



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:06 PM GMT

PDB ID : 3W4I
Title : Crystal Structure of human DAAO in complex with coumpound 8
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 : 2.50 Å(reported)

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

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

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

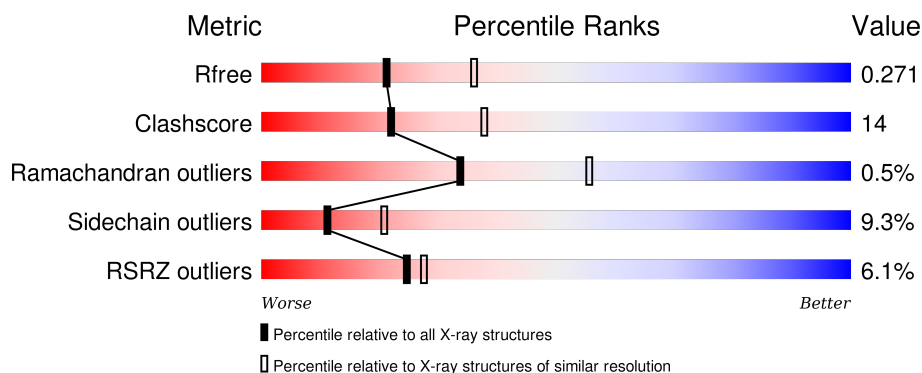
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	347	<div> <div>2%</div> <div>69%</div> <div>24%</div> <div>5%</div> <div>•</div> </div>
1	B	347	<div> <div>3%</div> <div>71%</div> <div>24%</div> <div>•••</div> </div>
1	C	347	<div> <div>9%</div> <div>71%</div> <div>21%</div> <div>5%</div> <div>••</div> </div>
1	D	347	<div> <div>10%</div> <div>66%</div> <div>29%</div> <div>••</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11176 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: $C_{27}H_{33}N_9O_{15}P_2$).



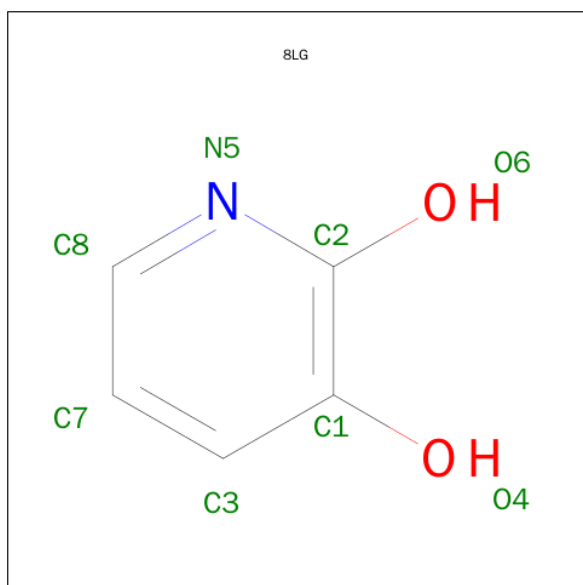
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

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 PYRIDINE-2,3-DIOL (three-letter code: 8LG) (formula: $C_5H_5NO_2$).

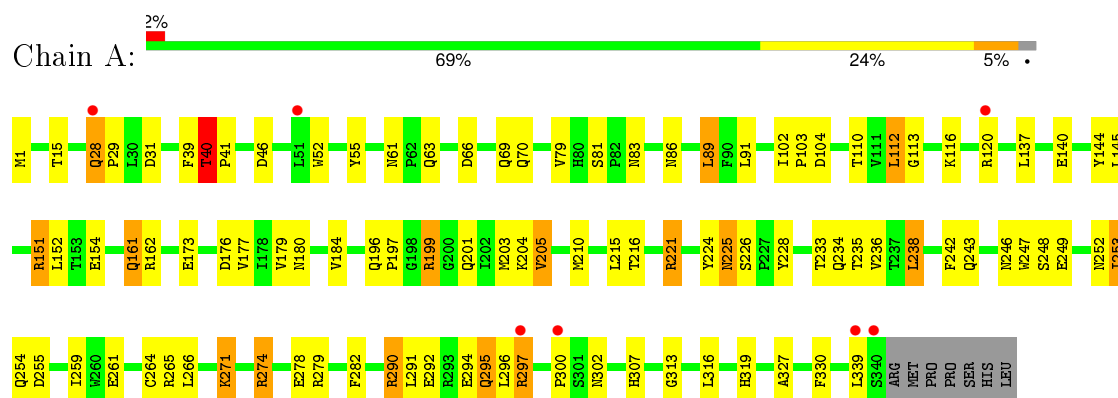


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	5	1	2		
3	B	1	Total	C	N	O	0	0
			8	5	1	2		
3	C	1	Total	C	N	O	0	0
			8	5	1	2		
3	D	1	Total	C	N	O	0	0
			8	5	1	2		

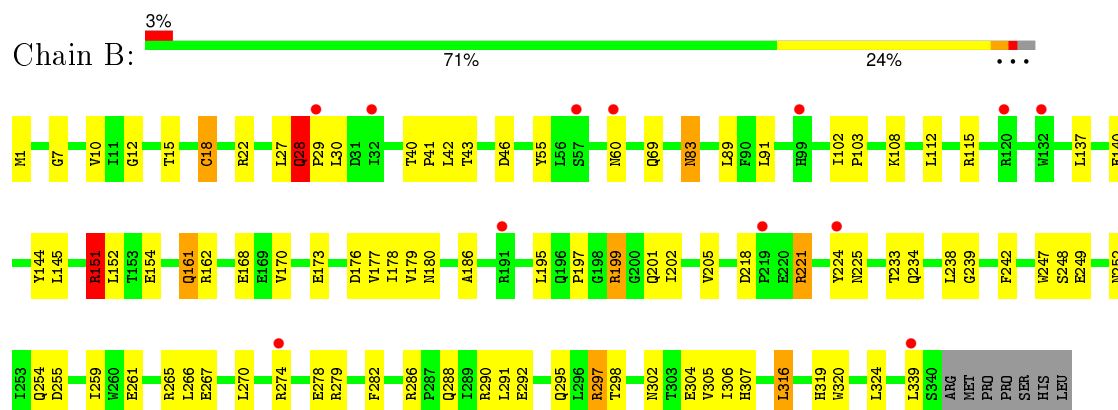
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

