Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:14 AM GMT

PDB ID	:	3LB8
Title	:	Crystal structure of the covalent putidaredoxin reductase-putidaredoxin complex
Authors	:	Sevrioukova, I.F.
Deposited on	:	2010-01-07
Resolution	:	2.60 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:

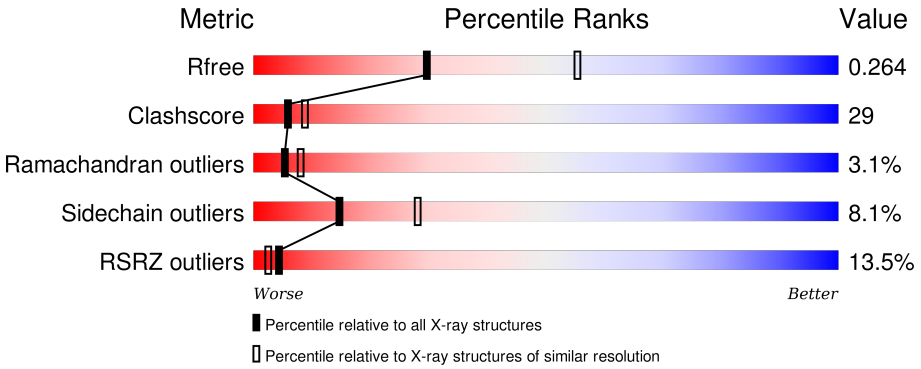
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	436	% 67% 25%
1	B	436	14% 51% 40%
2	C	106	18% 40% 47% 10%
2	D	106	54% 25% 53% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FES	D	107	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8063 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 Putidaredoxin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3186	2004	570	601	11			
1	B	417	Total	C	N	O	S	0	0	0
			3172	1995	568	598	11			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	LYS	-	EXPRESSION TAG	UNP P16640
A	424	ALA	-	EXPRESSION TAG	UNP P16640
A	425	GLU	-	EXPRESSION TAG	UNP P16640
A	426	LEU	-	EXPRESSION TAG	UNP P16640
A	427	SER	-	EXPRESSION TAG	UNP P16640
A	428	SER	-	EXPRESSION TAG	UNP P16640
A	429	ALA	-	EXPRESSION TAG	UNP P16640
A	430	PRO	-	EXPRESSION TAG	UNP P16640
A	431	ARG	-	EXPRESSION TAG	UNP P16640
A	432	HIS	-	EXPRESSION TAG	UNP P16640
A	433	HIS	-	EXPRESSION TAG	UNP P16640
A	434	HIS	-	EXPRESSION TAG	UNP P16640
A	435	HIS	-	EXPRESSION TAG	UNP P16640
A	436	HIS	-	EXPRESSION TAG	UNP P16640
A	437	HIS	-	EXPRESSION TAG	UNP P16640
B	423	LYS	-	EXPRESSION TAG	UNP P16640
B	424	ALA	-	EXPRESSION TAG	UNP P16640
B	425	GLU	-	EXPRESSION TAG	UNP P16640
B	426	LEU	-	EXPRESSION TAG	UNP P16640
B	427	SER	-	EXPRESSION TAG	UNP P16640
B	428	SER	-	EXPRESSION TAG	UNP P16640
B	429	ALA	-	EXPRESSION TAG	UNP P16640
B	430	PRO	-	EXPRESSION TAG	UNP P16640
B	431	ARG	-	EXPRESSION TAG	UNP P16640
B	432	HIS	-	EXPRESSION TAG	UNP P16640

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Chain	Residue	Modelled	Actual	Comment	Reference
B	433	HIS	-	EXPRESSION TAG	UNP P16640
B	434	HIS	-	EXPRESSION TAG	UNP P16640
B	435	HIS	-	EXPRESSION TAG	UNP P16640
B	436	HIS	-	EXPRESSION TAG	UNP P16640
B	437	HIS	-	EXPRESSION TAG	UNP P16640

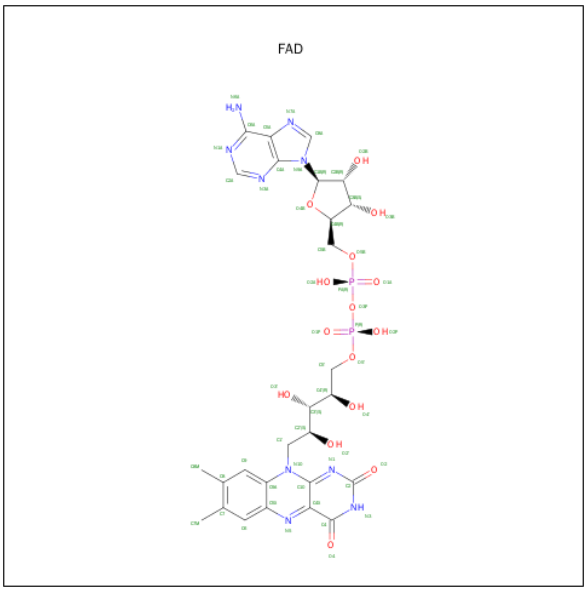
- Molecule 2 is a protein called Putidaredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	104	Total	C	N	O	S	0	0	0
			770	472	132	159	7			
2	D	103	Total	C	N	O	S	0	0	0
			759	466	128	158	7			

There are 4 discrepancies between the modelled and reference sequences:

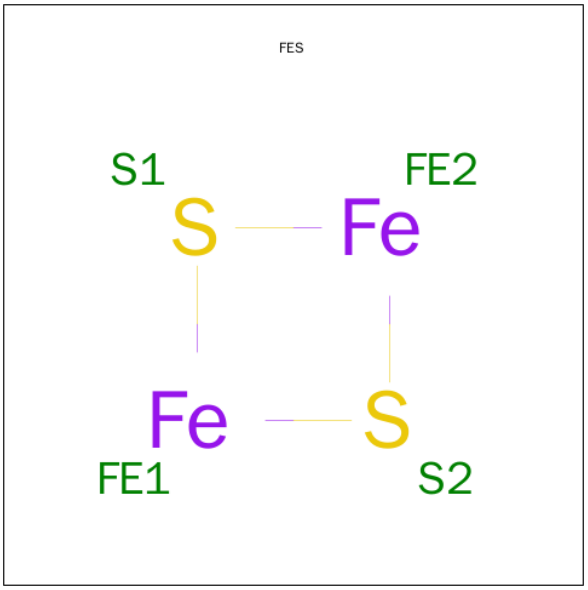
Chain	Residue	Modelled	Actual	Comment	Reference
C	73	SER	CYS	ENGINEERED	UNP P00259
C	85	SER	CYS	ENGINEERED	UNP P00259
D	73	SER	CYS	ENGINEERED	UNP P00259
D	85	SER	CYS	ENGINEERED	UNP P00259

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is water.

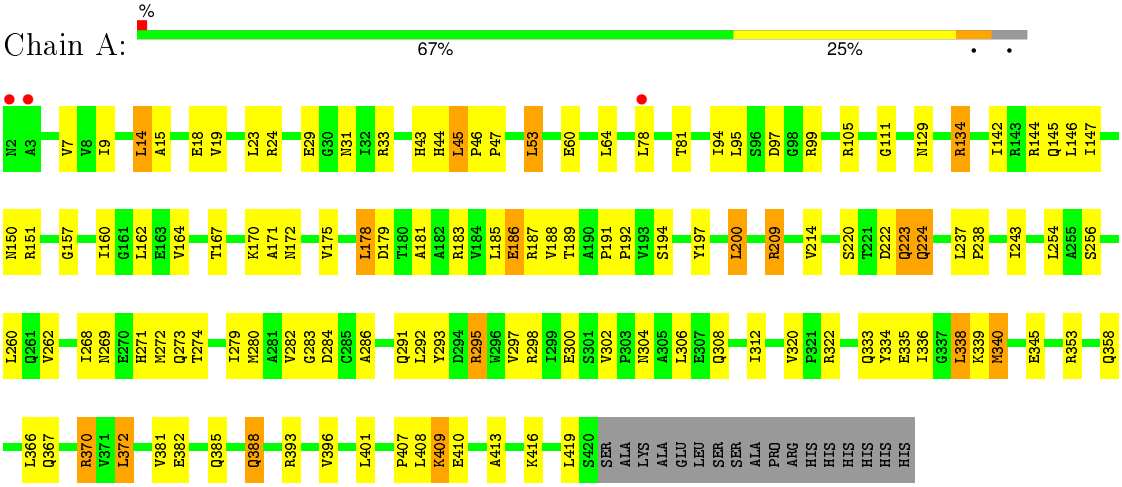
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		
5	B	11	Total	O	0	0
			11	11		
5	C	2	Total	O	0	0
			2	2		

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.

