Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:06 PM GMT

PDB ID	:	3W4J
Title	:	Crystal Structure of human DAAO in complex with coumpound 12
Authors	:	Hondo, T.; Warizaya, M.; Niimi, T.; Namatame, I.; Yamaguchi, T.; Nakanishi, K.; Hamajima, T.; Harada, K.; Sakashita, H.; Matsumoto, Y.; Orita, M.; Watanabe, T.; Takeuchi, M.
Deposited on	:	2013-01-09
Resolution	:	2.74 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:

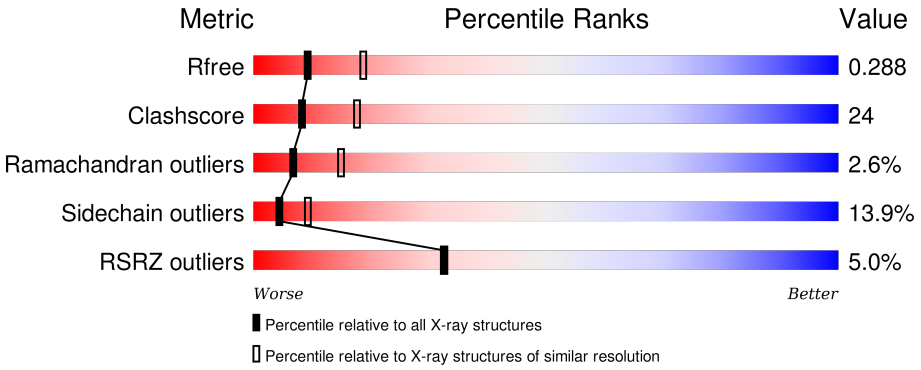
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.74 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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	347	2% 56% 34% 7%
1	B	347	2% 51% 38% 7%
1	C	347	8% 52% 37% 8%
1	D	347	8% 51% 38% 9%

2 Entry composition (i)

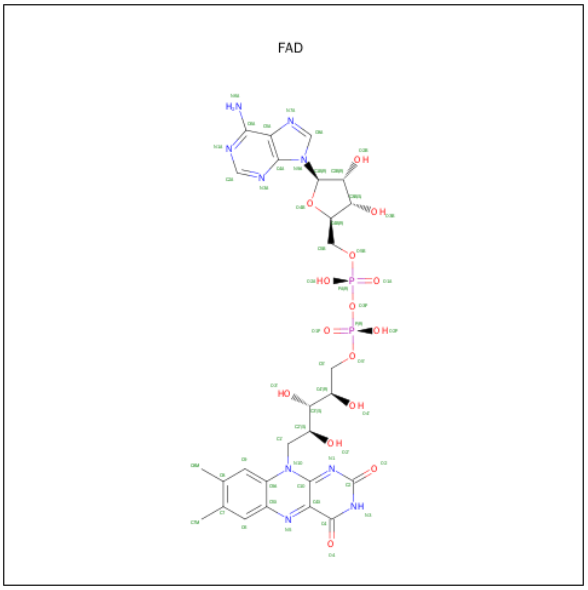
There are 3 unique types of molecules in this entry. The entry contains 11208 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			
1	B	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			
1	C	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			
1	D	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			

- 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		

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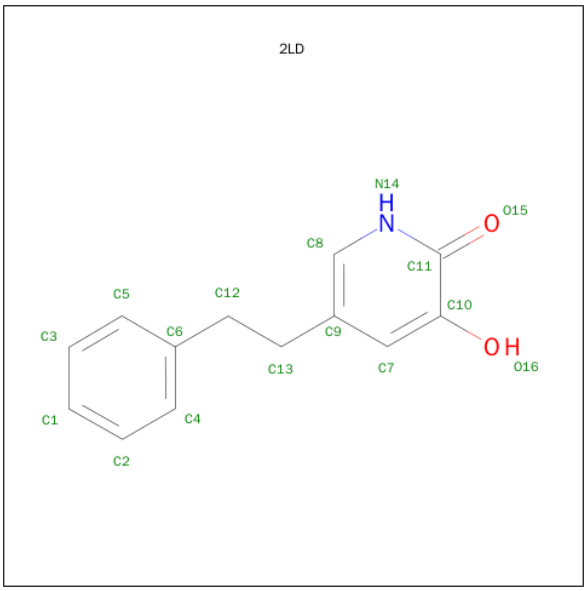
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 3-HYDROXY-5-(2-PHENYLETHYL)PYRIDIN-2(1H)-ONE (three-letter code: 2LD) (formula: $C_{13}H_{13}NO_2$).



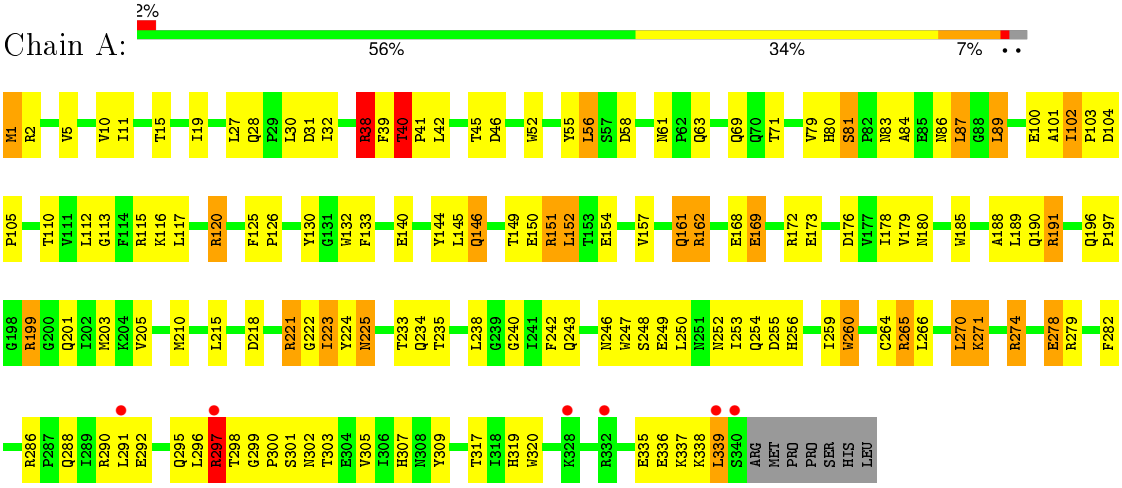
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	13	1	2		
3	B	1	Total	C	N	O	0	0
			16	13	1	2		
3	C	1	Total	C	N	O	0	0
			16	13	1	2		
3	D	1	Total	C	N	O	0	0
			16	13	1	2		

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.

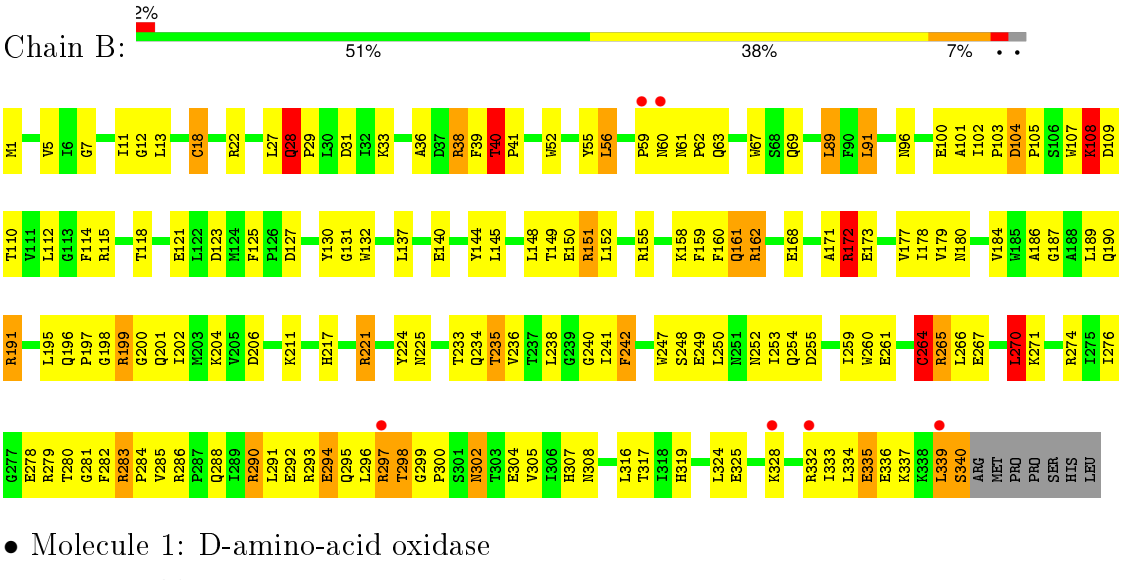
- Molecule 1: D-amino-acid oxidase

Chain A:



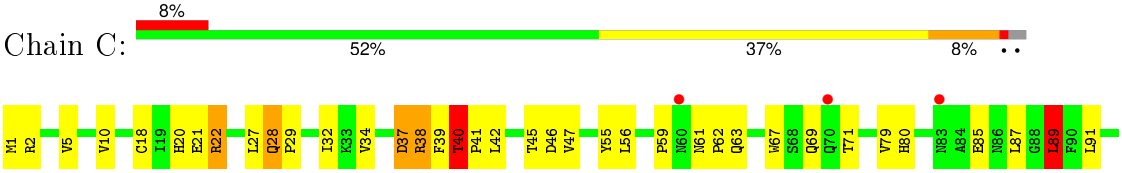
- Molecule 1: D-amino-acid oxidase

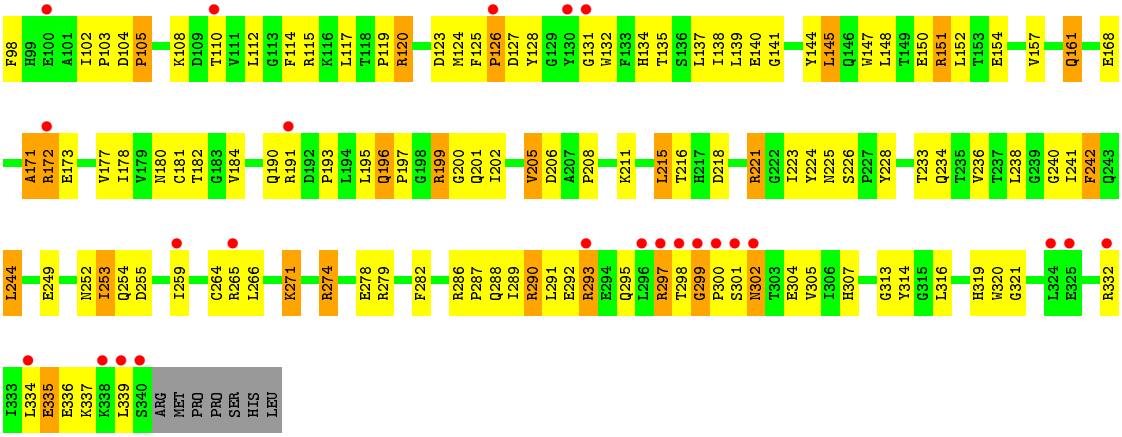
Chain B:



- Molecule 1: D-amino-acid oxidase

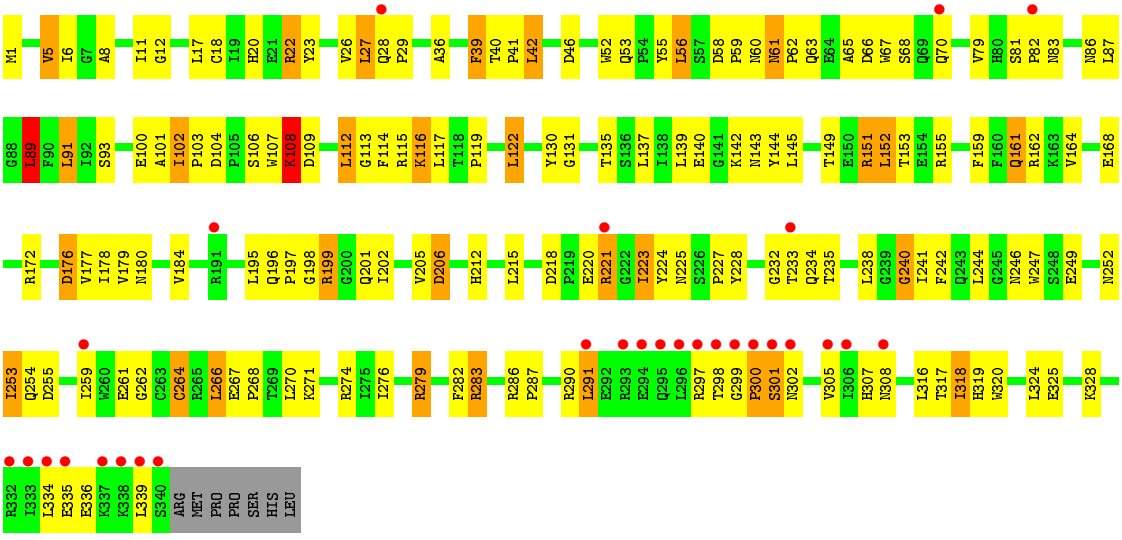
Chain C:





- Molecule 1: D-amino-acid oxidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	149.25Å 182.32Å 50.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.74 46.40 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.74) 97.6 (46.40-2.74)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.210 , 0.290 0.211 , 0.288	Depositor DCC
R_{free} test set	1824 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	59.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	10 of 36536 reflections (0.027%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11208	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.67 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7704e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 2LD, 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	1.10	5/2810 (0.2%)	1.14	10/3824 (0.3%)
1	B	1.09	5/2810 (0.2%)	1.11	14/3824 (0.4%)
1	C	0.99	2/2810 (0.1%)	1.00	5/3824 (0.1%)
1	D	0.97	0/2810	1.01	6/3824 (0.2%)
All	All	1.04	12/11240 (0.1%)	1.07	35/15296 (0.2%)

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	D	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	TRP	CB-CG	-7.66	1.36	1.50
1	C	181	CYS	CB-SG	-7.29	1.69	1.82
1	B	18	CYS	CB-SG	-6.90	1.70	1.82
1	A	100	GLU	CB-CG	6.35	1.64	1.52
1	A	185	TRP	CE3-CZ3	6.04	1.48	1.38
1	B	150	GLU	CB-CG	-5.96	1.40	1.52
1	B	236	VAL	CB-CG2	-5.90	1.40	1.52
1	B	264	CYS	CB-SG	-5.74	1.72	1.81
1	C	211	LYS	CE-NZ	-5.47	1.35	1.49
1	A	278	GLU	CD-OE2	5.44	1.31	1.25
1	B	260	TRP	CB-CG	-5.28	1.40	1.50
1	A	100	GLU	CG-CD	5.12	1.59	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	199	ARG	NE-CZ-NH1	-12.78	113.91	120.30
1	A	199	ARG	NE-CZ-NH2	11.32	125.96	120.30
1	B	199	ARG	NE-CZ-NH1	-9.63	115.48	120.30
1	B	206	ASP	CB-CG-OD1	8.56	126.00	118.30
1	D	199	ARG	NE-CZ-NH1	-8.33	116.14	120.30
1	C	89	LEU	CA-CB-CG	7.84	133.34	115.30
1	C	199	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	A	189	LEU	CA-CB-CG	7.23	131.93	115.30
1	A	270	LEU	CA-CB-CG	7.23	131.93	115.30
1	B	199	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	C	40	THR	N-CA-C	6.67	129.00	111.00
1	B	91	LEU	CB-CG-CD1	-6.63	99.72	111.00
1	A	38	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	B	40	THR	N-CA-C	6.43	128.36	111.00
1	B	283	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	A	339	LEU	CA-CB-CG	6.25	129.68	115.30
1	B	290	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	162	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	40	THR	C-N-CD	5.87	140.74	128.40
1	B	206	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	B	89	LEU	CB-CA-C	-5.87	99.05	110.20
1	D	89	LEU	CA-CB-CG	5.77	128.56	115.30
1	C	199	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	40	THR	N-CA-C	5.72	126.45	111.00
1	C	37	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	B	250	LEU	CA-CB-CG	5.59	128.15	115.30
1	D	291	LEU	CA-CB-CG	5.56	128.09	115.30
1	D	199	ARG	CG-CD-NE	-5.50	100.25	111.80
1	B	270	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	58	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	339	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	38	ARG	CG-CD-NE	5.27	122.86	111.80
1	B	40	THR	CB-CA-C	-5.24	97.47	111.60
1	D	6	ILE	CB-CA-C	-5.14	101.32	111.60
1	D	206	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	39	PHE	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	2733	0	2680	125	0
1	B	2733	0	2680	126	0
1	C	2733	0	2680	161	0
1	D	2733	0	2680	144	0
2	A	53	0	31	3	0
2	B	53	0	31	0	0
2	C	53	0	31	4	0
2	D	53	0	31	1	0
3	A	16	0	13	1	0
3	B	16	0	12	1	0
3	C	16	0	13	1	0
3	D	16	0	13	5	0
All	All	11208	0	10895	536	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 24.