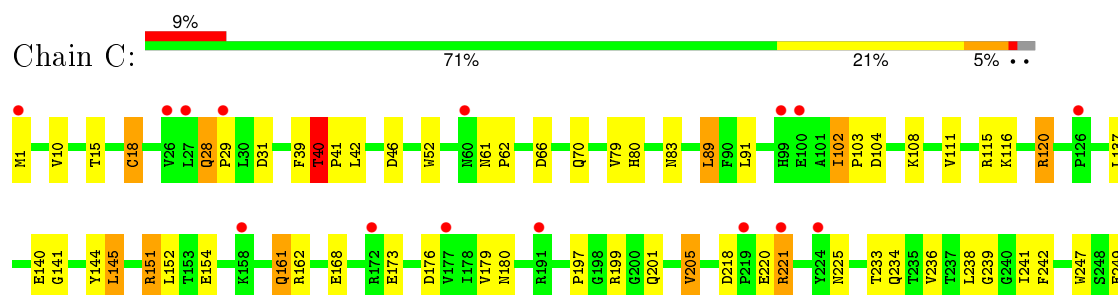
• Molecule 1: D-amino-acid oxidase

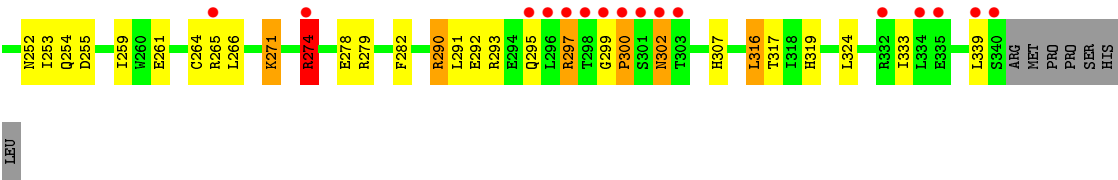


• Molecule 1: D-amino-acid oxidase

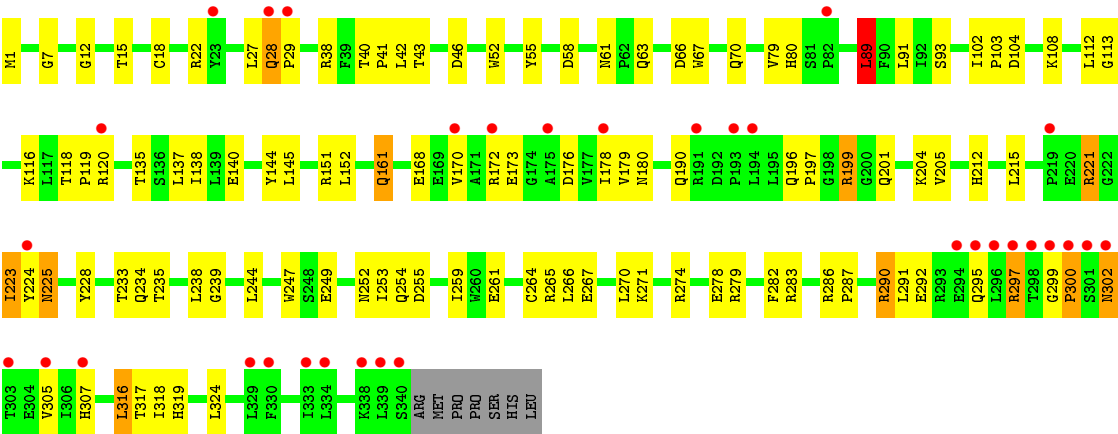


• Molecule 1: D-amino-acid oxidase





● Molecule 1: D-amino-acid oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	148.70 Å 181.53 Å 50.61 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.93 – 2.50 46.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.93-2.50) 96.0 (46.93-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.236 , 0.273 0.236 , 0.271	Depositor DCC
R_{free} test set	2350 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 46480 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11176	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 21.78 % 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 6.5320e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8LG, 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	0.68	0/2810	0.75	3/3824 (0.1%)
1	B	0.66	1/2810 (0.0%)	0.74	3/3824 (0.1%)
1	C	0.60	1/2810 (0.0%)	0.69	4/3824 (0.1%)
1	D	0.62	0/2810	0.71	2/3824 (0.1%)
All	All	0.64	2/11240 (0.0%)	0.72	12/15296 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18	CYS	CB-SG	-5.38	1.73	1.81
1	B	18	CYS	CB-SG	-5.01	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	ARG	NE-CZ-NH1	-7.71	116.45	120.30
1	B	151	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	40	THR	N-CA-C	6.07	127.38	111.00
1	C	40	THR	N-CA-C	6.00	127.20	111.00
1	C	89	LEU	CA-CB-CG	5.68	128.38	115.30
1	D	89	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	199	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	B	199	ARG	NE-CZ-NH2	5.43	123.01	120.30
1	A	112	LEU	CA-CB-CG	5.33	127.56	115.30
1	C	274	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	274	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	D	199	ARG	NE-CZ-NH1	-5.04	117.78	120.30

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	2733	0	2680	83	0
1	B	2733	0	2680	78	0
1	C	2733	0	2680	79	0
1	D	2733	0	2680	84	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	8	0	4	1	0
3	B	8	0	4	0	0
3	C	8	0	4	0	0
3	D	8	0	4	1	0
All	All	11176	0	10860	306	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 14.