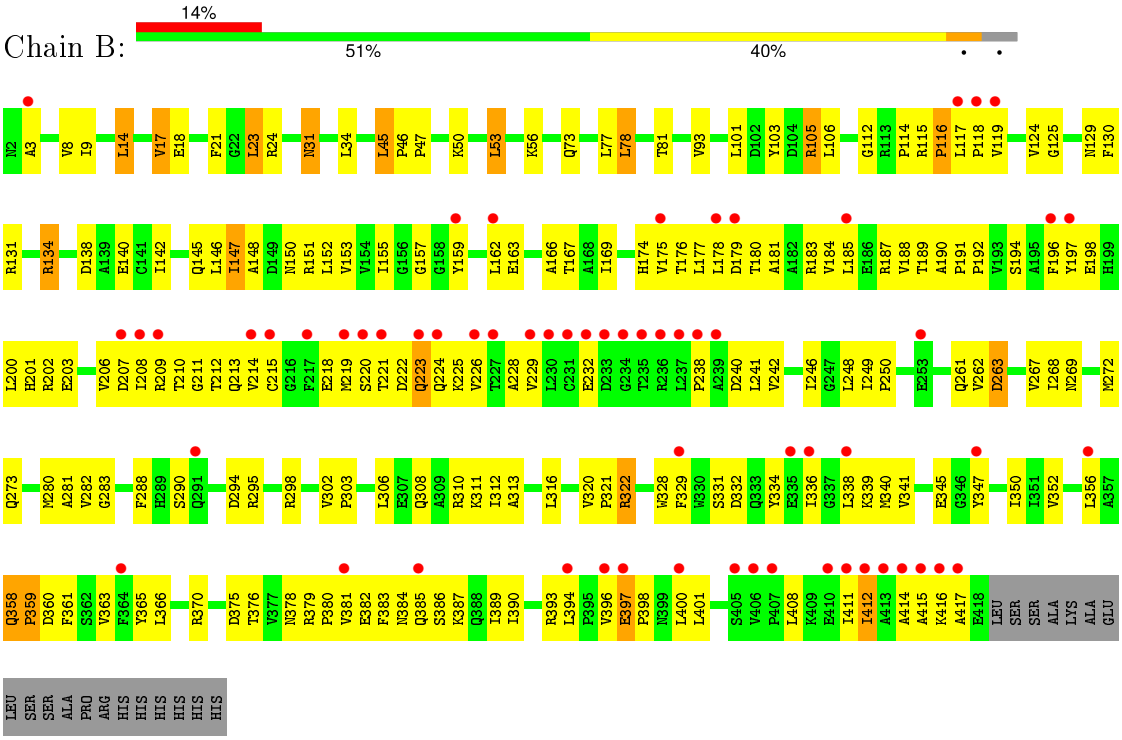
- Molecule 1: Putidaredoxin reductase

Chain A:



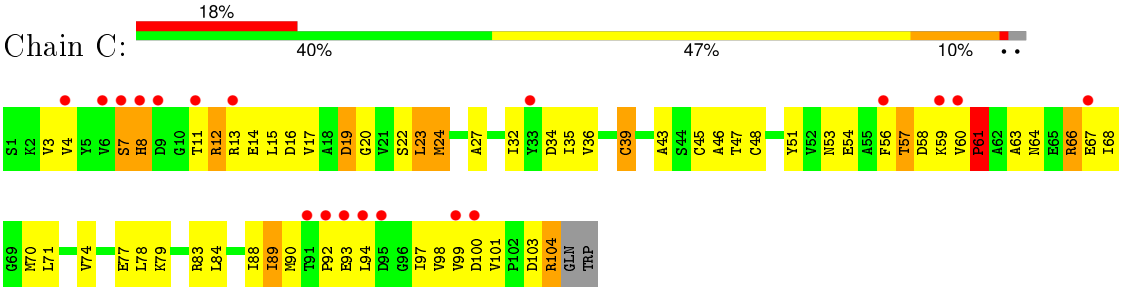
- Molecule 1: Putidaredoxin reductase

Chain B:



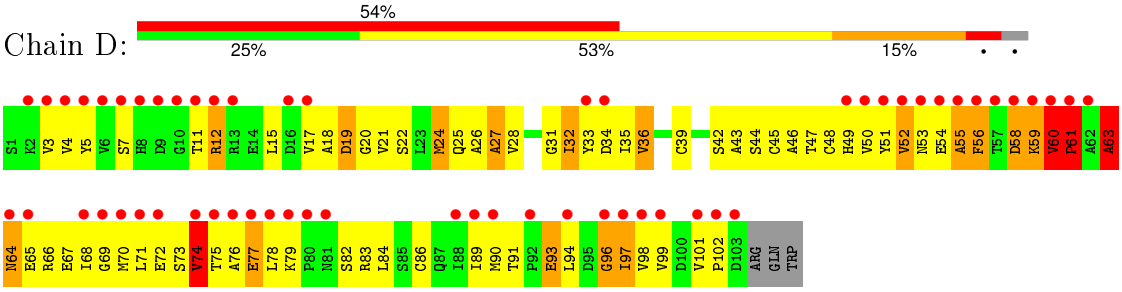
• Molecule 2: Putidaredoxin

Chain C:



• Molecule 2: Putidaredoxin

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.60Å 103.40Å 167.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 2.60 49.41 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.50-2.60) 97.7 (49.41-2.37)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.37Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.244 , 0.272 0.241 , 0.264	Depositor DCC
R_{free} test set	1842 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	1.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 61.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 47149 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8063	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: FES, 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	0/3240	0.69	1/4410 (0.0%)
1	B	0.34	0/3226	0.63	1/4391 (0.0%)
2	C	0.42	0/779	0.66	0/1058
2	D	0.54	0/768	0.93	3/1044 (0.3%)
All	All	0.42	0/8013	0.69	5/10903 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	61	PRO	CA-N-CD	-12.09	94.57	111.50
1	A	409	LYS	CD-CE-NZ	-5.55	98.93	111.70
2	D	63	ALA	N-CA-C	5.42	125.65	111.00
1	B	3	ALA	N-CA-C	5.20	125.05	111.00
2	D	60	VAL	CB-CA-C	5.05	121.00	111.40

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	3186	0	3212	107	0
1	B	3172	0	3197	202	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	770	0	752	65	0
2	D	759	0	739	97	0
3	A	53	0	31	1	0
3	B	53	0	31	1	0
4	C	4	0	0	1	0
4	D	4	0	0	2	0
5	A	49	0	0	3	0
5	B	11	0	0	1	0
5	C	2	0	0	0	0
All	All	8063	0	7962	458	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 29.