All (536) 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:1:MET:HE1	1:A:176:ASP:HB2	1.30	1.14
1:B:221:ARG:HH21	1:B:221:ARG:CB	1.62	1.13
1:A:1:MET:CE	1:A:176:ASP:HB2	1.79	1.12
1:D:221:ARG:HB2	1:D:221:ARG:HH21	1.09	1.10
1:C:264:CYS:HB3	1:C:271:LYS:HZ2	1.17	1.09
1:D:22:ARG:HG3	1:D:22:ARG:HH21	1.04	1.08
1:D:221:ARG:NH2	1:D:221:ARG:HB2	1.69	1.08
1:C:264:CYS:HB3	1:C:271:LYS:NZ	1.68	1.07
1:D:264:CYS:SG	1:D:271:LYS:HD2	1.97	1.04
1:C:274:ARG:HA	1:C:274:ARG:HE	1.18	1.03
1:C:264:CYS:SG	1:C:271:LYS:HD3	1.99	1.03
1:A:290:ARG:HD2	1:A:292:GLU:OE2	1.61	1.01
1:A:221:ARG:HB2	1:A:221:ARG:CZ	1.92	0.98
1:D:297:ARG:HA	1:D:302:ASN:HB3	1.44	0.97
1:D:22:ARG:HH21	1:D:22:ARG:CG	1.78	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ARG:HG3	1:D:283:ARG:HH21	1.29	0.97
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.06	0.95
1:B:264:CYS:SG	1:B:271:LYS:HG3	2.09	0.92
1:A:335:GLU:HG2	1:A:336:GLU:N	1.84	0.92
1:B:55:TYR:HE1	1:B:224:TYR:OH	1.50	0.92
1:D:283:ARG:NE	3:D:402:2LD:O15	2.01	0.92
1:B:290:ARG:HD2	1:B:292:GLU:OE2	1.70	0.92
1:B:180:ASN:HD22	1:B:307:HIS:HD2	1.00	0.91
1:A:55:TYR:HE1	1:A:224:TYR:HH	1.18	0.91
1:D:22:ARG:HG3	1:D:22:ARG:NH2	1.77	0.89
1:C:221:ARG:NH2	1:C:221:ARG:HB2	1.88	0.89
1:A:55:TYR:CE1	1:A:224:TYR:OH	2.23	0.89
1:D:55:TYR:HE1	1:D:224:TYR:OH	1.57	0.88
1:B:221:ARG:HH21	1:B:221:ARG:HB3	1.37	0.88
1:A:55:TYR:HE1	1:A:224:TYR:OH	1.53	0.88
1:B:221:ARG:HB2	1:B:221:ARG:HH21	1.37	0.87
1:A:180:ASN:HD22	1:A:307:HIS:CD2	1.92	0.87
1:B:264:CYS:HB3	1:B:271:LYS:HE3	1.54	0.86
1:C:2:ARG:HH21	1:C:2:ARG:HG2	1.38	0.86
1:C:40:THR:HG23	1:C:41:PRO:HD3	1.59	0.85
1:B:180:ASN:HD22	1:B:307:HIS:CD2	1.92	0.84
1:A:297:ARG:HA	1:A:302:ASN:HB3	1.57	0.84
1:C:264:CYS:SG	1:C:271:LYS:CD	2.66	0.83
1:C:39:PHE:O	1:C:41:PRO:HD2	1.79	0.81
1:B:40:THR:O	1:B:40:THR:OG1	1.88	0.81
1:C:252:ASN:HD22	1:C:255:ASP:H	1.27	0.81
1:D:91:LEU:HD23	1:D:137:LEU:HD23	1.62	0.81
1:C:120:ARG:HE	1:C:120:ARG:HA	1.44	0.81
1:B:221:ARG:NH2	1:B:221:ARG:CB	2.43	0.80
1:D:59:PRO:HG2	1:D:65:ALA:HB2	1.63	0.80
1:D:252:ASN:HD21	1:D:254:GLN:HB2	1.45	0.80
1:D:55:TYR:HE1	1:D:224:TYR:HH	0.80	0.80
1:C:28:GLN:HB3	1:C:29:PRO:HD3	1.62	0.79
1:B:91:LEU:HD23	1:B:137:LEU:HD23	1.65	0.79
1:B:59:PRO:HG2	1:B:62:PRO:HA	1.63	0.79
1:B:252:ASN:HD22	1:B:255:ASP:H	1.31	0.79
1:C:38:ARG:NH2	2:C:401:FAD:H2B	1.98	0.79
1:C:61:ASN:HD21	1:C:63:GLN:HE21	1.28	0.78
1:C:199:ARG:HH12	1:C:201:GLN:HE21	1.32	0.77
1:C:151:ARG:HH11	1:C:154:GLU:CD	1.88	0.77
1:D:255:ASP:O	1:D:259:ILE:HG13	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CE	1:A:176:ASP:CB	2.62	0.76
1:B:33:LYS:HG2	1:B:160:PHE:HE1	1.50	0.76
1:B:221:ARG:NH2	1:B:221:ARG:HB3	2.00	0.76
1:D:223:ILE:HG13	1:D:224:TYR:CD2	2.21	0.75
1:B:11:ILE:CG2	1:B:308:ASN:ND2	2.50	0.74
1:B:55:TYR:HE1	1:B:224:TYR:HH	0.75	0.74
1:D:102:ILE:HG12	1:D:103:PRO:HD2	1.69	0.74
1:C:289:ILE:HD11	1:C:314:TYR:HE2	1.53	0.73
1:D:221:ARG:NH2	1:D:221:ARG:CB	2.50	0.72
1:A:69:GLN:NE2	1:A:110:THR:OG1	2.21	0.72
1:D:283:ARG:NH2	1:D:283:ARG:HG3	2.03	0.72
1:C:150:GLU:O	1:C:154:GLU:HG2	1.89	0.72
1:B:161:GLN:HG3	1:D:249:GLU:O	1.90	0.72
1:B:335:GLU:HG3	1:B:336:GLU:H	1.54	0.72
1:C:199:ARG:HG3	1:C:282:PHE:CE1	2.24	0.72
1:B:264:CYS:CB	1:B:271:LYS:HE3	2.20	0.71
1:A:335:GLU:HG2	1:A:336:GLU:H	1.54	0.71
1:C:40:THR:CG2	1:C:41:PRO:HD3	2.20	0.71
1:C:274:ARG:HA	1:C:274:ARG:NE	2.01	0.70
1:C:252:ASN:ND2	1:C:255:ASP:H	1.88	0.70
1:C:105:PRO:HD2	1:C:108:LYS:HB3	1.74	0.70
1:B:144:TYR:OH	1:B:319:HIS:HE1	1.73	0.70
1:A:221:ARG:HB2	1:A:221:ARG:NH2	2.07	0.69
1:A:199:ARG:HD2	1:A:248:SER:O	1.92	0.69
1:C:40:THR:O	1:C:40:THR:OG1	2.11	0.69
1:B:199:ARG:HG3	1:B:282:PHE:CE1	2.28	0.69
1:C:102:ILE:HG13	1:C:103:PRO:HD2	1.75	0.69
1:B:11:ILE:HG22	1:B:308:ASN:ND2	2.08	0.68
1:B:28:GLN:HB3	1:B:29:PRO:HD3	1.75	0.68
1:A:291:LEU:HA	1:A:307:HIS:O	1.93	0.68
1:B:298:THR:HG23	1:B:298:THR:O	1.92	0.68
1:C:264:CYS:HB3	1:C:271:LYS:HZ3	1.58	0.68
1:B:286:ARG:HG2	1:B:288:GLN:O	1.94	0.68
1:A:274:ARG:HD2	1:D:274:ARG:HH12	1.58	0.68
1:C:38:ARG:HH22	2:C:401:FAD:H2B	1.56	0.68
1:C:140:GLU:OE1	1:C:233:THR:HB	1.94	0.68
1:A:5:VAL:HG22	1:A:179:VAL:HB	1.77	0.67
1:D:18:CYS:SG	1:D:324:LEU:HD23	2.34	0.67
1:D:55:TYR:HE1	1:D:224:TYR:CZ	2.12	0.67
1:B:293:ARG:HD3	1:B:333:ILE:HD11	1.76	0.67
1:D:27:LEU:HD21	1:D:339:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ASN:ND2	1:B:307:HIS:HD2	1.84	0.66
1:C:199:ARG:HG3	1:C:282:PHE:HE1	1.61	0.66
1:B:91:LEU:HD23	1:B:137:LEU:CD2	2.25	0.66
1:C:79:VAL:HG13	1:C:80:HIS:CD2	2.31	0.66
1:C:172:ARG:HH12	1:C:299:GLY:HA3	1.61	0.66
1:A:264:CYS:HB3	1:A:271:LYS:NZ	2.11	0.65
1:B:249:GLU:H	1:D:161:GLN:HE21	1.42	0.65
1:A:252:ASN:HD22	1:A:255:ASP:H	1.45	0.65
1:C:2:ARG:NH2	1:C:2:ARG:HG2	2.11	0.65
1:D:102:ILE:CG1	1:D:103:PRO:HD2	2.27	0.65
1:B:39:PHE:O	1:B:41:PRO:HD2	1.95	0.65
1:C:140:GLU:OE1	1:C:233:THR:CG2	2.45	0.65
1:A:15:THR:HG21	1:A:179:VAL:HG11	1.79	0.65
1:C:91:LEU:HD23	1:C:137:LEU:CD2	2.28	0.64
1:D:201:GLN:HE22	1:D:252:ASN:H	1.44	0.64
1:A:252:ASN:HD21	1:A:254:GLN:HB2	1.61	0.64
1:D:91:LEU:HD23	1:D:137:LEU:CD2	2.26	0.64
1:A:264:CYS:CB	1:A:271:LYS:HZ2	2.11	0.64
1:A:218:ASP:OD2	1:A:221:ARG:NH1	2.30	0.64
1:C:199:ARG:HH12	1:C:201:GLN:NE2	1.95	0.63
1:B:177:VAL:HG22	1:B:304:GLU:HB2	1.79	0.63
1:B:27:LEU:HD21	1:B:334:LEU:HD21	1.80	0.63
1:A:105:PRO:HD3	1:A:132:TRP:CZ2	2.34	0.63
1:B:233:THR:HG23	1:B:234:GLN:HG2	1.79	0.63
1:C:221:ARG:HB2	1:C:221:ARG:HH21	1.63	0.63
1:A:140:GLU:OE1	1:A:233:THR:HB	1.98	0.63
1:C:10:VAL:HB	1:C:45:THR:HG21	1.81	0.62
1:A:286:ARG:HH21	1:A:286:ARG:HG2	1.65	0.62
1:C:274:ARG:HE	1:C:274:ARG:CA	2.04	0.62
1:B:264:CYS:SG	1:B:271:LYS:HE3	2.40	0.62
1:A:61:ASN:HD21	1:A:63:GLN:NE2	1.97	0.62
1:B:297:ARG:HA	1:B:302:ASN:HB3	1.81	0.62
1:A:10:VAL:HB	1:A:45:THR:HG21	1.82	0.62
1:D:39:PHE:O	1:D:41:PRO:HD2	1.99	0.61
1:A:1:MET:HG2	1:A:27:LEU:HD13	1.81	0.61
1:D:252:ASN:ND2	1:D:254:GLN:HB2	2.13	0.61
1:A:144:TYR:OH	1:A:319:HIS:HE1	1.83	0.61
1:B:225:ASN:HA	1:B:240:GLY:O	2.00	0.61
1:B:255:ASP:O	1:B:259:ILE:HG13	2.01	0.61
1:A:101:ALA:HA	1:A:130:TYR:CD2	2.35	0.61
1:A:178:ILE:HB	1:A:305:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LYS:HD2	1:B:235:THR:HG21	1.82	0.60
1:A:201:GLN:HE22	1:A:252:ASN:H	1.47	0.60
1:C:91:LEU:HD23	1:C:137:LEU:HD23	1.81	0.60
1:B:107:TRP:O	1:B:109:ASP:N	2.35	0.60
1:D:117:LEU:HD12	1:D:131:GLY:HA3	1.82	0.60
1:A:56:LEU:H	1:A:56:LEU:HD22	1.66	0.60
1:A:40:THR:O	1:A:40:THR:OG1	2.18	0.60
1:B:144:TYR:OH	1:B:319:HIS:CE1	2.55	0.60
1:A:264:CYS:SG	1:A:271:LYS:HD3	2.42	0.60
1:C:40:THR:HG23	1:C:41:PRO:CD	2.31	0.59
1:C:144:TYR:OH	1:C:319:HIS:HE1	1.85	0.59
1:C:286:ARG:HD3	1:C:288:GLN:O	2.02	0.59
1:A:52:TRP:HE3	1:A:52:TRP:O	1.85	0.59
1:C:293:ARG:NH1	1:C:336:GLU:OE1	2.36	0.59
1:A:286:ARG:HG2	1:A:288:GLN:O	2.02	0.59
1:B:278:GLU:O	1:B:279:ARG:HG2	2.03	0.59
1:B:242:PHE:C	1:B:242:PHE:CD1	2.76	0.59
1:D:197:PRO:HG3	1:D:247:TRP:CE2	2.38	0.59
1:A:221:ARG:CB	1:A:221:ARG:CZ	2.73	0.58
1:D:297:ARG:HD3	1:D:297:ARG:H	1.67	0.58
1:A:61:ASN:HB2	1:A:288:GLN:OE1	2.03	0.58
1:A:161:GLN:HG3	1:C:249:GLU:O	2.02	0.58
1:C:180:ASN:HB3	1:C:307:HIS:HD2	1.68	0.58
1:B:5:VAL:HG22	1:B:179:VAL:HB	1.84	0.58
1:D:318:ILE:O	1:D:319:HIS:C	2.41	0.58
1:C:221:ARG:HB2	1:C:221:ARG:CZ	2.32	0.58
1:D:41:PRO:HB2	1:D:42:LEU:HD23	1.84	0.58
1:A:140:GLU:OE1	1:A:233:THR:CG2	2.52	0.58
1:C:141:GLY:O	1:C:145:LEU:HB2	2.04	0.58
1:C:178:ILE:HB	1:C:305:VAL:HG22	1.86	0.57
1:A:113:GLY:HA3	1:B:115:ARG:NH1	2.19	0.57
1:B:151:ARG:O	1:B:155:ARG:HG3	2.04	0.57
1:B:202:ILE:O	1:B:278:GLU:HG3	2.03	0.57
1:B:168:GLU:O	1:B:172:ARG:HD3	2.04	0.57
1:C:114:PHE:HZ	1:C:132:TRP:CD1	2.22	0.57
1:B:28:GLN:HB3	1:B:29:PRO:CD	2.35	0.57
1:C:216:THR:HG1	1:C:226:SER:HG	1.51	0.57
1:D:5:VAL:HG13	1:D:179:VAL:HB	1.86	0.57
1:D:23:TYR:HA	1:D:26:VAL:HG22	1.86	0.57
1:A:260:TRP:CD1	1:A:260:TRP:C	2.77	0.57
