Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:29 AM GMT

PDB ID	:	2XAS
Title	:	CRYSTAL STRUCTURE OF LSD1-COREST IN COMPLEX WITH A TRANYLCYPROMINE DERIVATIVE (MC2580, 14E)
Authors	:	Binda, C.; Valente, S.; Romanenghi, M.; Pilotto, S.; Cirilli, R.; Karytinos, A.; Ciossani, G.; Botrugno, O.A.; Forneris, F.; Tardugno, M.; Edmondson, D.E.; Minucci, S.; Mattevi, A.; Mai, A.
Deposited on	:	2010-03-31
Resolution	:	3.20 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:

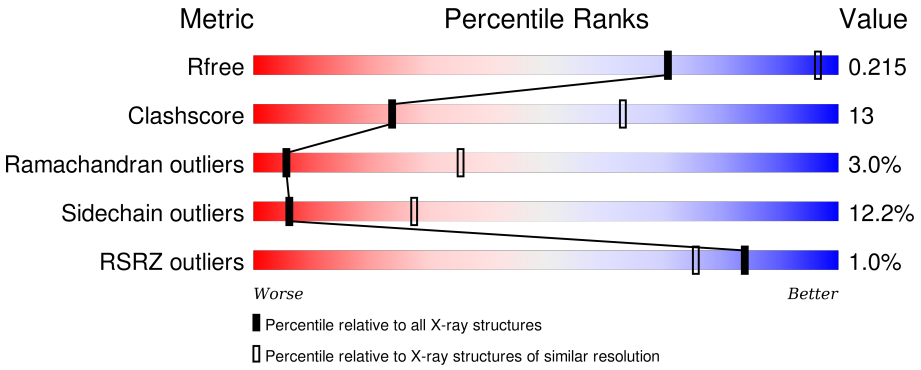
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	852	% 52% 23% • 22%
2	B	482	14% 12% • 72%

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
4	M80	A	901	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6378 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.

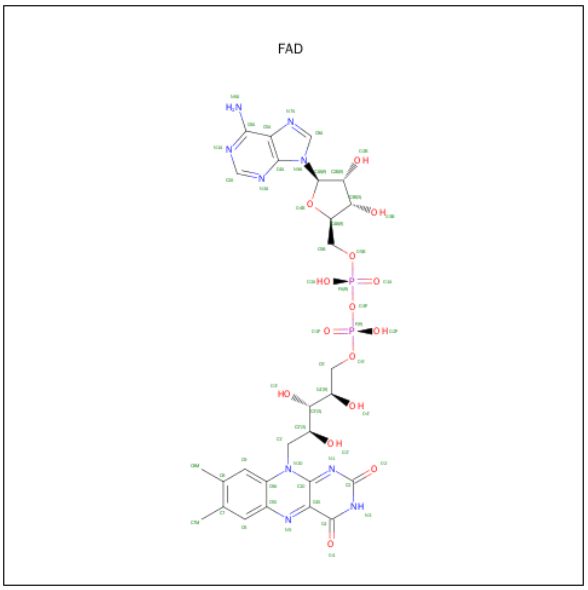
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5217	3324	906	967	20			

- Molecule 2 is a protein called REST COREPRESSOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

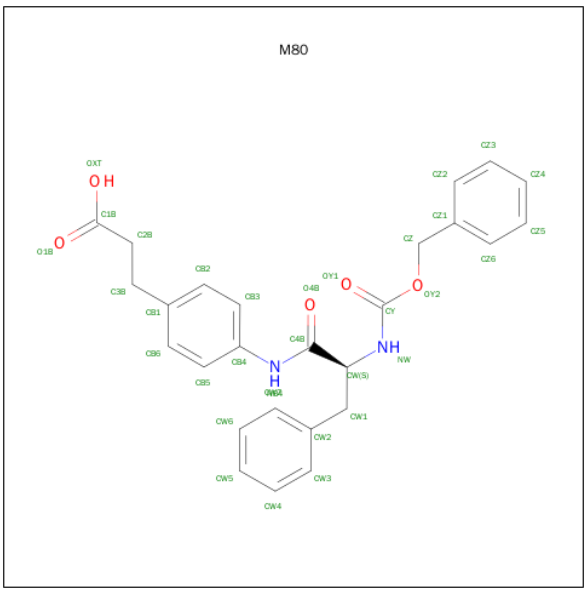
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is 3-[4-({N-[(BENZYLOXY)CARBONYL]-L-PHENYLALANYL}AMINO)PHE

NYL]PROPANOIC ACID (three-letter code: M80) (formula: $C_{26}H_{26}N_2O_5$).



