WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:17 PM GMT

PDB ID	:	1OAD
Title	:	GLUCOSE ISOMERASE FROM STREPTOMYCES RUBIGINOSUS IN P21212 CRYSTAL FORM
Authors	:	Ramagopal, U.A.; Dauter, M.; Dauter, Z.
Deposited on	:	2003-01-08
Resolution	:	1.50 Å(reported)

The following versions of software and data (see references (i)) 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 1.50 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.
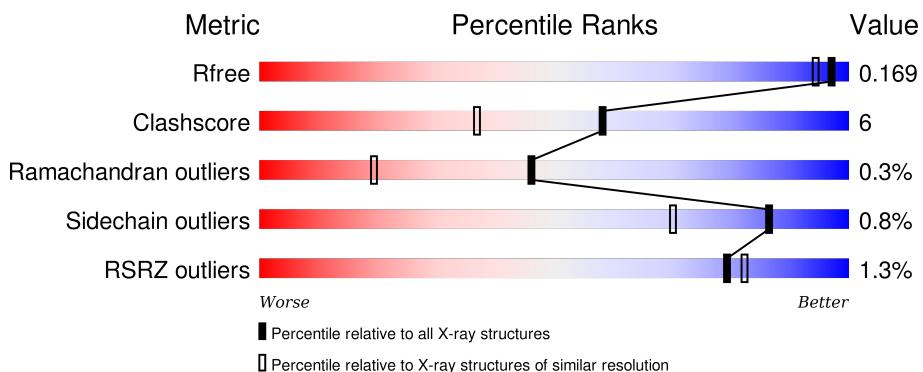
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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 <=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	388	69% 28%
1	B	388	2% 69% 29%
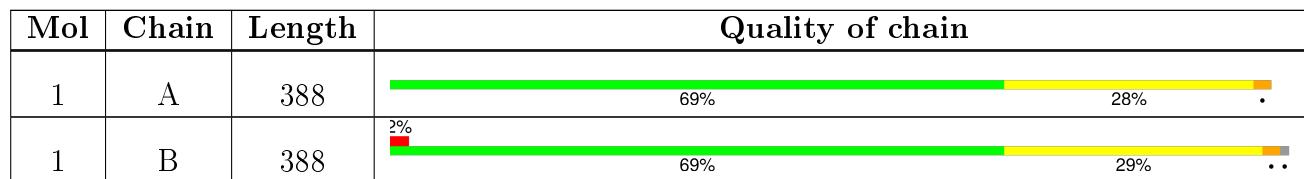
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MRD	A	394	-	-	-	X
5	MQD	A	395	-	-	-	X
5	MQD	B	395	-	-	-	X
6	TRS	A	396	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7120 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 XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total 3060	C 1922	N 552	O 577	S 9	0	5	0
1	B	386	Total 3095	C 1941	N 560	O 585	S 9	0	13	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	GLN	CONFLICT	UNP P24300
B	21	GLU	GLN	CONFLICT	UNP P24300

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).
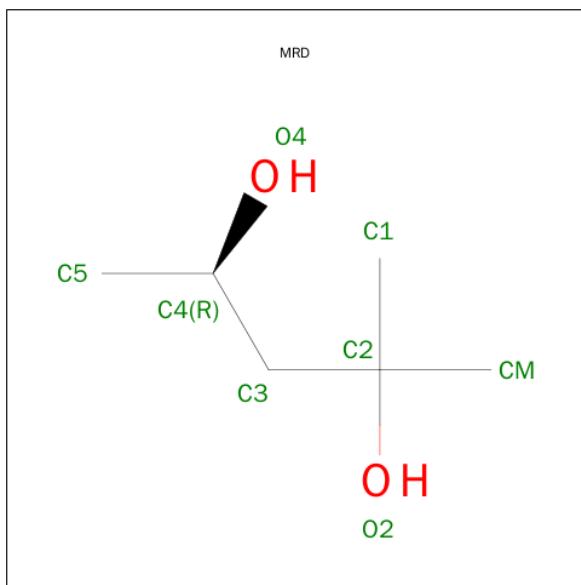
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 8	C 6	O 2	0	0
4	B	1	Total 8	C 6	O 2	0	0