All (306) 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:274:ARG:NH2	1:D:274:ARG:HH12	1.26	1.33
1:A:274:ARG:NH2	1:D:274:ARG:NH1	1.98	1.08
1:D:102:ILE:HG12	1:D:103:PRO:HD2	1.37	1.06
1:B:55:TYR:HE1	1:B:224:TYR:OH	1.39	1.06
1:C:1:MET:HE3	1:C:176:ASP:HB2	1.45	0.95
1:B:28:GLN:HB3	1:B:29:PRO:HD3	1.49	0.94
1:D:180:ASN:HD22	1:D:307:HIS:HD2	1.10	0.93
1:B:180:ASN:HD22	1:B:307:HIS:HD2	1.04	0.93
1:B:102:ILE:HG13	1:B:103:PRO:HD2	1.51	0.93
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.07	0.92
1:C:102:ILE:HG13	1:C:103:PRO:HD2	1.52	0.92
1:B:91:LEU:HD23	1:B:137:LEU:HD23	1.51	0.91
1:B:55:TYR:CE1	1:B:224:TYR:OH	2.19	0.91
1:C:28:GLN:HB3	1:C:29:PRO:HD3	1.53	0.89
1:A:264:CYS:HB3	1:A:271:LYS:NZ	1.87	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:HH21	1:D:274:ARG:NH1	1.64	0.88
1:A:274:ARG:HH21	1:D:274:ARG:HH12	0.88	0.86
1:B:1:MET:HE3	1:B:176:ASP:HB2	1.58	0.86
1:D:264:CYS:SG	1:D:271:LYS:HD2	2.16	0.86
1:A:102:ILE:HG13	1:A:103:PRO:HD2	1.59	0.84
1:D:102:ILE:CG1	1:D:103:PRO:HD2	2.07	0.84
1:A:28:GLN:HB3	1:A:29:PRO:HD3	1.59	0.84
1:B:91:LEU:HD23	1:B:137:LEU:CD2	2.07	0.83
1:D:28:GLN:HB3	1:D:29:PRO:HD3	1.60	0.83
1:A:201:GLN:HE22	1:A:252:ASN:H	1.28	0.82
1:D:102:ILE:HG12	1:D:103:PRO:CD	2.10	0.82
1:C:151:ARG:NH1	1:C:154:GLU:OE2	2.12	0.82
1:A:104:ASP:OD1	1:A:116:LYS:HE2	1.81	0.81
1:B:180:ASN:HD22	1:B:307:HIS:CD2	1.95	0.81
1:C:180:ASN:HD22	1:C:307:HIS:HD2	1.27	0.80
1:A:274:ARG:HH22	1:D:274:ARG:NH1	1.80	0.79
1:A:180:ASN:HD22	1:A:307:HIS:CD2	1.98	0.77
1:B:249:GLU:H	1:D:161:GLN:HE21	1.32	0.77
1:A:264:CYS:HB3	1:A:271:LYS:HZ2	1.46	0.76
1:A:161:GLN:HE21	1:C:249:GLU:H	1.31	0.76
1:B:252:ASN:HD21	1:B:254:GLN:HB2	1.51	0.75
1:D:201:GLN:HE22	1:D:252:ASN:H	1.33	0.74
1:C:1:MET:CE	1:C:176:ASP:HB2	2.15	0.74
1:B:140:GLU:OE1	1:B:233:THR:HG22	1.87	0.74
1:B:255:ASP:O	1:B:259:ILE:HG12	1.88	0.74
1:A:290:ARG:HD2	1:A:292:GLU:OE2	1.88	0.72
1:B:161:GLN:HE21	1:D:249:GLU:H	1.36	0.72
1:D:221:ARG:NH2	1:D:221:ARG:HB2	2.04	0.72
1:B:151:ARG:NH1	1:B:154:GLU:OE2	2.20	0.71
1:C:225:ASN:ND2	1:C:242:PHE:H	1.88	0.71
1:C:41:PRO:HG2	1:C:42:LEU:HG	1.71	0.71
1:C:221:ARG:NH2	1:C:221:ARG:HB2	2.06	0.70
1:C:225:ASN:HD22	1:C:242:PHE:H	1.39	0.70
1:B:201:GLN:HE22	1:B:252:ASN:H	1.37	0.70
1:C:252:ASN:HD22	1:C:255:ASP:H	1.39	0.70
1:D:221:ARG:HB2	1:D:221:ARG:HH21	1.57	0.70
1:C:201:GLN:HE22	1:C:252:ASN:H	1.39	0.69
1:D:223:ILE:HD12	1:D:224:TYR:H	1.57	0.69
1:D:255:ASP:O	1:D:259:ILE:HG12	1.93	0.69
1:B:140:GLU:OE1	1:B:233:THR:CG2	2.40	0.68
1:B:102:ILE:HG13	1:B:103:PRO:CD	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ASN:HD22	1:D:255:ASP:H	1.42	0.68
1:B:41:PRO:HG2	1:B:42:LEU:HG	1.75	0.68
1:D:1:MET:HG2	1:D:27:LEU:HD13	1.76	0.68
1:A:1:MET:CE	1:A:176:ASP:HB2	2.23	0.68
1:B:40:THR:O	1:B:40:THR:OG1	2.08	0.68
1:B:221:ARG:HB2	1:B:221:ARG:HH21	1.59	0.68
1:B:55:TYR:HE1	1:B:224:TYR:CZ	2.11	0.67
1:B:28:GLN:HB3	1:B:29:PRO:CD	2.24	0.67
1:A:252:ASN:HD21	1:A:254:GLN:HB2	1.59	0.67
1:D:1:MET:HE3	1:D:176:ASP:HB2	1.76	0.67
1:A:291:LEU:HA	1:A:307:HIS:O	1.95	0.67
1:A:151:ARG:NH1	1:A:154:GLU:OE2	2.26	0.66
1:D:201:GLN:NE2	1:D:252:ASN:H	1.93	0.66
1:B:144:TYR:OH	1:B:319:HIS:HE1	1.78	0.66
1:B:233:THR:HG23	1:B:234:GLN:HG2	1.78	0.65
1:A:40:THR:HG23	1:A:41:PRO:HD3	1.78	0.65
1:A:40:THR:O	1:A:40:THR:OG1	2.14	0.65
1:D:233:THR:HG23	1:D:234:GLN:HG2	1.77	0.65
1:D:283:ARG:NE	3:D:402:8LG:O6	2.26	0.65
1:A:233:THR:HG23	1:A:234:GLN:HG2	1.80	0.64
1:C:91:LEU:HD23	1:C:137:LEU:HD23	1.80	0.64
1:A:249:GLU:H	1:C:161:GLN:HE21	1.47	0.63
1:C:102:ILE:HG13	1:C:103:PRO:CD	2.28	0.63