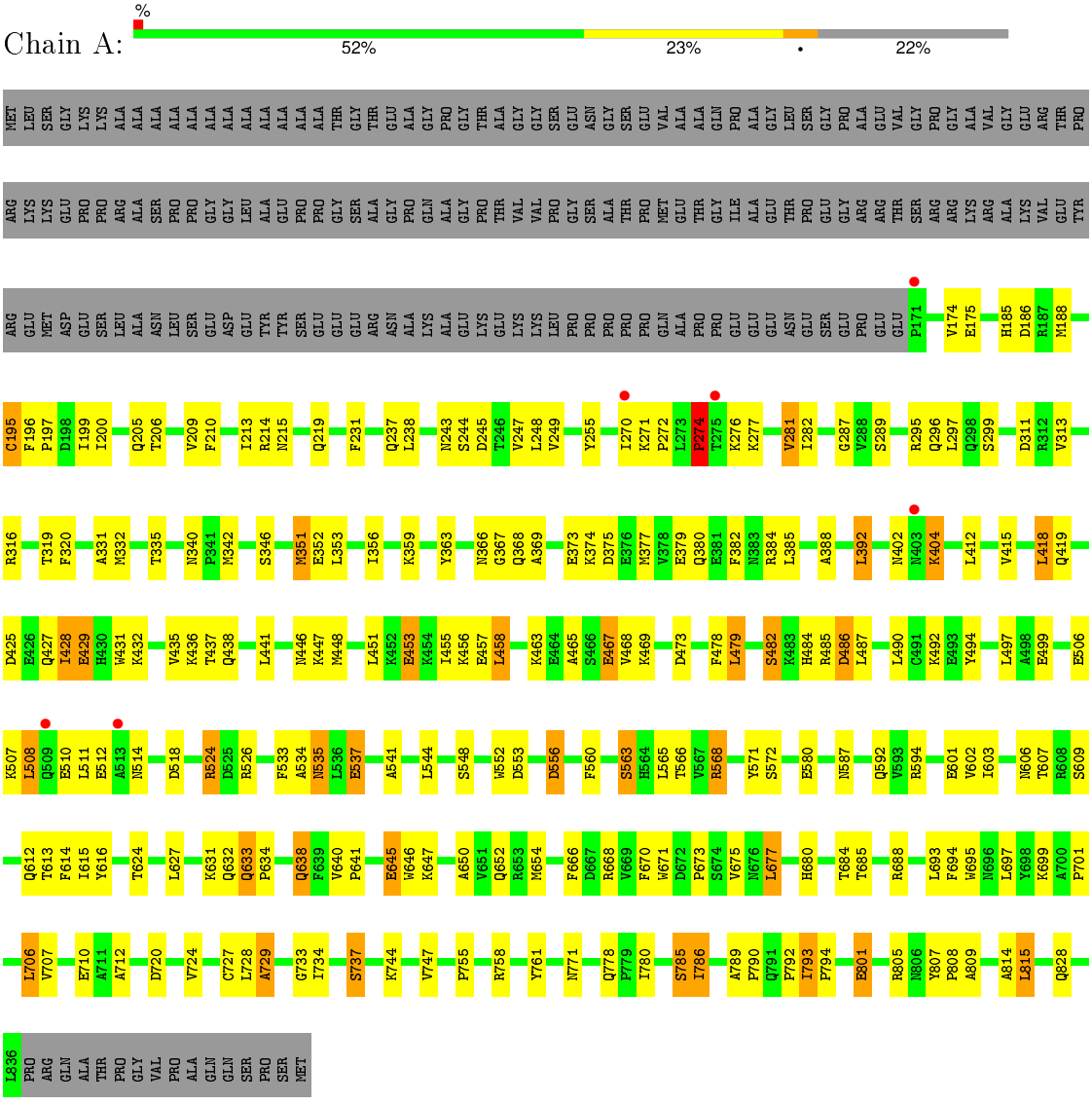
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	32	26	2	4	0	0

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.