- Molecule 5 is 2-METHYLPENTANE-1,2,4-TRIOL (three-letter code: MQD) (formula: $C_6H_{14}O_3$).
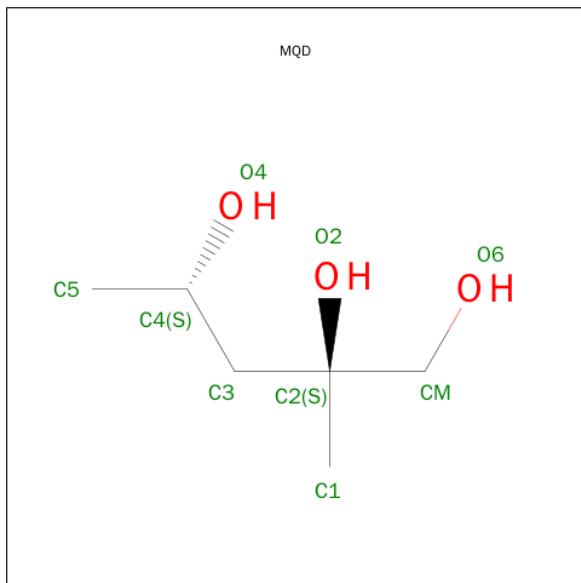
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 9	C 6	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 9	C 6	O 3	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).
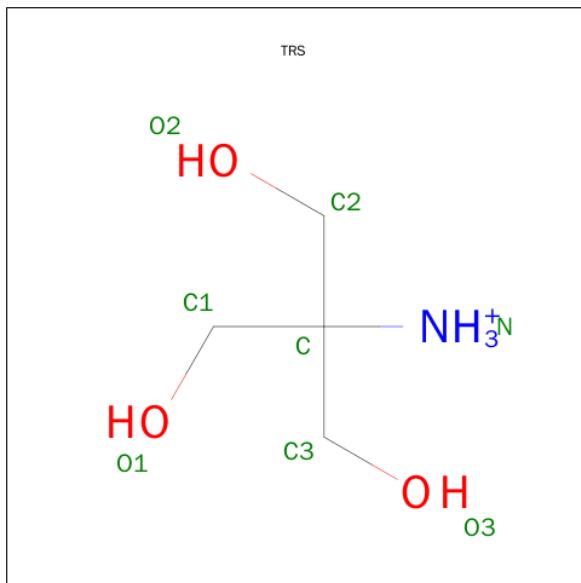
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 8	C 4	N 1	O 3	0	0

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).
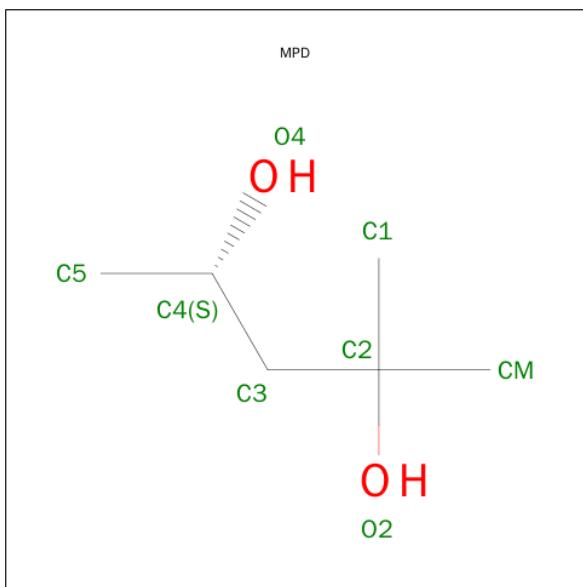
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 8	C 6	O 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	474	Total 474	O 474	1	0
8	B	437	Total 437	O 437	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: XYLOSE ISOMERASE
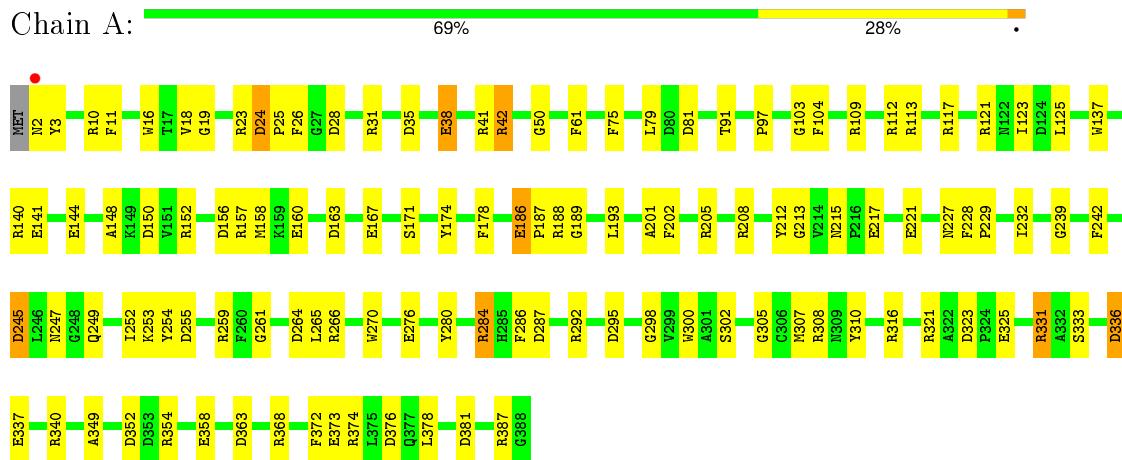
- Molecule 1: XYLOSE ISOMERASE
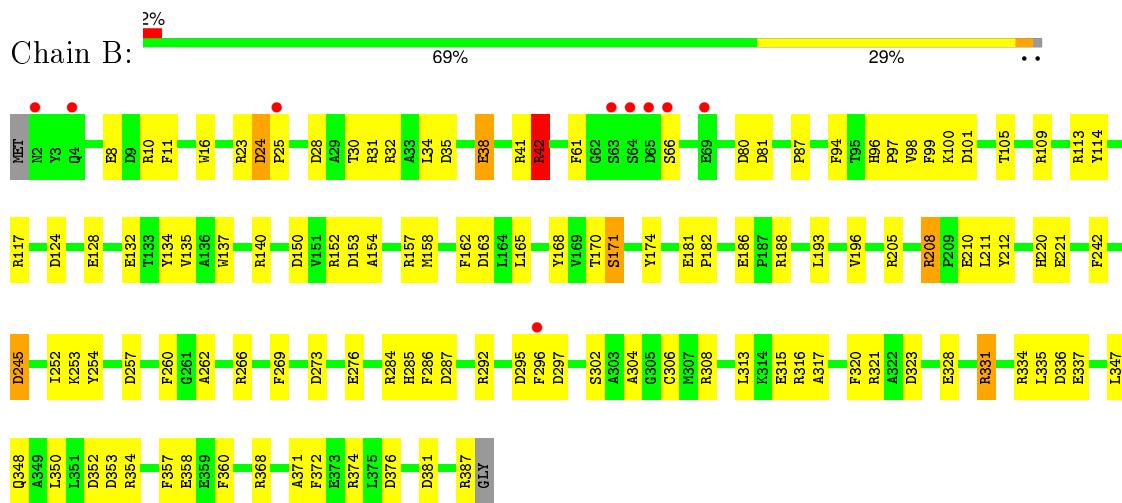
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.45Å 129.59Å 78.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 19.87 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-1.50) 98.0 (19.87-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.71 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.163 , 0.186 0.151 , 0.169	Depositor DCC
R_{free} test set	7880 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 157058 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7120	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MQD, MN, MPD, MRD, TRS

