



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:30 AM GMT

PDB ID : 2D0V
Title : Crystal structure of methanol dehydrogenase from *Hyphomicrobium denitrificans*
Authors : Nojiri, M.; Hira, D.; Yamaguchi, K.; Suzuki, S.
Deposited on : 2005-08-09
Resolution : 2.49 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

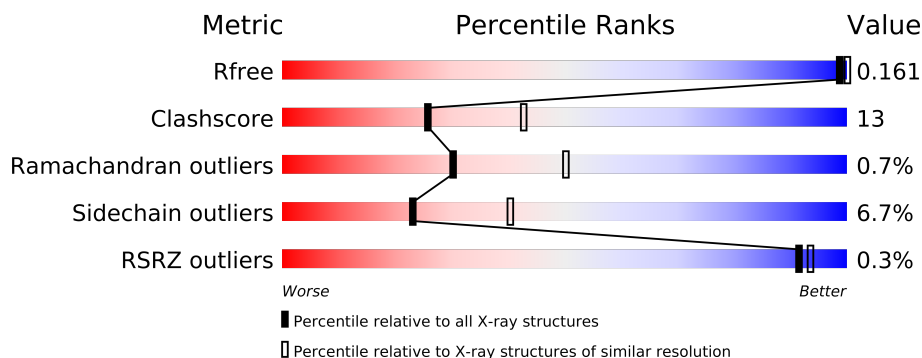
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.49 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	597	
1	D	597	
1	I	597	
2	B	72	
2	E	72	
2	J	72	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CA	A	775	-	X
4	PQQ	A	601	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	PQQ	D	601	-	X
4	PQQ	I	601	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16491 atoms, of which 0 are hydrogen and 0 are deuterium.

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 methanol dehydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4668	2962	797	889	20			
1	D	597	Total	C	N	O	S	0	0	0
			4668	2962	797	889	20			
1	I	595	Total	C	N	O	S	0	0	0
			4655	2954	794	887	20			

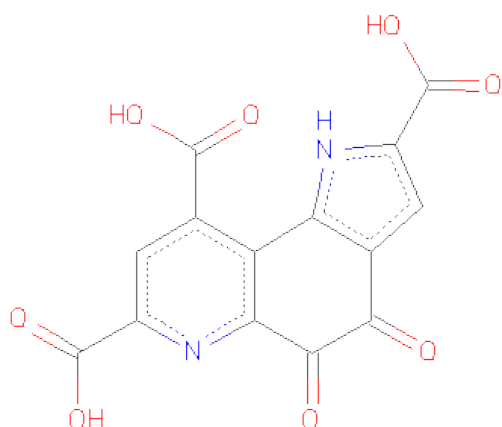
- Molecule 2 is a protein called methanol dehydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	70	Total	C	N	O	S	0	0	0
			572	359	105	106	2			
2	E	68	Total	C	N	O	S	0	0	0
			554	347	101	104	2			
2	J	70	Total	C	N	O	S	0	0	0
			572	359	105	106	2			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: C₁₄H₆N₂O₈).



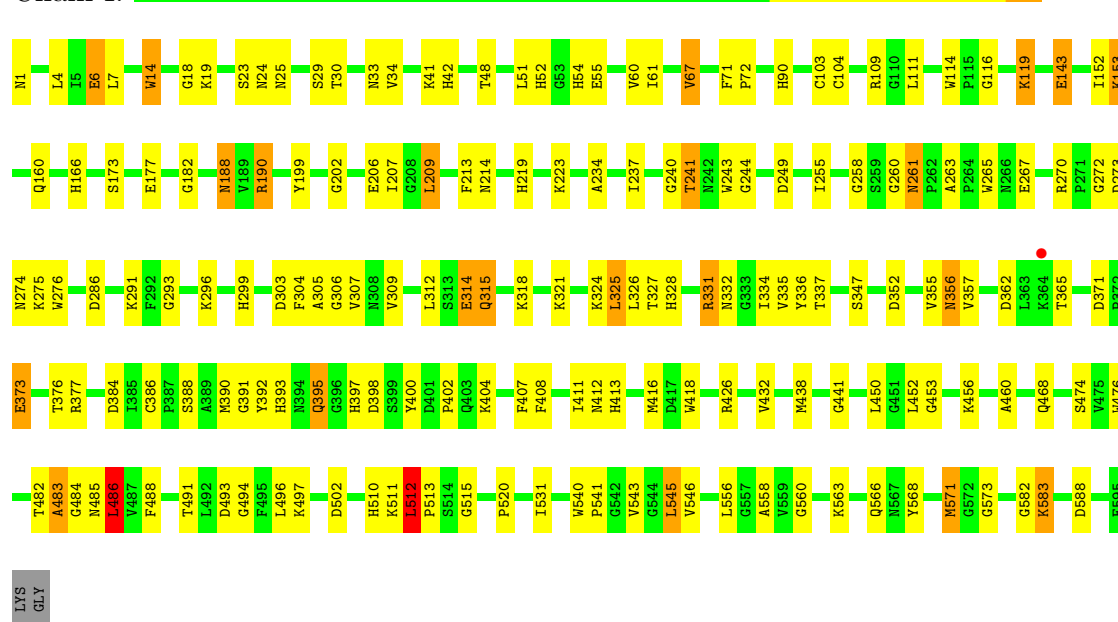
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	14	2	8		
4	D	1	Total	C	N	O	0	0
			24	14	2	8		
4	I	1	Total	C	N	O	0	0
			24	14	2	8		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	278	Total	O	0	0
			278	278		
5	B	31	Total	O	0	0
			31	31		
5	D	188	Total	O	0	0
			188	188		
5	E	31	Total	O	0	0
			31	31		
5	I	171	Total	O	0	0
			171	171		
5	J	28	Total	O	0	0
			28	28		

- Molecule 1: methanol dehydrogenase large subunit

Chain I:



- Molecule 2: methanol dehydrogenase small subunit

Chain B:



- Molecule 2: methanol dehydrogenase small subunit

Chain E:



- Molecule 2: methanol dehydrogenase small subunit

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	291.32Å 64.00Å 109.94Å 90.00° 105.74° 90.00°	Depositor
Resolution (Å)	44.60 – 2.49 44.60 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.60-2.49) 95.4 (44.60-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.149 , 0.247 0.162 , 0.161	Depositor DCC
R_{free} test set	6603 reflections (11.23%)	DCC
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 16.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 65421 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16491	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQQ, CA

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	1.30	12/4803 (0.2%)	1.17	21/6534 (0.3%)
1	D	1.28	12/4803 (0.2%)	1.16	22/6534 (0.3%)
1	I	1.26	10/4790 (0.2%)	1.14	20/6518 (0.3%)
2	B	1.36	4/589 (0.7%)	1.18	6/789 (0.8%)
2	E	1.26	1/571 (0.2%)	1.10	1/767 (0.1%)
2	J	1.33	2/589 (0.3%)	1.06	1/789 (0.1%)
All	All	1.28	41/16145 (0.3%)	1.15	71/21931 (0.3%)