All (458) 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:D:59:LYS:O	2:D:60:VAL:HG23	1.39	1.21
2:D:36:VAL:HG23	2:D:47:THR:HB	1.32	1.07
1:A:338:LEU:HB3	1:A:340:MET:HE1	1.42	1.02
2:C:48:CYS:SG	2:C:84:LEU:HD22	2.01	0.99
1:B:396:VAL:HG11	1:B:401:LEU:HD21	1.49	0.95
2:D:24:MET:HG3	2:D:48:CYS:CB	1.98	0.93
2:D:52:VAL:HG13	2:D:97:ILE:HG23	1.50	0.92
1:B:269:ASN:HD21	1:B:273:GLN:HE21	1.20	0.88
1:B:117:LEU:HD12	1:B:118:PRO:HD2	1.53	0.88
2:D:22:SER:HB2	2:D:86:CYS:HA	1.55	0.88
2:C:51:TYR:HB2	2:C:100:ASP:HB2	1.57	0.87
1:B:339:LYS:NZ	2:D:66:ARG:HH21	1.72	0.86
1:B:280:MET:HE1	1:B:312:ILE:HG23	1.58	0.86
1:A:19:VAL:O	1:A:23:LEU:HB2	1.76	0.85
1:B:201:HIS:HB2	1:B:208:ILE:HD11	1.58	0.85
1:B:358:GLN:O	1:B:358:GLN:HG2	1.77	0.84
2:D:24:MET:HG3	2:D:48:CYS:HB2	1.57	0.84
1:B:215:CYS:HB3	1:B:232:GLU:HG2	1.60	0.84
2:D:7:SER:HB2	2:D:11:THR:HG23	1.60	0.83
1:B:322:ARG:HB3	1:B:322:ARG:HH11	1.43	0.82
2:C:89:ILE:HD12	2:C:89:ILE:H	1.44	0.82
1:B:196:PHE:CZ	1:B:359:PRO:HG3	2.16	0.81
1:A:183:ARG:HG2	1:A:186:GLU:HG2	1.62	0.81
1:B:177:LEU:HD23	1:B:178:LEU:N	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:ASP:HB3	2:C:101:VAL:HG11	1.64	0.80
2:C:3:VAL:HG22	2:C:90:MET:HE2	1.64	0.79
1:B:250:PRO:HD3	1:B:298:ARG:NH2	1.98	0.77
2:D:27:ALA:HB1	2:D:35:ILE:HD11	1.64	0.77
1:B:129:ASN:HA	1:B:145:GLN:HE22	1.50	0.77
1:A:188:VAL:HG23	1:A:189:THR:HG23	1.66	0.77
2:C:17:VAL:HG12	2:C:19:ASP:H	1.48	0.77
1:A:385:GLN:HE22	1:A:409:LYS:HG3	1.50	0.77
1:B:283:GLY:H	1:B:308:GLN:NE2	1.81	0.76
1:A:407:PRO:HB2	1:A:410:GLU:HG3	1.65	0.76
1:B:125:GLY:HA2	1:B:130:PHE:HD2	1.50	0.76
1:B:224:GLN:O	1:B:225:LYS:HG2	1.85	0.76
2:C:13:ARG:HG3	2:C:15:LEU:HD11	1.69	0.75
2:D:17:VAL:HG13	2:D:90:MET:HG2	1.66	0.75
1:B:394:LEU:HB3	1:B:415:ALA:HB1	1.69	0.74
2:D:58:ASP:O	2:D:59:LYS:O	2.06	0.74
1:B:396:VAL:O	1:B:398:PRO:HD3	1.88	0.73
1:A:283:GLY:H	1:A:308:GLN:NE2	1.85	0.73
2:C:13:ARG:HG3	2:C:15:LEU:CD1	2.19	0.72
1:B:412:ILE:HD11	1:B:416:LYS:HE3	1.72	0.72
1:B:183:ARG:HE	1:B:191:PRO:HG3	1.55	0.72
1:B:280:MET:CE	1:B:312:ILE:HG23	2.21	0.70
1:B:73:GLN:HA	1:B:73:GLN:HE21	1.55	0.70
1:B:347:TYR:CE1	1:B:350:ILE:HG23	2.27	0.70
1:B:339:LYS:NZ	2:D:66:ARG:NH2	2.39	0.70
2:C:39:CYS:HB3	2:C:45:CYS:SG	2.30	0.70
1:B:192:PRO:HB3	1:B:356:LEU:HD11	1.72	0.70
2:C:3:VAL:HG22	2:C:90:MET:CE	2.22	0.70
1:B:183:ARG:HD2	1:B:194:SER:HB2	1.72	0.70
1:B:339:LYS:HZ2	2:D:66:ARG:HH21	1.39	0.69
2:D:82:SER:O	2:D:83:ARG:HD2	1.92	0.69
1:A:338:LEU:HB3	1:A:340:MET:CE	2.22	0.69
2:D:19:ASP:CG	2:D:20:GLY:H	1.96	0.69
1:B:322:ARG:NH1	1:B:322:ARG:HB3	2.07	0.68
1:B:370:ARG:NH1	1:B:393:ARG:HH12	1.91	0.68
1:B:159:TYR:OH	1:B:188:VAL:HG11	1.92	0.68
1:A:385:GLN:NE2	1:A:409:LYS:HG3	2.09	0.68
1:A:81:THR:HG21	1:A:95:LEU:HD13	1.76	0.68
1:B:115:ARG:HD2	1:B:246:ILE:O	1.93	0.68
1:A:254:LEU:HB2	5:A:440:HOH:O	1.94	0.68
1:B:14:LEU:HD11	1:B:302:VAL:HG13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:VAL:HG21	1:B:387:LYS:HA	1.75	0.67
1:A:7:VAL:HG12	1:A:31:ASN:O	1.94	0.67
2:D:36:VAL:CG2	2:D:47:THR:HB	2.18	0.67
1:B:339:LYS:HZ1	2:D:66:ARG:NH2	1.92	0.67
2:C:8:HIS:O	2:C:11:THR:HG22	1.95	0.67
1:B:187:ARG:HG3	1:B:188:VAL:HG23	1.78	0.66
1:B:159:TYR:HE1	1:B:188:VAL:HG21	1.60	0.66
1:A:340:MET:HB3	5:A:442:HOH:O	1.94	0.65
1:B:125:GLY:HA2	1:B:130:PHE:CD2	2.31	0.65
2:C:60:VAL:HG22	2:C:83:ARG:HH12	1.61	0.65
1:A:183:ARG:CG	1:A:186:GLU:HG2	2.26	0.65
1:B:370:ARG:NH1	1:B:393:ARG:NH1	2.44	0.65
2:C:34:ASP:CB	2:C:101:VAL:HG11	2.27	0.64
1:B:396:VAL:HG13	1:B:411:ILE:HG21	1.79	0.64
1:B:339:LYS:HZ1	2:D:66:ARG:HH21	1.42	0.64
2:C:23:LEU:HD23	2:C:99:VAL:HG11	1.79	0.64
1:B:46:PRO:HB2	1:B:47:PRO:HD3	1.78	0.64
1:B:78:LEU:HD22	1:B:81:THR:OG1	1.98	0.64
2:D:5:TYR:CE1	2:D:15:LEU:HD12	2.32	0.64
2:D:59:LYS:O	2:D:60:VAL:CG2	2.32	0.64
2:D:89:ILE:N	2:D:89:ILE:HD12	2.11	0.64
1:B:183:ARG:HD2	1:B:194:SER:CB	2.28	0.64
1:B:196:PHE:CE1	1:B:359:PRO:HG3	2.32	0.64
1:B:114:PRO:HD3	1:B:134:ARG:HG3	1.80	0.63
2:D:45:CYS:O	2:D:46:ALA:HB3	1.98	0.63
1:B:202:ARG:HG3	1:B:202:ARG:HH11	1.62	0.63
1:B:201:HIS:HB3	1:B:206:VAL:HB	1.81	0.63
2:D:12:ARG:H	2:D:12:ARG:HD2	1.63	0.63
1:A:170:LYS:HD3	1:A:170:LYS:O	1.98	0.63
2:D:3:VAL:HG22	2:D:90:MET:CE	2.29	0.63
2:D:3:VAL:CG2	2:D:17:VAL:HG12	2.29	0.63
2:D:24:MET:HG3	2:D:48:CYS:HB3	1.79	0.62
1:B:219:MET:SD	1:B:223:GLN:HG3	2.40	0.62
1:A:197:TYR:OH	1:A:338:LEU:HD22	2.00	0.62
1:B:306:LEU:O	1:B:310:ARG:HG2	1.98	0.62
1:B:153:VAL:HG11	1:B:229:VAL:HG21	1.81	0.62
2:D:63:ALA:HB2	2:D:83:ARG:NE	2.15	0.61
1:A:293:TYR:O	1:A:295:ARG:HG2	2.00	0.61
1:B:396:VAL:HG22	1:B:411:ILE:HG22	1.81	0.61
2:D:43:ALA:HA	4:D:107:FES:S2	2.41	0.61
1:B:116:PRO:O	1:B:246:ILE:HD11	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:VAL:HG23	1:B:308:GLN:HB3	1.83	0.60
2:C:12:ARG:HG2	2:C:12:ARG:HH11	1.66	0.60
1:A:200:LEU:HD11	1:A:336:ILE:HD12	1.82	0.60
1:B:221:THR:C	1:B:223:GLN:H	2.05	0.60
1:B:115:ARG:HG3	1:B:115:ARG:HH11	1.66	0.60
1:B:151:ARG:HE	1:B:238:PRO:HG2	1.66	0.59
2:D:78:LEU:HD13	2:D:79:LYS:N	2.17	0.59
1:A:274:THR:HG23	1:A:279:ILE:O	2.02	0.59
1:A:53:LEU:CD1	1:A:167:THR:HG21	2.32	0.59
1:B:201:HIS:CB	1:B:208:ILE:HD11	2.32	0.59
1:A:144:ARG:NH1	1:B:140:GLU:OE1	2.32	0.59
1:B:112:GLY:HA3	1:B:248:LEU:HD21	1.83	0.59
1:B:202:ARG:NH1	1:B:208:ILE:HB	2.18	0.58
2:C:64:ASN:OD1	2:C:66:ARG:HB2	2.02	0.58
2:C:71:LEU:O	2:C:74:VAL:HG22	2.03	0.58
2:C:17:VAL:HG11	2:C:90:MET:HB3	1.84	0.58
1:B:176:THR:HG23	1:B:207:ASP:O	2.03	0.58
2:D:4:VAL:HB	2:D:98:VAL:HG23	1.84	0.58
2:D:94:LEU:O	2:D:94:LEU:HD23	2.03	0.58
1:B:280:MET:HG3	5:B:442:HOH:O	2.02	0.58
1:B:268:ILE:HA	1:B:273:GLN:O	2.04	0.58
2:C:48:CYS:SG	2:C:84:LEU:CD2	2.86	0.58
1:B:269:ASN:HD21	1:B:273:GLN:NE2	1.97	0.58
2:C:60:VAL:HG13	2:C:60:VAL:O	2.03	0.58
2:D:96:GLY:O	2:D:98:VAL:N	2.31	0.58
1:B:152:LEU:HB3	1:B:175:VAL:HB	1.86	0.58
2:C:4:VAL:HB	2:C:98:VAL:HG22	1.85	0.58
2:C:27:ALA:CB	2:C:35:ILE:HD11	2.34	0.57
1:B:150:ASN:HD22	1:B:240:ASP:CG	2.08	0.57
1:B:105:ARG:HG2	1:B:316:LEU:HD22	1.84	0.57
1:B:119:VAL:HG21	1:B:214:VAL:CG1	2.34	0.57
1:A:385:GLN:NE2	1:A:409:LYS:CG	2.68	0.57
1:A:147:ILE:O	1:A:150:ASN:HB2	2.05	0.57
1:A:178:LEU:CD2	1:A:209:ARG:HG3	2.35	0.57
1:B:376:THR:HG23	1:B:379:ARG:HB2	1.85	0.57
1:B:282:VAL:HB	1:B:312:ILE:CD1	2.34	0.56
1:A:381:VAL:O	1:A:385:GLN:HG3	2.04	0.56
1:B:396:VAL:CG1	1:B:401:LEU:HD21	2.29	0.56
1:A:282:VAL:HG23	1:A:308:GLN:CB	2.36	0.56
2:C:89:ILE:H	2:C:89:ILE:CD1	2.09	0.56
1:B:363:VAL:HB	1:B:375:ASP:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:GLU:O	2:D:71:LEU:HG	2.05	0.56
2:C:43:ALA:HA	4:C:107:FES:S2	2.46	0.56
2:D:101:VAL:HG13	2:D:102:PRO:HD2	1.88	0.56
1:B:302:VAL:HB	1:B:303:PRO:HD3	1.88	0.56
1:A:396:VAL:HG11	1:A:401:LEU:HD21	1.87	0.56
1:B:331:SER:O	1:B:338:LEU:HD12	2.05	0.56