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	1.35	9/3158 (0.3%)	2.40	139/4270 (3.3%)
1	B	1.24	3/3231 (0.1%)	2.29	142/4368 (3.3%)
All	All	1.30	12/6389 (0.2%)	2.35	281/8638 (3.3%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	GLU	CD-OE2	8.56	1.35	1.25
1	B	140	ARG	NE-CZ	7.97	1.43	1.33
1	B	157	ARG	CZ-NH2	6.68	1.41	1.33
1	B	321	ARG	CZ-NH2	6.05	1.41	1.33
1	A	373	GLU	CD-OE2	5.74	1.31	1.25
1	A	213	GLY	CA-C	5.63	1.60	1.51
1	A	109	ARG	CZ-NH2	5.55	1.40	1.33
1	A	333	SER	CB-OG	5.33	1.49	1.42
1	A	201	ALA	C-O	5.19	1.33	1.23
1	A	217	GLU	CB-CG	5.12	1.61	1.52
1	A	103	GLY	CA-C	5.07	1.59	1.51
1	A	113	ARG	NE-CZ	5.02	1.39	1.33

All (281) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	157	ARG	NE-CZ-NH1	27.21	133.91	120.30
1	A	109	ARG	NE-CZ-NH1	26.24	133.42	120.30
1	A	205	ARG	NE-CZ-NH2	-22.58	109.01	120.30
1	A	292	ARG	NE-CZ-NH1	-22.27	109.17	120.30
1	A	109	ARG	NE-CZ-NH2	-21.50	109.55	120.30
1	B	321	ARG	NE-CZ-NH1	19.41	130.00	120.30
1	A	321	ARG	NE-CZ-NH2	-19.00	110.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	205	ARG	NE-CZ-NH2	-18.36	111.12	120.30
1	B	157	ARG	NE-CZ-NH2	-17.62	111.49	120.30
1	B	387	ARG	NE-CZ-NH1	17.28	128.94	120.30
1	A	113	ARG	NE-CZ-NH2	-17.23	111.68	120.30
1	B	266	ARG	NE-CZ-NH1	17.04	128.82	120.30
1	A	387	ARG	NE-CZ-NH1	17.02	128.81	120.30
1	A	295	ASP	CB-CG-OD1	16.66	133.29	118.30
1	B	266	ARG	NE-CZ-NH2	-16.00	112.30	120.30
1	A	212	TYR	CB-CG-CD1	15.96	130.57	121.00
1	B	374	ARG	NE-CZ-NH1	-15.54	112.53	120.30
1	A	331	ARG	NE-CZ-NH2	-14.81	112.89	120.30
1	B	31	ARG	NE-CZ-NH2	13.89	127.25	120.30
1	A	368	ARG	NE-CZ-NH1	-13.68	113.46	120.30
1	B	140	ARG	NE-CZ-NH2	-13.65	113.48	120.30
1	A	286	PHE	CB-CG-CD1	13.24	130.07	120.80
1	B	109	ARG	NE-CZ-NH1	13.23	126.92	120.30
1	A	212	TYR	CB-CG-CD2	-13.20	113.08	121.00
1	A	292	ARG	NE-CZ-NH2	13.12	126.86	120.30
1	B	368	ARG	NE-CZ-NH1	-13.07	113.76	120.30
1	A	280	TYR	CB-CG-CD1	12.90	128.74	121.00
1	A	31	ARG	NE-CZ-NH1	12.76	126.68	120.30
1	A	321	ARG	NE-CZ-NH1	12.75	126.67	120.30
1	B	208[A]	ARG	NE-CZ-NH2	-12.56	114.02	120.30
1	B	208[B]	ARG	NE-CZ-NH2	-12.56	114.02	120.30
1	B	42[A]	ARG	CD-NE-CZ	12.13	140.59	123.60
1	B	42[B]	ARG	CD-NE-CZ	12.13	140.59	123.60
1	B	113	ARG	NE-CZ-NH2	-12.04	114.28	120.30
1	A	24	ASP	CB-CG-OD1	-11.96	107.54	118.30
1	A	157	ARG	NE-CZ-NH1	11.85	126.22	120.30
1	A	41	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	B	387	ARG	NE-CZ-NH2	-11.44	114.58	120.30
1	B	114	TYR	CB-CG-CD1	11.34	127.80	121.00
1	B	336	ASP	CB-CG-OD1	11.16	128.34	118.30
1	A	323	ASP	CB-CG-OD1	10.99	128.19	118.30
1	A	368	ARG	NE-CZ-NH2	10.81	125.71	120.30
1	A	163	ASP	CB-CG-OD1	10.72	127.95	118.30
1	B	140	ARG	NH1-CZ-NH2	10.71	131.18	119.40
1	B	337	GLU	OE1-CD-OE2	-10.56	110.62	123.30
1	A	376	ASP	CB-CG-OD2	10.52	127.76	118.30
1	A	264	ASP	CB-CG-OD1	10.46	127.71	118.30
1	B	117	ARG	NE-CZ-NH1	-10.45	115.08	120.30
1	A	205	ARG	NH1-CZ-NH2	10.44	130.88	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	A	81	ASP	CB-CG-OD2	10.36	127.63	118.30
1	B	308	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	B	292	ARG	NE-CZ-NH2	10.27	125.44	120.30
1	B	292	ARG	NE-CZ-NH1	-10.27	115.17	120.30
1	B	316	ARG	NE-CZ-NH2	-10.27	115.17	120.30
1	B	212	TYR	CB-CG-CD2	-10.03	114.98	121.00
1	B	140	ARG	NE-CZ-NH1	-9.92	115.34	120.30
1	A	373	GLU	OE1-CD-OE2	-9.86	111.47	123.30
1	B	354	ARG	NE-CZ-NH1	9.77	125.18	120.30
1	B	211	LEU	O-C-N	9.65	138.13	122.70
1	A	188	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	208	ARG	NE-CZ-NH1	-9.59	115.51	120.30