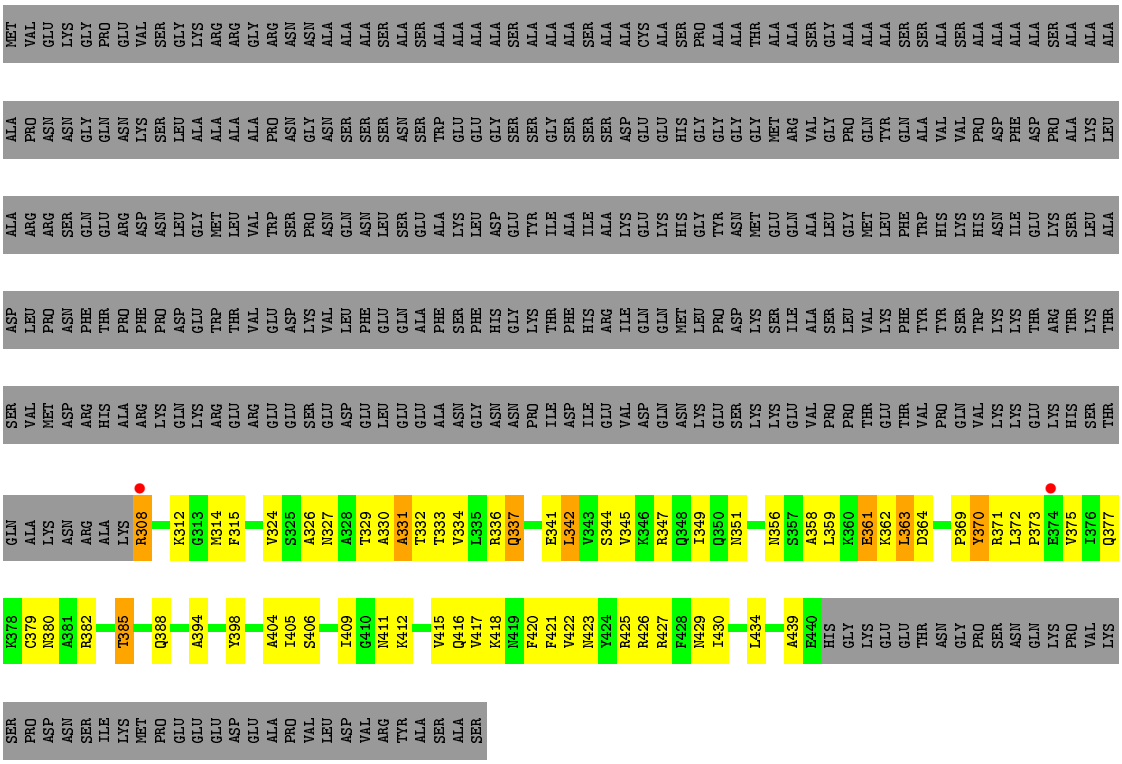
- Molecule 1: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1

Chain A:



- Molecule 2: REST COREPRESSOR 1

Chain B:


MET VAL GLU LYS GLY PRO GLU VAL SER GLY LYS ARG ARG GLY ARG ASN ASN ALA ALA ALA SER ALA SER ALA ALA ALA ALA ALA SER ALA ALA ALA CYS ALA SER PRO ALA ALA THR ALA ALA SER GLY ALA ALA ALA SER SER ALA SER ALA ALA ALA ALA SER ALA SER ALA ALA PRO ASN ASN GLY GLN ASN LYS SER LEU ALA ALA ALA PRO ASN GLY ASN SER SER SER ASN SER TRP GLU GLU GLY SER SER GLY SER SER SER ASP GLU GLU HIS GLY GLY GLY GLY MET ARG VAL GLY PRO GLN TYR GLN ALA VAL VAL PRO ASP PHE ASP PRO ALA LYS LEU ALA ARG ARG SER GLN GLU ARG ASP ASN LEU GLY MET LEU VAL TRP SER PRO ASN GLN ASN LEU SER GLU ALA LYS LEU ASP GLU GLN LYS HIS GLY TYR ASN MET GLU GLN ALA LEU GLY MET LEU PHE TRP HIS LYS HIS ASN ILE GLU LYS SER LEU ALA ASP LEU PRO ASN PHE THR PRO PHE PRO ASP GLU TRP THR VAL GLU ASP LYS VAL LEU PHE GLU GLN ALA PHE SER PHE HIS GLY LYS THR PHE HIS ARG ILE GLN GLN MET LEU PRO ASP LYS SER ILE ALA SER LEU VAL LYS PHE TYR TYR SER TRP LYS LYS THR ARG THR LYS THR SER VAL MET ASP ARG HIS ALA ARG LYS GLN LYS ARG GLU ARG GLU GLU SER GLU ASP GLU LEU GLU GLU ALA ASN GLY ASN ASN PRO ILE ASP ILE GLU VAL ASP GLN ASN LYS GLU SER LYS LYS GLU VAL PRO PRO THR GLU THR VAL PRO GLN VAL LYS LYS GLU LYS HIS SER THR GLN ALA LYS LYS R308 K312 G313 M314 F315 V324 S325 A326 N327 A328 T329 A330 A331 T332 T333 V334 L335 R336 Q337 E341 L342 V343 S344 V345 K346 R347 Q348 I349 Q350 N351 N356 S357 A358 L359 K360 E361 K362 L363 D364 P369 Y370 R371 L372 P373 E374 V375 I376 Q377 R378 C379 N380 A381 R382 T386 Q388 A394 Y398 A404 I405 S406 I409 G410 N411 K412 V415 Q416 V417 K418 N419 F420 F421 V422 N423 Y424 R425 R426 R427 F428 N429 I430 L434 A439 E440 HIS GLY LYS GLU GLU THR ASN GLY PRO SER ASN GLN LYS PRO VAL LYS SER PRO ASP ASN SER ILE LYS MET PRO GLU GLU GLU ASP GLU ALA PRO VAL LEU ASP VAL ARG TYR ALA SER ALA SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	118.32Å 179.69Å 235.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.40 – 3.20 71.40 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.40-3.20) 99.8 (71.40-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0090	Depositor
R, R_{free}	0.200 , 0.220 0.198 , 0.215	Depositor DCC
R_{free} test set	803 reflections (1.97%)	DCC
Wilson B-factor (Å^2)	82.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 41633 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6378	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 3.31% 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: M80, 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	0.69	1/5331 (0.0%)	0.78	3/7232 (0.0%)
2	B	0.60	0/1091	0.69	0/1471
All	All	0.68	1/6422 (0.0%)	0.76	3/8703 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	CYS	CB-SG	-5.01	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	815	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	281	VAL	CB-CA-C	-5.21	101.50	111.40
1	A	316	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	792	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5217	0	5252	137	0
2	B	1076	0	1091	43	0
3	A	53	0	31	6	0
4	A	32	0	25	8	0
All	All	6378	0	6399	169	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 13.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:GLU:OE1	1:A:453:GLU:HA	1.54	1.07
1:A:384:ARG:HB3	2:B:314:MET:HE1	1.52	0.92
1:A:755:PRO:HA	1:A:758:ARG:NH1	1.91	0.86
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.11	0.84
1:A:510:GLU:HG3	1:A:511:LEU:HD23	1.60	0.83
1:A:807:TYR:N	1:A:808:PRO:HD3	2.00	0.76
1:A:794:PRO:HD2	1:A:828:GLN:NE2	2.01	0.75
1:A:801:GLU:CG	1:A:809:ALA:HA	2.16	0.75
1:A:456:LYS:HA	2:B:370:TYR:HE1	1.50	0.74
1:A:353:LEU:HB3	1:A:565:LEU:HD23	1.69	0.73
1:A:671:TRP:O	1:A:673:PRO:HD3	1.88	0.73