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	1	1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	143	GLU	CG-CD	8.78	1.65	1.51
1	I	314	GLU	CG-CD	8.68	1.65	1.51
2	J	42	GLU	CG-CD	8.17	1.64	1.51
1	D	39	GLN	CG-CD	7.89	1.69	1.51
1	I	143	GLU	CD-OE2	6.88	1.33	1.25
1	I	143	GLU	CG-CD	6.73	1.62	1.51
1	A	276	TRP	CB-CG	6.64	1.62	1.50
1	A	489	TYR	CD1-CE1	6.58	1.49	1.39
1	A	446	ARG	CG-CD	-6.50	1.35	1.51
1	D	265	TRP	CE3-CZ3	6.37	1.49	1.38
1	A	581	ASP	CB-CG	6.26	1.65	1.51
2	B	7	LYS	CD-CE	6.24	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	LYS	CD-CE	6.22	1.66	1.51
1	A	369	VAL	CB-CG1	6.16	1.65	1.52
2	B	42	GLU	CG-CD	6.14	1.61	1.51
1	I	206	GLU	CG-CD	6.11	1.61	1.51
1	D	196	TRP	CB-CG	6.09	1.61	1.50
1	D	421	PHE	CE2-CZ	6.04	1.48	1.37
2	B	56	GLU	CG-CD	5.99	1.60	1.51
1	A	116	GLY	N-CA	5.98	1.55	1.46
1	D	418	TRP	CB-CG	5.92	1.60	1.50
1	I	314	GLU	CB-CG	5.87	1.63	1.52
1	I	143	GLU	CD-OE1	5.86	1.32	1.25
2	J	42	GLU	CD-OE1	5.82	1.32	1.25
1	D	419	GLU	CG-CD	5.79	1.60	1.51
1	A	373	GLU	CG-CD	5.68	1.60	1.51
1	I	199	TYR	CD2-CE2	5.62	1.47	1.39
2	E	42	GLU	CG-CD	5.52	1.60	1.51
1	I	543	VAL	CB-CG1	-5.41	1.41	1.52
1	I	55	GLU	CG-CD	5.37	1.60	1.51
1	D	348	ALA	CA-CB	5.35	1.63	1.52
1	A	314	GLU	CD-OE2	5.33	1.31	1.25
1	D	142	GLU	CG-CD	5.31	1.59	1.51
1	D	437	TRP	CE3-CZ3	5.25	1.47	1.38
2	B	1	TYR	CE1-CZ	5.19	1.45	1.38
1	I	568	TYR	CB-CG	-5.14	1.44	1.51
1	A	276	TRP	N-CA	-5.11	1.36	1.46
1	D	304	PHE	CD1-CE1	5.08	1.49	1.39
1	D	294	TYR	CD2-CE2	5.03	1.46	1.39
1	A	142	GLU	CG-CD	5.03	1.59	1.51
1	A	206	GLU	CB-CG	-5.02	1.42	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ARG	NE-CZ-NH2	-13.46	113.57	120.30
1	A	190	ARG	NE-CZ-NH1	11.79	126.20	120.30
1	A	446	ARG	NE-CZ-NH1	-9.81	115.39	120.30
1	D	167	ASP	CB-CG-OD1	9.02	126.42	118.30
1	A	275	LYS	C-N-CA	8.58	143.15	121.70
1	D	452	LEU	CA-CB-CG	8.41	134.65	115.30
1	D	79	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	D	275	LYS	C-N-CA	8.22	142.25	121.70
1	I	452	LEU	CA-CB-CG	8.22	134.20	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	324	LYS	CD-CE-NZ	7.81	129.66	111.70
1	D	79	ASP	CB-CG-OD1	7.80	125.32	118.30
1	I	588	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	401	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	D	275	LYS	CA-C-N	-7.53	100.63	117.20
1	A	415	CYS	CA-CB-SG	-7.47	100.55	114.00
1	A	275	LYS	CA-C-N	-7.21	101.33	117.20
1	I	190	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	A	276	TRP	CB-CA-C	6.82	124.04	110.40
1	I	286	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	452	LEU	CA-CB-CG	6.73	130.78	115.30
1	I	209	LEU	CB-CG-CD1	-6.63	99.73	111.00
1	I	571	MET	CG-SD-CE	6.62	110.79	100.20
1	A	181	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	286	ASP	CB-CG-OD1	6.52	124.17	118.30
1	D	197	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	D	545	LEU	CA-CB-CG	6.44	130.12	115.30
1	D	65	MET	CG-SD-CE	6.42	110.48	100.20
1	I	275	LYS	CA-C-N	-6.37	103.19	117.20
2	B	7	LYS	CD-CE-NZ	6.26	126.10	111.70
2	B	50	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	446	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	D	551	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	99	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	181	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	D	398	ASP	CB-CG-OD1	5.95	123.65	118.30
1	I	273	ASP	CB-CG-OD1	5.94	123.64	118.30
1	I	486	LEU	CA-CB-CG	5.88	128.82	115.30
1	D	255	ILE	CB-CA-C	-5.77	100.07	111.60
2	B	50	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	I	14	TRP	N-CA-C	-5.75	95.46	111.00
1	I	286	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	417	ASP	CB-CG-OD1	-5.74	113.13	118.30
1	A	275	LYS	O-C-N	5.72	131.85	122.70
1	D	437	TRP	N-CA-C	-5.70	95.61	111.00
2	B	2	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	587	ASP	CB-CG-OD1	-5.62	113.24	118.30
2	J	54	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	B	29	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	I	588	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	D	283	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	D	78	LEU	CA-CB-CG	5.47	127.89	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	409	MET	CG-SD-CE	5.47	108.95	100.20
2	E	67	ASP	N-CA-C	5.44	125.68	111.00
1	I	512	LEU	CA-CB-CG	5.43	127.80	115.30
1	A	117	ASP	CB-CG-OD1	5.37	123.14	118.30
1	I	249	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	351	LEU	CB-CG-CD1	-5.35	101.91	111.00
1	I	67	VAL	CB-CA-C	5.33	121.52	111.40
1	I	275	LYS	C-N-CA	5.32	135.00	121.70
1	D	349	ASP	CB-CG-OD1	-5.32	113.51	118.30
2	B	54	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	I	190	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	D	331	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	119	LYS	CD-CE-NZ	5.20	123.66	111.70
1	D	417	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	A	588	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	I	276	TRP	CB-CA-C	5.13	120.67	110.40
1	I	450	LEU	CA-CB-CG	5.07	126.97	115.30
1	D	551	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	D	275	LYS	O-C-N	5.04	130.76	122.70
1	A	512	LEU	CA-CB-CG	5.01	126.81	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	276	TRP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	ARG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4668	0	4426	112	0
1	D	4668	0	4426	107	0
1	I	4655	0	4410	140	0
2	B	572	0	553	19	0
2	E	554	0	527	23	0
2	J	572	0	553	24	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
4	A	24	0	3	5	0
4	D	24	0	3	5	0
4	I	24	0	3	4	0
5	A	278	0	0	15	0
5	B	31	0	0	2	0
5	D	188	0	0	10	0
5	E	31	0	0	3	0
5	I	171	0	0	13	0
5	J	28	0	0	1	0
All	All	16491	0	14904	413	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (413) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:447:GLN:HG3	5:A:903:HOH:O	1.63	0.97
1:I:314:GLU:HG2	5:I:942:HOH:O	1.74	0.87
1:D:211:ASP:HB3	5:D:793:HOH:O	1.74	0.86
1:I:540:TRP:CZ3	4:I:601:PQQ:O4	2.32	0.83
1:A:51:LEU:O	1:A:52:HIS:HB2	1.78	0.83