1	A	140	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	B	42[A]	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	B	42[B]	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	A	316	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	A	24	ASP	OD1-CG-OD2	9.19	140.77	123.30
1	B	348	GLN	O-C-N	9.16	137.36	122.70
1	B	337	GLU	CG-CD-OE1	9.14	136.57	118.30
1	A	121	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	A	308	ARG	NE-CZ-NH1	-9.02	115.79	120.30
1	B	42[A]	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	B	42[B]	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	157	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	B	376	ASP	CB-CG-OD2	8.97	126.38	118.30
1	A	221	GLU	OE1-CD-OE2	8.96	134.06	123.30
1	B	212	TYR	CB-CG-CD1	8.89	126.33	121.00
1	A	202	PHE	CB-CG-CD1	8.88	127.02	120.80
1	A	336	ASP	CB-CG-OD1	8.88	126.29	118.30
1	B	109	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	B	205	ARG	NH1-CZ-NH2	8.69	128.96	119.40
1	B	321	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	99	PHE	CB-CG-CD1	-8.44	114.89	120.80
1	A	141	GLU	OE1-CD-OE2	-8.43	113.19	123.30
1	A	287	ASP	CB-CG-OD1	8.41	125.87	118.30
1	A	266	ARG	CD-NE-CZ	8.41	135.37	123.60
1	A	217	GLU	CG-CD-OE1	8.38	135.06	118.30
1	A	372	PHE	CB-CG-CD2	-8.19	115.07	120.80
1	A	286	PHE	CB-CG-CD2	-8.16	115.09	120.80
1	B	221	GLU	OE1-CD-OE2	8.12	133.04	123.30
1	B	113	ARG	NE-CZ-NH1	8.09	124.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	B	181	GLU	OE1-CD-OE2	-7.92	113.80	123.30
1	B	306	CYS	O-C-N	7.90	135.34	122.70
1	B	150	ASP	CB-CG-OD2	7.85	125.37	118.30
1	A	24	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	259	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	B	163	ASP	CB-CG-OD2	7.77	125.29	118.30
1	A	152	ARG	NE-CZ-NH1	-7.75	116.43	120.30
1	B	11	PHE	CB-CG-CD2	-7.73	115.39	120.80
1	A	298	GLY	O-C-N	7.71	135.04	122.70
1	B	257	ASP	CB-CG-OD1	7.66	125.19	118.30
1	B	162	PHE	CB-CG-CD2	-7.61	115.47	120.80
1	A	387	ARG	NH1-CZ-NH2	-7.58	111.06	119.40
1	A	245	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	B	242	PHE	CB-CG-CD2	-7.56	115.51	120.80
1	A	325	GLU	OE1-CD-OE2	-7.54	114.26	123.30
1	A	104	PHE	CB-CG-CD2	-7.52	115.53	120.80
1	A	254	TYR	CB-CG-CD1	-7.51	116.50	121.00
1	A	261	GLY	O-C-N	7.49	134.69	122.70
1	A	113	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	260	PHE	CB-CG-CD1	7.47	126.03	120.80
1	B	245	ASP	N-CA-CB	-7.41	97.26	110.60
1	B	331	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	31	ARG	NH1-CZ-NH2	-7.29	111.38	119.40
1	A	253[A]	LYS	CD-CE-NZ	7.29	128.46	111.70
1	A	253[B]	LYS	CD-CE-NZ	7.29	128.46	111.70
1	A	323	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	B	152	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	24	ASP	CB-CA-C	7.19	124.78	110.40
1	A	354	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	28	ASP	CB-CG-OD1	7.13	124.72	118.30
1	B	257	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	B	196	VAL	CA-C-N	7.09	130.38	116.20
1	A	213	GLY	O-C-N	7.08	134.03	122.70
1	B	295	ASP	CB-CG-OD1	7.04	124.64	118.30
1	B	253[A]	LYS	CD-CE-NZ	7.04	127.89	111.70
1	B	253[B]	LYS	CD-CE-NZ	7.04	127.89	111.70
1	B	124	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	374	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	B	260	PHE	O-C-N	6.99	135.09	123.20
1	A	300	TRP	CD1-CG-CD2	-6.99	100.71	106.30
1	A	381	ASP	CB-CG-OD2	6.98	124.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	GLU	OE1-CD-OE2	-6.98	114.92	123.30