1:B:61:ASN:HD21	1:B:63:GLN:HE21	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:PHE:CZ	1:C:132:TRP:CD1	2.93	0.56
1:D:264:CYS:HG	1:D:271:LYS:HD2	1.67	0.56
1:D:252:ASN:HD22	1:D:255:ASP:H	1.53	0.56
1:D:58:ASP:OD1	1:D:106:SER:HB3	2.06	0.56
1:A:1:MET:HG2	1:A:27:LEU:CD1	2.35	0.56
1:D:102:ILE:CD1	1:D:103:PRO:HD2	2.35	0.56
1:C:79:VAL:HG21	1:C:91:LEU:HG	1.87	0.56
1:C:242:PHE:CD1	1:C:242:PHE:C	2.79	0.56
1:B:199:ARG:HG3	1:B:282:PHE:HE1	1.70	0.56
1:A:1:MET:HE3	1:A:176:ASP:CB	2.36	0.56
1:C:120:ARG:HB3	1:D:112:LEU:CD1	2.36	0.56
1:C:177:VAL:HG22	1:C:304:GLU:HB2	1.88	0.56
1:D:107:TRP:O	1:D:109:ASP:N	2.39	0.56
1:D:201:GLN:NE2	1:D:252:ASN:H	2.04	0.55
1:C:224:TYR:HB2	1:C:242:PHE:HD2	1.70	0.55
1:B:55:TYR:CE1	1:B:224:TYR:OH	2.38	0.55
1:D:232:GLY:N	1:D:235:THR:O	2.35	0.55
1:A:210:MET:HE3	1:A:210:MET:HA	1.89	0.55
1:D:283:ARG:CG	1:D:283:ARG:NH2	2.67	0.55
1:C:39:PHE:O	1:C:41:PRO:CD	2.53	0.55
1:C:150:GLU:HG3	1:C:151:ARG:NH2	2.22	0.55
1:C:224:TYR:HD2	1:C:242:PHE:CD2	2.24	0.55
1:C:69:GLN:NE2	1:C:110:THR:OG1	2.40	0.55
1:B:18:CYS:SG	1:B:324:LEU:HD23	2.47	0.55
1:D:198:GLY:O	1:D:283:ARG:HG3	2.07	0.55
1:D:223:ILE:O	1:D:224:TYR:HB2	2.06	0.55
1:C:233:THR:HG23	1:C:234:GLN:N	2.22	0.54
1:C:289:ILE:HD11	1:C:314:TYR:CE2	2.38	0.54
1:D:40:THR:O	1:D:46:ASP:OD2	2.25	0.54
1:A:27:LEU:HD12	1:A:30:LEU:HD13	1.88	0.54
1:C:55:TYR:HE1	1:C:224:TYR:HH	1.54	0.54
1:A:335:GLU:CG	1:A:336:GLU:N	2.63	0.54
1:B:27:LEU:HD11	1:B:334:LEU:HD11	1.89	0.54
1:C:20:HIS:C	1:C:22:ARG:H	2.11	0.54
1:C:287:PRO:O	1:C:288:GLN:HB3	2.07	0.54
1:D:36:ALA:HB3	1:D:39:PHE:CZ	2.43	0.54
1:C:201:GLN:HE22	1:C:252:ASN:H	1.56	0.54
1:C:27:LEU:HD11	1:C:334:LEU:HD21	1.89	0.54
1:D:104:ASP:OD2	1:D:108:LYS:NZ	2.41	0.54
1:C:225:ASN:ND2	1:C:242:PHE:H	2.06	0.54
1:C:184:VAL:HG21	1:C:197:PRO:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ALA:O	1:C:172:ARG:C	2.47	0.53
1:C:264:CYS:CB	1:C:271:LYS:NZ	2.58	0.53
1:C:120:ARG:HB3	1:D:112:LEU:HD13	1.90	0.53
1:A:197:PRO:HG3	1:A:247:TRP:CE2	2.44	0.53
1:A:199:ARG:NH2	1:A:250:LEU:O	2.41	0.53
1:D:268:PRO:C	1:D:270:LEU:H	2.12	0.53
1:A:255:ASP:O	1:A:259:ILE:HG12	2.08	0.53
1:C:32:ILE:HB	1:C:157:VAL:HG22	1.91	0.53
1:A:233:THR:HG23	1:A:234:GLN:HG2	1.91	0.53
1:D:151:ARG:O	1:D:155:ARG:HD2	2.09	0.53
1:C:297:ARG:HA	1:C:302:ASN:HD22	1.74	0.52
1:D:178:ILE:HB	1:D:305:VAL:HG22	1.91	0.52
1:C:201:GLN:NE2	1:C:252:ASN:H	2.07	0.52
1:D:112:LEU:N	1:D:112:LEU:CD2	2.73	0.52
1:B:140:GLU:OE1	1:B:233:THR:CG2	2.57	0.52
1:C:89:LEU:HA	1:C:138:ILE:O	2.10	0.52
1:B:337:LYS:HB3	1:B:339:LEU:HD13	1.90	0.52
1:D:297:ARG:HG3	1:D:302:ASN:HD22	1.75	0.52
1:A:61:ASN:OD1	1:A:63:GLN:HB2	2.10	0.52
1:C:278:GLU:O	1:C:279:ARG:HG2	2.08	0.52
1:A:150:GLU:HG3	1:A:151:ARG:NH2	2.24	0.52
1:A:297:ARG:HB2	1:A:297:ARG:CZ	2.40	0.52
1:D:112:LEU:HD22	1:D:112:LEU:N	2.24	0.52
1:C:144:TYR:OH	1:C:319:HIS:CE1	2.63	0.52
1:C:27:LEU:HD11	1:C:334:LEU:CD2	2.40	0.52
1:A:296:LEU:O	1:A:302:ASN:HB2	2.10	0.52
1:A:274:ARG:HD2	1:D:274:ARG:NH1	2.23	0.52
1:D:233:THR:HG23	1:D:234:GLN:HG2	1.92	0.52
1:B:199:ARG:HH12	1:B:201:GLN:NE2	2.08	0.52
1:A:120:ARG:HA	1:A:120:ARG:HE	1.75	0.52
1:D:264:CYS:SG	1:D:271:LYS:CD	2.86	0.51
1:C:221:ARG:CB	1:C:221:ARG:CZ	2.88	0.51
1:B:161:GLN:HE21	1:D:249:GLU:H	1.58	0.51
1:D:267:GLU:O	1:D:270:LEU:HB2	2.11	0.51
1:A:199:ARG:NH1	1:A:255:ASP:OD2	2.42	0.51
1:C:172:ARG:HH12	1:C:299:GLY:CA	2.23	0.51
1:C:242:PHE:HD1	1:C:242:PHE:C	2.14	0.51
1:A:146:GLN:O	1:A:149:THR:HB	2.10	0.51
1:B:335:GLU:HG3	1:B:336:GLU:N	2.24	0.51
1:D:41:PRO:CB	1:D:42:LEU:HD23	2.41	0.51
1:B:242:PHE:HD1	1:B:242:PHE:C	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HH21	2:A:401:FAD:H2B	1.75	0.51
1:D:283:ARG:CD	3:D:402:2LD:O15	2.58	0.51
1:D:42:LEU:N	1:D:42:LEU:HD23	2.26	0.51
1:C:37:ASP:HB3	1:C:38:ARG:NH1	2.26	0.51
1:D:196:GLN:HB2	1:D:197:PRO:HD2	1.93	0.51
1:A:115:ARG:HG3	1:A:116:LYS:N	2.25	0.51
1:B:316:LEU:O	1:B:319:HIS:HD2	1.94	0.50
1:B:96:ASN:O	1:B:131:GLY:HA3	2.11	0.50
1:B:335:GLU:HA	1:B:340:SER:HB3	1.93	0.50
1:C:20:HIS:O	1:C:22:ARG:N	2.40	0.50
1:D:22:ARG:CG	1:D:22:ARG:NH2	2.49	0.50
1:C:40:THR:O	1:C:46:ASP:OD2	2.29	0.50
1:C:140:GLU:OE1	1:C:233:THR:CB	2.59	0.50
1:C:290:ARG:HD2	1:C:292:GLU:OE2	2.11	0.50
1:A:38:ARG:HH21	2:A:401:FAD:C2B	2.24	0.50
1:C:332:ARG:O	1:C:335:GLU:HG3	2.12	0.50
1:C:112:LEU:HB2	1:C:135:THR:HB	1.93	0.50
1:B:274:ARG:NH1	1:C:274:ARG:HD2	2.26	0.50
1:B:204:LYS:HD2	1:B:235:THR:CG2	2.41	0.50
1:C:105:PRO:HD2	1:C:105:PRO:O	2.11	0.50
1:D:87:LEU:N	1:D:87:LEU:HD12	2.27	0.50
1:D:1:MET:HE1	1:D:177:VAL:HG23	1.94	0.50
1:A:243:GLN:NE2	1:A:246:ASN:HD22	2.09	0.50
1:B:36:ALA:HB3	1:B:39:PHE:CZ	2.47	0.50
1:A:256:HIS:C	1:A:256:HIS:CD2	2.85	0.50
1:C:201:GLN:HE22	1:C:252:ASN:HB3	1.77	0.49
1:D:52:TRP:CD1	1:D:317:THR:HG23	2.47	0.49
1:B:33:LYS:HG2	1:B:160:PHE:CE1	2.40	0.49
1:A:42:LEU:HD21	1:C:279:ARG:NH2	2.27	0.49
1:B:178:ILE:HB	1:B:305:VAL:HG22	1.95	0.49
1:A:144:TYR:OH	1:A:319:HIS:CE1	2.65	0.49
1:A:117:LEU:HD21	1:A:133:PHE:HB2	1.93	0.49
1:C:2:ARG:CG	1:C:2:ARG:NH2	2.75	0.49
1:A:52:TRP:O	1:A:52:TRP:CE3	2.65	0.49
1:C:184:VAL:HA	1:C:195:LEU:HD11	1.94	0.49
1:B:325:GLU:HA	1:B:325:GLU:OE1	2.13	0.49
1:D:228:TYR:OH	3:D:402:2LD:O16	2.30	0.49
1:C:1:MET:HB3	1:C:29:PRO:O	2.12	0.49
1:C:105:PRO:O	1:C:105:PRO:CD	2.61	0.49
1:B:298:THR:O	1:B:298:THR:CG2	2.60	0.49
1:D:318:ILE:O	1:D:320:TRP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HD11	1:B:217:HIS:CE1	2.48	0.49
1:A:249:GLU:H	1:C:161:GLN:NE2	2.11	0.49
1:B:199:ARG:HD2	1:B:248:SER:O	2.12	0.49
1:B:115:ARG:NH2	1:B:121:GLU:OE2	2.35	0.49
1:B:291:LEU:HA	1:B:307:HIS:O	2.12	0.48
1:A:61:ASN:HD21	1:A:63:GLN:HE21	1.60	0.48
1:D:83:ASN:O	1:D:86:ASN:N	2.46	0.48
1:B:158:LYS:HA	1:B:158:LYS:HE2	1.95	0.48
1:A:71:THR:HA	1:A:320:TRP:HB3	1.95	0.48
1:B:149:THR:HG23	1:B:159:PHE:HE1	1.77	0.48
1:C:120:ARG:NE	1:C:120:ARG:HA	2.21	0.48
1:D:116:LYS:HD2	1:D:130:TYR:OH	2.12	0.48
1:C:115:ARG:NH1	1:D:113:GLY:HA3	2.29	0.48
1:B:69:GLN:OE1	1:B:110:THR:HG23	2.14	0.48
1:A:249:GLU:H	1:C:161:GLN:HE21	1.62	0.48
1:C:140:GLU:OE1	1:C:233:THR:HG21	2.14	0.48
1:C:233:THR:HG23	1:C:234:GLN:HG2	1.95	0.48
1:A:40:THR:CG2	1:A:41:PRO:HD3	2.44	0.48
1:A:169:GLU:O	1:A:173:GLU:HG2	2.14	0.48
1:A:1:MET:HE1	1:A:176:ASP:CB	2.21	0.47
1:D:55:TYR:HE1	1:D:224:TYR:CE2	2.31	0.47
1:D:1:MET:HE1	1:D:176:ASP:HB2	1.96	0.47
1:A:79:VAL:HA	1:A:89:LEU:HD13	1.96	0.47
1:C:39:PHE:C	1:C:41:PRO:HD2	2.34	0.47
1:C:98:PHE:HZ	1:C:132:TRP:CZ3	2.32	0.47
1:D:241:ILE:HD13	1:D:241:ILE:HA	1.62	0.47
1:B:299:GLY:O	1:B:300:PRO:C	2.53	0.47
1:B:286:ARG:HD3	1:B:288:GLN:O	2.13	0.47
1:B:149:THR:HG23	1:B:159:PHE:CE1	2.49	0.47
1:B:184:VAL:N	1:B:284:PRO:HB3	2.29	0.47
1:B:101:ALA:HA	1:B:130:TYR:CD2	2.49	0.47
1:C:28:GLN:HB3	1:C:29:PRO:CD	2.37	0.47
1:A:278:GLU:O	1:A:279:ARG:HG2	2.15	0.47
1:D:266:LEU:O	1:D:266:LEU:HD22	2.14	0.47
1:A:162:ARG:O	1:A:162:ARG:HG3	2.14	0.47
1:C:264:CYS:CB	1:C:271:LYS:HZ2	2.07	0.47
1:D:206:ASP:HB2	1:D:276:ILE:HD11	1.97	0.47
1:C:91:LEU:HD23	1:C:137:LEU:HD21	1.97	0.47
1:A:117:LEU:CD2	1:A:133:PHE:HB2	2.45	0.47
1:D:264:CYS:HB3	1:D:271:LYS:NZ	2.30	0.47
1:C:180:ASN:CB	1:C:307:HIS:HD2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:PHE:O	1:D:115:ARG:HB3	2.15	0.47
1:A:104:ASP:OD1	1:A:116:LYS:HE2	2.14	0.47
1:C:241:ILE:HD13	1:C:255:ASP:HB3	1.97	0.47
1:D:59:PRO:HG2	1:D:65:ALA:CB	2.41	0.47
1:C:38:ARG:NH2	2:C:401:FAD:C2B	2.74	0.47
1:A:140:GLU:OE1	1:A:233:THR:CB	2.62	0.47
1:D:81:SER:HB2	1:D:82:PRO:HD2	1.96	0.47
1:D:17:LEU:HB2	1:D:152:LEU:HD11	1.96	0.47
1:A:83:ASN:O	1:A:86:ASN:N	2.48	0.47
1:C:223:ILE:O	1:C:224:TYR:HB2	2.15	0.46
1:D:119:PRO:HA	1:D:122:LEU:HD12	1.97	0.46
1:B:186:ALA:HB3	1:B:195:LEU:HD22	1.98	0.46
1:D:224:TYR:HB2	1:D:242:PHE:CD2	2.50	0.46
1:A:40:THR:HG23	1:A:41:PRO:HD3	1.97	0.46
1:B:202:ILE:C	1:B:202:ILE:HD12	2.36	0.46
1:D:67:TRP:CH2	1:D:291:LEU:HD23	2.50	0.46
1:A:190:GLN:O	1:A:191:ARG:C	2.54	0.46