2:J:69:LYS:C	2:J:70:LYS:HD3	1.99	0.82
1:A:447:GLN:CG	5:A:903:HOH:O	2.25	0.82
1:A:143:GLU:HG3	5:A:816:HOH:O	1.79	0.81
1:D:510:HIS:HE1	1:I:42:HIS:ND1	1.79	0.80
5:A:790:HOH:O	2:B:32:HIS:HD2	1.64	0.80
1:I:540:TRP:CE3	4:I:601:PQQ:O4	2.35	0.79
1:A:356:ASN:HD21	1:A:386:CYS:H	1.29	0.79
1:D:484:GLY:O	1:D:485:ASN:HB2	1.82	0.79
5:A:847:HOH:O	2:B:32:HIS:HE1	1.67	0.77
1:D:540:TRP:CZ3	4:D:601:PQQ:O4	2.37	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:21:GLU:HB2	5:J:118:HOH:O	1.85	0.77
1:A:52:HIS:O	1:A:54:HIS:HD2	1.67	0.76
1:I:583:LYS:NZ	1:I:583:LYS:HB2	2.01	0.76
5:D:797:HOH:O	2:E:32:HIS:HD2	1.68	0.76
1:I:314:GLU:CG	5:I:942:HOH:O	2.33	0.76
1:A:191:THR:OG1	1:A:193:GLU:HB2	1.86	0.75
1:D:109:ARG:HE	1:D:395:GLN:HE21	1.33	0.75
1:I:314:GLU:HB3	5:I:942:HOH:O	1.86	0.74
1:I:482:THR:C	1:I:484:GLY:H	1.89	0.74
1:I:296:LYS:HZ3	1:I:328:HIS:HE1	1.36	0.74
1:A:134:VAL:HG22	1:A:146:LYS:HG3	1.69	0.73
1:D:532:ALA:HB1	1:D:575:LEU:HD11	1.70	0.73
2:E:36:GLU:O	2:E:39:LYS:HG3	1.88	0.73
1:I:109:ARG:HE	1:I:395:GLN:HE21	1.37	0.73
1:D:584:ASN:HB2	1:D:585:PRO:HD2	1.71	0.72
1:I:296:LYS:NZ	1:I:328:HIS:HE1	1.88	0.72
1:A:33:ASN:HA	1:A:486:LEU:HD22	1.72	0.71
1:I:261:ASN:H	1:I:305:ALA:HA	1.54	0.71
1:A:595:GLU:O	1:A:597:GLY:N	2.22	0.70
1:D:540:TRP:CE3	4:D:601:PQQ:O4	2.44	0.70
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.56	0.70
1:I:390:MET:HE3	1:I:558:ALA:HB2	1.73	0.70
1:I:34:VAL:HG22	1:I:486:LEU:HD13	1.72	0.70
1:I:260:GLY:HA2	1:I:306:GLY:H	1.56	0.69
1:D:214:ASN:HD21	1:D:293:GLY:H	1.39	0.69
1:A:540:TRP:CE3	4:A:601:PQQ:O4	2.45	0.69
1:I:240:GLY:HA2	1:I:260:GLY:O	1.93	0.68
1:D:219:HIS:HE1	5:D:795:HOH:O	1.75	0.68
2:J:20:PRO:HB2	2:J:22:LYS:O	1.94	0.68
2:E:11:ASN:HD22	2:E:11:ASN:C	1.98	0.67
1:I:30:THR:HG22	1:I:483:ALA:O	1.93	0.67
1:I:371:ASP:OD2	1:I:373:GLU:HB2	1.95	0.67
1:I:152:ILE:HG23	5:I:826:HOH:O	1.94	0.67
2:J:69:LYS:C	2:J:70:LYS:CD	2.63	0.67
1:A:18:GLY:HA2	1:A:25:ASN:HD21	1.60	0.66
1:A:243:TRP:CZ2	4:A:601:PQQ:C6A	2.78	0.66
1:A:356:ASN:ND2	1:A:386:CYS:H	1.93	0.66
1:I:314:GLU:CB	5:I:942:HOH:O	2.43	0.66
2:B:60:LYS:NZ	2:B:60:LYS:HB2	2.11	0.66
1:D:595:GLU:O	1:D:596:LYS:HB2	1.95	0.65
1:A:219:HIS:H	1:A:219:HIS:CD2	2.14	0.65
1:A:426:ARG:HB3	1:A:429:GLN:HG3	1.78	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:510:HIS:CE1	1:I:42:HIS:ND1	2.64	0.65
1:I:356:ASN:C	1:I:356:ASN:HD22	2.00	0.65
1:A:438:MET:HB2	1:A:561:ALA:HB2	1.80	0.64
1:A:595:GLU:C	1:A:597:GLY:H	2.01	0.64
2:B:33:ASP:OD2	2:B:35:LYS:HG2	1.96	0.64
1:D:397:HIS:HD2	1:D:398:ASP:O	1.80	0.64
1:A:309:VAL:O	1:A:328:HIS:HD2	1.80	0.64
1:D:590:ASN:O	1:D:596:LYS:HG2	1.98	0.64
1:I:267:GLU:OE2	1:I:299:HIS:HE1	1.81	0.63
2:B:35:LYS:HB3	2:B:35:LYS:NZ	2.14	0.63
1:I:237:ILE:HG13	1:I:237:ILE:O	1.97	0.63
1:D:41:LYS:HB2	1:D:582:GLY:N	2.14	0.63
1:D:243:TRP:CZ2	4:D:601:PQQ:C6A	2.83	0.62
1:I:52:HIS:O	1:I:54:HIS:HD2	1.82	0.62
1:D:229:THR:O	1:D:272:GLY:HA3	1.99	0.62
1:A:404:LYS:NZ	1:A:502:ASP:OD1	2.33	0.62
1:A:512:LEU:HB3	1:A:513:PRO:HD2	1.81	0.62
1:A:323:ARG:HH11	1:A:323:ARG:CG	2.12	0.62
1:I:188:ASN:HB2	5:I:925:HOH:O	1.98	0.61
1:A:143:GLU:CG	5:A:816:HOH:O	2.45	0.61
1:I:177:GLU:HB2	5:I:926:HOH:O	2.00	0.61
1:I:14:TRP:CH2	1:I:19:LYS:HB2	2.36	0.61
2:J:70:LYS:HD3	2:J:70:LYS:N	2.15	0.61
1:A:14:TRP:CZ2	1:A:19:LYS:HB2	2.36	0.60
1:A:238:GLY:O	1:A:262:PRO:HA	2.01	0.60
1:A:44:TRP:CZ2	1:A:577:VAL:HG21	2.36	0.60
1:D:270:ARG:HH21	1:D:274:ASN:ND2	1.99	0.60
1:A:52:HIS:O	1:A:54:HIS:CD2	2.54	0.60
1:D:326:LEU:O	1:D:337:THR:HG23	2.02	0.59
1:A:14:TRP:CE3	1:A:19:LYS:HG3	2.37	0.59
2:J:23:ILE:CD1	2:J:30:PRO:HD3	2.32	0.59
1:I:14:TRP:CZ2	1:I:19:LYS:HB2	2.37	0.59
1:D:215:SER:HA	5:D:890:HOH:O	2.03	0.59
1:D:194:GLN:NE2	5:D:881:HOH:O	2.32	0.59
1:I:391:GLY:O	1:I:412:ASN:HB2	2.02	0.59
1:I:393:HIS:NE2	1:I:398:ASP:OD2	2.30	0.59
1:A:51:LEU:O	1:A:52:HIS:CB	2.50	0.58
1:A:496:LEU:HD13	1:A:508:TRP:HZ3	1.68	0.58
1:A:19:LYS:HE3	1:A:26:TYR:O	2.03	0.58
1:I:335:VAL:O	1:I:335:VAL:HG13	2.03	0.58
1:I:356:ASN:ND2	1:I:386:CYS:H	2.00	0.58
1:I:356:ASN:HD21	1:I:386:CYS:H	1.51	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:236:LYS:NZ	2:B:38:ASN:HD21	2.01	0.58
1:D:41:LYS:HG2	1:D:581:ASP:HA	1.86	0.57
2:E:57:HIS:HE1	2:E:63:LYS:NZ	2.03	0.57
1:D:42:HIS:ND1	1:I:510:HIS:HE1	2.01	0.57
1:A:18:GLY:HA2	1:A:25:ASN:ND2	2.19	0.57
1:A:219:HIS:H	1:A:219:HIS:HD2	1.53	0.57
1:D:170:ILE:HD13	1:D:186:ALA:HB2	1.87	0.57
1:D:205:ALA:HA	5:D:913:HOH:O	2.04	0.57
1:I:352:ASP:O	1:I:355:VAL:HG23	2.05	0.56
1:I:583:LYS:HZ2	1:I:583:LYS:HB2	1.68	0.56
1:I:482:THR:C	1:I:484:GLY:N	2.56	0.56
1:A:92:PRO:HA	5:A:984:HOH:O	2.04	0.56
1:D:457:ALA:O	1:D:465:TYR:HA	2.06	0.56
1:A:314:GLU:HG2	1:A:322:LYS:HD2	1.86	0.56
2:J:1:TYR:CD1	2:J:14:GLU:HG2	2.41	0.56
1:D:31:GLN:NE2	1:D:527:GLY:O	2.30	0.56
1:D:584:ASN:O	1:D:587:ASP:HB2	2.05	0.56
2:J:16:LYS:O	2:J:19:PHE:HB2	2.05	0.56
1:D:296:LYS:HZ1	1:D:306:GLY:HA3	1.69	0.56
1:I:274:ASN:ND2	1:I:299:HIS:HA	2.21	0.55
1:I:453:GLY:HA3	1:I:474:SER:HA	1.87	0.55
1:I:173:SER:O	1:I:241:THR:HB	2.06	0.55
1:I:219:HIS:H	1:I:219:HIS:CD2	2.23	0.55
1:A:540:TRP:CZ3	4:A:601:PQQ:O4	2.59	0.55
1:I:296:LYS:HZ3	1:I:328:HIS:CE1	2.22	0.55
1:I:261:ASN:OD1	1:I:303:ASP:OD2	2.25	0.55
1:D:128:GLN:NE2	1:D:134:VAL:HG21	2.22	0.55
1:D:356:ASN:HD21	1:D:386:CYS:H	1.54	0.55
1:I:258:GLY:HA3	1:I:306:GLY:O	2.06	0.55
1:D:202:GLY:O	1:D:226:GLY:HA3	2.07	0.55
1:I:51:LEU:O	1:I:52:HIS:HB2	2.06	0.54
1:A:270:ARG:HH21	1:A:274:ASN:ND2	2.04	0.54
1:A:317:ASP:HA	1:A:461:ILE:HD12	1.89	0.54
1:A:546:VAL:HG22	1:A:571:MET:SD	2.48	0.54
1:I:400:TYR:CE2	1:I:402:PRO:HA	2.42	0.54
1:D:207:ILE:HD13	1:D:276:TRP:HD1	1.72	0.54
2:E:23:ILE:HD12	2:E:30:PRO:HD3	1.89	0.54
1:I:362:ASP:OD1	1:I:365:THR:N	2.39	0.54
1:D:420:PRO:HA	1:D:434:ALA:HA	1.90	0.54
1:A:173:SER:HB3	1:A:183:HIS:CE1	2.43	0.54
1:I:18:GLY:HA2	1:I:25:ASN:ND2	2.23	0.53
1:A:109:ARG:HE	1:A:395:GLN:HE21	1.55	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:60:LYS:HZ2	2:B:60:LYS:HB2	1.73	0.53
2:E:15:PRO:HB3	2:E:20:PRO:O	2.09	0.53