1	A	340	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	358	GLU	OE1-CD-OE2	-6.89	115.03	123.30
1	A	242	PHE	CB-CG-CD2	-6.88	115.98	120.80
1	A	310	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	A	349	ALA	O-C-N	6.84	133.65	122.70
1	B	101	ASP	CB-CG-OD1	6.83	124.45	118.30
1	B	374	ARG	NE-CZ-NH2	6.83	123.71	120.30
1	A	217	GLU	OE1-CD-OE2	-6.78	115.16	123.30
1	A	305	GLY	O-C-N	6.76	133.51	122.70
1	A	174	TYR	CB-CG-CD2	6.75	125.05	121.00
1	B	273	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	B	368	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	A	28	ASP	CB-CG-OD1	6.65	124.29	118.30
1	B	114	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	B	269	PHE	CB-CG-CD1	-6.57	116.20	120.80
1	B	317	ALA	O-C-N	6.57	133.21	122.70
1	A	208	ARG	NH1-CZ-NH2	6.56	126.61	119.40
1	A	280	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	B	353	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	A	331	ARG	NH1-CZ-NH2	6.41	126.45	119.40
1	A	373	GLU	CG-CD-OE1	6.39	131.09	118.30
1	B	260	PHE	CG-CD1-CE1	6.36	127.80	120.80
1	A	178	PHE	CB-CG-CD2	-6.35	116.36	120.80
1	B	134	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	A	254	TYR	CB-CG-CD2	6.30	124.78	121.00
1	B	105	THR	O-C-N	6.29	132.77	122.70
1	A	280	TYR	CG-CD1-CE1	6.29	126.33	121.30
1	A	137	TRP	CE2-CD2-CG	-6.26	102.29	107.30
1	A	42	ARG	CD-NE-CZ	6.23	132.32	123.60
1	A	270	TRP	CE2-CD2-CG	6.22	112.27	107.30
1	A	302	SER	N-CA-CB	-6.21	101.18	110.50
1	B	38[A]	GLU	CA-CB-CG	6.20	127.03	113.40
1	B	38[B]	GLU	CA-CB-CG	6.20	127.03	113.40
1	B	302	SER	O-C-N	6.20	132.62	122.70
1	B	347	LEU	O-C-N	-6.18	112.81	122.70
1	A	242	PHE	CD1-CE1-CZ	-6.18	112.69	120.10
1	B	320	PHE	CG-CD1-CE1	6.16	127.57	120.80
1	B	374	ARG	CD-NE-CZ	-6.16	114.98	123.60
1	A	239	GLY	CA-C-O	6.16	131.68	120.60
1	A	276	GLU	OE1-CD-OE2	-6.14	115.93	123.30
1	B	371	ALA	CA-C-O	6.13	132.97	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	154	ALA	O-C-N	6.12	132.50	122.70
1	B	358	GLU	OE1-CD-OE2	-6.11	115.96	123.30
1	B	171	SER	O-C-N	-6.09	112.95	122.70
1	B	24	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	B	174	TYR	CB-CG-CD1	6.07	124.64	121.00
1	A	205	ARG	CG-CD-NE	-6.03	99.13	111.80
1	A	286	PHE	CG-CD1-CE1	6.03	127.43	120.80
1	B	260	PHE	CZ-CE2-CD2	6.03	127.33	120.10
1	B	313	LEU	O-C-N	6.01	132.31	122.70
1	A	300	TRP	CG-CD1-NE1	5.99	116.09	110.10
1	A	156	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	247	ASN	OD1-CG-ND2	5.96	135.61	121.90
1	A	117	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	16	TRP	NE1-CE2-CZ2	-5.96	123.85	130.40
1	A	276	GLU	CG-CD-OE2	5.94	130.19	118.30
1	A	23	ARG	O-C-N	-5.94	113.20	122.70
1	B	286	PHE	CB-CG-CD2	-5.94	116.64	120.80
1	B	135	VAL	O-C-N	5.93	132.19	122.70
1	A	259	ARG	NH1-CZ-NH2	5.92	125.91	119.40
1	B	101	ASP	OD1-CG-OD2	-5.91	112.07	123.30
1	B	254	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	B	320	PHE	CB-CG-CD1	5.88	124.92	120.80
1	B	94	PHE	CB-CG-CD1	5.88	124.92	120.80
1	B	297	ASP	CB-CG-OD1	5.86	123.58	118.30
1	B	352	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	295	ASP	OD1-CG-OD2	-5.85	112.19	123.30
1	A	123	ILE	O-C-N	5.80	131.98	122.70
1	B	316	ARG	NH1-CZ-NH2	5.80	125.78	119.40
1	A	3	TYR	CB-CG-CD2	5.78	124.47	121.00
1	B	334	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	307	MET	CA-C-O	5.75	132.19	120.10
1	B	101	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	262	ALA	O-C-N	-5.73	113.45	123.20
1	A	292	ARG	O-C-N	5.70	131.82	122.70
1	B	181	GLU	CG-CD-OE1	5.69	129.68	118.30