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.24	0.71
1:A:548:SER:O	1:A:552:TRP:HB3	1.92	0.70
3:A:900:FAD:C4X	4:A:901:M80:H3B1	2.21	0.69
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.74	0.69
1:A:563:SER:O	1:A:565:LEU:HD12	1.91	0.69
4:A:901:M80:HB3	4:A:901:M80:O4B	1.93	0.69
1:A:418:LEU:HD11	2:B:324:VAL:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.26	0.66
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.62	0.64
1:A:447:LYS:HD3	1:A:497:LEU:HD21	1.80	0.64
1:A:801:GLU:HG2	1:A:809:ALA:HA	1.80	0.64
1:A:418:LEU:CD1	2:B:324:VAL:HG21	2.27	0.64
1:A:366:ASN:OD1	1:A:367:GLY:N	2.31	0.64
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.81	0.63
1:A:693:LEU:HD12	1:A:694:PHE:N	2.13	0.63
1:A:458:LEU:HD12	1:A:487:LEU:HD12	1.80	0.63
1:A:693:LEU:HD12	1:A:694:PHE:H	1.63	0.62
1:A:807:TYR:N	1:A:808:PRO:CD	2.63	0.61
3:A:900:FAD:C10	4:A:901:M80:H3B1	2.29	0.61
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.81	0.60
1:A:478:PHE:O	1:A:482:SER:HB3	2.01	0.60
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.82	0.60
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.65	0.60
1:A:384:ARG:HB3	2:B:314:MET:CE	2.29	0.60
3:A:900:FAD:C4	4:A:901:M80:HB6	2.32	0.60
2:B:370:TYR:N	2:B:370:TYR:HD2	2.00	0.60
2:B:418:LYS:O	2:B:421:PHE:HB2	2.02	0.59
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.85	0.58
2:B:370:TYR:CD2	2:B:370:TYR:N	2.71	0.58
1:A:448:MET:HB3	2:B:363:LEU:HD11	1.85	0.57
1:A:627:LEU:O	1:A:631:LYS:HG3	2.03	0.57
1:A:606:ASN:HD22	1:A:609:SER:H	1.50	0.57
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.86	0.56
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.70	0.56
2:B:417:VAL:O	2:B:420:PHE:HB3	2.06	0.55
1:A:188:MET:SD	1:A:200:ILE:HG13	2.46	0.55
1:A:366:ASN:OD1	1:A:368:GLN:N	2.40	0.55
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.40	0.54
1:A:448:MET:HG3	1:A:497:LEU:HD23	1.89	0.54
1:A:647:LYS:HE3	1:A:780:ILE:HD11	1.88	0.54
1:A:356:ILE:HG22	1:A:356:ILE:O	2.07	0.54
1:A:340:ASN:OD1	1:A:342:MET:N	2.40	0.54
1:A:473:ASP:OD1	1:A:473:ASP:C	2.46	0.54
1:A:385:LEU:O	1:A:388:ALA:HB3	2.08	0.54
1:A:456:LYS:HA	2:B:370:TYR:CD1	2.43	0.53
1:A:456:LYS:HE3	2:B:370:TYR:OH	2.09	0.53
2:B:362:LYS:C	2:B:364:ASP:H	2.12	0.53
1:A:463:LYS:O	1:A:467:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:PHE:HE2	2:B:434:LEU:HD11	1.72	0.53
1:A:311:ASP:OD1	1:A:311:ASP:N	2.37	0.53
1:A:789:ALA:HB1	1:A:790:PRO:HD2	1.90	0.53
1:A:458:LEU:CD1	1:A:487:LEU:HD12	2.39	0.52
1:A:455:ILE:HD11	1:A:490:LEU:O	2.10	0.52
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.10	0.52
3:A:900:FAD:C4X	4:A:901:M80:C3B	2.88	0.51
1:A:650:ALA:O	1:A:654:MET:HG3	2.09	0.51
1:A:456:LYS:CA	2:B:370:TYR:HE1	2.22	0.51
1:A:771:ASN:HA	1:A:805:ARG:NH1	2.26	0.51
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.41	0.51
2:B:425:ARG:HA	2:B:430:ILE:HG13	1.94	0.50
1:A:755:PRO:HA	1:A:758:ARG:HH12	1.71	0.50
1:A:645:GLU:HG3	1:A:646:TRP:N	2.27	0.50
2:B:308:ARG:HH11	2:B:308:ARG:HA	1.77	0.50
1:A:209:VAL:O	1:A:213:ILE:HG13	2.12	0.49
2:B:369:PRO:C	2:B:370:TYR:HD2	2.15	0.49
2:B:358:ALA:O	2:B:361:GLU:HB2	2.13	0.48
1:A:374:LYS:O	1:A:375:ASP:C	2.49	0.48
1:A:494:TYR:CD2	1:A:494:TYR:O	2.65	0.48
1:A:374:LYS:O	1:A:377:MET:N	2.47	0.48
1:A:695:TRP:HE1	1:A:706:LEU:HD22	1.77	0.48
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.49	0.48
2:B:426:ARG:HB2	2:B:427:ARG:HG3	1.94	0.48
1:A:633:GLN:OE1	1:A:634:PRO:HA	2.14	0.48
1:A:553:ASP:O	1:A:556:ASP:HB2	2.14	0.48
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.44	0.47
1:A:374:LYS:HE2	1:A:524:ARG:HH12	1.80	0.47
1:A:685:THR:O	1:A:688:ARG:HG2	2.14	0.47
1:A:666:PHE:O	1:A:701:PRO:HG2	2.14	0.47
1:A:335:THR:HG21	4:A:901:M80:HB4	1.80	0.47