1:I:24:ASN:O	1:I:25:ASN:C	2.47	0.53
1:A:89:GLN:NE2	5:A:936:HOH:O	2.42	0.53
1:A:380:HIS:HE1	5:A:814:HOH:O	1.92	0.52
1:D:583:LYS:HA	1:D:587:ASP:OD1	2.10	0.52
2:B:35:LYS:HZ3	2:B:35:LYS:HB3	1.72	0.52
1:A:580:LEU:HB2	5:A:797:HOH:O	2.08	0.52
1:D:29:SER:OG	1:D:524:GLU:OE1	2.22	0.52
2:J:33:ASP:OD2	2:J:35:LYS:HB2	2.09	0.52
1:A:496:LEU:HD13	1:A:508:TRP:CZ3	2.43	0.52
1:A:175:GLY:N	4:A:601:PQQ:O7B	2.32	0.52
1:A:512:LEU:HB3	1:A:513:PRO:CD	2.40	0.52
2:J:23:ILE:HD12	2:J:30:PRO:HD3	1.92	0.52
1:A:114:TRP:HZ2	1:A:190:ARG:NH2	2.08	0.52
1:D:249:ASP:C	1:D:249:ASP:OD2	2.48	0.52
1:I:33:ASN:HA	1:I:486:LEU:HD22	1.92	0.51
2:B:35:LYS:CB	2:B:35:LYS:NZ	2.73	0.51
1:I:71:PHE:CD2	1:I:72:PRO:HA	2.45	0.51
1:I:390:MET:CE	1:I:558:ALA:HB2	2.40	0.51
1:D:45:SER:O	1:I:511:LYS:NZ	2.44	0.51
1:A:314:GLU:CG	1:A:322:LYS:HD2	2.40	0.51
1:A:382:GLY:O	1:A:417:ASP:HA	2.10	0.51
1:A:272:GLY:O	1:A:299:HIS:CD2	2.64	0.51
1:D:238:GLY:O	1:D:262:PRO:HA	2.10	0.51
1:D:488:PHE:CE2	1:D:498:ALA:HB2	2.46	0.51
1:I:327:THR:HA	1:I:336:TYR:O	2.11	0.50
1:I:1:ASN:N	1:I:166:HIS:H	2.09	0.50
1:I:202:GLY:O	1:I:207:ILE:HD12	2.11	0.50
1:A:230:TRP:CE2	1:A:274:ASN:HA	2.46	0.50
1:D:337:THR:C	1:D:338:LEU:HD12	2.31	0.50
1:I:214:ASN:HD21	1:I:293:GLY:H	1.60	0.50
1:A:194:GLN:NE2	5:A:836:HOH:O	2.38	0.50
1:A:272:GLY:O	1:A:299:HIS:HD2	1.94	0.50
1:I:397:HIS:HD2	1:I:398:ASP:O	1.94	0.50
1:I:173:SER:HB2	1:I:241:THR:HG22	1.94	0.50
1:I:411:ILE:CG2	1:I:412:ASN:N	2.75	0.49
1:D:408:PHE:CZ	1:D:501:SER:HB2	2.47	0.49
1:D:270:ARG:HH21	1:D:274:ASN:HD21	1.59	0.49
1:D:244:GLY:HA3	1:D:307:VAL:O	2.12	0.49
1:A:418:TRP:CD1	1:A:418:TRP:C	2.84	0.49
2:J:68:VAL:O	2:J:68:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:546:VAL:HG22	1:I:571:MET:SD	2.53	0.49
1:I:60:VAL:O	1:I:61:ILE:HD13	2.12	0.49
1:A:305:ALA:O	1:A:331:ARG:HG3	2.11	0.49
1:D:291:LYS:HD3	5:D:906:HOH:O	2.11	0.49
1:A:33:ASN:CA	1:A:486:LEU:HD22	2.40	0.49
1:I:90:HIS:HE2	1:I:143:GLU:CD	2.16	0.49
1:A:120:THR:HG22	1:A:121:PRO:HD2	1.94	0.49
1:A:296:LYS:NZ	1:A:328:HIS:HE1	2.11	0.49
1:D:274:ASN:HD22	1:D:299:HIS:HA	1.77	0.49
2:E:54:ARG:HB3	2:E:64:TRP:CZ2	2.47	0.49
2:J:69:LYS:O	2:J:70:LYS:HD2	2.12	0.49
2:E:29:ASP:OD2	2:E:31:LYS:N	2.38	0.49
1:I:265:TRP:CD2	1:I:432:VAL:HG13	2.48	0.49
1:I:48:THR:OG1	1:I:54:HIS:HE1	1.96	0.48
1:A:278:MET:HE1	1:A:304:PHE:C	2.33	0.48
1:I:512:LEU:HB3	1:I:513:PRO:CD	2.42	0.48
1:D:51:LEU:O	1:D:52:HIS:HB2	2.13	0.48
2:J:1:TYR:HD1	2:J:14:GLU:HG2	1.77	0.48
1:D:356:ASN:ND2	1:D:386:CYS:H	2.11	0.48
2:E:57:HIS:CE1	2:E:61:THR:HG21	2.48	0.48
1:D:114:TRP:CD2	1:D:189:VAL:HG21	2.48	0.48
2:E:56:GLU:HG2	5:E:638:HOH:O	2.13	0.48
1:I:303:ASP:CG	1:I:303:ASP:O	2.52	0.48
1:A:214:ASN:HD21	1:A:293:GLY:H	1.61	0.48
1:I:25:ASN:OD1	1:I:397:HIS:CD2	2.66	0.48
1:D:55:GLU:OE1	4:D:601:PQQ:O2A	2.31	0.48
2:E:63:LYS:HG3	2:E:63:LYS:O	2.14	0.48
1:I:315:GLN:HG3	1:I:325:LEU:CD1	2.44	0.48
1:D:52:HIS:O	1:D:54:HIS:HD2	1.97	0.47
2:E:30:PRO:O	2:E:31:LYS:C	2.52	0.47
1:A:185:THR:HG22	1:A:186:ALA:N	2.29	0.47
1:I:545:LEU:C	1:I:545:LEU:HD12	2.34	0.47
1:I:243:TRP:CZ2	4:I:601:PQQ:C6A	2.97	0.47
1:I:296:LYS:HZ1	1:I:306:GLY:HA3	1.78	0.47
1:I:305:ALA:O	1:I:331:ARG:HG3	2.14	0.47
1:I:272:GLY:HA2	2:J:13:TRP:CB	2.44	0.47
2:E:57:HIS:HE1	2:E:63:LYS:HZ1	1.61	0.47
1:I:510:HIS:HD2	5:I:825:HOH:O	1.97	0.47
1:A:117:ASP:OD1	1:A:190:ARG:CZ	2.62	0.47
1:D:304:PHE:O	1:D:305:ALA:C	2.53	0.47
1:D:1:ASN:N	1:D:166:HIS:H	2.13	0.47
1:A:440:PRO:HA	1:A:452:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:584:ASN:OD1	1:D:586:TYR:HB2	2.15	0.47
1:A:146:LYS:HE3	5:A:820:HOH:O	2.14	0.47
1:D:272:GLY:O	1:D:299:HIS:CD2	2.67	0.47
1:D:53:GLY:CA	1:D:517:ILE:HD11	2.44	0.47
1:I:219:HIS:HE1	5:I:816:HOH:O	1.97	0.47
2:B:60:LYS:CB	2:B:60:LYS:NZ	2.77	0.47
1:D:53:GLY:HA3	1:D:517:ILE:HD11	1.97	0.47
1:D:255:ILE:HD13	1:D:255:ILE:HG21	1.55	0.47
2:B:16:LYS:O	2:B:17:PRO:C	2.52	0.46
1:A:114:TRP:CZ2	1:A:190:ARG:NH2	2.83	0.46
1:I:408:PHE:HA	1:I:456:LYS:O	2.15	0.46
1:I:491:THR:OG1	1:I:493:ASP:OD2	2.27	0.46
1:A:356:ASN:HD22	1:A:356:ASN:C	2.19	0.46
1:D:243:TRP:CE2	1:D:307:VAL:HG21	2.50	0.46
1:I:407:PHE:CE2	1:I:460:ALA:HB2	2.50	0.46
1:A:267:GLU:HB2	1:A:299:HIS:CE1	2.50	0.46
1:I:545:LEU:O	1:I:545:LEU:HD12	2.16	0.46
1:D:157:THR:O	1:D:174:SER:HB2	2.15	0.46
2:B:31:LYS:HE3	5:B:84:HOH:O	2.14	0.46
1:I:566:GLN:H	1:I:566:GLN:HG2	1.46	0.46
1:D:185:THR:OG1	1:D:197:ARG:HD2	2.15	0.46
2:E:29:ASP:HA	2:E:30:PRO:HD2	1.65	0.46
2:E:56:GLU:HA	5:E:638:HOH:O	2.15	0.46
1:I:234:ALA:HB2	5:I:868:HOH:O	2.14	0.46
1:D:25:ASN:O	1:D:480:LEU:HD12	2.16	0.46
1:I:583:LYS:HZ3	1:I:583:LYS:HB2	1.79	0.46
1:A:219:HIS:N	1:A:219:HIS:CD2	2.81	0.46
1:D:400:TYR:O	1:D:402:PRO:HD3	2.16	0.46
1:I:476:TRP:CD2	1:I:541:PRO:HG2	2.51	0.45
1:D:42:HIS:ND1	1:I:510:HIS:CE1	2.84	0.45
1:A:36:ASN:ND2	1:A:580:LEU:HD11	2.31	0.45
1:A:326:LEU:O	1:A:337:THR:HA	2.16	0.45
1:I:390:MET:HG3	1:I:438:MET:SD	2.57	0.45
1:I:356:ASN:HD22	1:I:357:VAL:N	2.14	0.45
1:I:272:GLY:O	1:I:299:HIS:HB2	2.16	0.45
1:D:267:GLU:OE2	1:D:299:HIS:HE1	1.99	0.45
1:A:267:GLU:OE2	1:A:299:HIS:HE1	1.99	0.45
1:A:185:THR:HG23	1:A:197:ARG:HB2	1.98	0.45
1:I:318:LYS:HG2	5:I:821:HOH:O	2.15	0.45
1:I:560:GLY:O	1:I:563:LYS:HG2	2.16	0.45
2:B:12:CYS:O	2:B:13:TRP:C	2.55	0.45
1:I:103:CYS:SG	1:I:104:CYS:N	2.89	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:304:PHE:CD2	1:I:332:ASN:HB3	2.52	0.45
1:A:540:TRP:HB2	4:A:601:PQQ:C3	2.47	0.45
2:E:11:ASN:ND2	2:E:11:ASN:C	2.68	0.45
1:D:361:VAL:HA	1:D:368:PRO:HA	1.98	0.45
1:A:368:PRO:HG2	5:A:821:HOH:O	2.16	0.45
2:J:36:GLU:OE1	2:J:39:LYS:NZ	2.35	0.45
1:A:125:ILE:HG22	1:A:162:PRO:HG2	1.98	0.45
1:D:160:GLN:OE1	1:D:172:GLY:N	2.49	0.45
1:A:283:ARG:NH1	1:A:290:MET:HE2	2.32	0.45
1:A:438:MET:HG3	1:A:557:GLY:O	2.16	0.44
1:A:257:TYR:HA	1:A:310:ILE:HD12	1.99	0.44
1:I:14:TRP:CZ3	1:I:19:LYS:HD2	2.52	0.44
1:I:209:LEU:HD22	1:I:213:PHE:CD1	2.53	0.44
1:I:18:GLY:HA2	1:I:25:ASN:HD21	1.80	0.44
1:A:236:LYS:HZ3	2:B:38:ASN:HD21	1.65	0.44
1:I:119:LYS:HE3	1:I:119:LYS:HB2	1.78	0.44