1:A:243:GLN:HE21	1:A:246:ASN:HD22	1.64	0.46
1:D:17:LEU:HB2	1:D:152:LEU:CD1	2.45	0.46
1:C:218:ASP:OD1	1:C:218:ASP:C	2.54	0.46
1:A:222:GLY:O	1:A:225:ASN:HB2	2.15	0.46
1:A:199:ARG:HG3	1:A:282:PHE:CE1	2.51	0.46
1:C:190:GLN:O	1:C:191:ARG:C	2.53	0.46
1:C:332:ARG:HA	1:C:335:GLU:CG	2.46	0.46
1:A:125:PHE:O	1:A:126:PRO:C	2.54	0.46
1:B:283:ARG:HH21	1:B:283:ARG:HG3	1.81	0.46
1:C:47:VAL:O	1:C:47:VAL:HG12	2.14	0.46
1:D:53:GLN:HG2	3:D:402:2LD:H9	1.97	0.46
1:C:196:GLN:CD	1:C:244:LEU:HD21	2.37	0.46
1:C:199:ARG:NH1	1:C:201:GLN:HE21	2.08	0.45
1:D:139:LEU:HD11	1:D:144:TYR:CD1	2.51	0.45
1:B:7:GLY:O	1:B:12:GLY:HA3	2.16	0.45
1:A:298:THR:HG22	1:A:302:ASN:HA	1.98	0.45
1:D:140:GLU:OE1	1:D:233:THR:HB	2.17	0.45
1:D:162:ARG:O	2:D:401:FAD:H2A	2.17	0.45
1:B:123:ASP:C	1:B:125:PHE:H	2.19	0.45
1:A:242:PHE:C	1:A:243:GLN:HG3	2.37	0.45
1:D:227:PRO:CG	1:D:262:GLY:HA3	2.47	0.45
1:C:10:VAL:HB	1:C:45:THR:CG2	2.46	0.45
1:B:198:GLY:O	1:B:283:ARG:HG3	2.17	0.45
1:B:233:THR:HG23	1:B:234:GLN:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD22	1:C:42:LEU:HD22	1.98	0.45
1:A:223:ILE:HG23	1:A:223:ILE:O	2.16	0.45
1:C:215:LEU:HD23	1:C:215:LEU:N	2.32	0.45
1:C:205:VAL:HG12	1:C:236:VAL:HB	1.98	0.45
1:C:117:LEU:HG	1:C:131:GLY:O	2.17	0.45
1:D:102:ILE:HD13	1:D:103:PRO:HD2	1.99	0.45
1:C:233:THR:CG2	1:C:234:GLN:N	2.79	0.45
1:C:316:LEU:O	1:C:319:HIS:HD2	1.99	0.45
1:C:291:LEU:HA	1:C:307:HIS:O	2.17	0.45
1:C:27:LEU:HD11	1:C:334:LEU:HD11	1.99	0.45
1:A:10:VAL:HG13	1:A:11:ILE:HD13	2.00	0.44
1:D:144:TYR:OH	1:D:319:HIS:CE1	2.70	0.44
1:B:168:GLU:O	1:B:172:ARG:HB2	2.18	0.44
1:A:10:VAL:HB	1:A:45:THR:CG2	2.46	0.44
1:C:224:TYR:HB2	1:C:242:PHE:CD2	2.50	0.44
1:A:215:LEU:HD13	3:A:402:2LD:C6	2.47	0.44
1:D:67:TRP:HB2	1:D:318:ILE:HD11	1.99	0.44
1:C:5:VAL:O	1:C:34:VAL:HA	2.18	0.44
1:D:297:ARG:HG3	1:D:302:ASN:ND2	2.32	0.44
1:B:140:GLU:OE1	1:B:233:THR:HB	2.17	0.44
1:A:38:ARG:HD2	2:A:401:FAD:O2B	2.17	0.44
1:B:13:LEU:HB2	1:B:148:LEU:HD13	1.97	0.44
1:A:252:ASN:ND2	1:A:255:ASP:H	2.13	0.44
1:D:55:TYR:CE1	1:D:224:TYR:CE2	3.05	0.44
1:C:119:PRO:O	1:C:120:ARG:C	2.55	0.44
1:C:71:THR:OG1	1:C:320:TRP:HB3	2.18	0.44
1:B:293:ARG:NH2	1:B:304:GLU:OE1	2.42	0.44
1:D:180:ASN:ND2	1:D:307:HIS:HD2	2.15	0.44
1:B:161:GLN:HG3	1:D:249:GLU:C	2.39	0.44
1:D:36:ALA:HB3	1:D:39:PHE:CE1	2.53	0.44
1:D:40:THR:O	1:D:40:THR:OG1	2.31	0.44
1:B:171:ALA:O	1:B:172:ARG:C	2.56	0.44
1:C:114:PHE:HA	1:C:134:HIS:HB3	2.00	0.44
1:B:197:PRO:HG3	1:B:247:TRP:CE2	2.52	0.44
1:A:265:ARG:HB2	1:A:265:ARG:HE	1.36	0.44
1:B:265:ARG:HB2	1:B:265:ARG:HE	1.49	0.44
1:C:264:CYS:SG	1:C:271:LYS:HD2	2.54	0.43
1:D:40:THR:CG2	1:D:41:PRO:HD3	2.48	0.43
1:A:39:PHE:O	1:A:41:PRO:HD2	2.16	0.43
1:C:224:TYR:HD2	1:C:242:PHE:CE2	2.36	0.43
1:B:198:GLY:H	1:B:285:VAL:HG23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:GLU:O	1:B:270:LEU:HB2	2.18	0.43
1:A:102:ILE:HG13	1:A:103:PRO:HD2	1.99	0.43
1:D:11:ILE:HG21	1:D:308:ASN:O	2.18	0.43
1:C:200:GLY:HA2	1:C:241:ILE:O	2.18	0.43
1:A:274:ARG:HH21	1:D:274:ARG:HH12	1.66	0.43
1:C:69:GLN:CD	1:C:110:THR:HG23	2.39	0.43
1:A:87:LEU:HB3	1:A:89:LEU:HB2	1.98	0.43
1:C:59:PRO:HG2	1:C:62:PRO:HA	2.00	0.43
1:A:298:THR:HG21	1:A:303:THR:HG23	1.99	0.43
1:B:332:ARG:HA	1:B:335:GLU:HG2	2.00	0.43
1:A:161:GLN:NE2	1:C:249:GLU:H	2.16	0.43
1:D:68:SER:N	1:D:318:ILE:HG13	2.33	0.43
1:B:104:ASP:OD2	1:B:108:LYS:NZ	2.50	0.43
1:B:105:PRO:HG2	1:B:108:LYS:H	1.82	0.43
1:A:152:LEU:HD12	1:A:157:VAL:HG21	1.99	0.43
1:A:199:ARG:HH12	1:A:201:GLN:NE2	2.17	0.43
1:B:38:ARG:NH1	1:B:249:GLU:OE2	2.52	0.43
1:D:199:ARG:HG3	1:D:282:PHE:CE1	2.54	0.43
1:D:56:LEU:HG	1:D:56:LEU:H	1.47	0.43
1:C:206:ASP:OD1	1:C:208:PRO:HD3	2.18	0.43
1:C:191:ARG:NH1	1:C:193:PRO:HG3	2.33	0.43
1:D:240:GLY:O	1:D:241:ILE:HD13	2.19	0.43
1:B:252:ASN:HD21	1:B:254:GLN:HB2	1.84	0.43
1:C:139:LEU:HD21	1:C:144:TYR:CE2	2.54	0.43
1:C:190:GLN:OE1	1:C:290:ARG:NH1	2.52	0.43
1:D:55:TYR:CE1	1:D:224:TYR:OH	2.42	0.42
1:D:299:GLY:HA3	1:D:300:PRO:HD3	1.87	0.42
1:D:218:ASP:OD2	1:D:221:ARG:NH2	2.47	0.42
1:A:264:CYS:CB	1:A:271:LYS:NZ	2.73	0.42
1:D:268:PRO:C	1:D:270:LEU:N	2.71	0.42
1:A:83:ASN:O	1:A:84:ALA:C	2.57	0.42
1:B:102:ILE:HG12	1:B:103:PRO:O	2.18	0.42
1:D:202:ILE:HD11	1:D:279:ARG:HB2	2.01	0.42
1:D:67:TRP:HB3	1:D:318:ILE:HG12	2.01	0.42
1:B:332:ARG:O	1:B:335:GLU:HG3	2.20	0.42
1:C:104:ASP:N	1:C:104:ASP:OD1	2.52	0.42
1:C:196:GLN:CG	1:C:244:LEU:HD21	2.49	0.42
1:D:325:GLU:HA	1:D:328:LYS:HG3	2.02	0.42
1:C:253:ILE:HG22	1:C:254:GLN:NE2	2.35	0.42
1:D:286:ARG:HG2	1:D:287:PRO:HD2	2.01	0.42
1:D:112:LEU:HB2	1:D:135:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:ARG:HA	1:C:335:GLU:HG2	2.01	0.42
1:B:190:GLN:NE2	1:B:294:GLU:OE1	2.53	0.42
1:C:202:ILE:O	1:C:278:GLU:HG3	2.20	0.42
1:A:309:TYR:C	1:A:309:TYR:CD1	2.92	0.42
1:D:61:ASN:CG	1:D:63:GLN:HE21	2.22	0.42
1:B:249:GLU:H	1:D:161:GLN:HG3	1.85	0.42
1:D:66:ASP:O	1:D:70:GLN:HG3	2.20	0.42
1:B:202:ILE:O	1:B:202:ILE:HD12	2.20	0.42
1:D:1:MET:HA	1:D:176:ASP:OD1	2.20	0.42
1:B:114:PHE:C	1:B:114:PHE:CD1	2.94	0.42
1:C:39:PHE:HE2	1:C:161:GLN:HA	1.84	0.41
1:B:61:ASN:HB2	1:B:288:GLN:NE2	2.35	0.41
1:C:233:THR:CG2	1:C:234:GLN:H	2.34	0.41
2:C:401:FAD:H1'1	2:C:401:FAD:H9	1.78	0.41
1:A:15:THR:HG22	1:A:19:ILE:HD12	2.02	0.41
1:D:8:ALA:CB	1:D:39:PHE:CD1	3.03	0.41
1:A:40:THR:HG23	1:A:41:PRO:CD	2.50	0.41
1:A:150:GLU:HG3	1:A:151:ARG:HH22	1.85	0.41
1:C:67:TRP:HB3	1:C:321:GLY:HA3	2.02	0.41
1:C:147:TRP:O	1:C:148:LEU:C	2.57	0.41
1:B:249:GLU:N	1:D:161:GLN:HG3	2.34	0.41
1:D:53:GLN:HG2	3:D:402:2LD:C3	2.50	0.41
1:D:149:THR:HG23	1:D:159:PHE:CE1	2.56	0.41
1:A:41:PRO:HB2	1:A:42:LEU:HD23	2.02	0.41
1:C:286:ARG:HG2	1:C:287:PRO:HD2	2.01	0.41
1:A:52:TRP:CD1	1:A:317:THR:HG23	2.55	0.41
1:B:118:THR:OG1	1:B:121:GLU:HG3	2.20	0.41
1:D:300:PRO:HB2	1:D:301:SER:H	1.77	0.41
1:C:228:TYR:CZ	3:C:402:2LD:H3	2.55	0.41
1:A:1:MET:HE3	1:A:176:ASP:CG	2.41	0.41
1:B:249:GLU:H	1:D:161:GLN:NE2	2.14	0.41
1:D:100:GLU:O	1:D:101:ALA:C	2.58	0.41
1:D:20:HIS:CE1	1:D:155:ARG:HB3	2.55	0.41
1:D:61:ASN:HA	1:D:62:PRO:HD3	1.92	0.41
1:B:276:ILE:HA	1:B:276:ILE:HD13	1.84	0.41
1:D:59:PRO:CG	1:D:65:ALA:HB2	2.42	0.41
1:B:280:THR:HG22	1:B:281:GLY:N	2.34	0.41
1:B:67:TRP:CH2	1:B:291:LEU:HD23	2.56	0.41
1:D:223:ILE:HG13	1:D:224:TYR:CG	2.54	0.41
1:C:1:MET:CB	1:C:29:PRO:O	2.69	0.41
1:C:61:ASN:OD1	1:C:63:GLN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:PHE:O	1:B:41:PRO:CD	2.65	0.41
1:A:133:PHE:CD2	1:A:133:PHE:C	2.94	0.41
1:D:79:VAL:HA	1:D:89:LEU:CD1	2.50	0.41
3:B:402:2LD:H6	3:B:402:2LD:H2	1.81	0.41
1:B:200:GLY:HA2	1:B:241:ILE:O	2.21	0.41
1:D:253:ILE:CG2	1:D:254:GLN:N	2.83	0.41
1:D:1:MET:CE	1:D:176:ASP:HB2	2.50	0.41
1:A:80:HIS:C	1:A:81:SER:O	2.55	0.41
1:B:161:GLN:NE2	1:D:249:GLU:H	2.18	0.40
1:D:199:ARG:HB2	1:D:246:ASN:HB3	2.02	0.40
1:C:126:PRO:O	1:C:128:TYR:N	2.54	0.40
1:A:40:THR:O	1:A:46:ASP:OD2	2.39	0.40
1:C:139:LEU:HD11	1:C:144:TYR:CD1	2.56	0.40
1:C:224:TYR:CZ	1:C:313:GLY:HA3	2.56	0.40
1:A:252:ASN:ND2	1:A:254:GLN:HB2	2.33	0.40
1:B:100:GLU:HA	1:B:100:GLU:OE1	2.22	0.40
1:D:161:GLN:O	1:D:162:ARG:HB3	2.22	0.40
1:B:1:MET:HG2	1:B:27:LEU:HD22	2.04	0.40
1:D:40:THR:HG23	1:D:41:PRO:HD3	2.02	0.40
1:A:39:PHE:O	1:A:41:PRO:CD	2.70	0.40
1:D:334:LEU:C	1:D:336:GLU:H	2.25	0.40
1:A:203:MET:HE3	1:A:203:MET:HB2	1.97	0.40
1:C:123:ASP:O	1:C:125:PHE:N	2.55	0.40
1:B:233:THR:CG2	1:B:234:GLN:N	2.85	0.40
1:C:98:PHE:HZ	1:C:132:TRP:CH2	2.39	0.40
1:D:93:SER:O	1:D:212:HIS:HA	2.22	0.40
1:B:187:GLY:C	1:B:189:LEU:H	2.24	0.40
1:B:52:TRP:CD1	1:B:317:THR:HG23	2.57	0.40
1:C:56:LEU:HD23	1:C:56:LEU:N	2.37	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	338/347 (97%)	298 (88%)	33 (10%)	7 (2%)	9 21
1	B	338/347 (97%)	295 (87%)	34 (10%)	9 (3%)	6 14
1	C	338/347 (97%)	292 (86%)	35 (10%)	11 (3%)	5 10
1	D	338/347 (97%)	289 (86%)	41 (12%)	8 (2%)	7 17
All	All	1352/1388 (97%)	1174 (87%)	143 (11%)	35 (3%)	7 15