1:B:261:GLN:HG2	1:B:267:VAL:HG21	1.86	0.55
1:B:261:GLN:HG2	1:B:267:VAL:CG2	2.37	0.55
2:D:53:ASN:ND2	2:D:55:ALA:HB3	2.22	0.55
2:D:32:ILE:CG2	2:D:35:ILE:HG12	2.37	0.54
1:A:282:VAL:HG23	1:A:308:GLN:HB3	1.89	0.54
2:C:45:CYS:O	2:C:46:ALA:HB3	2.06	0.54
1:A:142:ILE:O	1:A:146:LEU:HD13	2.08	0.54
1:B:328:TRP:O	1:B:329:PHE:HB3	2.06	0.54
1:B:376:THR:OG1	1:B:383:PHE:HB2	2.08	0.54
2:C:35:ILE:HG23	2:C:101:VAL:HG13	1.90	0.54
1:B:157:GLY:HA3	1:B:179:ASP:OD2	2.08	0.54
1:B:192:PRO:HB3	1:B:356:LEU:CD1	2.38	0.53
1:B:73:GLN:HA	1:B:73:GLN:NE2	2.22	0.53
1:A:222:ASP:OD1	1:A:224:GLN:HB2	2.08	0.53
2:D:32:ILE:HG22	2:D:35:ILE:HG12	1.90	0.53
1:B:352:VAL:HG11	1:B:356:LEU:HG	1.89	0.53
2:C:3:VAL:CG2	2:C:90:MET:HE2	2.37	0.53
1:B:311:LYS:HG3	1:B:321:PRO:HB3	1.91	0.53
1:B:93:VAL:HG12	1:B:101:LEU:HB2	1.89	0.53
1:A:53:LEU:HD12	1:A:167:THR:HG21	1.89	0.53
1:B:336:ILE:HG23	1:B:378:ASN:ND2	2.23	0.53
1:B:166:ALA:HA	1:B:334:TYR:CZ	2.43	0.53
1:A:18:GLU:HG2	1:A:306:LEU:HD23	1.89	0.53
2:C:13:ARG:HG2	2:C:13:ARG:HH11	1.73	0.53
2:C:14:GLU:C	2:C:15:LEU:HD12	2.29	0.53
1:B:17:VAL:HA	1:B:34:LEU:HD11	1.91	0.53
1:B:282:VAL:HG23	1:B:308:GLN:CB	2.39	0.53
1:B:152:LEU:HG	1:B:175:VAL:HG23	1.91	0.53
2:D:42:SER:O	2:D:43:ALA:HB3	2.09	0.53
1:A:111:GLY:HA2	1:A:284:ASP:HB2	1.92	0.52
2:D:17:VAL:CG2	2:D:21:VAL:HB	2.38	0.52
2:D:98:VAL:O	2:D:98:VAL:HG22	2.09	0.52
2:D:91:THR:HG22	2:D:93:GLU:H	1.74	0.52
1:A:97:ASP:OD2	1:A:99:ARG:NE	2.42	0.52
2:D:49:HIS:CD2	2:D:50:VAL:N	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ILE:O	1:B:150:ASN:HB2	2.09	0.52
1:B:31:ASN:N	1:B:31:ASN:HD22	2.08	0.52
2:D:45:CYS:O	2:D:46:ALA:CB	2.58	0.52
2:D:46:ALA:HB3	2:D:74:VAL:HG23	1.92	0.52
1:B:210:THR:O	1:B:212:THR:N	2.42	0.52
2:D:53:ASN:C	2:D:55:ALA:H	2.13	0.52
2:D:84:LEU:HD13	4:D:107:FES:S2	2.49	0.52
1:B:151:ARG:HA	1:B:174:HIS:O	2.09	0.52
1:B:196:PHE:HZ	1:B:359:PRO:HG3	1.72	0.51
1:A:43:HIS:HD2	1:A:44:HIS:O	1.93	0.51
1:A:333:GLN:O	1:A:334:TYR:HB2	2.10	0.51
1:A:157:GLY:HA3	1:A:179:ASP:OD2	2.10	0.51
2:D:64:ASN:O	2:D:68:ILE:HG13	2.11	0.51
2:D:3:VAL:HG22	2:D:90:MET:HE3	1.91	0.51
1:B:119:VAL:HG21	1:B:214:VAL:HG12	1.93	0.51
1:B:23:LEU:HD13	1:B:313:ALA:HA	1.92	0.51
1:B:336:ILE:HA	1:B:378:ASN:HD21	1.74	0.51
1:A:129:ASN:HA	1:A:145:GLN:HE22	1.75	0.51
1:B:8:VAL:O	1:B:106:LEU:HD12	2.10	0.51
1:B:142:ILE:O	1:B:146:LEU:HD13	2.11	0.51
2:D:83:ARG:HH11	2:D:83:ARG:HG3	1.76	0.51
1:A:286:ALA:O	1:A:298:ARG:HG3	2.11	0.51
2:C:77:GLU:OE2	2:C:79:LYS:HG2	2.10	0.51
2:D:59:LYS:C	2:D:60:VAL:HG23	2.24	0.51
1:B:310:ARG:HH12	2:D:36:VAL:CG1	2.24	0.51
2:D:34:ASP:CB	2:D:101:VAL:HG11	2.41	0.51
1:B:18:GLU:HG2	1:B:306:LEU:HD23	1.93	0.50
1:B:115:ARG:NH1	1:B:115:ARG:HG3	2.25	0.50
2:C:8:HIS:HB2	2:C:34:ASP:OD1	2.11	0.50
1:B:221:THR:C	1:B:223:GLN:N	2.63	0.50
1:B:179:ASP:OD1	1:B:181:ALA:HB3	2.10	0.50
2:D:60:VAL:O	2:D:61:PRO:C	2.50	0.50
1:B:396:VAL:HG13	1:B:411:ILE:CG2	2.40	0.50
1:B:219:MET:CB	1:B:225:LYS:O	2.59	0.50
1:A:191:PRO:N	1:A:192:PRO:HD2	2.26	0.50
1:B:282:VAL:HG23	1:B:308:GLN:HE21	1.76	0.50
2:D:53:ASN:HD22	2:D:56:PHE:H	1.60	0.50
2:D:56:PHE:N	2:D:56:PHE:CD1	2.78	0.50
1:B:9:ILE:HB	1:B:34:LEU:HD23	1.94	0.50
1:A:197:TYR:CE2	1:A:338:LEU:HD22	2.46	0.50
1:A:320:VAL:HG13	1:A:320:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ARG:HG2	1:B:151:ARG:HH11	1.77	0.50
1:B:209:ARG:O	1:B:212:THR:HG22	2.11	0.49
1:B:152:LEU:HD12	1:B:241:LEU:O	2.11	0.49
1:A:187:ARG:NH1	1:A:345:GLU:OE1	2.45	0.49
1:A:269:ASN:OD1	1:A:271:HIS:N	2.43	0.49
1:B:370:ARG:O	1:B:370:ARG:HG3	2.11	0.49
1:B:191:PRO:HB2	1:B:192:PRO:HD3	1.93	0.49
1:B:151:ARG:HG2	1:B:151:ARG:NH1	2.28	0.49
1:B:310:ARG:NH1	2:D:36:VAL:HG11	2.28	0.49
1:B:223:GLN:HG2	1:B:224:GLN:H	1.78	0.49
1:B:183:ARG:HH11	1:B:183:ARG:HG3	1.76	0.49
2:D:34:ASP:HB3	2:D:101:VAL:CG1	2.42	0.49
1:A:144:ARG:HD3	1:B:140:GLU:OE1	2.12	0.49
1:B:295:ARG:NH2	1:B:345:GLU:HB3	2.28	0.49
2:D:51:TYR:HE2	2:D:82:SER:HG	1.59	0.49
2:C:60:VAL:O	2:C:61:PRO:C	2.50	0.49
1:A:151:ARG:HE	1:A:238:PRO:HG2	1.77	0.48
1:A:367:GLN:HB2	1:A:372:LEU:CD2	2.43	0.48
2:C:63:ALA:HB2	2:C:83:ARG:HE	1.76	0.48
1:B:290:SER:O	1:B:294:ASP:HA	2.13	0.48
2:C:24:MET:O	2:C:24:MET:HE2	2.12	0.48
1:A:385:GLN:O	1:A:388:GLN:HG3	2.13	0.48
1:B:117:LEU:HD13	1:B:246:ILE:HD13	1.95	0.48
2:D:19:ASP:CG	2:D:20:GLY:N	2.65	0.48
2:D:34:ASP:HB3	2:D:101:VAL:HG11	1.95	0.48
2:D:22:SER:CB	2:D:86:CYS:HA	2.34	0.48
1:B:207:ASP:OD1	1:B:209:ARG:HD2	2.13	0.48
1:B:341:VAL:HG22	1:B:390:ILE:HD12	1.95	0.48
1:B:380:PRO:O	2:D:70:MET:HE1	2.13	0.48
1:B:340:MET:C	1:B:383:PHE:HE1	2.16	0.48
2:C:22:SER:HA	2:C:88:ILE:O	2.13	0.48
2:C:20:GLY:N	2:C:90:MET:O	2.46	0.48
2:D:93:GLU:HG2	2:D:94:LEU:N	2.28	0.48
2:D:65:GLU:HA	2:D:68:ILE:HD12	1.96	0.48
2:D:28:VAL:HG11	2:D:36:VAL:O	2.14	0.48
2:D:101:VAL:CG1	2:D:102:PRO:HD2	2.44	0.48
1:A:14:LEU:HD11	1:A:302:VAL:HG13	1.96	0.48
2:D:58:ASP:O	2:D:59:LYS:C	2.47	0.47
1:B:177:LEU:O	1:B:178:LEU:HD23	2.14	0.47
2:C:60:VAL:CG2	2:C:83:ARG:HH12	2.25	0.47
1:B:45:LEU:N	1:B:46:PRO:CD	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:VAL:HB	2:D:99:VAL:HB	1.96	0.47
1:A:298:ARG:NH2	1:A:300:GLU:OE2	2.46	0.47
1:B:282:VAL:HB	1:B:312:ILE:HD12	1.96	0.47
1:B:210:THR:C	1:B:212:THR:H	2.18	0.47
1:B:262:VAL:HG12	1:B:263:ASP:N	2.29	0.47
1:A:171:ALA:O	1:A:172:ASN:HB2	2.14	0.47
2:C:63:ALA:HB2	2:C:83:ARG:NE	2.28	0.47
2:C:64:ASN:O	2:C:68:ILE:HG13	2.14	0.47
1:A:178:LEU:HD23	1:A:209:ARG:HG3	1.95	0.47
2:C:48:CYS:SG	2:C:84:LEU:HB3	2.54	0.47
2:D:78:LEU:C	2:D:78:LEU:HD13	2.35	0.47
1:B:365:TYR:C	1:B:366:LEU:HD12	2.34	0.47
2:D:45:CYS:HB2	2:D:47:THR:HG23	1.97	0.47
2:D:22:SER:HB2	2:D:86:CYS:CA	2.38	0.47
2:C:35:ILE:CG2	2:C:101:VAL:HG13	2.45	0.47
1:B:151:ARG:NE	1:B:238:PRO:HG2	2.30	0.47
1:A:396:VAL:CG1	1:A:401:LEU:HD21	2.45	0.47
1:A:271:HIS:HB2	1:A:273:GLN:HE21	1.79	0.47
1:B:412:ILE:O	1:B:412:ILE:HD13	2.15	0.47
1:A:280:MET:HE1	1:A:312:ILE:HG23	1.96	0.47
2:C:83:ARG:HG3	2:C:83:ARG:HH11	1.79	0.47
1:B:248:LEU:HG	1:B:249:ILE:N	2.29	0.47
1:A:366:LEU:N	1:A:366:LEU:HD12	2.30	0.46
1:A:178:LEU:HD21	1:A:237:LEU:CD1	2.46	0.46
3:B:449:FAD:H1'1	3:B:449:FAD:H9	1.71	0.46
2:D:24:MET:CB	2:D:86:CYS:HB3	2.46	0.46
1:B:159:TYR:O	1:B:163:GLU:HG3	2.15	0.46
1:A:53:LEU:HD13	1:A:167:THR:HG21	1.98	0.46
2:D:56:PHE:N	2:D:56:PHE:HD1	2.13	0.46
1:B:184:VAL:O	1:B:185:LEU:HB2	2.14	0.46
2:D:24:MET:HB3	2:D:86:CYS:HB3	1.98	0.46
1:B:50:LYS:HE3	1:B:163:GLU:OE2	2.16	0.46
1:A:181:ALA:HB1	1:A:186:GLU:HG3	1.97	0.46
1:B:129:ASN:CA	1:B:145:GLN:HE22	2.24	0.46
1:B:190:ALA:N	1:B:365:TYR:OH	2.48	0.46
1:B:310:ARG:NH2	2:D:36:VAL:HG11	2.31	0.46
1:A:222:ASP:O	1:A:223:GLN:HB2	2.15	0.46
1:B:103:TYR:O	1:B:103:TYR:CD1	2.69	0.46
2:C:92:PRO:C	2:C:94:LEU:H	2.19	0.46
1:A:268:ILE:HD12	1:A:272:MET:HA	1.96	0.46