2:J:67:ASP:OD1	2:J:67:ASP:C	2.56	0.44
1:D:33:ASN:OD1	1:D:35:ASP:HB2	2.17	0.44
1:D:458:TYR:CE2	1:D:460:ALA:HA	2.53	0.44
1:A:329:PRO:HA	1:A:335:VAL:HA	1.99	0.44
1:I:188:ASN:ND2	1:I:190:ARG:H	2.16	0.44
1:A:532:ALA:HB1	1:A:575:LEU:HD11	1.99	0.44
1:D:271:PRO:HB2	2:E:13:TRP:CH2	2.52	0.44
1:I:404:LYS:HD3	1:I:502:ASP:OD1	2.17	0.44
1:A:114:TRP:CZ3	1:A:116:GLY:HA2	2.53	0.44
1:A:537:VAL:HG22	1:A:538:GLY:H	1.83	0.44
1:A:595:GLU:C	1:A:597:GLY:N	2.66	0.44
1:D:197:ARG:NH2	2:E:44:ARG:HD3	2.33	0.44
1:D:428:GLY:N	5:D:783:HOH:O	2.51	0.44
1:I:267:GLU:OE1	1:I:377:ARG:HA	2.18	0.44
1:D:401:ASP:O	1:D:405:GLN:N	2.51	0.44
1:D:34:VAL:HG11	1:D:500:ASN:ND2	2.33	0.44
1:D:414:ILE:HD11	1:D:474:SER:OG	2.18	0.44
1:I:41:LYS:HB2	1:I:582:GLY:N	2.32	0.44
1:D:383:THR:HG22	1:D:417:ASP:CG	2.38	0.44
1:I:540:TRP:HB2	4:I:601:PQQ:C3	2.48	0.43
1:D:421:PHE:CE1	1:D:433:GLY:HA2	2.53	0.43
1:D:522:THR:HA	1:D:530:TYR:O	2.17	0.43
1:I:34:VAL:HG21	1:I:485:ASN:HB2	2.00	0.43
1:D:298:PRO:O	1:D:299:HIS:C	2.56	0.43
1:D:387:PRO:HB3	1:D:392:TYR:CD2	2.53	0.43
1:I:412:ASN:OD1	1:I:474:SER:HB3	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:520:PRO:HD3	5:I:785:HOH:O	2.17	0.43
1:D:411:ILE:CG2	1:D:412:ASN:N	2.81	0.43
1:D:256:TYR:HA	1:D:281:THR:O	2.18	0.43
2:J:30:PRO:HG2	2:J:31:LYS:H	1.83	0.43
1:D:151:ASP:OD2	1:D:153:LYS:HB2	2.18	0.43
1:I:388:SER:HA	1:I:416:MET:CE	2.48	0.43
1:I:540:TRP:N	1:I:541:PRO:CD	2.81	0.43
1:I:296:LYS:HZ1	1:I:306:GLY:CA	2.32	0.43
2:J:68:VAL:CG1	2:J:68:VAL:O	2.66	0.43
1:A:414:ILE:HG12	1:A:452:LEU:HD12	2.01	0.43
1:I:476:TRP:CZ2	1:I:541:PRO:HD3	2.54	0.43
1:D:243:TRP:CH2	4:D:601:PQQ:C9A	3.01	0.43
1:A:44:TRP:CE2	1:A:577:VAL:HG21	2.53	0.43
1:D:296:LYS:NZ	1:D:328:HIS:HE1	2.17	0.43
1:I:400:TYR:HB2	1:I:407:PHE:CD1	2.54	0.43
1:D:37:VAL:HG11	1:D:507:VAL:HG21	2.00	0.43
1:A:233:ASP:HB3	1:A:236:LYS:HD2	2.01	0.43
1:A:537:VAL:HG22	1:A:538:GLY:N	2.34	0.43
1:A:229:THR:HB	1:A:273:ASP:H	1.84	0.43
2:E:40:GLN:HG3	5:E:267:HOH:O	2.19	0.43
2:B:32:HIS:HB3	2:B:37:LEU:CD1	2.48	0.43
1:A:40:LEU:O	1:A:41:LYS:HD3	2.19	0.43
2:B:69:LYS:O	2:B:70:LYS:HG3	2.19	0.43
1:D:371:ASP:OD2	1:D:373:GLU:HB2	2.18	0.43
1:I:315:GLN:HG3	1:I:325:LEU:HD12	2.01	0.43
1:I:153:LYS:HD3	1:I:153:LYS:HA	1.87	0.43
1:D:540:TRP:O	1:D:543:VAL:HG22	2.19	0.43
1:I:182:GLY:HA2	1:I:241:THR:HA	2.01	0.43
1:A:337:THR:C	1:A:338:LEU:HD12	2.40	0.43
2:J:23:ILE:HD12	2:J:28:TYR:O	2.18	0.42
1:A:270:ARG:NH2	1:A:274:ASN:ND2	2.66	0.42
1:A:466:LYS:NZ	1:A:502:ASP:O	2.51	0.42
2:J:29:ASP:HA	2:J:30:PRO:HD2	1.79	0.42
1:I:488:PHE:HA	1:I:497:LYS:O	2.19	0.42
2:J:69:LYS:O	2:J:70:LYS:CD	2.67	0.42
1:I:304:PHE:O	1:I:305:ALA:C	2.57	0.42
1:I:456:LYS:HE2	1:I:468:GLN:HB2	2.00	0.42
1:A:244:GLY:HA3	1:A:307:VAL:O	2.19	0.42
1:D:248:TYR:CD1	1:D:254:LEU:O	2.73	0.42
1:D:99:ARG:HE	1:D:99:ARG:HB2	1.48	0.42
1:I:114:TRP:CZ3	1:I:116:GLY:HA2	2.54	0.42
1:A:275:LYS:HE3	1:A:295:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:180:VAL:O	1:A:239:GLY:HA2	2.18	0.42
1:D:7:LEU:HB3	1:D:15:VAL:HG11	2.00	0.42
2:B:32:HIS:HB3	2:B:37:LEU:HD11	2.00	0.42
1:I:392:TYR:O	1:I:411:ILE:HG23	2.20	0.42
1:I:274:ASN:HD22	1:I:299:HIS:HA	1.83	0.42
1:I:244:GLY:HA3	1:I:307:VAL:O	2.20	0.42
2:B:9:PRO:HD2	5:B:198:HOH:O	2.20	0.42
1:I:309:VAL:O	1:I:328:HIS:HD2	2.03	0.42
2:E:39:LYS:HE2	2:E:39:LYS:HB3	1.81	0.42
2:E:6:CYS:HB3	2:E:8:ALA:O	2.19	0.42
1:D:19:LYS:NZ	5:D:896:HOH:O	2.53	0.42
1:I:356:ASN:C	1:I:356:ASN:ND2	2.70	0.42
1:D:274:ASN:ND2	1:D:299:HIS:HA	2.35	0.42
1:D:114:TRP:HA	1:D:115:PRO:HD3	1.83	0.42
1:D:245:TRP:HB2	1:D:309:VAL:HA	2.01	0.41
1:D:42:HIS:CB	1:I:42:HIS:HB3	2.49	0.41
1:I:334:ILE:HB	1:I:336:TYR:CE1	2.55	0.41
2:E:54:ARG:HB3	2:E:64:TRP:CE2	2.55	0.41
1:I:376:THR:O	1:I:377:ARG:HB3	2.20	0.41
1:A:534:MET:HG2	5:A:778:HOH:O	2.20	0.41
1:I:494:GLY:HA2	1:I:515:GLY:HA2	2.03	0.41
1:I:397:HIS:CD2	1:I:398:ASP:O	2.73	0.41
1:A:462:THR:HG21	5:A:809:HOH:O	2.20	0.41
1:D:540:TRP:N	1:D:541:PRO:CD	2.84	0.41
1:D:397:HIS:CD2	1:D:397:HIS:C	2.94	0.41
1:I:326:LEU:O	1:I:337:THR:HA	2.21	0.41
1:D:283:ARG:CZ	1:D:290:MET:HE2	2.51	0.41
1:D:68:HIS:CE1	1:D:110:GLY:HA2	2.55	0.41
1:A:309:VAL:HG22	1:A:310:ILE:N	2.36	0.41
1:D:267:GLU:HG2	1:D:301:GLU:HG2	2.03	0.41
1:I:223:LYS:HZ2	1:I:223:LYS:HB3	1.86	0.41
1:A:401:ASP:HA	1:A:402:PRO:HD3	1.75	0.41
1:A:256:TYR:HA	1:A:281:THR:O	2.21	0.41
2:J:33:ASP:OD2	2:J:33:ASP:C	2.59	0.41
1:D:35:ASP:HB2	5:D:867:HOH:O	2.20	0.41
1:A:296:LYS:HZ3	1:A:328:HIS:HE1	1.69	0.41
1:A:36:ASN:O	1:A:39:GLN:HB2	2.20	0.41
1:D:3:LYS:HB2	1:D:115:PRO:HG2	2.01	0.41
1:I:223:LYS:HG3	5:I:830:HOH:O	2.21	0.41
1:A:476:TRP:CZ2	1:A:541:PRO:HD3	2.56	0.41
1:I:418:TRP:C	1:I:418:TRP:CD1	2.94	0.41
2:J:11:ASN:HD22	2:J:11:ASN:C	2.25	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:34:VAL:HG23	1:I:34:VAL:H	1.52	0.41
1:A:236:LYS:HZ2	2:B:38:ASN:HD21	1.68	0.41
1:I:1:ASN:H1	1:I:166:HIS:H	1.68	0.41
1:A:280:ILE:O	1:A:293:GLY:HA2	2.21	0.41
1:D:180:VAL:O	1:D:239:GLY:HA2	2.21	0.41
1:I:6:GLU:HG3	1:I:7:LEU:N	2.35	0.41
1:I:413:HIS:CD2	1:I:441:GLY:HA3	2.56	0.40
1:A:103:CYS:SG	1:A:104:CYS:N	2.94	0.40
1:I:263:ALA:O	1:I:270:ARG:HD3	2.21	0.40
1:D:181:ARG:HD3	1:D:181:ARG:HH11	1.74	0.40
1:D:296:LYS:HE3	1:D:296:LYS:HB2	1.90	0.40
2:E:23:ILE:HD12	2:E:30:PRO:CD	2.50	0.40
1:I:411:ILE:HG22	1:I:412:ASN:N	2.36	0.40
1:I:512:LEU:HB3	1:I:513:PRO:HD2	2.04	0.40
1:I:4:LEU:HD23	1:I:4:LEU:HA	1.89	0.40
1:A:95:ASP:OD2	1:A:96:PRO:HD2	2.22	0.40
1:I:407:PHE:HE2	1:I:460:ALA:HB2	1.87	0.40
1:A:378:MET:HA	1:A:420:PRO:HG2	2.04	0.40
1:D:323:ARG:NH1	1:D:339:ASP:OD2	2.53	0.40
2:J:32:HIS:O	2:J:34:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	595/597 (100%)	561 (94%)	32 (5%)	2 (0%)	50 73
1	D	595/597 (100%)	537 (90%)	53 (9%)	5 (1%)	27 46
1	I	593/597 (99%)	546 (92%)	43 (7%)	4 (1%)	30 50
2	B	68/72 (94%)	63 (93%)	5 (7%)	0	100 100
2	E	66/72 (92%)	60 (91%)	5 (8%)	1 (2%)	15 25
2	J	68/72 (94%)	60 (88%)	6 (9%)	2 (3%)	7 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1985/2007 (99%)	1827 (92%)	144 (7%)	14 (1%)	30 50

