	GOL	1	0
5	B	607	GOL	3	0
5	B	608	GOL	2	0
2	C	601	FAD	7	0
3	C	602	1PE	4	0
5	C	604	GOL	1	0
2	D	601	FAD	5	0
3	D	602	1PE	14	0
4	D	603	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	569/597 (95%)	0.14	26 (4%)	36	40	21, 41, 77, 126	0
1	B	559/597 (93%)	0.14	29 (5%)	31	35	20, 41, 69, 98	0
1	C	571/597 (95%)	0.06	20 (3%)	48	52	19, 38, 66, 107	0
1	D	568/597 (95%)	0.20	34 (5%)	25	29	18, 46, 79, 109	0
All	All	2267/2388 (94%)	0.14	109 (4%)	34	38	18, 41, 74, 126	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	VAL	6.6
1	A	441	LEU	6.4
1	A	8	ALA	6.1
1	A	448	GLU	6.0
1	C	341	VAL	5.7
1	C	8	ALA	5.6
1	D	170	ALA	5.6
1	A	439	GLU	5.0
1	B	451	ASP	4.9
1	C	342	LYS	4.7
1	A	430	LEU	4.7
1	C	451	ASP	4.4
1	D	8	ALA	4.3
1	A	451	ASP	4.2
1	B	428	LEU	4.0
1	D	520	GLU	4.0
1	D	449	VAL	4.0
1	B	425	LYS	3.9
1	A	431	LEU	3.8
1	B	553	ASN	3.8
1	D	167	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	450	GLY	3.7
1	B	8	ALA	3.7
1	D	481	LYS	3.7
1	C	336	LEU	3.7
1	D	338	GLU	3.6
1	A	434	ALA	3.5
1	D	451	ASP	3.4
1	A	338	GLU	3.3
1	D	452	GLU	3.3
1	D	241	LEU	3.3
1	D	441	LEU	3.2
1	C	448	GLU	3.2
1	D	339	GLU	3.2
1	C	337	SER	3.2
1	B	452	GLU	3.2
1	A	432	GLN	3.2
1	A	452	GLU	3.1
1	B	427	GLU	3.1
1	D	166	ALA	3.1
1	B	274	VAL	3.1
1	A	339	GLU	3.1
1	C	170	ALA	3.0
1	B	426	GLY	3.0
1	C	555	ASP	3.0
1	A	259	PHE	2.9
1	B	554	GLY	2.9
1	C	481	LYS	2.9
1	D	435	GLN	2.9
1	B	558	ARG	2.9
1	D	84	GLU	2.9
1	B	133	LYS	2.9
1	D	200	ASP	2.8
1	D	179	GLY	2.8
1	D	18	GLU	2.8
1	D	431	LEU	2.8
1	D	244	LYS	2.8
1	D	342	LYS	2.8
1	A	22	ASP	2.7
1	C	335	THR	2.7
1	D	476	ALA	2.7
1	B	339	GLU	2.7
1	C	334	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	423	ALA	2.7
1	D	437	LEU	2.7
1	D	168	LEU	2.7
1	C	343	ASP	2.6
1	C	259[A]	PHE	2.6
1	B	421	ARG	2.6
1	D	203	HIS	2.6
1	B	552	GLU	2.6
1	C	22	ASP	2.6
1	B	481	LYS	2.6
1	A	84	GLU	2.5
1	B	368	VAL	2.5
1	A	337	SER	2.5
1	B	168	LEU	2.5
1	A	435	GLN	2.4
1	C	552	GLU	2.4
1	D	341	VAL	2.4
1	C	339	GLU	2.4
1	A	440	GLU	2.3
1	B	171	GLU	2.3
1	A	18	GLU	2.3
1	D	171	GLU	2.3
1	A	429	PRO	2.3
1	D	85	TYR	2.2
1	D	176	VAL	2.2
1	A	336	LEU	2.2
1	B	269	LEU	2.2
1	B	555	ASP	2.1
1	D	554	GLY	2.1
1	B	364	PHE	2.1
1	C	167	ARG	2.1
1	A	269[A]	LEU	2.1
1	B	265	GLY	2.1
1	B	271	VAL	2.1
1	B	404[A]	PHE	2.1
1	B	363	VAL	2.1
1	A	296	GLN	2.1
1	D	450	GLY	2.1
1	D	434	ALA	2.1
1	C	202	GLU	2.1
1	C	110	ILE	2.0
1	D	169	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	481	LYS	2.0
1	B	270	GLY	2.0
1	B	448	GLU	2.0
1	D	174	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	B	607	6/6	0.48	0.64	63.79	82,84,85,85	0
3	1PE	A	602	16/16	0.89	0.43	8.70	68,72,77,78	0
3	1PE	B	602	16/16	0.79	0.41	7.82	71,73,75,76	0
3	1PE	D	602	16/16	0.78	0.38	7.59	70,72,74,74	0
3	1PE	C	602	16/16	0.80	0.36	7.19	65,71,74,74	0
5	GOL	B	606	6/6	0.74	0.25	4.02	80,80,81,81	0
6	SO4	B	604	5/5	0.83	0.16	2.83	119,119,120,120	0
6	SO4	A	606	5/5	0.67	0.30	2.02	183,183,183,183	0
4	PEG	B	603	7/7	0.71	0.16	1.53	74,75,76,76	0
2	FAD	A	601	53/53	0.95	0.13	1.13	28,34,42,46	0
2	FAD	D	601	53/53	0.94	0.14	1.13	32,38,44,46	0
4	PEG	C	603	7/7	0.83	0.14	0.89	72,72,74,74	0
5	GOL	C	606	6/6	0.94	0.13	0.85	62,67,67,67	0
2	FAD	B	601	53/53	0.94	0.13	0.67	29,37,44,46	0
4	PEG	D	603	7/7	0.74	0.15	0.66	67,69,71,73	0
2	FAD	C	601	53/53	0.96	0.12	0.66	23,32,37,39	0
5	GOL	C	604	6/6	0.83	0.16	0.56	87,88,88,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	PEG	A	603	7/7	0.88	0.10	-0.33	67,67,70,73	0
5	GOL	B	608	6/6	0.73	0.41	-	78,83,84,85	0
5	GOL	A	604	6/6	0.64	0.28	-	85,86,87,87	0
5	GOL	B	605	6/6	0.95	0.11	-	81,82,84,85	0
5	GOL	C	605	6/6	0.59	0.27	-	98,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.