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.97	0.47
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.28	0.47
1:A:710:GLU:OE1	1:A:710:GLU:HA	2.15	0.47
1:A:363:TYR:CD2	1:A:734:ILE:HG12	2.49	0.47
1:A:465:ALA:CB	1:A:479:LEU:HD23	2.45	0.46
2:B:337:GLN:HA	2:B:337:GLN:HE21	1.80	0.46
1:A:340:ASN:HB2	1:A:560:PHE:CD2	2.51	0.46
1:A:319:THR:HB	1:A:572:SER:HB3	1.96	0.46
1:A:195:CYS:HB2	1:A:196:PHE:CD1	2.51	0.46
1:A:601:GLU:HA	1:A:616:TYR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:ALA:O	2:B:398:TYR:N	2.46	0.46
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.31	0.46
1:A:592:GLN:HG3	1:A:638:GLN:HB3	1.98	0.46
1:A:346:SER:HA	1:A:351:MET:SD	2.56	0.46
1:A:534:ALA:HA	1:A:537:GLU:HG3	1.98	0.45
2:B:329:THR:C	2:B:331:ALA:N	2.69	0.45
1:A:379:GLU:O	1:A:382:PHE:HB3	2.17	0.45
1:A:392:LEU:HD11	1:A:415:VAL:CG2	2.47	0.45
2:B:361:GLU:O	2:B:364:ASP:HB2	2.16	0.45
1:A:435:VAL:HG23	1:A:436:LYS:H	1.81	0.45
2:B:406:SER:OG	2:B:412:LYS:O	2.30	0.45
1:A:446:ASN:OD1	2:B:359:LEU:HD11	2.17	0.44
1:A:720:ASP:O	1:A:724:VAL:HG23	2.17	0.44
1:A:352:GLU:HB2	1:A:568:ARG:HB3	1.98	0.44
2:B:385:THR:HA	2:B:388:GLN:HG3	1.98	0.44
2:B:421:PHE:O	2:B:425:ARG:HB2	2.16	0.44
1:A:419:GLN:HE22	2:B:315:PHE:H	1.65	0.44
1:A:613:THR:HG22	1:A:614:PHE:N	2.31	0.44
1:A:427:GLN:O	1:A:431:TRP:HD1	2.01	0.44
1:A:185:HIS:CE1	1:A:186:ASP:HB3	2.53	0.44
1:A:174:VAL:HG12	1:A:219:GLN:OE1	2.17	0.44
2:B:362:LYS:O	2:B:364:ASP:N	2.50	0.44
1:A:175:GLU:HG2	1:A:185:HIS:ND1	2.33	0.44
1:A:794:PRO:CD	1:A:828:GLN:NE2	2.75	0.43
1:A:563:SER:O	1:A:565:LEU:CD1	2.65	0.43
1:A:412:LEU:HD13	1:A:533:PHE:CE1	2.53	0.43
1:A:214:ARG:HD2	1:A:215:ASN:OD1	2.18	0.43
1:A:707:VAL:O	1:A:712:ALA:HB2	2.18	0.43
2:B:333:THR:HG22	2:B:334:VAL:N	2.33	0.43
2:B:415:VAL:O	2:B:418:LYS:N	2.51	0.43
1:A:603:ILE:HG12	1:A:615:ILE:HD13	2.00	0.43
1:A:465:ALA:HB1	1:A:479:LEU:HD23	2.00	0.43
1:A:670:PHE:CD1	1:A:670:PHE:C	2.92	0.43
1:A:587:ASN:HB3	1:A:607:THR:OG1	2.18	0.43
1:A:196:PHE:N	1:A:197:PRO:CD	2.81	0.43
1:A:331:ALA:HA	3:A:900:FAD:C4X	2.48	0.43
1:A:761:TYR:CE2	4:A:901:M80:H3B2	2.53	0.43
1:A:427:GLN:NE2	1:A:518:ASP:HA	2.34	0.43
1:A:707:VAL:HG12	1:A:712:ALA:HA	2.00	0.43
1:A:506:GLU:C	1:A:508:LEU:H	2.22	0.43
1:A:205:GLN:O	1:A:209:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ARG:NH2	1:A:580:GLU:O	2.52	0.43
1:A:801:GLU:HG2	1:A:809:ALA:CA	2.47	0.43
1:A:541:ALA:HB2	1:A:761:TYR:CZ	2.54	0.42
1:A:761:TYR:CZ	4:A:901:M80:H3B2	2.53	0.42
1:A:728:LEU:O	1:A:729:ALA:C	2.57	0.42
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.54	0.42
1:A:677:LEU:HB2	1:A:693:LEU:HD11	2.01	0.42
1:A:270:ILE:O	1:A:272:PRO:HD3	2.19	0.42
1:A:640:VAL:O	1:A:640:VAL:HG12	2.19	0.42
1:A:640:VAL:HA	1:A:641:PRO:HA	1.89	0.42
1:A:670:PHE:HD1	1:A:670:PHE:O	2.02	0.42
2:B:377:GLN:OE1	2:B:411:ASN:HB3	2.18	0.42
1:A:535:ASN:HA	1:A:535:ASN:HD22	1.66	0.42
1:A:289:SER:HB3	1:A:814:ALA:HB1	2.01	0.42
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.75	0.42
2:B:342:LEU:O	2:B:345:VAL:N	2.53	0.42
1:A:320:PHE:CD1	1:A:747:VAL:HG21	2.56	0.41
1:A:404:LYS:HG2	1:A:404:LYS:H	1.68	0.41
1:A:331:ALA:HA	3:A:900:FAD:N5	2.35	0.41
2:B:415:VAL:O	2:B:416:GLN:C	2.58	0.41
2:B:405:ILE:O	2:B:409:ILE:HG13	2.21	0.41
2:B:380:ASN:O	2:B:416:GLN:NE2	2.51	0.41
1:A:485:ARG:HD2	2:B:404:ALA:HA	2.02	0.41
1:A:428:ILE:HG22	1:A:429:GLU:N	2.35	0.41
1:A:244:SER:OG	1:A:245:ASP:N	2.54	0.41
1:A:786:ILE:HD12	1:A:786:ILE:H	1.86	0.41
1:A:451:LEU:HA	1:A:451:LEU:HD12	1.90	0.41
1:A:594:ARG:HA	1:A:640:VAL:O	2.21	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	664/852 (78%)	572 (86%)	75 (11%)	17 (3%)	7 40
2	B	131/482 (27%)	104 (79%)	20 (15%)	7 (5%)	2 19
All	All	795/1334 (60%)	676 (85%)	95 (12%)	24 (3%)	5 35