1	B	220	HIS	O-C-N	-5.68	113.60	122.70
1	A	298	GLY	CA-C-O	-5.66	110.41	120.60
1	A	148	ALA	O-C-N	5.66	131.75	122.70
1	A	363	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	372	PHE	CB-CG-CD1	-5.64	116.85	120.80
1	A	286	PHE	CZ-CE2-CD2	5.63	126.85	120.10
1	B	137	TRP	CE2-CD2-CG	-5.60	102.82	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	255	ASP	OD1-CG-OD2	5.57	133.88	123.30
1	B	287	ASP	O-C-N	5.56	131.59	122.70
1	A	245	ASP	CB-CG-OD1	5.55	123.29	118.30
1	B	323	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	352	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	B	31	ARG	NH1-CZ-NH2	-5.53	113.32	119.40
1	B	100	LYS	O-C-N	-5.52	113.86	122.70
1	B	381	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	112	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	357	PHE	CB-CG-CD1	-5.47	116.97	120.80
1	A	261	GLY	CA-C-O	-5.46	110.77	120.60
1	A	150	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	156	ASP	CB-CG-OD1	5.44	123.20	118.30
1	B	304	ALA	O-C-N	-5.44	113.96	123.20
1	B	210	GLU	CG-CD-OE1	5.43	129.17	118.30
1	A	215	ASN	O-C-N	5.42	131.40	121.10
1	B	31	ARG	CD-NE-CZ	5.42	131.19	123.60
1	B	321	ARG	O-C-N	5.39	131.33	122.70
1	B	205	ARG	CG-CD-NE	-5.39	100.48	111.80
1	A	300	TRP	O-C-N	-5.39	114.08	122.70
1	B	348	GLN	CA-C-O	-5.38	108.81	120.10
1	B	11	PHE	CG-CD2-CE2	-5.36	114.90	120.80
1	B	165	LEU	O-C-N	5.36	132.32	123.20
1	A	144	GLU	OE1-CD-OE2	5.35	129.72	123.30
1	A	38	GLU	CA-CB-CG	5.35	125.17	113.40
1	A	259	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	B	23	ARG	O-C-N	-5.34	114.15	122.70
1	A	378	LEU	O-C-N	-5.31	114.21	122.70
1	A	152	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	B	308	ARG	NH1-CZ-NH2	5.26	125.19	119.40
1	A	259	ARG	O-C-N	-5.26	114.28	122.70
1	A	79	LEU	O-C-N	5.25	131.10	122.70
1	B	336	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	B	358	GLU	CG-CD-OE1	5.24	128.78	118.30
1	A	239	GLY	O-C-N	-5.24	114.32	122.70
1	B	360	PHE	CB-CG-CD2	-5.24	117.13	120.80
1	B	168	TYR	CB-CG-CD2	5.23	124.14	121.00
1	B	276	GLU	CG-CD-OE2	5.23	128.76	118.30
1	B	242	PHE	CB-CG-CD1	5.22	124.46	120.80
1	A	18	VAL	O-C-N	-5.22	114.32	123.20
1	B	211	LEU	CA-C-O	-5.22	109.13	120.10
1	A	11	PHE	O-C-N	-5.22	114.35	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	HIS	O-C-N	5.20	131.02	122.70
1	A	19	GLY	O-C-N	5.17	130.98	122.70
1	A	363	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	B	16	TRP	CH2-CZ2-CE2	-5.13	112.27	117.40
1	B	153	ASP	CA-C-O	5.13	130.87	120.10
1	B	188	ARG	CD-NE-CZ	5.12	130.78	123.60
1	A	265	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	B	80	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	16	TRP	CD1-NE1-CE2	-5.11	104.40	109.00
1	B	182	PRO	N-CA-CB	5.10	109.42	103.30
1	A	75	PHE	CB-CG-CD1	5.10	124.37	120.80
1	B	350	LEU	O-C-N	-5.10	114.54	122.70
1	A	189	GLY	CA-C-O	5.09	129.76	120.60
1	B	208[A]	ARG	NH1-CZ-NH2	5.08	124.99	119.40
1	B	208[B]	ARG	NH1-CZ-NH2	5.08	124.99	119.40
1	B	245	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	315	GLU	O-C-N	-5.07	114.59	122.70
1	A	50	GLY	O-C-N	5.03	130.75	122.70
1	A	188	ARG	NH1-CZ-NH2	-5.03	113.86	119.40
1	A	249	GLN	CG-CD-OE1	5.02	131.64	121.60
1	A	125	LEU	O-C-N	-5.01	114.69	122.70
1	A	284	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3060	0	2925	33	0
1	B	3095	0	2955	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	8	0	14	0	0
5	A	9	0	14	1	0
5	B	9	0	14	0	0
6	A	8	0	12	0	0
7	B	8	0	14	5	0
8	A	474	0	0	11	1
8	B	437	0	0	11	0
All	All	7120	0	5962	72	1