1:B:197:TYR:O	1:B:200:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:VAL:CG1	2:D:90:MET:HG2	2.41	0.46
1:B:414:ALA:O	1:B:417:ALA:HB3	2.16	0.46
1:A:292:LEU:O	1:A:370:ARG:NH2	2.49	0.46
1:A:260:LEU:O	1:A:262:VAL:HG23	2.15	0.46
1:A:297:VAL:HG22	1:A:298:ARG:N	2.31	0.46
1:B:290:SER:O	1:B:294:ASP:N	2.49	0.45
2:D:69:GLY:O	2:D:72:GLU:HG3	2.15	0.45
1:A:339:LYS:N	1:A:340:MET:HE3	2.31	0.45
1:A:7:VAL:O	1:A:7:VAL:HG13	2.16	0.45
1:A:134:ARG:HH11	1:A:134:ARG:HG2	1.80	0.45
2:D:74:VAL:HG12	2:D:74:VAL:O	2.16	0.45
1:B:129:ASN:HD21	1:B:226:VAL:HB	1.82	0.45
2:C:103:ASP:O	2:C:104:ARG:C	2.55	0.45
1:B:272:MET:HG3	1:B:312:ILE:HG13	1.98	0.45
2:D:27:ALA:HB1	2:D:35:ILE:CD1	2.39	0.45
2:C:13:ARG:CG	2:C:15:LEU:HD11	2.44	0.45
1:B:183:ARG:NH1	1:B:194:SER:OG	2.49	0.45
1:B:361:PHE:C	1:B:379:ARG:HD2	2.37	0.45
1:A:164:VAL:HG11	1:A:243:ILE:HD13	1.99	0.45
1:B:280:MET:HE3	1:B:312:ILE:HG12	1.99	0.45
1:A:9:ILE:HD13	1:A:19:VAL:HG22	1.98	0.45
1:B:145:GLN:O	1:B:147:ILE:HG22	2.16	0.45
2:D:96:GLY:C	2:D:98:VAL:H	2.18	0.45
1:A:413:ALA:HA	1:A:416:LYS:HE2	1.98	0.45
1:B:412:ILE:HA	1:B:415:ALA:HB3	1.98	0.45
1:A:367:GLN:HB2	1:A:372:LEU:HD21	1.99	0.45
3:A:449:FAD:H9	3:A:449:FAD:H1'1	1.74	0.45
2:C:74:VAL:HG21	2:C:78:LEU:HD23	1.99	0.45
2:D:76:ALA:O	2:D:78:LEU:N	2.50	0.44
1:B:322:ARG:NH1	1:B:322:ARG:CB	2.77	0.44
1:B:198:GLU:HA	1:B:208:ILE:CD1	2.48	0.44
2:C:17:VAL:HG11	2:C:90:MET:CB	2.47	0.44
1:B:192:PRO:O	1:B:356:LEU:HD22	2.17	0.44
1:A:147:ILE:HD12	1:A:147:ILE:N	2.32	0.44
1:B:124:VAL:HG22	1:B:219:MET:CE	2.47	0.44
2:C:54:GLU:HA	2:C:57:THR:OG1	2.17	0.44
1:A:162:LEU:HD11	1:A:185:LEU:HD21	2.00	0.44
1:B:53:LEU:CD1	1:B:167:THR:HG21	2.48	0.44
1:B:358:GLN:HB3	1:B:358:GLN:HE21	1.57	0.44
1:B:112:GLY:HA3	1:B:248:LEU:CD2	2.48	0.44
1:A:151:ARG:HG2	1:A:151:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:27:ALA:HA	2:C:32:ILE:HD12	1.99	0.44
1:B:268:ILE:HD11	1:B:288:PHE:HB3	2.00	0.44
1:B:219:MET:HA	1:B:226:VAL:HA	2.00	0.44
1:A:353:ARG:NE	1:A:382:GLU:OE2	2.44	0.44
2:D:74:VAL:C	2:D:76:ALA:H	2.21	0.43
1:A:81:THR:CG2	1:A:95:LEU:HD13	2.47	0.43
1:B:202:ARG:HG3	1:B:202:ARG:NH1	2.29	0.43
1:A:381:VAL:HA	2:C:70:MET:CE	2.48	0.43
2:C:71:LEU:O	2:C:74:VAL:HG13	2.18	0.43
2:C:7:SER:HB2	2:C:34:ASP:OD2	2.19	0.43
1:B:45:LEU:H	1:B:46:PRO:CD	2.31	0.43
2:D:70:MET:HB2	2:D:84:LEU:HD11	1.99	0.43
1:B:310:ARG:HH12	2:D:36:VAL:HG11	1.83	0.43
2:D:45:CYS:SG	2:D:47:THR:OG1	2.65	0.43
2:D:74:VAL:CG1	2:D:76:ALA:HB3	2.49	0.43
1:B:269:ASN:ND2	1:B:273:GLN:HB2	2.33	0.43
2:D:98:VAL:O	2:D:98:VAL:HG13	2.18	0.43
1:B:185:LEU:CD2	1:B:197:TYR:HE1	2.31	0.43
1:A:381:VAL:HA	2:C:70:MET:HE1	2.00	0.43
1:B:218:GLU:N	1:B:228:ALA:O	2.52	0.43
1:A:419:LEU:N	1:A:419:LEU:HD12	2.33	0.43
1:B:250:PRO:HD3	1:B:298:ARG:HH21	1.80	0.43
2:D:51:TYR:OH	2:D:77:GLU:O	2.36	0.43
1:B:386:SER:O	1:B:389:ILE:HB	2.19	0.43
1:A:183:ARG:NH1	1:A:194:SER:OG	2.46	0.43
1:A:46:PRO:HB2	1:A:47:PRO:HD3	2.01	0.43
2:C:74:VAL:HG23	2:C:74:VAL:O	2.19	0.43
1:A:304:ASN:O	1:A:308:GLN:HG3	2.19	0.43
2:D:22:SER:C	2:D:24:MET:H	2.21	0.43
1:B:166:ALA:HA	1:B:334:TYR:CE2	2.54	0.43
1:B:381:VAL:HG12	1:B:385:GLN:NE2	2.34	0.43
1:B:268:ILE:CG2	1:B:281:ALA:HB3	2.48	0.42
1:A:14:LEU:O	1:A:18:GLU:HB2	2.19	0.42
1:A:134:ARG:HD3	1:A:134:ARG:O	2.18	0.42
1:A:60:GLU:OE2	1:B:56:LYS:NZ	2.49	0.42
1:B:177:LEU:HD23	1:B:178:LEU:H	1.76	0.42
1:B:169:ILE:HG13	1:B:206:VAL:HG22	2.01	0.42
2:C:27:ALA:HB1	2:C:35:ILE:HD11	2.01	0.42
1:A:162:LEU:CD1	1:A:185:LEU:HD21	2.49	0.42
2:D:46:ALA:CB	2:D:74:VAL:CG2	2.97	0.42
1:A:45:LEU:N	1:A:46:PRO:CD	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:ALA:O	2:D:74:VAL:HG21	2.20	0.42
1:B:347:TYR:CD1	1:B:347:TYR:C	2.93	0.42
1:B:331:SER:O	1:B:338:LEU:HB2	2.20	0.42
1:A:282:VAL:HG23	1:A:308:GLN:HB2	2.01	0.42
2:D:7:SER:HB2	2:D:11:THR:CG2	2.42	0.42
1:A:282:VAL:HB	1:A:312:ILE:CD1	2.50	0.42
1:B:412:ILE:HD11	1:B:416:LYS:HB3	2.00	0.42
1:B:188:VAL:HG12	1:B:189:THR:HG23	2.00	0.42
1:B:382:GLU:HB3	1:B:408:LEU:HD23	2.02	0.42
1:B:131:ARG:HH11	1:B:138:ASP:HA	1.85	0.42
1:A:33:ARG:HD2	5:A:462:HOH:O	2.18	0.42
2:C:67:GLU:HG3	2:C:84:LEU:HD12	2.02	0.41
1:B:162:LEU:HD23	1:B:177:LEU:CD1	2.50	0.41
1:B:130:PHE:HA	1:B:242:VAL:O	2.20	0.41
1:A:160:ILE:O	1:A:164:VAL:HG23	2.20	0.41
2:D:25:GLN:HG3	2:D:26:ALA:N	2.35	0.41
1:B:180:THR:HG22	1:B:213:GLN:HA	2.01	0.41
2:C:56:PHE:O	2:C:58:ASP:N	2.54	0.41
2:C:90:MET:HE1	2:C:97:ILE:HG21	2.01	0.41
1:A:282:VAL:HB	1:A:312:ILE:HD12	2.03	0.41
1:A:178:LEU:HD22	1:A:209:ARG:HG3	2.02	0.41
1:A:220:SER:C	1:A:222:ASP:N	2.73	0.41
1:B:17:VAL:HG23	1:B:21:PHE:CD1	2.55	0.41
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.86	0.41
1:A:408:LEU:HA	1:A:408:LEU:HD12	1.84	0.41
1:A:15:ALA:O	1:A:19:VAL:HG13	2.20	0.41
2:D:3:VAL:HG21	2:D:17:VAL:HG12	1.98	0.41
1:A:283:GLY:H	1:A:308:GLN:HE21	1.63	0.41
1:B:183:ARG:NE	1:B:191:PRO:HG3	2.28	0.41
1:A:44:HIS:CE1	1:A:64:LEU:HD23	2.55	0.41
1:A:419:LEU:CD1	1:A:419:LEU:H	2.33	0.41
2:C:67:GLU:HG2	2:C:71:LEU:HG	2.02	0.41
2:C:56:PHE:CZ	2:C:97:ILE:HA	2.56	0.41
1:B:415:ALA:C	1:B:417:ALA:H	2.23	0.41
1:A:272:MET:HE1	1:A:308:GLN:HB3	2.03	0.41
1:A:280:MET:CE	1:A:312:ILE:HG23	2.49	0.41
1:A:197:TYR:CZ	1:A:338:LEU:HD22	2.56	0.41
2:C:3:VAL:HG11	2:C:23:LEU:HG	2.02	0.41
1:B:147:ILE:HG12	1:B:150:ASN:OD1	2.21	0.41
1:B:397:GLU:HB3	1:B:400:LEU:HD12	2.03	0.41
1:A:197:TYR:HE2	1:A:338:LEU:CD2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLY:H	1:B:308:GLN:HE22	1.65	0.41
1:B:358:GLN:O	1:B:360:ASP:N	2.53	0.41
1:A:209:ARG:H	1:A:209:ARG:HG2	1.69	0.41
1:B:376:THR:CB	1:B:383:PHE:HB2	2.51	0.41
2:C:59:LYS:HA	2:C:59:LYS:HD2	1.88	0.41
2:C:36:VAL:HG23	2:C:47:THR:HB	2.02	0.41
2:D:46:ALA:HB1	2:D:74:VAL:CG2	2.51	0.40
2:C:67:GLU:OE2	2:C:71:LEU:HD11	2.20	0.40
1:B:162:LEU:HD22	1:B:201:HIS:CD2	2.56	0.40
1:B:201:HIS:CE1	1:B:334:TYR:HE1	2.39	0.40
1:B:73:GLN:CA	1:B:73:GLN:HE21	2.19	0.40
1:B:155:ILE:O	1:B:155:ILE:HG22	2.21	0.40
1:B:223:GLN:HE21	1:B:224:GLN:NE2	2.20	0.40
1:B:153:VAL:CG1	1:B:229:VAL:HG21	2.49	0.40
1:A:162:LEU:HD11	1:A:185:LEU:CD2	2.51	0.40
1:B:213:GLN:HE21	1:B:213:GLN:HB3	1.58	0.40
2:D:31:GLY:O	2:D:33:TYR:N	2.54	0.40
1:B:73:GLN:CA	1:B:73:GLN:NE2	2.83	0.40
1:A:145:GLN:HA	1:A:147:ILE:CD1	2.51	0.40
1:B:320:VAL:HG13	1:B:320:VAL:O	2.21	0.40
2:D:53:ASN:HD22	2:D:55:ALA:HB3	1.87	0.40
2:C:67:GLU:HG3	2:C:84:LEU:HG	2.04	0.40
1:B:345:GLU:C	1:B:345:GLU:OE2	2.60	0.40
1:B:53:LEU:HD13	1:B:167:THR:HG21	2.03	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	417/436 (96%)	389 (93%)	28 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	415/436 (95%)	364 (88%)	44 (11%)	7 (2%)	11 22
2	C	102/106 (96%)	81 (79%)	16 (16%)	5 (5%)	3 3
2	D	101/106 (95%)	64 (63%)	17 (17%)	20 (20%)	0 0
All	All	1035/1084 (96%)	898 (87%)	105 (10%)	32 (3%)	5 8