1:C:180:ASN:HD22	1:C:307:HIS:CD2	2.13	0.63
1:A:144:TYR:OH	1:A:319:HIS:HE1	1.81	0.63
1:D:297:ARG:HA	1:D:302:ASN:HB3	1.82	0.62
1:D:180:ASN:HD22	1:D:307:HIS:CD2	2.03	0.62
1:A:102:ILE:HG13	1:A:103:PRO:CD	2.28	0.62
1:C:201:GLN:NE2	1:C:252:ASN:H	1.96	0.62
1:A:297:ARG:HA	1:A:302:ASN:HB3	1.80	0.62
1:A:252:ASN:HD22	1:A:255:ASP:H	1.47	0.62
1:A:1:MET:HE3	1:A:176:ASP:HB2	1.82	0.62
1:A:201:GLN:NE2	1:A:252:ASN:H	1.97	0.61
1:B:221:ARG:HB2	1:B:221:ARG:NH2	2.15	0.61
1:C:28:GLN:HB3	1:C:29:PRO:CD	2.27	0.61
1:B:252:ASN:HD22	1:B:255:ASP:H	1.46	0.61
1:A:61:ASN:HD21	1:A:63:GLN:HE21	1.48	0.61
1:C:140:GLU:OE1	1:C:233:THR:CG2	2.49	0.61
1:C:239:GLY:HA2	1:C:259:ILE:HD12	1.82	0.61
1:B:1:MET:CE	1:B:176:ASP:HB2	2.29	0.60
1:B:274:ARG:HH12	1:C:274:ARG:CZ	2.13	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:GLU:O	1:C:279:ARG:HG2	2.00	0.60
1:C:79:VAL:HG13	1:C:80:HIS:CD2	2.35	0.60
1:D:180:ASN:ND2	1:D:307:HIS:HD2	1.91	0.60
1:C:140:GLU:OE2	1:C:233:THR:HG22	2.02	0.60
1:D:140:GLU:OE1	1:D:233:THR:HG22	2.01	0.60
1:A:39:PHE:O	1:A:41:PRO:HD2	2.02	0.60
1:C:140:GLU:OE1	1:C:233:THR:HG22	2.02	0.60
1:D:197:PRO:HG3	1:D:247:TRP:CE2	2.36	0.59
1:B:252:ASN:ND2	1:B:254:GLN:HB2	2.17	0.59
1:A:40:THR:O	1:A:46:ASP:OD2	2.19	0.59
1:B:298:THR:HG23	1:B:298:THR:O	2.01	0.59
1:A:28:GLN:HB3	1:A:29:PRO:CD	2.32	0.59
1:A:264:CYS:HB3	1:A:271:LYS:HZ3	1.65	0.58
1:A:161:GLN:NE2	1:C:249:GLU:H	2.00	0.58
1:B:291:LEU:HA	1:B:307:HIS:O	2.03	0.58
1:C:252:ASN:HD21	1:C:254:GLN:HB2	1.67	0.58
1:A:249:GLU:O	1:C:161:GLN:HG3	2.03	0.58
1:B:55:TYR:CE1	1:B:224:TYR:CE2	2.92	0.57
1:C:120:ARG:HE	1:C:120:ARG:HA	1.69	0.57
1:C:291:LEU:HA	1:C:307:HIS:O	2.05	0.57
1:D:40:THR:O	1:D:46:ASP:OD2	2.23	0.57
1:B:18:CYS:SG	1:B:324:LEU:HD23	2.45	0.57
1:B:286:ARG:HD3	1:B:288:GLN:O	2.05	0.57
1:D:140:GLU:OE1	1:D:233:THR:CG2	2.53	0.56
1:B:201:GLN:NE2	1:B:252:ASN:H	2.02	0.56
1:C:151:ARG:HH11	1:C:154:GLU:CD	2.05	0.56
1:C:91:LEU:HD23	1:C:137:LEU:CD2	2.35	0.56
1:A:197:PRO:HG3	1:A:247:TRP:CE2	2.40	0.56
1:B:274:ARG:HH12	1:C:274:ARG:NH2	2.04	0.56
1:A:221:ARG:HB2	1:A:221:ARG:NH2	2.21	0.55
1:B:161:GLN:NE2	1:D:249:GLU:H	2.05	0.55
1:D:55:TYR:HE1	1:D:224:TYR:HE2	1.54	0.55
1:D:144:TYR:OH	1:D:319:HIS:HE1	1.89	0.55
1:C:241:ILE:HD13	1:C:255:ASP:HB3	1.89	0.55
1:B:83:ASN:OD1	1:B:83:ASN:N	2.40	0.54
1:B:297:ARG:HA	1:B:302:ASN:HB3	1.89	0.54
1:D:144:TYR:OH	1:D:319:HIS:CE1	2.61	0.54
1:C:199:ARG:HG3	1:C:282:PHE:CE1	2.42	0.54
1:A:91:LEU:HD23	1:A:137:LEU:HD23	1.90	0.54
1:A:264:CYS:SG	1:A:271:LYS:HD3	2.47	0.54
1:A:1:MET:HE1	1:A:176:ASP:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:LEU:O	1:C:319:HIS:HD2	1.91	0.54
1:D:91:LEU:HD23	1:D:137:LEU:HD23	1.90	0.54
1:A:252:ASN:ND2	1:A:254:GLN:HB2	2.23	0.54
1:D:190:GLN:OE1	1:D:290:ARG:NH1	2.40	0.53
1:A:102:ILE:CG1	1:A:103:PRO:HD2	2.36	0.53
1:D:201:GLN:HE22	1:D:252:ASN:N	2.04	0.53
1:A:180:ASN:ND2	1:A:307:HIS:HD2	1.91	0.53
1:C:274:ARG:HE	1:C:274:ARG:CA	2.19	0.53
1:D:40:THR:O	1:D:40:THR:OG1	2.22	0.53
1:B:55:TYR:HE1	1:B:224:TYR:CE2	2.26	0.53
1:A:225:ASN:ND2	1:A:242:PHE:O	2.42	0.52
1:C:40:THR:OG1	1:C:40:THR:O	2.25	0.52
1:C:225:ASN:HD22	1:C:242:PHE:N	2.06	0.52
1:A:205:VAL:HG12	1:A:236:VAL:HB	1.90	0.52
1:A:327:ALA:O	1:A:330:PHE:HB3	2.09	0.52
1:B:40:THR:O	1:B:46:ASP:OD2	2.28	0.52
1:D:252:ASN:HD21	1:D:254:GLN:HB2	1.74	0.52
1:A:255:ASP:O	1:A:259:ILE:HG12	2.09	0.51
1:B:218:ASP:OD2	1:B:221:ARG:NH2	2.43	0.51
1:C:115:ARG:NH1	1:D:113:GLY:HA3	2.26	0.51
1:A:140:GLU:OE1	1:A:233:THR:HG22	2.11	0.51
1:C:140:GLU:CD	1:C:233:THR:HG22	2.30	0.51