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 6.

All (72) 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:B:132[B]:GLU:HG3	8:B:2187:HOH:O	1.28	1.26
1:A:10[B]:ARG:HH21	1:A:284:ARG:NH1	1.35	1.24
1:A:10[B]:ARG:NH2	1:A:284:ARG:NH1	1.86	1.23
1:A:10[B]:ARG:HH21	1:A:284:ARG:CZ	1.64	1.09
1:B:132[B]:GLU:OE2	8:B:2188:HOH:O	1.77	1.00
8:A:2036:HOH:O	1:B:25:PRO:HB3	1.63	0.96
1:B:35:ASP:HB3	1:B:38[A]:GLU:HG3	1.48	0.94
1:A:160[A]:GLU:OE2	8:A:2253:HOH:O	1.85	0.94
1:B:61:PHE:CE2	8:B:2154:HOH:O	2.21	0.94
1:A:331:ARG:HB3	7:B:396:MPD:H13	1.51	0.93
1:B:96:HIS:HD2	1:B:98:VAL:H	1.09	0.92
1:A:10[B]:ARG:NH2	1:A:284:ARG:CZ	2.28	0.90
1:A:42:ARG:HG2	8:A:2064:HOH:O	1.72	0.86
1:A:61:PHE:CE2	8:A:2191:HOH:O	2.32	0.82
1:A:42:ARG:HD2	8:A:2078:HOH:O	1.85	0.77
8:A:2036:HOH:O	1:B:25:PRO:CB	2.25	0.75
1:B:61:PHE:HE2	8:B:2154:HOH:O	1.63	0.75
1:A:10[B]:ARG:NH2	1:A:284:ARG:HH12	1.83	0.74
1:B:96:HIS:CD2	1:B:98:VAL:H	2.00	0.74
1:B:328[A]:GLU:HG3	8:B:2364:HOH:O	1.89	0.71
1:A:2:ASN:N	8:A:2001:HOH:O	2.24	0.71
1:A:336:ASP:OD2	7:B:396:MPD:CM	2.41	0.68
1:A:61:PHE:CD2	8:A:2096:HOH:O	2.47	0.67
1:A:337:GLU:OE2	7:B:396:MPD:H51	1.95	0.66
1:B:10[B]:ARG:NH2	1:B:284:ARG:NH1	2.44	0.66
1:B:132[A]:GLU:HG3	8:B:2187:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128[A]:GLU:OE2	8:B:2177:HOH:O	2.14	0.64
1:A:24:ASP:HB2	1:A:25:PRO:CD	2.29	0.62
1:A:10[B]:ARG:CZ	1:A:284:ARG:NH1	2.63	0.61
1:A:336:ASP:OD2	7:B:396:MPD:HM1	2.02	0.59
1:B:61:PHE:CD2	8:B:2075:HOH:O	2.52	0.59
1:A:61:PHE:HE2	8:A:2191:HOH:O	1.77	0.59
1:B:87:PRO:O	1:B:132[B]:GLU:OE2	2.20	0.59
1:B:10[B]:ARG:HH21	1:B:284:ARG:CZ	2.15	0.58
1:B:32:ARG:HG2	1:B:296:PHE:HE2	1.72	0.55
1:A:336:ASP:OD2	7:B:396:MPD:HM3	2.06	0.55
1:A:42:ARG:NH2	8:A:2072:HOH:O	2.20	0.54
1:B:328[B]:GLU:OE1	1:B:331:ARG:NH2	2.28	0.54
1:B:10[B]:ARG:HH21	1:B:284:ARG:NH1	2.07	0.52
1:B:41[B]:ARG:HH12	1:B:81:ASP:HB2	1.77	0.50
1:B:132[A]:GLU:OE2	8:B:2187:HOH:O	2.18	0.50
1:A:24:ASP:HB2	1:A:25:PRO:HD2	1.94	0.50
1:A:24:ASP:CB	1:A:25:PRO:CD	2.89	0.49
1:B:32:ARG:HG2	1:B:296:PHE:CE2	2.47	0.49
1:B:96:HIS:CD2	1:B:97:PRO:HD2	2.47	0.49
1:B:10[B]:ARG:NH2	1:B:284:ARG:CZ	2.75	0.49
1:A:42:ARG:NE	8:A:2072:HOH:O	2.38	0.48
1:B:170:THR:HG21	1:B:208[A]:ARG:CZ	2.44	0.48
1:B:132[B]:GLU:CD	8:B:2188:HOH:O	2.38	0.48
5:A:395:MQD:H4	5:A:395:MQD:HMC1	1.62	0.47
1:B:24:ASP:HB2	1:B:25:PRO:HD2	1.96	0.46
1:A:158[B]:MET:SD	1:A:193:LEU:HD11	2.55	0.46
1:B:158[B]:MET:SD	1:B:193:LEU:HD11	2.55	0.46
1:A:97:PRO:HB3	1:B:30:THR:HG22	1.98	0.46
1:A:35:ASP:HB3	1:A:38:GLU:HG3	1.98	0.46
1:B:132[A]:GLU:CG	8:B:2187:HOH:O	2.61	0.46
1:B:24:ASP:HB2	1:B:25:PRO:CD	2.45	0.45
1:B:170:THR:HG21	1:B:208[A]:ARG:NH1	2.32	0.45
1:A:252:ILE:HG22	1:B:252:ILE:HG22	1.97	0.45
1:A:24:ASP:HB2	1:A:25:PRO:HD3	1.99	0.45
1:A:25:PRO:HB2	1:A:26:PHE:CD1	2.53	0.44
1:B:8:GLU:H	1:B:8:GLU:CD	2.21	0.43
1:B:34:LEU:HD21	1:B:296:PHE:CE1	2.53	0.43
1:B:335:LEU:HD13	1:B:335:LEU:HA	1.96	0.43
1:A:186:GLU:HA	1:A:187:PRO:HA	1.95	0.42
1:A:228:PHE:CZ	1:A:232:ILE:HD11	2.55	0.41
1:A:227:ASN:OD1	1:A:229:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:HIS:CG	1:B:97:PRO:HD2	2.56	0.40
1:A:167:GLU:O	1:A:171:SER:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2136:HOH:O	8:A:2233:HOH:O[2_665]	2.08	0.12