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	61	PRO
2	D	19	ASP
2	D	52	VAL
2	D	59	LYS
2	D	77	GLU
2	D	97	ILE
1	B	148	ALA
1	B	211	GLY
1	B	223	GLN
1	B	359	PRO
2	D	18	ALA
2	D	58	ASP
2	D	63	ALA
2	D	74	VAL
2	D	93	GLU
1	B	220	SER
1	B	263	ASP
2	C	7	SER
2	C	57	THR
2	D	60	VAL
2	D	96	GLY
1	B	116	PRO
2	D	54	GLU
2	D	64	ASN
2	D	73	SER
2	D	75	THR
2	D	27	ALA
2	C	19	ASP
2	C	93	GLU
2	D	55	ALA
2	D	61	PRO
2	D	32	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	335/349 (96%)	306 (91%)	29 (9%)	13 24
1	B	333/349 (95%)	313 (94%)	20 (6%)	24 47
2	C	87/89 (98%)	76 (87%)	11 (13%)	5 10
2	D	86/89 (97%)	78 (91%)	8 (9%)	11 21
All	All	841/876 (96%)	773 (92%)	68 (8%)	15 28

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	24	ARG
1	A	29	GLU
1	A	45	LEU
1	A	53	LEU
1	A	78	LEU
1	A	94	ILE
1	A	105	ARG
1	A	134	ARG
1	A	175	VAL
1	A	178	LEU
1	A	186	GLU
1	A	200	LEU
1	A	209	ARG
1	A	214	VAL
1	A	223	GLN
1	A	224	GLN
1	A	256	SER
1	A	291	GLN
1	A	295	ARG
1	A	322	ARG
1	A	335	GLU
1	A	338	LEU
1	A	340	MET