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	297	ARG
1	B	40	THR
1	B	108	LYS
1	C	40	THR
1	C	127	ASP
1	D	335	GLU
1	A	299	GLY
1	B	191	ARG
1	C	21	GLU
1	C	124	MET
1	C	299	GLY
1	D	12	GLY
1	D	108	LYS
1	D	220	GLU
1	D	300	PRO
1	A	188	ALA
1	A	223	ILE
1	B	127	ASP
1	C	126	PRO
1	C	171	ALA
1	B	28	GLN
1	B	253	ILE
1	B	298	THR
1	C	300	PRO
1	D	223	ILE
1	A	300	PRO
1	B	172	ARG
1	C	105	PRO
1	B	104	ASP
1	D	29	PRO
1	A	240	GLY
1	C	28	GLN

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Mol	Chain	Res	Type
1	C	240	GLY
1	D	240	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	292/299 (98%)	250 (86%)	42 (14%)	4 8
1	B	292/299 (98%)	255 (87%)	37 (13%)	5 12
1	C	292/299 (98%)	254 (87%)	38 (13%)	5 11
1	D	292/299 (98%)	247 (85%)	45 (15%)	3 7
All	All	1168/1196 (98%)	1006 (86%)	162 (14%)	4 9

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	28	GLN
1	A	31	ASP
1	A	32	ILE
1	A	38	ARG
1	A	56	LEU
1	A	81	SER
1	A	87	LEU
1	A	89	LEU
1	A	102	ILE
1	A	112	LEU
1	A	120	ARG
1	A	145	LEU
1	A	146	GLN
1	A	151	ARG
1	A	152	LEU
1	A	154	GLU
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	162	ARG
1	A	168	GLU
1	A	169	GLU
1	A	172	ARG
1	A	191	ARG
1	A	196	GLN
1	A	205	VAL
1	A	221	ARG
1	A	225	ASN
1	A	235	THR
1	A	238	LEU
1	A	253	ILE
1	A	265	ARG
1	A	266	LEU
1	A	270	LEU
1	A	271	LYS
1	A	274	ARG
1	A	295	GLN
1	A	297	ARG
1	A	301	SER
1	A	337	LYS
1	A	338	LYS
1	A	339	LEU
1	B	22	ARG
1	B	28	GLN
1	B	31	ASP
1	B	38	ARG
1	B	56	LEU
1	B	60	ASN
1	B	89	LEU
1	B	108	LYS
1	B	112	LEU
1	B	132	TRP
1	B	145	LEU
1	B	151	ARG
1	B	152	LEU
1	B	161	GLN
1	B	162	ARG
1	B	172	ARG
1	B	173	GLU
1	B	191	ARG
1	B	196	GLN