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	390/388 (100%)	379 (97%)	10 (3%)	1 (0%)	46	19
1	B	397/388 (102%)	387 (98%)	9 (2%)	1 (0%)	46	19
All	All	787/776 (101%)	766 (97%)	19 (2%)	2 (0%)	46	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLU
1	B	186	GLU

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	307/304 (101%)	305 (99%)	2 (1%)	88	73
1	B	315/304 (104%)	311 (99%)	4 (1%)	76	50
All	All	622/608 (102%)	616 (99%)	6 (1%)	86	62

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	THR
1	A	245	ASP
1	B	42[A]	ARG
1	B	42[B]	ARG
1	B	66	SER
1	B	245	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4	GLN
1	B	96	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)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	MRD	A	394	-	6,7,7	0.63	0	7,10,10	0.71	0
5	MQD	A	395	3	8,8,8	0.74	0	2,11,11	1.08	0
6	TRS	A	396	-	7,7,7	1.04	0	9,9,9	2.18	2 (22%)
4	MRD	B	394	-	6,7,7	0.47	0	7,10,10	0.83	0
5	MQD	B	395	3	8,8,8	0.87	1 (12%)	2,11,11	0.88	0
7	MPD	B	396	-	6,7,7	0.50	0	7,10,10	1.88	2 (28%)

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	MRD	A	394	-	-	0/5/5/5	0/0/0/0
5	MQD	A	395	3	-	0/8/8/8	0/0/0/0
6	TRS	A	396	-	-	0/9/9/9	0/0/0/0
4	MRD	B	394	-	-	0/5/5/5	0/0/0/0
5	MQD	B	395	3	-	0/8/8/8	0/0/0/0
7	MPD	B	396	-	-	0/5/5/5	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	395	MQD	C1-C2	2.07	1.54	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	396	TRS	C3-C-C1	-3.53	103.14	110.78
7	B	396	MPD	O2-C2-CM	2.71	118.03	108.09
7	B	396	MPD	O2-C2-C1	3.44	120.72	108.09
6	A	396	TRS	C3-C-N	4.77	116.78	108.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	395	MQD	1	0
7	B	396	MPD	5	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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	387/388 (99%)	-0.17	1 (0%)	94 95	9, 13, 24, 34	0
1	B	386/388 (99%)	-0.10	9 (2%)	64 67	10, 14, 27, 44	0
All	All	773/776 (99%)	-0.13	10 (1%)	79 82	9, 13, 26, 44	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	64	SER	3.3
1	B	25	PRO	2.6
1	B	65	ASP	2.6
1	B	2	ASN	2.5
1	B	69	GLU	2.5
1	B	296	PHE	2.2
1	A	2	ASN	2.2
1	B	63	SER	2.1
1	B	4	GLN	2.1
1	B	66	SER	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.

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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
5	MQD	B	395	9/9	0.90	0.15	8.27	21,24,25,29	0
5	MQD	A	395	9/9	0.92	0.14	5.94	18,25,27,27	0
6	TRS	A	396	8/8	0.72	0.27	4.22	28,30,32,35	0
4	MRD	A	394	8/8	0.75	0.17	2.28	24,31,38,38	0
4	MRD	B	394	8/8	0.90	0.13	0.89	21,27,32,34	0
3	MG	A	392	1/1	0.99	0.07	-0.14	11,11,11,11	0
3	MG	B	392	1/1	0.99	0.06	-1.18	12,12,12,12	0
2	MN	B	390	1/1	0.99	0.04	-3.28	14,14,14,14	0
2	MN	A	390	1/1	1.00	0.05	-3.68	14,14,14,14	0
7	MPD	B	396	8/8	0.83	0.26	-	5,20,28,33	8

6.5 Other polymers (i)

There are no such residues in this entry.