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Mol	Chain	Res	Type
1	A	358	GLN
1	A	370	ARG
1	A	372	LEU
1	A	388	GLN
1	A	393	ARG
1	B	14	LEU
1	B	17	VAL
1	B	23	LEU
1	B	24	ARG
1	B	31	ASN
1	B	45	LEU
1	B	53	LEU
1	B	77	LEU
1	B	78	LEU
1	B	105	ARG
1	B	134	ARG
1	B	147	ILE
1	B	203	GLU
1	B	222	ASP
1	B	322	ARG
1	B	332	ASP
1	B	358	GLN
1	B	384	ASN
1	B	397	GLU
1	B	412	ILE
2	C	8	HIS
2	C	12	ARG
2	C	16	ASP
2	C	23	LEU
2	C	24	MET
2	C	39	CYS
2	C	53	ASN
2	C	61	PRO
2	C	66	ARG
2	C	89	ILE
2	C	104	ARG
2	D	12	ARG
2	D	24	MET
2	D	36	VAL
2	D	39	CYS
2	D	44	SER
2	D	56	PHE

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Mol	Chain	Res	Type
2	D	61	PRO
2	D	74	VAL

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	4	ASN
1	A	43	HIS
1	A	145	GLN
1	A	224	GLN
1	A	273	GLN
1	A	308	GLN
1	A	358	GLN
1	A	385	GLN
1	A	388	GLN
1	B	2	ASN
1	B	31	ASN
1	B	43	HIS
1	B	73	GLN
1	B	91	GLN
1	B	92	GLN
1	B	145	GLN
1	B	150	ASN
1	B	213	GLN
1	B	224	GLN
1	B	273	GLN
1	B	304	ASN
1	B	308	GLN
1	B	358	GLN
1	B	378	ASN
1	B	384	ASN
1	B	388	GLN
2	D	25	GLN
2	D	30	ASN
2	D	53	ASN

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FAD	A	449	-	48,58,58	2.44	19 (39%)	54,89,89	2.53	17 (31%)
3	FAD	B	449	-	48,58,58	2.50	19 (39%)	54,89,89	2.47	14 (25%)
4	FES	C	107	2	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	D	107	2	0,4,4	0.00	-	0,4,4	0.00	-