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Mol	Chain	Res	Type
1	B	211	LYS
1	B	221	ARG
1	B	235	THR
1	B	238	LEU
1	B	242	PHE
1	B	261	GLU
1	B	264	CYS
1	B	265	ARG
1	B	266	LEU
1	B	270	LEU
1	B	294	GLU
1	B	295	GLN
1	B	296	LEU
1	B	297	ARG
1	B	302	ASN
1	B	328	LYS
1	B	335	GLU
1	B	340	SER
1	C	18	CYS
1	C	22	ARG
1	C	38	ARG
1	C	85	GLU
1	C	87	LEU
1	C	89	LEU
1	C	120	ARG
1	C	145	LEU
1	C	151	ARG
1	C	152	LEU
1	C	161	GLN
1	C	168	GLU
1	C	172	ARG
1	C	173	GLU
1	C	182	THR
1	C	196	GLN
1	C	205	VAL
1	C	215	LEU
1	C	221	ARG
1	C	238	LEU
1	C	242	PHE
1	C	244	LEU
1	C	253	ILE
1	C	259	ILE

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Mol	Chain	Res	Type
1	C	265	ARG
1	C	266	LEU
1	C	271	LYS
1	C	274	ARG
1	C	290	ARG
1	C	293	ARG
1	C	295	GLN
1	C	297	ARG
1	C	298	THR
1	C	301	SER
1	C	302	ASN
1	C	335	GLU
1	C	337	LYS
1	C	339	LEU
1	D	5	VAL
1	D	22	ARG
1	D	27	LEU
1	D	28	GLN
1	D	42	LEU
1	D	56	LEU
1	D	60	ASN
1	D	61	ASN
1	D	89	LEU
1	D	91	LEU
1	D	102	ILE
1	D	108	LYS
1	D	112	LEU
1	D	116	LYS
1	D	122	LEU
1	D	142	LYS
1	D	143	ASN
1	D	145	LEU
1	D	151	ARG
1	D	152	LEU
1	D	153	THR
1	D	161	GLN
1	D	164	VAL
1	D	168	GLU
1	D	172	ARG
1	D	176	ASP
1	D	184	VAL
1	D	195	LEU

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Mol	Chain	Res	Type
1	D	205	VAL
1	D	215	LEU
1	D	221	ARG
1	D	225	ASN
1	D	238	LEU
1	D	244	LEU
1	D	253	ILE
1	D	261	GLU
1	D	264	CYS
1	D	266	LEU
1	D	279	ARG
1	D	283	ARG
1	D	290	ARG
1	D	298	THR
1	D	301	SER
1	D	316	LEU
1	D	318	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	63	GLN
1	A	69	GLN
1	A	134	HIS
1	A	161	GLN
1	A	196	GLN
1	A	201	GLN
1	A	243	GLN
1	A	252	ASN
1	A	307	HIS
1	A	319	HIS
1	B	24	HIS
1	B	28	GLN
1	B	53	GLN
1	B	60	ASN
1	B	63	GLN
1	B	96	ASN
1	B	161	GLN
1	B	201	GLN
1	B	225	ASN
1	B	243	GLN

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Mol	Chain	Res	Type
1	B	252	ASN
1	B	288	GLN
1	B	295	GLN
1	B	307	HIS
1	B	308	ASN
1	B	319	HIS
1	C	63	GLN
1	C	69	GLN
1	C	80	HIS
1	C	134	HIS
1	C	161	GLN
1	C	201	GLN
1	C	225	ASN
1	C	243	GLN
1	C	252	ASN
1	C	254	GLN
1	C	302	ASN
1	C	307	HIS
1	C	319	HIS
1	D	63	GLN
1	D	80	HIS
1	D	161	GLN
1	D	180	ASN
1	D	201	GLN
1	D	225	ASN
1	D	243	GLN
1	D	252	ASN
1	D	288	GLN
1	D	302	ASN
1	D	307	HIS
1	D	319	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	A	401	-	48,58,58	1.37	4 (8%)	54,89,89	3.23	18 (33%)
3	2LD	A	402	-	17,17,17	1.54	4 (23%)	19,22,22	1.78	5 (26%)
2	FAD	B	401	-	48,58,58	1.52	8 (16%)	54,89,89	2.50	12 (22%)
3	2LD	B	402	-	17,17,17	1.55	4 (23%)	19,22,22	1.64	4 (21%)
2	FAD	C	401	-	48,58,58	1.70	8 (16%)	54,89,89	2.32	11 (20%)
3	2LD	C	402	-	17,17,17	1.54	4 (23%)	19,22,22	1.79	5 (26%)
2	FAD	D	401	-	48,58,58	1.56	9 (18%)	54,89,89	2.54	14 (25%)
3	2LD	D	402	-	17,17,17	1.55	4 (23%)	19,22,22	1.77	5 (26%)

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	401	-	-	0/30/50/50	0/6/6/6
3	2LD	A	402	-	-	0/5/5/5	0/2/2/2
2	FAD	B	401	-	-	0/30/50/50	0/6/6/6
3	2LD	B	402	-	-	0/5/5/5	0/2/2/2
2	FAD	C	401	-	-	0/30/50/50	0/6/6/6
3	2LD	C	402	-	-	0/5/5/5	0/2/2/2
2	FAD	D	401	-	-	0/30/50/50	0/6/6/6
3	2LD	D	402	-	-	0/5/5/5	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FAD	C10-N10	-7.18	1.30	1.39
2	A	401	FAD	C10-N10	-5.03	1.33	1.39
2	D	401	FAD	C10-N10	-4.61	1.33	1.39
2	B	401	FAD	C10-N10	-4.59	1.33	1.39
2	C	401	FAD	C9A-N10	-4.57	1.32	1.38
2	D	401	FAD	C9A-N10	-3.99	1.33	1.38
3	B	402	2LD	C8-C9	-2.77	1.33	1.38
2	C	401	FAD	C6-C5X	-2.74	1.37	1.41
3	D	402	2LD	C8-C9	-2.64	1.34	1.38
3	C	402	2LD	C8-C9	-2.62	1.34	1.38
3	A	402	2LD	C8-C9	-2.62	1.34	1.38
2	A	401	FAD	C1'-N10	-2.53	1.45	1.48
2	D	401	FAD	C6-C5X	-2.43	1.38	1.41
2	A	401	FAD	C9A-N10	-2.32	1.35	1.38
2	B	401	FAD	C6-C5X	-2.32	1.38	1.41
2	C	401	FAD	C4X-C10	-2.22	1.36	1.41
2	D	401	FAD	C8M-C8	-2.19	1.46	1.51
2	C	401	FAD	C4A-N3A	-2.06	1.32	1.35
2	C	401	FAD	C9-C9A	-2.03	1.36	1.40
2	C	401	FAD	C4-C4X	2.02	1.45	1.41
2	B	401	FAD	C2A-N3A	2.06	1.35	1.32
2	B	401	FAD	C10-N1	2.12	1.39	1.35
3	C	402	2LD	C7-C9	2.15	1.43	1.39
3	A	402	2LD	C7-C9	2.19	1.43	1.39
2	D	401	FAD	C4-N3	2.20	1.37	1.33
3	D	402	2LD	C7-C9	2.21	1.43	1.39
2	D	401	FAD	C10-N1	2.38	1.39	1.35
2	D	401	FAD	O4B-C1B	2.43	1.44	1.41
3	B	402	2LD	C7-C9	2.50	1.43	1.39
2	D	401	FAD	C2'-C3'	2.72	1.59	1.53
3	B	402	2LD	C11-N14	2.85	1.38	1.33
2	B	401	FAD	C5'-C4'	2.91	1.56	1.51
2	A	401	FAD	O4B-C1B	3.05	1.45	1.41
3	D	402	2LD	C11-N14	3.17	1.39	1.33
2	B	401	FAD	C4-C4X	3.18	1.47	1.41
3	A	402	2LD	C11-N14	3.19	1.39	1.33
3	C	402	2LD	C11-N14	3.20	1.39	1.33
3	C	402	2LD	C11-C10	3.36	1.49	1.40
3	A	402	2LD	C11-C10	3.36	1.49	1.40
3	D	402	2LD	C11-C10	3.38	1.49	1.40
2	B	401	FAD	O4B-C1B	3.40	1.45	1.41
2	C	401	FAD	O4B-C1B	3.45	1.45	1.41
2	D	401	FAD	C4-C4X	3.51	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	2LD	C11-C10	3.52	1.49	1.40
2	B	401	FAD	C4-N3	3.57	1.39	1.33