1:D:43:THR:O	1:D:46:ASP:HB2	2.10	0.51
1:D:290:ARG:HD2	1:D:292:GLU:OE2	2.11	0.51
1:D:196:GLN:HG3	1:D:244:LEU:HD22	1.93	0.51
1:B:199:ARG:HG3	1:B:282:PHE:CE1	2.45	0.51
1:C:52:TRP:HE3	1:C:52:TRP:O	1.94	0.51
1:B:170:VAL:O	1:B:173:GLU:HG3	2.10	0.50
1:A:216:THR:O	1:A:226:SER:HB3	2.12	0.50
1:B:55:TYR:CE1	1:B:224:TYR:CZ	2.93	0.50
1:C:10:VAL:HG21	1:C:316:LEU:HD13	1.94	0.50
1:D:79:VAL:HA	1:D:89:LEU:HD13	1.92	0.50
1:C:66:ASP:O	1:C:70:GLN:HG3	2.12	0.49
1:C:79:VAL:HG21	1:C:91:LEU:HG	1.94	0.49
1:A:221:ARG:HB2	1:A:221:ARG:CZ	2.42	0.49
1:D:15:THR:HG21	1:D:179:VAL:HG11	1.94	0.49
1:D:7:GLY:O	1:D:12:GLY:HA3	2.12	0.49
1:A:79:VAL:HA	1:A:89:LEU:HD13	1.95	0.49
1:D:55:TYR:HE1	1:D:224:TYR:CE2	2.30	0.49
1:A:199:ARG:NH1	1:A:255:ASP:OD2	2.46	0.49
1:C:255:ASP:O	1:C:259:ILE:HG12	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:TYR:OH	1:B:319:HIS:CE1	2.62	0.49
1:D:215:LEU:HD22	1:D:228:TYR:HB2	1.94	0.49
1:C:233:THR:HG23	1:C:234:GLN:HG2	1.95	0.49
1:B:197:PRO:HG3	1:B:247:TRP:CE2	2.48	0.49
1:B:199:ARG:HD2	1:B:248:SER:O	2.12	0.48
1:C:201:GLN:HE22	1:C:252:ASN:N	2.08	0.48
1:D:178:ILE:HB	1:D:305:VAL:HG22	1.94	0.48
1:A:151:ARG:HH11	1:A:154:GLU:CD	2.15	0.48
1:C:221:ARG:HB2	1:C:221:ARG:HH21	1.75	0.48
1:D:278:GLU:O	1:D:279:ARG:HG2	2.12	0.48
1:C:180:ASN:ND2	1:C:307:HIS:HD2	2.05	0.48
1:C:197:PRO:HG3	1:C:247:TRP:CE2	2.48	0.48
1:D:291:LEU:HA	1:D:307:HIS:O	2.13	0.48
1:C:144:TYR:OH	1:C:319:HIS:HE1	1.97	0.48
1:B:201:GLN:HE22	1:B:252:ASN:N	2.08	0.48
1:A:294:GLU:OE2	1:A:307:HIS:HE1	1.98	0.47
1:A:66:ASP:O	1:A:70:GLN:HG3	2.14	0.47
1:B:290:ARG:HD2	1:B:292:GLU:OE2	2.15	0.47
1:C:18:CYS:SG	1:C:324:LEU:HD23	2.54	0.47
1:A:41:PRO:O	1:A:279:ARG:NH1	2.47	0.47
1:C:52:TRP:CE3	1:C:52:TRP:O	2.68	0.47
1:C:218:ASP:OD1	1:C:220:GLU:N	2.47	0.47
1:D:170:VAL:O	1:D:173:GLU:HG3	2.15	0.46
1:A:215:LEU:HD22	1:A:228:TYR:HB2	1.97	0.46
1:B:199:ARG:HH12	1:B:201:GLN:NE2	2.14	0.46
1:B:267:GLU:O	1:B:270:LEU:HB2	2.15	0.46
1:B:202:ILE:O	1:B:278:GLU:HG3	2.15	0.46
1:B:10:VAL:HG21	1:B:316:LEU:HD13	1.98	0.46
1:C:290:ARG:HD2	1:C:292:GLU:OE2	2.16	0.46
1:A:243:GLN:NE2	1:A:246:ASN:HD22	2.14	0.46
1:C:28:GLN:CB	1:C:29:PRO:HD3	2.36	0.46
1:B:249:GLU:H	1:D:161:GLN:NE2	2.08	0.45
1:D:225:ASN:HD22	1:D:225:ASN:HA	1.51	0.45
1:B:242:PHE:C	1:B:242:PHE:CD1	2.90	0.45
1:A:140:GLU:OE1	1:A:233:THR:CG2	2.63	0.45
1:C:52:TRP:CD1	1:C:317:THR:HG23	2.51	0.45
1:A:274:ARG:HD2	1:D:274:ARG:HH22	1.82	0.45
1:B:91:LEU:HD23	1:B:137:LEU:HD21	1.93	0.45
1:A:278:GLU:O	1:A:279:ARG:HG2	2.16	0.45
1:A:15:THR:HG21	1:A:179:VAL:HG11	1.99	0.45
1:D:223:ILE:HD12	1:D:224:TYR:N	2.28	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LEU:HD22	1:D:42:LEU:HD22	1.99	0.45
1:D:104:ASP:OD1	1:D:116:LYS:HE2	2.17	0.45
1:A:61:ASN:HD21	1:A:63:GLN:NE2	2.13	0.44
1:C:293:ARG:HD3	1:C:333:ILE:HD11	1.98	0.44
1:B:278:GLU:O	1:B:279:ARG:HG2	2.17	0.44
1:D:79:VAL:HG13	1:D:80:HIS:CD2	2.53	0.44
1:B:186:ALA:HB3	1:B:195:LEU:HD22	1.99	0.44
1:C:297:ARG:HA	1:C:302:ASN:HB3	2.00	0.44
1:D:18:CYS:SG	1:D:324:LEU:HD23	2.57	0.44
1:B:239:GLY:HA2	1:B:259:ILE:HD12	2.00	0.44
1:A:1:MET:HE1	1:A:177:VAL:HG23	1.99	0.44
1:D:239:GLY:HA2	1:D:259:ILE:HD12	1.99	0.44
1:B:27:LEU:HD13	1:B:30:LEU:HD13	1.98	0.44
1:C:264:CYS:SG	1:C:271:LYS:HD2	2.58	0.44
1:D:112:LEU:HB2	1:D:135:THR:HB	1.98	0.44
1:D:204:LYS:HD2	1:D:235:THR:HG21	2.00	0.44
1:A:296:LEU:O	1:A:302:ASN:HB2	2.18	0.43
1:D:89:LEU:HA	1:D:138:ILE:O	2.18	0.43
1:D:286:ARG:HG2	1:D:287:PRO:HD2	2.00	0.43
1:C:1:MET:HE3	1:C:176:ASP:CB	2.33	0.43
1:C:199:ARG:HH12	1:C:201:GLN:NE2	2.16	0.43