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	729	ALA
1	A	793	ILE
1	A	468	VAL
1	A	486	ASP
1	A	737	SER
1	A	785	SER
1	A	801	GLU
2	B	341	GLU
2	B	363	LEU
1	A	274	PRO
1	A	369	ALA
1	A	425	ASP
1	A	507	LYS
2	B	326	ALA
2	B	331	ALA
2	B	373	PRO
2	B	439	ALA
1	A	733	GLY
1	A	499	GLU
2	B	429	ASN
1	A	287	GLY
1	A	508	LEU
1	A	428	ILE
1	A	313	VAL

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	566/699 (81%)	502 (89%)	64 (11%)	7 31
2	B	117/395 (30%)	98 (84%)	19 (16%)	3 14
All	All	683/1094 (62%)	600 (88%)	83 (12%)	6 27

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	THR
1	A	237	GLN
1	A	247	VAL
1	A	255	TYR
1	A	271	LYS
1	A	274	PRO
1	A	276	LYS
1	A	277	LYS
1	A	281	VAL
1	A	296	GLN
1	A	299	SER
1	A	332	MET
1	A	351	MET
1	A	359	LYS
1	A	373	GLU
1	A	380	GLN
1	A	392	LEU
1	A	402	ASN
1	A	404	LYS
1	A	418	LEU
1	A	429	GLU
1	A	432	LYS
1	A	437	THR
1	A	438	GLN
1	A	453	GLU
1	A	457	GLU
1	A	458	LEU
1	A	467	GLU
1	A	469	LYS
1	A	479	LEU
1	A	482	SER
1	A	492	LYS
1	A	512	GLU
1	A	514	ASN
1	A	524	ARG