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	266	ASN
2	E	67	ASP
1	I	261	ASN
1	I	331	ARG
1	D	587	ASP
1	D	595	GLU
1	I	483	ALA
1	A	70	SER
1	A	105	ASP
1	D	105	ASP
1	D	276	TRP
2	J	35	LYS
2	J	68	VAL
1	I	573	GLY

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	487/487 (100%)	457 (94%)	30 (6%)	26 45
1	D	487/487 (100%)	461 (95%)	26 (5%)	32 54
1	I	486/487 (100%)	457 (94%)	29 (6%)	27 47
2	B	60/62 (97%)	50 (83%)	10 (17%)	3 6
2	E	58/62 (94%)	53 (91%)	5 (9%)	15 27
2	J	60/62 (97%)	50 (83%)	10 (17%)	3 6
All	All	1638/1647 (100%)	1528 (93%)	110 (7%)	23 40

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	67	VAL
1	A	78	LEU
1	A	93	LYS
1	A	118	ASP
1	A	119	LYS
1	A	120	THR
1	A	142	GLU
1	A	223	LYS
1	A	267	GLU
1	A	312	LEU
1	A	322	LYS
1	A	323	ARG
1	A	356	ASN
1	A	357	VAL
1	A	395	GLN
1	A	418	TRP
1	A	426	ARG
1	A	438	MET
1	A	439	TYR
1	A	455	ILE
1	A	464	GLU
1	A	468	GLN
1	A	486	LEU
1	A	496	LEU
1	A	511	LYS
1	A	512	LEU
1	A	556	LEU
1	A	580	LEU
1	A	596	LYS
2	B	7	LYS
2	B	11	ASN
2	B	31	LYS
2	B	35	LYS
2	B	39	LYS
2	B	53	ASN
2	B	59	LYS
2	B	63	LYS
2	B	69	LYS
2	B	70	LYS
1	D	23	SER
1	D	34	VAL
1	D	67	VAL