1:D:40:THR:HG23	1:D:41:PRO:HD3	2.00	0.43
1:A:144:TYR:OH	1:A:319:HIS:CE1	2.67	0.43
2:B:401:FAD:O2'	2:B:401:FAD:C9	2.67	0.43
1:A:52:TRP:HE3	1:A:52:TRP:O	2.00	0.43
1:D:79:VAL:HA	1:D:89:LEU:CD1	2.48	0.43
1:C:39:PHE:O	1:C:41:PRO:HD2	2.18	0.43
1:C:199:ARG:NH1	1:C:255:ASP:OD2	2.52	0.43
1:C:15:THR:HG21	1:C:179:VAL:HG11	2.00	0.43
1:D:52:TRP:CD1	1:D:317:THR:HG23	2.54	0.43
1:D:299:GLY:HA3	1:D:300:PRO:HD2	1.86	0.43
1:D:93:SER:O	1:D:212:HIS:HA	2.19	0.43
1:B:55:TYR:HE1	1:B:224:TYR:HH	0.61	0.42
1:B:170:VAL:HA	1:B:173:GLU:HG2	2.01	0.42
1:D:244:LEU:HD23	1:D:244:LEU:HA	1.91	0.42
1:C:253:ILE:HA	1:C:253:ILE:HD13	1.86	0.42
1:A:313:GLY:O	3:A:402:8LG:N5	2.53	0.42
1:C:104:ASP:OD1	1:C:116:LYS:HE2	2.19	0.42
1:D:267:GLU:O	1:D:270:LEU:HB2	2.19	0.42
1:A:39:PHE:O	1:A:41:PRO:CD	2.66	0.42
1:A:55:TYR:HE1	1:A:224:TYR:HE2	1.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:TRP:HB2	1:D:318:ILE:HD11	2.00	0.42
1:B:180:ASN:ND2	1:B:307:HIS:HD2	1.90	0.42
1:A:199:ARG:HG3	1:A:282:PHE:CE1	2.54	0.42
1:A:113:GLY:HA3	1:B:115:ARG:NH1	2.34	0.42
1:B:177:VAL:HG22	1:B:304:GLU:HB2	2.01	0.42
1:A:204:LYS:HD2	1:A:235:THR:HG21	2.02	0.42
1:D:28:GLN:HB3	1:D:29:PRO:CD	2.35	0.42
1:A:203:MET:HB3	1:A:238:LEU:HB2	2.02	0.42
1:C:205:VAL:HG12	1:C:236:VAL:HB	2.02	0.42
1:C:242:PHE:CD1	1:C:242:PHE:C	2.94	0.42
1:B:151:ARG:HD3	1:B:151:ARG:HH21	1.60	0.41
1:A:253:ILE:HG22	1:A:254:GLN:N	2.35	0.41
1:C:52:TRP:CE2	1:C:317:THR:HG23	2.54	0.41
1:D:79:VAL:HG13	1:D:80:HIS:HD2	1.85	0.41
1:D:204:LYS:HD2	1:D:235:THR:CG2	2.49	0.41
1:A:28:GLN:CB	1:A:29:PRO:HD3	2.40	0.41
1:C:221:ARG:HB2	1:C:221:ARG:CZ	2.50	0.41
1:D:297:ARG:HG3	1:D:302:ASN:HD22	1.83	0.41
1:B:286:ARG:CZ	1:B:290:ARG:HB2	2.50	0.41
1:A:55:TYR:HE1	1:A:224:TYR:CE2	2.38	0.41
1:D:199:ARG:HG3	1:D:282:PHE:CE1	2.55	0.41
1:C:61:ASN:HA	1:C:62:PRO:HD2	1.93	0.41
1:A:69:GLN:NE2	1:A:110:THR:HG23	2.36	0.41
1:B:225:ASN:ND2	1:B:242:PHE:H	2.19	0.41
1:B:178:ILE:HB	1:B:305:VAL:HG22	2.02	0.41
1:C:199:ARG:HH12	1:C:201:GLN:HE21	1.68	0.41
1:B:316:LEU:O	1:B:319:HIS:HD2	2.04	0.41
1:C:40:THR:O	1:C:46:ASP:OD2	2.39	0.41
1:B:15:THR:HG21	1:B:179:VAL:HG11	2.02	0.41
1:D:199:ARG:NH1	1:D:255:ASP:OD2	2.54	0.41
1:B:298:THR:O	1:B:298:THR:CG2	2.67	0.41
1:B:7:GLY:O	1:B:12:GLY:HA3	2.21	0.41
1:A:295:GLN:H	1:A:295:GLN:HG2	1.71	0.41
1:B:319:HIS:CG	1:B:320:TRP:N	2.89	0.41
1:C:144:TYR:OH	1:C:319:HIS:CE1	2.73	0.41
1:C:141:GLY:O	1:C:145:LEU:HB2	2.21	0.40
1:A:210:MET:HE2	1:A:210:MET:HB3	1.98	0.40
1:D:61:ASN:HD21	1:D:63:GLN:NE2	2.20	0.40
1:D:118:THR:HB	1:D:119:PRO:HD2	2.02	0.40
1:D:66:ASP:O	1:D:70:GLN:HG3	2.21	0.40
1:A:199:ARG:HD2	1:A:248:SER:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:THR:O	1:B:46:ASP:HB2	2.21	0.40
1:D:316:LEU:HD13	1:D:316:LEU:HA	1.96	0.40
1:A:83:ASN:O	1:A:86:ASN:N	2.55	0.40
1:C:299:GLY:HA3	1:C:300:PRO:HD2	1.86	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%)	313 (93%)	23 (7%)	2 (1%)	30	50
1	B	338/347 (97%)	315 (93%)	22 (6%)	1 (0%)	46	68
1	C	338/347 (97%)	316 (94%)	19 (6%)	3 (1%)	21	37
1	D	338/347 (97%)	317 (94%)	20 (6%)	1 (0%)	46	68
All	All	1352/1388 (97%)	1261 (93%)	84 (6%)	7 (0%)	34	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	C	40	THR
1	B	28	GLN
1	C	300	PRO
1	D	300	PRO
1	A	300	PRO
1	C	111	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	292/299 (98%)	263 (90%)	29 (10%)	10	18
1	B	292/299 (98%)	267 (91%)	25 (9%)	13	24
1	C	292/299 (98%)	264 (90%)	28 (10%)	10	19
1	D	292/299 (98%)	265 (91%)	27 (9%)	11	21
All	All	1168/1196 (98%)	1059 (91%)	109 (9%)	11	21