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
3	FAD	A	449	-	-	0/30/50/50	0/6/6/6
3	FAD	B	449	-	-	0/30/50/50	0/6/6/6
4	FES	C	107	2	-	0/0/4/4	0/1/1/1
4	FES	D	107	2	-	0/0/4/4	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	449	FAD	C10-N10	-4.14	1.34	1.39
3	A	449	FAD	PA-O2A	-4.07	1.37	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	449	FAD	PA-O2A	-3.86	1.38	1.54
3	A	449	FAD	P-O2P	-3.57	1.39	1.54
3	B	449	FAD	P-O2P	-3.33	1.40	1.54
3	A	449	FAD	P-O5'	-2.67	1.46	1.59
3	B	449	FAD	P-O5'	-2.35	1.48	1.59
3	A	449	FAD	C2'-C3'	-2.21	1.49	1.53
3	A	449	FAD	O3B-C3B	-2.13	1.37	1.43
3	B	449	FAD	C9A-C5X	2.02	1.46	1.42
3	A	449	FAD	C9-C9A	2.09	1.45	1.40
3	B	449	FAD	O5'-C5'	2.09	1.53	1.44
3	A	449	FAD	C5X-N5	2.10	1.38	1.35
3	B	449	FAD	C2A-N1A	2.17	1.38	1.33
3	B	449	FAD	O4B-C4B	2.19	1.50	1.45
3	B	449	FAD	C6-C5X	2.22	1.45	1.41
3	A	449	FAD	C2A-N3A	2.25	1.36	1.32
3	A	449	FAD	O4B-C4B	2.26	1.50	1.45
3	B	449	FAD	C4A-N3A	2.27	1.38	1.35
3	B	449	FAD	C9-C9A	2.39	1.46	1.40
3	B	449	FAD	C4-C4X	2.43	1.46	1.41
3	B	449	FAD	C2A-N3A	2.53	1.36	1.32
3	B	449	FAD	C5X-N5	2.56	1.39	1.35
3	A	449	FAD	C2A-N1A	2.58	1.38	1.33
3	A	449	FAD	C4-C4X	2.63	1.46	1.41
3	A	449	FAD	C8-C7	3.06	1.49	1.41
3	A	449	FAD	C4A-N3A	3.08	1.40	1.35
3	A	449	FAD	O4B-C1B	3.21	1.45	1.41
3	A	449	FAD	C4-N3	3.25	1.39	1.33
3	B	449	FAD	C8-C7	3.47	1.50	1.41
3	A	449	FAD	C4X-N5	3.80	1.39	1.33
3	B	449	FAD	C4X-N5	3.82	1.39	1.33
3	B	449	FAD	C4-N3	4.08	1.40	1.33
3	B	449	FAD	O4B-C1B	4.41	1.46	1.41
3	A	449	FAD	C4X-C10	4.68	1.49	1.41
3	B	449	FAD	C4X-C10	6.21	1.52	1.41
3	A	449	FAD	C9A-N10	8.61	1.50	1.38
3	B	449	FAD	C9A-N10	8.78	1.50	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	449	FAD	C1'-N10-C9A	-6.54	111.52	118.86
3	A	449	FAD	C1'-N10-C9A	-6.02	112.10	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	449	FAD	C4X-C10-N10	-5.99	116.99	120.52
3	A	449	FAD	C4-C4X-C10	-5.30	116.55	119.94
3	B	449	FAD	N3A-C2A-N1A	-4.73	125.27	128.89
3	A	449	FAD	N3A-C2A-N1A	-4.73	125.28	128.89
3	A	449	FAD	C4X-C4-N3	-4.67	117.20	123.59
3	B	449	FAD	C4X-C4-N3	-4.47	117.48	123.59
3	A	449	FAD	C4X-C10-N10	-4.38	117.94	120.52
3	A	449	FAD	C4B-O4B-C1B	-4.18	105.13	109.72
3	B	449	FAD	C4-C4X-C10	-3.97	117.40	119.94
3	B	449	FAD	C4B-O4B-C1B	-3.40	105.98	109.72
3	A	449	FAD	C1'-C2'-C3'	-2.90	101.53	109.82
3	B	449	FAD	O5'-P-O1P	-2.75	98.92	109.62
3	A	449	FAD	O5'-P-O1P	-2.75	98.92	109.62
3	B	449	FAD	C1'-C2'-C3'	-2.54	102.56	109.82
3	A	449	FAD	O5B-C5B-C4B	-2.01	101.72	109.12
3	A	449	FAD	C4X-N5-C5X	2.04	119.10	116.76
3	A	449	FAD	O2B-C2B-C3B	2.07	118.56	111.83
3	A	449	FAD	C4A-C5A-N7A	2.35	111.64	109.48
3	B	449	FAD	C2A-N1A-C6A	2.36	122.99	118.77
3	B	449	FAD	C4A-C5A-N7A	2.43	111.71	109.48
3	A	449	FAD	C2A-N1A-C6A	2.45	123.14	118.77
3	A	449	FAD	O2'-C2'-C3'	2.59	115.53	109.02
3	B	449	FAD	O2'-C2'-C3'	2.67	115.72	109.02
3	B	449	FAD	P-O3P-PA	2.98	141.09	132.73
3	A	449	FAD	P-O3P-PA	3.67	143.03	132.73
3	B	449	FAD	O3P-P-O5'	5.57	117.70	102.94
3	A	449	FAD	O3P-P-O5'	6.31	119.67	102.94
3	A	449	FAD	C4-N3-C2	7.87	122.05	115.25
3	B	449	FAD	C4-N3-C2	8.02	122.18	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	449	FAD	1	0
3	B	449	FAD	1	0
4	C	107	FES	1	0
4	D	107	FES	2	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	419/436 (96%)	0.02	3 (0%) 89 87	34, 53, 68, 94	0
1	B	417/436 (95%)	0.82	62 (14%) 3 2	43, 84, 121, 129	0
2	C	104/106 (98%)	1.07	19 (18%) 2 1	64, 94, 115, 121	0
2	D	103/106 (97%)	2.56	57 (55%) 0 0	100, 117, 129, 140	0
All	All	1043/1084 (96%)	0.70	141 (13%) 4 2	34, 66, 121, 140	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	60	VAL	9.0
2	D	33	TYR	7.9
1	B	237	LEU	7.9
2	D	97	ILE	7.5
2	D	56	PHE	7.1
2	D	3	VAL	6.7
2	D	94	LEU	6.2
1	B	406	VAL	6.1
2	D	9	ASP	6.1
2	D	59	LYS	6.0
2	C	59	LYS	5.5
2	D	58	ASP	5.5
2	D	10	GLY	5.4
1	B	219	MET	5.1
1	A	2	ASN	5.0
2	C	91	THR	4.9
1	B	231	CYS	4.7
2	D	65	GLU	4.7
2	D	8	HIS	4.7
1	B	235	THR	4.7
1	B	119	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
2	C	8	HIS	4.5
2	D	88	ILE	4.5
1	B	159	TYR	4.4
2	D	5	TYR	4.2
2	C	100	ASP	4.2
1	B	227	THR	4.2
2	D	17	VAL	4.1
1	B	416	LYS	4.1
2	D	62	ALA	4.1
2	D	75	THR	4.1
1	B	179	ASP	4.0
1	B	217	PHE	4.0
2	D	103	ASP	4.0
2	D	74	VAL	4.0
2	D	80	PRO	4.0
1	B	232	GLU	3.9
1	B	238	PRO	3.9
2	C	4	VAL	3.9
1	B	411	ILE	3.8
1	B	412	ILE	3.8
2	C	56	PHE	3.8
2	C	94	LEU	3.8
1	B	3	ALA	3.8
2	D	98	VAL	3.8
2	D	102	PRO	3.7
1	B	229	VAL	3.7
2	D	72	GLU	3.7
2	D	76	ALA	3.7
1	B	224	GLN	3.6
2	D	52	VAL	3.6
1	B	414	ALA	3.6
2	D	13	ARG	3.5
2	D	92	PRO	3.5
2	D	71	LEU	3.5
1	B	239	ALA	3.4
2	D	64	ASN	3.4
1	B	410	GLU	3.3
2	D	50	VAL	3.3
1	B	338	LEU	3.3
2	D	68	ILE	3.3
2	C	60	VAL	3.3
1	B	405	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	101	VAL	3.3
1	B	178	LEU	3.2
2	D	61	PRO	3.2
1	B	226	VAL	3.2
1	B	234	GLY	3.2
1	B	356	LEU	3.2
2	D	79	LYS	3.2
1	B	236	ARG	3.2
2	D	69	GLY	3.2
2	D	70	MET	3.1
1	B	381	VAL	3.1
1	B	117	LEU	3.1
2	C	33	TYR	3.0
1	B	230	LEU	3.0
2	D	57	THR	3.0
2	C	9	ASP	3.0
1	B	417	ALA	3.0
2	D	89	ILE	3.0
2	D	11	THR	3.0
1	B	385	GLN	2.9
2	D	4	VAL	2.9
2	D	90	MET	2.9
1	B	196	PHE	2.9
2	D	34	ASP	2.9
2	D	81	ASN	2.9
2	D	16	ASP	2.9
2	D	54	GLU	2.9
1	B	209	ARG	2.8
2	D	78	LEU	2.8
2	D	53	ASN	2.8
1	B	335	GLU	2.8
2	D	51	TYR	2.8
2	C	99	VAL	2.8
1	B	364	PHE	2.7
2	D	99	VAL	2.7
1	B	329	PHE	2.7
1	B	185	LEU	2.7
2	D	2	LYS	2.6
1	B	253	GLU	2.6
1	B	397	GLU	2.6
1	B	118	PRO	2.6
1	B	415	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	77	GLU	2.6
2	D	55	ALA	2.6
1	B	223	GLN	2.6
2	D	6	VAL	2.6
1	B	214	VAL	2.5
1	B	407	PRO	2.5
1	B	175	VAL	2.5
1	B	291	GLN	2.5
1	B	396	VAL	2.4
2	D	96	GLY	2.4
2	C	67	GLU	2.4
1	B	208	ILE	2.4
2	D	12	ARG	2.4
1	B	233	ASP	2.3
2	C	95	ASP	2.3
1	B	162	LEU	2.3
1	B	413	ALA	2.3
2	C	93	GLU	2.3
1	B	400	LEU	2.3
2	D	7	SER	2.3
2	D	49	HIS	2.2
1	B	336	ILE	2.2
1	B	220	SER	2.2
1	A	78	LEU	2.2
1	B	197	TYR	2.2
1	B	207	ASP	2.2
2	C	11	THR	2.2
1	B	394	LEU	2.2
2	C	7	SER	2.2
1	A	3	ALA	2.2
2	C	6	VAL	2.1
2	C	92	PRO	2.1
2	C	13	ARG	2.1
1	B	347	TYR	2.1
1	B	215	CYS	2.0
1	B	221	THR	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, 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
3	FAD	B	449	53/53	0.94	0.24	0.78	52,57,62,65	0
3	FAD	A	449	53/53	0.97	0.19	0.15	26,44,48,52	0
4	FES	C	107	4/4	0.93	0.14	-1.21	67,69,70,71	0
4	FES	D	107	4/4	0.91	0.07	-3.63	109,109,109,109	0

6.5 Other polymers (i)

There are no such residues in this entry.