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Mol	Chain	Res	Type
1	D	78	LEU
1	D	119	LYS
1	D	153	LYS
1	D	193	GLU
1	D	237	ILE
1	D	312	LEU
1	D	322	LYS
1	D	356	ASN
1	D	364	LYS
1	D	367	LEU
1	D	395	GLN
1	D	406	LEU
1	D	418	TRP
1	D	426	ARG
1	D	436	LEU
1	D	452	LEU
1	D	466	LYS
1	D	486	LEU
1	D	496	LEU
1	D	512	LEU
1	D	556	LEU
1	D	563	LYS
1	D	581	ASP
2	E	11	ASN
2	E	22	LYS
2	E	35	LYS
2	E	37	LEU
2	E	49	GLU
1	I	6	GLU
1	I	23	SER
1	I	29	SER
1	I	67	VAL
1	I	111	LEU
1	I	119	LYS
1	I	153	LYS
1	I	160	GLN
1	I	188	ASN
1	I	241	THR
1	I	255	ILE
1	I	291	LYS
1	I	312	LEU
1	I	315	GLN

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Mol	Chain	Res	Type
1	I	321	LYS
1	I	325	LEU
1	I	347	SER
1	I	356	ASN
1	I	373	GLU
1	I	384	ASP
1	I	395	GLN
1	I	426	ARG
1	I	486	LEU
1	I	496	LEU
1	I	512	LEU
1	I	531	ILE
1	I	545	LEU
1	I	556	LEU
1	I	583	LYS
2	J	11	ASN
2	J	31	LYS
2	J	35	LYS
2	J	42	GLU
2	J	53	ASN
2	J	59	LYS
2	J	60	LYS
2	J	63	LYS
2	J	68	VAL
2	J	70	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	25	ASN
1	A	54	HIS
1	A	89	GLN
1	A	194	GLN
1	A	214	ASN
1	A	217	ASN
1	A	219	HIS
1	A	253	ASN
1	A	274	ASN
1	A	299	HIS
1	A	328	HIS
1	A	356	ASN

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Mol	Chain	Res	Type
1	A	380	HIS
1	A	395	GLN
1	A	397	HIS
1	A	405	GLN
1	A	525	HIS
2	B	11	ASN
2	B	32	HIS
2	B	38	ASN
2	B	53	ASN
2	B	57	HIS
1	D	11	ASN
1	D	25	ASN
1	D	54	HIS
1	D	128	GLN
1	D	194	GLN
1	D	214	ASN
1	D	217	ASN
1	D	219	HIS
1	D	253	ASN
1	D	274	ASN
1	D	299	HIS
1	D	328	HIS
1	D	356	ASN
1	D	395	GLN
1	D	397	HIS
1	D	468	GLN
1	D	510	HIS
1	D	525	HIS
2	E	11	ASN
2	E	32	HIS
2	E	57	HIS
1	I	11	ASN
1	I	54	HIS
1	I	89	GLN
1	I	214	ASN
1	I	217	ASN
1	I	219	HIS
1	I	253	ASN
1	I	274	ASN
1	I	299	HIS
1	I	328	HIS
1	I	356	ASN

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Mol	Chain	Res	Type
1	I	395	GLN
1	I	397	HIS
1	I	510	HIS
2	J	11	ASN
2	J	53	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
4	PQQ	A	601	3	26,26,26	3.87	11 (42%)	39,40,40	3.49	21 (53%)
4	PQQ	D	601	3	26,26,26	4.08	12 (46%)	39,40,40	2.93	14 (35%)
4	PQQ	I	601	3	26,26,26	3.39	11 (42%)	39,40,40	2.78	15 (38%)