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	31	ASP
1	A	81	SER
1	A	89	LEU
1	A	112	LEU
1	A	120	ARG
1	A	145	LEU
1	A	151	ARG
1	A	152	LEU
1	A	161	GLN
1	A	162	ARG
1	A	173	GLU
1	A	184	VAL
1	A	196	GLN
1	A	205	VAL
1	A	221	ARG
1	A	225	ASN
1	A	238	LEU
1	A	253	ILE
1	A	261	GLU
1	A	265	ARG
1	A	266	LEU
1	A	271	LYS
1	A	274	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	290	ARG
1	A	295	GLN
1	A	297	ARG
1	A	316	LEU
1	A	339	LEU
1	B	22	ARG
1	B	28	GLN
1	B	60	ASN
1	B	69	GLN
1	B	83	ASN
1	B	89	LEU
1	B	108	LYS
1	B	112	LEU
1	B	145	LEU
1	B	151	ARG
1	B	152	LEU
1	B	161	GLN
1	B	162	ARG
1	B	168	GLU
1	B	205	VAL
1	B	221	ARG
1	B	238	LEU
1	B	261	GLU
1	B	265	ARG
1	B	266	LEU
1	B	295	GLN
1	B	297	ARG
1	B	306	ILE
1	B	316	LEU
1	B	339	LEU
1	C	28	GLN
1	C	31	ASP
1	C	83	ASN
1	C	89	LEU
1	C	102	ILE
1	C	108	LYS
1	C	120	ARG
1	C	145	LEU
1	C	151	ARG
1	C	152	LEU
1	C	161	GLN
1	C	162	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	168	GLU
1	C	173	GLU
1	C	205	VAL
1	C	221	ARG
1	C	238	LEU
1	C	261	GLU
1	C	265	ARG
1	C	266	LEU
1	C	271	LYS
1	C	274	ARG
1	C	290	ARG
1	C	295	GLN
1	C	297	ARG
1	C	302	ASN
1	C	316	LEU
1	C	339	LEU
1	D	22	ARG
1	D	28	GLN
1	D	38	ARG
1	D	58	ASP
1	D	89	LEU
1	D	108	LYS
1	D	120	ARG
1	D	145	LEU
1	D	151	ARG
1	D	152	LEU
1	D	161	GLN
1	D	168	GLU
1	D	172	ARG
1	D	205	VAL
1	D	221	ARG
1	D	223	ILE
1	D	225	ASN
1	D	238	LEU
1	D	253	ILE
1	D	261	GLU
1	D	265	ARG
1	D	266	LEU
1	D	290	ARG
1	D	295	GLN
1	D	297	ARG
1	D	302	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	316	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	63	GLN
1	A	69	GLN
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	60	ASN
1	B	63	GLN
1	B	69	GLN
1	B	80	HIS
1	B	161	GLN
1	B	196	GLN
1	B	201	GLN
1	B	225	ASN
1	B	243	GLN
1	B	252	ASN
1	B	307	HIS
1	B	319	HIS
1	C	63	GLN
1	C	69	GLN
1	C	80	HIS
1	C	161	GLN
1	C	196	GLN
1	C	201	GLN
1	C	225	ASN
1	C	243	GLN
1	C	252	ASN
1	C	307	HIS
1	C	319	HIS
1	D	63	GLN
1	D	69	GLN
1	D	80	HIS
1	D	161	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	201	GLN
1	D	225	ASN
1	D	243	GLN
1	D	252	ASN
1	D	302	ASN
1	D	307	HIS
1	D	319	HIS