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Mol	Chain	Res	Type
1	A	526	ARG
1	A	535	ASN
1	A	537	GLU
1	A	556	ASP
1	A	563	SER
1	A	568	ARG
1	A	571	TYR
1	A	612	GLN
1	A	624	THR
1	A	632	GLN
1	A	633	GLN
1	A	638	GLN
1	A	645	GLU
1	A	652	GLN
1	A	668	ARG
1	A	675	VAL
1	A	677	LEU
1	A	680	HIS
1	A	684	THR
1	A	699	LYS
1	A	706	LEU
1	A	727	CYS
1	A	737	SER
1	A	744	LYS
1	A	778	GLN
1	A	785	SER
1	A	786	ILE
1	A	793	ILE
1	A	815	LEU
2	B	308	ARG
2	B	312	LYS
2	B	332	THR
2	B	336	ARG
2	B	337	GLN
2	B	342	LEU
2	B	344	SER
2	B	347	ARG
2	B	349	ILE
2	B	351	ASN
2	B	361	GLU
2	B	370	TYR
2	B	371	ARG

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Mol	Chain	Res	Type
2	B	375	VAL
2	B	379	CYS
2	B	382	ARG
2	B	385	THR
2	B	422	VAL
2	B	423	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	422	HIS
1	A	427	GLN
1	A	438	GLN
1	A	535	ASN
1	A	606	ASN
1	A	828	GLN
2	B	337	GLN
2	B	348	GLN
2	B	388	GLN
2	B	419	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

2 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	900	4	48,58,58	2.28	9 (18%)	54,89,89	3.15	10 (18%)
4	M80	A	901	3	34,34,35	1.45	1 (2%)	42,43,45	1.65	9 (21%)

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	900	4	-	0/30/50/50	0/6/6/6
4	M80	A	901	3	-	0/24/25/26	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C5'-C4'	2.15	1.54	1.51
3	A	900	FAD	C10-N10	3.22	1.42	1.39
3	A	900	FAD	C4X-C10	3.57	1.47	1.41
3	A	900	FAD	C9A-N10	3.82	1.44	1.38
3	A	900	FAD	C5X-N5	3.92	1.41	1.35
3	A	900	FAD	C4X-N5	4.47	1.40	1.33
3	A	900	FAD	O4-C4	4.98	1.36	1.24
4	A	901	M80	OY2-CY	7.33	1.50	1.35
3	A	900	FAD	C2A-N1A	7.74	1.48	1.33
3	A	900	FAD	C2A-N3A	8.04	1.46	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	900	FAD	N3A-C2A-N1A	-19.57	113.91	128.89
3	A	900	FAD	C4X-C10-N10	-3.99	118.17	120.52
3	A	900	FAD	C1B-N9A-C4A	-3.75	121.28	126.94
4	A	901	M80	OY1-CY-NW	-3.73	118.35	124.86
3	A	900	FAD	P-O3P-PA	-3.02	124.25	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	900	FAD	C4X-C4-N3	-2.92	119.59	123.59
4	A	901	M80	CB4-NB4-C4B	-2.88	122.22	127.40
4	A	901	M80	OY2-CY-OY1	-2.56	118.95	124.22
3	A	900	FAD	C4A-C5A-N7A	-2.34	107.32	109.48
4	A	901	M80	C2B-C3B-CB1	-2.18	107.20	113.04
3	A	900	FAD	C6-C5X-N5	-2.11	116.25	118.96
4	A	901	M80	CW-NW-CY	2.05	126.66	121.12
4	A	901	M80	CW2-CW1-CW	2.19	119.78	113.41
3	A	900	FAD	C2A-N1A-C6A	2.37	123.00	118.77
4	A	901	M80	OY2-CZ-CZ1	2.40	115.41	109.36
3	A	900	FAD	C5X-C9A-N10	3.45	120.24	117.62
4	A	901	M80	CZ-OY2-CY	4.24	126.01	115.91
4	A	901	M80	OY2-CY-NW	5.48	122.69	110.54
3	A	900	FAD	C4-N3-C2	6.74	121.08	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FAD	6	0
4	A	901	M80	8	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, 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	666/852 (78%)	0.13	6 (0%)	85	78	38, 70, 100, 113	0
2	B	133/482 (27%)	0.38	2 (1%)	76	63	68, 100, 114, 122	0
All	All	799/1334 (59%)	0.17	8 (1%)	84	75	38, 74, 108, 122	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	2.9
1	A	403	ASN	2.9
1	A	275	THR	2.4
1	A	270	ILE	2.3
2	B	308	ARG	2.3
1	A	509	GLN	2.2
1	A	513	ALA	2.0
2	B	374	GLU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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
4	M80	A	901	32/33	0.92	0.39	4.33	66,101,105,108	0
3	FAD	A	900	53/53	0.99	0.23	-0.36	37,45,63,64	0

6.5 Other polymers (i)

There are no such residues in this entry.