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	FAD	C4X-C4-N3	-6.55	114.64	123.59
2	B	401	FAD	C4X-C4-N3	-6.15	115.18	123.59
2	C	401	FAD	C4X-C4-N3	-5.71	115.78	123.59
2	B	401	FAD	C4X-C10-N10	-4.84	117.67	120.52
2	D	401	FAD	C4X-C4-N3	-4.79	117.04	123.59
2	D	401	FAD	C1B-N9A-C4A	-4.77	119.75	126.94
2	B	401	FAD	O3'-C3'-C4'	-4.58	97.22	108.75
2	A	401	FAD	C4X-C10-N10	-4.27	118.00	120.52
2	A	401	FAD	C4-C4X-N5	-4.17	113.66	118.72
2	A	401	FAD	C4X-N5-C5X	-4.01	112.14	116.76
3	C	402	2LD	C10-C11-N14	-3.73	116.39	121.47
3	A	402	2LD	C10-C11-N14	-3.70	116.43	121.47
3	D	402	2LD	C10-C11-N14	-3.66	116.48	121.47
2	D	401	FAD	C4-C4X-C10	-3.46	117.73	119.94
2	D	401	FAD	C4B-O4B-C1B	-3.40	105.99	109.72
2	A	401	FAD	O3'-C3'-C4'	-3.34	100.34	108.75
3	B	402	2LD	C10-C11-N14	-3.33	116.94	121.47
2	C	401	FAD	P-O3P-PA	-3.19	123.77	132.73
2	A	401	FAD	O3B-C3B-C2B	-2.92	102.32	111.83
2	C	401	FAD	O3'-C3'-C4'	-2.86	101.56	108.75
2	A	401	FAD	O4B-C1B-N9A	-2.78	102.28	108.10
2	B	401	FAD	O3P-PA-O5B	-2.74	95.67	102.94
2	C	401	FAD	C4X-N5-C5X	-2.73	113.62	116.76
2	B	401	FAD	O2P-P-O5'	-2.70	94.82	108.46
2	A	401	FAD	O2'-C2'-C3'	-2.66	102.32	109.02
2	D	401	FAD	C4X-C10-N10	-2.63	118.97	120.52
2	A	401	FAD	O3P-PA-O5B	-2.59	96.07	102.94
2	D	401	FAD	O3'-C3'-C4'	-2.54	102.34	108.75
2	B	401	FAD	C4B-O4B-C1B	-2.53	106.94	109.72
3	C	402	2LD	C9-C8-N14	-2.53	119.50	123.80
2	A	401	FAD	O3B-C3B-C4B	-2.51	103.52	111.05
3	A	402	2LD	C9-C8-N14	-2.50	119.55	123.80
3	D	402	2LD	C9-C8-N14	-2.49	119.57	123.80
2	A	401	FAD	N6A-C6A-N1A	-2.47	113.91	119.20
2	A	401	FAD	C4-C4X-C10	-2.34	118.44	119.94
2	D	401	FAD	O3B-C3B-C2B	-2.33	104.24	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	FAD	C4-C4X-C10	-2.33	118.45	119.94
3	A	402	2LD	C1-C2-C4	-2.30	116.82	120.19
3	C	402	2LD	C1-C2-C4	-2.28	116.85	120.19
2	D	401	FAD	C8M-C8-C9	-2.23	114.21	120.28
3	D	402	2LD	C1-C2-C4	-2.21	116.94	120.19
2	B	401	FAD	C4-C4X-N5	-2.15	116.11	118.72
2	C	401	FAD	O2B-C2B-C3B	-2.09	105.03	111.83
2	D	401	FAD	O2P-P-O3P	-2.09	95.63	105.09
2	D	401	FAD	C4X-N5-C5X	-2.06	114.40	116.76
2	B	401	FAD	N3A-C2A-N1A	2.18	130.56	128.89
2	A	401	FAD	C4B-O4B-C1B	2.23	112.17	109.72
2	C	401	FAD	O2A-PA-O3P	2.37	115.84	105.09
2	B	401	FAD	C5X-C9A-N10	2.48	119.50	117.62
3	B	402	2LD	C4-C6-C5	2.59	122.28	118.13
2	B	401	FAD	C6-C5X-C9A	2.62	122.43	118.98
3	B	402	2LD	C8-N14-C11	2.72	122.46	116.51
3	A	402	2LD	C7-C9-C8	2.82	119.65	116.57
2	D	401	FAD	C1'-C2'-C3'	2.82	117.89	109.82
3	D	402	2LD	C7-C9-C8	2.84	119.67	116.57
3	C	402	2LD	C7-C9-C8	2.89	119.72	116.57
2	C	401	FAD	O4B-C1B-N9A	2.91	114.19	108.10
3	B	402	2LD	C7-C9-C8	3.05	119.90	116.57
3	D	402	2LD	C8-N14-C11	3.34	123.81	116.51
3	A	402	2LD	C8-N14-C11	3.37	123.88	116.51
3	C	402	2LD	C8-N14-C11	3.39	123.92	116.51
2	A	401	FAD	N3A-C2A-N1A	3.63	131.67	128.89
2	C	401	FAD	C5X-C9A-N10	4.20	120.81	117.62
2	D	401	FAD	C1'-N10-C9A	4.29	123.68	118.86
2	A	401	FAD	C2B-C1B-N9A	4.44	121.07	114.29
2	C	401	FAD	C1'-N10-C9A	5.09	124.58	118.86
2	A	401	FAD	C5X-C9A-N10	5.37	121.70	117.62
2	A	401	FAD	C1'-N10-C9A	6.35	126.00	118.86
2	D	401	FAD	C5X-C9A-N10	6.80	122.78	117.62
2	B	401	FAD	C1'-N10-C9A	7.38	127.14	118.86
2	B	401	FAD	C4-N3-C2	10.12	124.00	115.25
2	C	401	FAD	C4-N3-C2	10.73	124.53	115.25
2	D	401	FAD	C4-N3-C2	11.66	125.32	115.25
2	A	401	FAD	C4-N3-C2	16.50	129.51	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	FAD	3	0
3	A	402	2LD	1	0
3	B	402	2LD	1	0
2	C	401	FAD	4	0
3	C	402	2LD	1	0
2	D	401	FAD	1	0
3	D	402	2LD	5	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	340/347 (97%)	0.09	6 (1%)	71	74	28, 48, 72, 89	0
1	B	340/347 (97%)	0.14	6 (1%)	71	74	29, 49, 73, 81	0
1	C	340/347 (97%)	0.39	27 (7%)	15	14	40, 58, 82, 100	0
1	D	340/347 (97%)	0.42	29 (8%)	13	12	39, 58, 84, 99	0
All	All	1360/1388 (97%)	0.26	68 (5%)	32	32	28, 53, 79, 100	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	339	LEU	11.2
1	D	339	LEU	10.2
1	C	300	PRO	7.6
1	D	297	ARG	7.4
1	C	340	SER	5.9
1	D	296	LEU	5.8
1	A	340	SER	5.8
1	D	295	GLN	5.6
1	D	340	SER	5.0
1	C	297	ARG	4.9
1	A	339	LEU	4.5
1	D	299	GLY	4.5
1	D	301	SER	4.2
1	C	299	GLY	3.6
1	C	338	LYS	3.6
1	D	82	PRO	3.5
1	C	301	SER	3.4
1	D	338	LYS	3.2
1	C	70	GLN	3.2
1	D	300	PRO	3.2
1	D	28	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	291	LEU	3.1
1	C	265	ARG	3.0
1	C	298	THR	2.9
1	C	83	ASN	2.8
1	C	334	LEU	2.8
1	D	70	GLN	2.8
1	C	131	GLY	2.7
1	C	302	ASN	2.7
1	A	328	LYS	2.7
1	D	302	ASN	2.7
1	D	191	ARG	2.7
1	C	110	THR	2.7
1	B	60	ASN	2.6
1	D	233	THR	2.6
1	D	294	GLU	2.6
1	D	308	ASN	2.6
1	C	191	ARG	2.6
1	C	325	GLU	2.5
1	C	293	ARG	2.5
1	D	334	LEU	2.5
1	C	172	ARG	2.5
1	C	60	ASN	2.4
1	B	59	PRO	2.4
1	D	293	ARG	2.4
1	D	335	GLU	2.4
1	D	333	ILE	2.4
1	B	297	ARG	2.4
1	C	100	GLU	2.4
1	C	130	TYR	2.3
1	D	259	ILE	2.3
1	A	291	LEU	2.3
1	B	339	LEU	2.3
1	C	324	LEU	2.3
1	D	305	VAL	2.2
1	C	296	LEU	2.2
1	B	328	LYS	2.2
1	A	297	ARG	2.1
1	D	332	ARG	2.1
1	A	332	ARG	2.1
1	B	332	ARG	2.1
1	C	332	ARG	2.1
1	D	221	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	126	PRO	2.0
1	C	259	ILE	2.0
1	D	337	LYS	2.0
1	D	298	THR	2.0
1	D	306	ILE	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	2LD	C	402	16/16	0.89	0.23	0.86	32,36,43,43	0
3	2LD	A	402	16/16	0.96	0.21	0.77	32,36,43,43	0
3	2LD	D	402	16/16	0.90	0.21	0.31	32,36,43,43	0
3	2LD	B	402	16/16	0.97	0.16	-0.39	34,39,45,45	0
2	FAD	A	401	53/53	0.97	0.15	-0.47	26,36,43,46	0
2	FAD	B	401	53/53	0.97	0.15	-0.48	29,34,44,50	0
2	FAD	C	401	53/53	0.97	0.16	-0.73	35,39,48,50	0
2	FAD	D	401	53/53	0.97	0.14	-0.96	31,39,49,52	0

6.5 Other polymers (i)

There are no such residues in this entry.