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
4	PQQ	A	601	3	-	0/10/28/28	0/0/3/3
4	PQQ	D	601	3	-	0/10/28/28	0/0/3/3
4	PQQ	I	601	3	-	0/10/28/28	0/0/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	PQQ	C9A-C6A	13.25	1.54	1.40
4	D	601	PQQ	C9A-C6A	12.72	1.53	1.40
4	I	601	PQQ	C9A-C6A	11.11	1.52	1.40
4	D	601	PQQ	C9-C9A	10.96	1.54	1.40
4	A	601	PQQ	C9-C9A	10.46	1.53	1.40
4	I	601	PQQ	C9-C9A	7.89	1.50	1.40
4	I	601	PQQ	C3A-C1A	6.23	1.50	1.40
4	D	601	PQQ	C3A-C1A	6.23	1.50	1.40
4	A	601	PQQ	C3A-C1A	6.13	1.50	1.40
4	D	601	PQQ	C6A-C5	6.06	1.56	1.49
4	D	601	PQQ	O5-C5	3.20	1.30	1.23
4	I	601	PQQ	C9A-C1A	-3.04	1.43	1.49
4	D	601	PQQ	C7-C7X	3.04	1.55	1.50
4	I	601	PQQ	C3-C3A	2.95	1.44	1.39
4	I	601	PQQ	C3A-C4	2.88	1.53	1.48
4	A	601	PQQ	C3-C3A	2.83	1.44	1.39
4	A	601	PQQ	C6A-C5	2.82	1.52	1.49
4	D	601	PQQ	C7-N6	2.76	1.38	1.34
4	I	601	PQQ	O5-C5	2.74	1.29	1.23
4	I	601	PQQ	C6A-C5	2.72	1.52	1.49
4	A	601	PQQ	C7-N6	2.68	1.38	1.34
4	D	601	PQQ	C6A-N6	2.68	1.39	1.34
4	A	601	PQQ	O5-C5	2.61	1.29	1.23
4	A	601	PQQ	C1A-N1	2.55	1.39	1.36
4	D	601	PQQ	C3A-C4	2.51	1.53	1.48
4	I	601	PQQ	O2B-C2X	-2.49	1.22	1.30
4	D	601	PQQ	C3-C3A	2.33	1.43	1.39
4	I	601	PQQ	O7B-C7X	-2.31	1.23	1.30
4	A	601	PQQ	C2-N1	2.25	1.39	1.36
4	A	601	PQQ	O7B-C7X	-2.20	1.23	1.30
4	D	601	PQQ	O2B-C2X	-2.17	1.23	1.30
4	A	601	PQQ	O2B-C2X	-2.14	1.23	1.30
4	D	601	PQQ	C9A-C1A	-2.09	1.45	1.49
4	I	601	PQQ	C3-C2	2.06	1.41	1.39

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	PQQ	C2X-C2-N1	13.33	127.14	116.85
4	D	601	PQQ	C2X-C2-N1	11.32	125.58	116.85
4	I	601	PQQ	C2X-C2-N1	9.46	124.15	116.85
4	A	601	PQQ	C9-C9A-C1A	8.19	129.95	122.52
4	D	601	PQQ	C6A-N6-C7	5.47	126.55	117.97
4	A	601	PQQ	O9A-C9X-C9	-4.86	109.61	121.82
4	D	601	PQQ	C9-C9A-C1A	4.76	126.84	122.52
4	A	601	PQQ	O2B-C2X-C2	4.68	125.00	113.39
4	I	601	PQQ	O4-C4-C5	-4.63	112.39	119.30
4	D	601	PQQ	C9A-C6A-N6	-4.46	116.71	123.37
4	A	601	PQQ	C3A-C3-C2	-4.44	104.05	109.86
4	I	601	PQQ	O9A-C9X-C9	-4.42	110.71	121.82
4	D	601	PQQ	O7B-C7X-C7	4.26	124.42	114.68
4	A	601	PQQ	C6A-N6-C7	4.22	124.60	117.97
4	D	601	PQQ	C3A-C1A-C9A	4.20	123.88	121.70
4	I	601	PQQ	O2B-C2X-C2	4.17	123.72	113.39
4	I	601	PQQ	C9-C9A-C1A	4.10	126.24	122.52
4	I	601	PQQ	O5-C5-C6A	3.94	126.34	122.24
4	A	601	PQQ	C9A-C9-C9X	3.78	127.09	121.77
4	I	601	PQQ	C3A-C4-C5	3.60	122.53	118.08
4	I	601	PQQ	C9A-C6A-N6	-3.52	118.11	123.37
4	I	601	PQQ	C9A-C9-C9X	3.48	126.67	121.77
4	A	601	PQQ	C9-C9A-C6A	-3.37	112.44	118.53
4	A	601	PQQ	C3A-C4-C5	3.35	122.22	118.08
4	D	601	PQQ	C3A-C3-C2	-3.34	105.49	109.86
4	A	601	PQQ	O7B-C7X-C7	3.24	122.08	114.68
4	D	601	PQQ	O7B-C7X-O7A	-3.18	116.13	123.35
4	D	601	PQQ	C1A-C9A-C6A	-3.15	116.94	119.78
4	I	601	PQQ	C3A-C3-C2	-3.14	105.75	109.86
4	I	601	PQQ	C6A-N6-C7	3.07	122.79	117.97
4	D	601	PQQ	C8-C7-C7X	3.02	125.10	119.55
4	I	601	PQQ	C9A-C6A-C5	2.91	123.70	121.02
4	D	601	PQQ	C5-C6A-N6	2.91	120.83	116.23
4	D	601	PQQ	O2B-C2X-C2	2.90	120.57	113.39
4	A	601	PQQ	C3A-C1A-N1	-2.79	102.12	106.96
4	A	601	PQQ	C3-C3A-C1A	2.78	110.32	106.65
4	A	601	PQQ	C9A-C6A-N6	-2.69	119.34	123.37
4	D	601	PQQ	O9A-C9X-C9	-2.69	115.06	121.82
4	A	601	PQQ	C8-C9-C9X	-2.68	109.80	117.79
4	D	601	PQQ	O9B-C9X-C9	2.53	123.03	115.47
4	I	601	PQQ	O2B-C2X-O2A	-2.48	117.72	123.35
4	A	601	PQQ	C1A-C9A-C6A	-2.41	117.61	119.78
4	A	601	PQQ	C3-C2-C2X	-2.37	121.19	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	PQQ	O4-C4-C3A	-2.36	117.46	121.58
4	A	601	PQQ	O9B-C9X-C9	2.35	122.49	115.47
4	A	601	PQQ	O7A-C7X-C7	-2.33	116.09	121.09
4	I	601	PQQ	C3-C3A-C4	2.27	134.96	132.29
4	A	601	PQQ	O2B-C2X-O2A	-2.15	118.47	123.35
4	A	601	PQQ	C9A-C6A-C5	2.15	122.99	121.02
4	I	601	PQQ	O4-C4-C3A	2.00	125.08	121.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	597/597 (100%)	-0.60	0 100 100	17, 28, 39, 55	0
1	D	597/597 (100%)	-0.40	3 (0%) 88 90	18, 32, 45, 61	0
1	I	595/597 (99%)	-0.33	1 (0%) 93 94	20, 34, 48, 57	0
2	B	70/72 (97%)	-0.35	0 100 100	26, 36, 48, 54	0
2	E	68/72 (94%)	0.06	1 (1%) 70 72	35, 49, 58, 68	0
2	J	70/72 (97%)	0.07	0 100 100	34, 47, 59, 68	0
All	All	1997/2007 (99%)	-0.40	5 (0%) 91 93	17, 32, 49, 68	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	68	VAL	4.3
1	D	307	VAL	2.3
1	D	421	PHE	2.2
1	D	305	ALA	2.2
1	I	364	LYS	2.2

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	PQQ	A	601	24/24	0.34	4.41	59,68,69,69	0
4	PQQ	D	601	24/24	0.36	4.19	69,77,78,78	0
4	PQQ	I	601	24/24	0.31	2.99	67,75,75,76	0
3	CA	A	775	1/1	0.18	2.59	55,55,55,55	1
3	CA	D	775	1/1	0.13	-0.92	49,49,49,49	1
3	CA	I	775	1/1	0.11	-1.27	49,49,49,49	1

6.5 Other polymers

There are no such residues in this entry.