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 ⓘ

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	1.40	7 (14%)	54,89,89	2.05	9 (16%)
3	8LG	A	402	-	7,8,8	1.19	1 (14%)	8,10,10	0.81	0
2	FAD	B	401	-	48,58,58	1.48	6 (12%)	54,89,89	2.90	13 (24%)
3	8LG	B	402	-	7,8,8	1.22	1 (14%)	8,10,10	1.10	1 (12%)
2	FAD	C	401	-	48,58,58	1.45	6 (12%)	54,89,89	2.31	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	8LG	C	402	-	7,8,8	1.24	1 (14%)	8,10,10	1.21	1 (12%)
2	FAD	D	401	-	48,58,58	1.50	8 (16%)	54,89,89	2.11	11 (20%)
3	8LG	D	402	-	7,8,8	1.21	1 (14%)	8,10,10	1.04	1 (12%)

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	8LG	A	402	-	-	0/0/0/0	0/1/1/1
2	FAD	B	401	-	-	0/30/50/50	0/6/6/6
3	8LG	B	402	-	-	0/0/0/0	0/1/1/1
2	FAD	C	401	-	-	0/30/50/50	0/6/6/6
3	8LG	C	402	-	-	0/0/0/0	0/1/1/1
2	FAD	D	401	-	-	0/30/50/50	0/6/6/6
3	8LG	D	402	-	-	0/0/0/0	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FAD	C10-N10	-5.83	1.32	1.39
2	B	401	FAD	C10-N10	-5.46	1.32	1.39
2	D	401	FAD	C10-N10	-4.20	1.34	1.39
2	A	401	FAD	C10-N10	-3.93	1.34	1.39
2	C	401	FAD	C9A-N10	-3.58	1.33	1.38
2	B	401	FAD	C9A-N10	-3.24	1.34	1.38
2	A	401	FAD	C4X-C10	-2.71	1.35	1.41
2	B	401	FAD	C5X-N5	-2.56	1.31	1.35
3	A	402	8LG	C3-C1	-2.46	1.35	1.39
3	C	402	8LG	C3-C1	-2.28	1.35	1.39
2	C	401	FAD	C4X-C10	-2.24	1.36	1.41
3	D	402	8LG	C3-C1	-2.24	1.35	1.39
3	B	402	8LG	C3-C1	-2.24	1.35	1.39
2	C	401	FAD	C6-C5X	-2.19	1.38	1.41
2	D	401	FAD	C4X-C10	-2.17	1.37	1.41
2	B	401	FAD	C4X-C10	-2.17	1.37	1.41
2	D	401	FAD	C6-C5X	-2.08	1.38	1.41
2	A	401	FAD	C9A-C5X	-2.06	1.38	1.42
2	D	401	FAD	O4B-C1B	2.27	1.44	1.41
2	A	401	FAD	C4-N3	2.32	1.37	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FAD	C1'-N10	2.41	1.50	1.48
2	A	401	FAD	C10-N1	2.43	1.39	1.35
2	B	401	FAD	C1'-N10	2.55	1.51	1.48
2	C	401	FAD	O4B-C1B	2.60	1.44	1.41
2	A	401	FAD	O4B-C1B	2.69	1.44	1.41
2	D	401	FAD	C10-N1	3.02	1.40	1.35
2	B	401	FAD	O4B-C1B	3.09	1.45	1.41
2	D	401	FAD	C4-N3	3.11	1.38	1.33
2	C	401	FAD	C4-C4X	3.14	1.47	1.41
2	A	401	FAD	C4-C4X	3.40	1.48	1.41
2	D	401	FAD	C4-C4X	4.25	1.49	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	FAD	C4X-C4-N3	-7.92	112.76	123.59
2	B	401	FAD	C4-C4X-N5	-7.53	109.58	118.72
2	B	401	FAD	C4X-C10-N10	-6.66	116.59	120.52
2	C	401	FAD	C4X-C4-N3	-5.68	115.82	123.59
2	D	401	FAD	C4-C4X-C10	-4.99	116.75	119.94
2	A	401	FAD	C4X-C10-N10	-3.37	118.53	120.52
2	B	401	FAD	C4B-O4B-C1B	-3.14	106.27	109.72
2	A	401	FAD	C4-C4X-C10	-3.03	118.00	119.94
2	D	401	FAD	C1B-N9A-C4A	-2.71	122.86	126.94
2	C	401	FAD	C4-C4X-C10	-2.65	118.25	119.94
2	B	401	FAD	C8M-C8-C7	-2.63	114.95	120.73
2	A	401	FAD	C4B-O4B-C1B	-2.62	106.84	109.72
3	C	402	8LG	C1-C2-N5	-2.58	120.86	123.40
3	B	402	8LG	C1-C2-N5	-2.39	121.05	123.40
2	B	401	FAD	O3P-PA-O5B	-2.39	96.60	102.94
2	D	401	FAD	C4B-O4B-C1B	-2.39	107.10	109.72
2	D	401	FAD	C4X-C10-N10	-2.36	119.13	120.52
2	D	401	FAD	C4X-C4-N3	-2.35	120.38	123.59
3	D	402	8LG	C1-C2-N5	-2.27	121.16	123.40
2	B	401	FAD	O3'-C3'-C4'	-2.26	103.06	108.75
2	C	401	FAD	C1B-N9A-C4A	-2.21	123.61	126.94
2	A	401	FAD	C4X-C4-N3	-2.16	120.63	123.59
2	A	401	FAD	C1B-N9A-C4A	-2.14	123.71	126.94
2	D	401	FAD	O3'-C3'-C4'	-2.10	103.45	108.75
2	B	401	FAD	C7M-C7-C8	-2.09	116.14	120.73
2	D	401	FAD	O3B-C3B-C2B	-2.08	105.05	111.83
2	D	401	FAD	O2'-C2'-C1'	-2.07	104.87	109.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FAD	O3B-C3B-C4B	-2.01	105.01	111.05
2	C	401	FAD	C2B-C1B-N9A	2.06	117.43	114.29
2	B	401	FAD	C7M-C7-C6	2.11	126.01	120.28
2	A	401	FAD	C7M-C7-C8	2.11	125.37	120.73
2	B	401	FAD	O2P-P-O1P	2.23	124.63	112.53
2	A	401	FAD	C4X-N5-C5X	2.45	119.59	116.76
2	D	401	FAD	C4-C4X-N5	2.60	121.88	118.72
2	C	401	FAD	C1'-N10-C9A	5.37	124.89	118.86
2	B	401	FAD	C4-C4X-C10	5.39	123.39	119.94
2	B	401	FAD	C5X-C9A-N10	6.53	122.58	117.62
2	A	401	FAD	C1'-N10-C9A	7.95	127.78	118.86
2	D	401	FAD	C1'-N10-C9A	8.02	127.87	118.86
2	D	401	FAD	C4-N3-C2	8.64	122.72	115.25
2	A	401	FAD	C4-N3-C2	8.68	122.75	115.25
2	B	401	FAD	C4-N3-C2	11.72	125.38	115.25
2	C	401	FAD	C4-N3-C2	13.25	126.70	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	8LG	1	0
2	B	401	FAD	1	0
3	D	402	8LG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/347 (97%)	0.34	7 (2%) 67 71	35, 52, 73, 90	0
1	B	340/347 (97%)	0.36	12 (3%) 48 53	36, 53, 74, 89	0
1	C	340/347 (97%)	0.59	31 (9%) 11 12	38, 55, 77, 93	0
1	D	340/347 (97%)	0.73	33 (9%) 10 10	38, 55, 77, 94	0
All	All	1360/1388 (97%)	0.50	83 (6%) 25 27	35, 54, 76, 94	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	339	LEU	14.2
1	D	300	PRO	13.0
1	C	300	PRO	9.6
1	D	299	GLY	8.6
1	C	340	SER	8.1
1	D	301	SER	8.1
1	D	339	LEU	7.8
1	D	340	SER	7.2
1	C	298	THR	7.1
1	D	296	LEU	6.9
1	C	301	SER	6.6
1	D	302	ASN	6.3
1	D	297	ARG	6.3
1	D	298	THR	5.9
1	C	297	ARG	5.7
1	D	172	ARG	5.6
1	D	194	LEU	5.6
1	C	299	GLY	5.4
1	D	28	GLN	4.9
1	D	82	PRO	4.4
1	D	305	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	193	PRO	3.6
1	C	100	GLU	3.5
1	B	191	ARG	3.4
1	A	297	ARG	3.4
1	B	219	PRO	3.4
1	C	296	LEU	3.3
1	C	29	PRO	3.3
1	D	219	PRO	3.3
1	D	338	LYS	3.2
1	A	339	LEU	3.2
1	D	333	ILE	3.2
1	C	1	MET	3.2
1	D	23	TYR	3.1
1	C	274	ARG	3.1
1	C	191	ARG	3.0
1	D	303	THR	3.0
1	C	26	VAL	3.0
1	C	60	ASN	2.9
1	A	120	ARG	2.9
1	D	170	VAL	2.9
1	C	303	THR	2.8
1	D	224	TYR	2.7
1	C	295	GLN	2.7
1	B	120	ARG	2.7
1	C	334	LEU	2.7
1	D	307	HIS	2.7
1	D	191	ARG	2.7
1	C	172	ARG	2.6
1	D	295	GLN	2.6
1	B	32	ILE	2.6
1	B	224	TYR	2.6
1	D	294	GLU	2.5
1	D	334	LEU	2.5
1	D	175	ALA	2.5
1	A	300	PRO	2.5
1	C	126	PRO	2.5
1	C	302	ASN	2.5
1	C	219	PRO	2.4
1	D	29	PRO	2.4
1	D	120	ARG	2.4
1	C	265	ARG	2.4
1	A	340	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	51	LEU	2.3
1	A	28	GLN	2.3
1	C	99	HIS	2.3
1	B	29	PRO	2.3
1	D	329	LEU	2.2
1	B	132	TRP	2.2
1	B	57	SER	2.2
1	D	330	PHE	2.2
1	C	158	LYS	2.2
1	C	221	ARG	2.2
1	D	178	ILE	2.2
1	C	27	LEU	2.1
1	B	339	LEU	2.1
1	B	274	ARG	2.1
1	C	332	ARG	2.1
1	C	224	TYR	2.0
1	B	60	ASN	2.0
1	B	99	HIS	2.0
1	C	177	VAL	2.0
1	C	335	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FAD	B	401	53/53	0.95	0.15	-0.14	32,39,47,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FAD	A	401	53/53	0.97	0.16	-0.16	33,40,47,48	0
2	FAD	C	401	53/53	0.97	0.14	-0.38	35,40,47,47	0
3	8LG	A	402	8/8	0.96	0.17	-0.52	32,35,36,36	0
3	8LG	C	402	8/8	0.94	0.14	-0.82	33,35,36,37	0
2	FAD	D	401	53/53	0.97	0.14	-0.87	33,42,48,48	0
3	8LG	B	402	8/8	0.95	0.14	-0.88	33,35,36,36	0
3	8LG	D	402	8/8	0.97	0.12	-1.10	33,35,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.