Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2024 – 03:16 PM EST

PDB ID	:	1EC7
Title	:	E. COLI GLUCARATE DEHYDRATASE NATIVE ENZYME
Authors	:	Gulick, A.M.; Hubbard, B.K.; Gerlt, J.A.; Rayment, I.
Deposited on	:	2000-01-25
Resolution	:	1.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

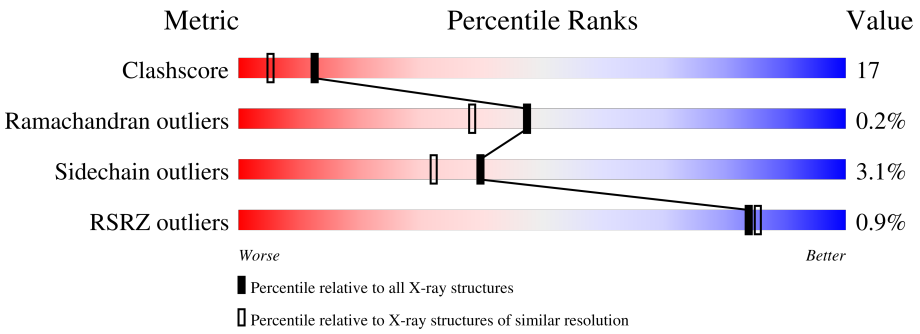
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	446	62% 29% 5% •
1	B	446	63% 31% 5% •
1	C	446	67% 26% • •
1	D	446	60% 32% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14443 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.

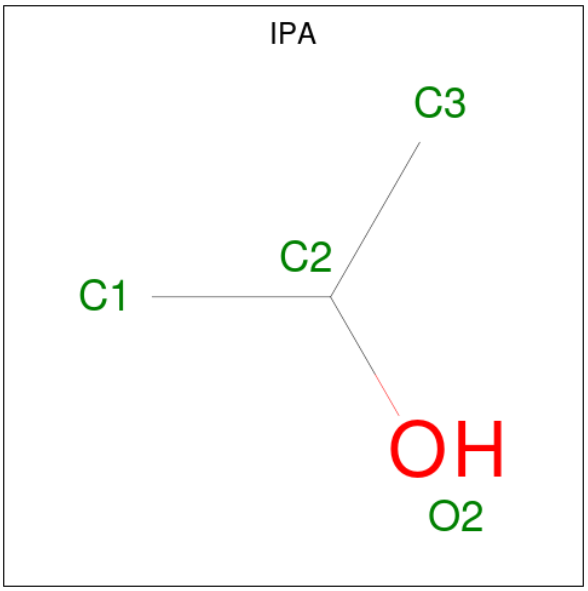
- Molecule 1 is a protein called GLUCARATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	3300	2091	571	617	21	0	0	0
1	B	440	3398	2151	597	629	21	0	0	0
1	C	428	3309	2096	576	616	21	0	1	0
1	D	431	3314	2098	576	619	21	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	3	1	0	0
			Total	C	O		
3	C	1	4	3	1	0	0
			Total	C	O		
3	D	1	4	3	1	0	0
			Total	C	O		
3	D	1	4	3	1	0	0

- Molecule 4 is water.

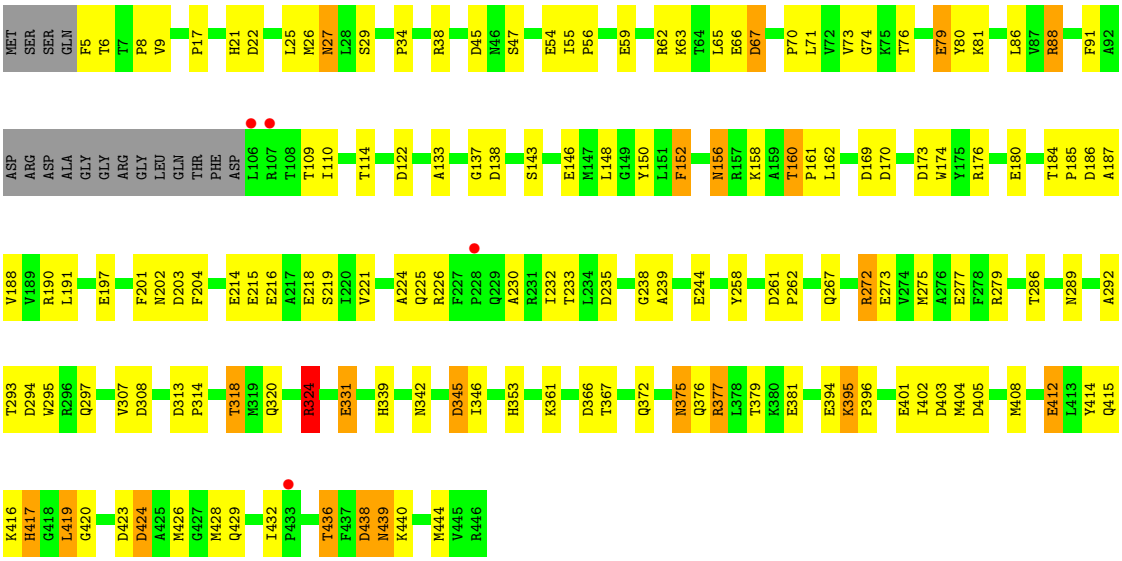
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	312	312	312	0	0
			Total	O		
4	B	232	232	232	0	0
			Total	O		
4	C	304	304	304	0	0
			Total	O		
4	D	254	254	254	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

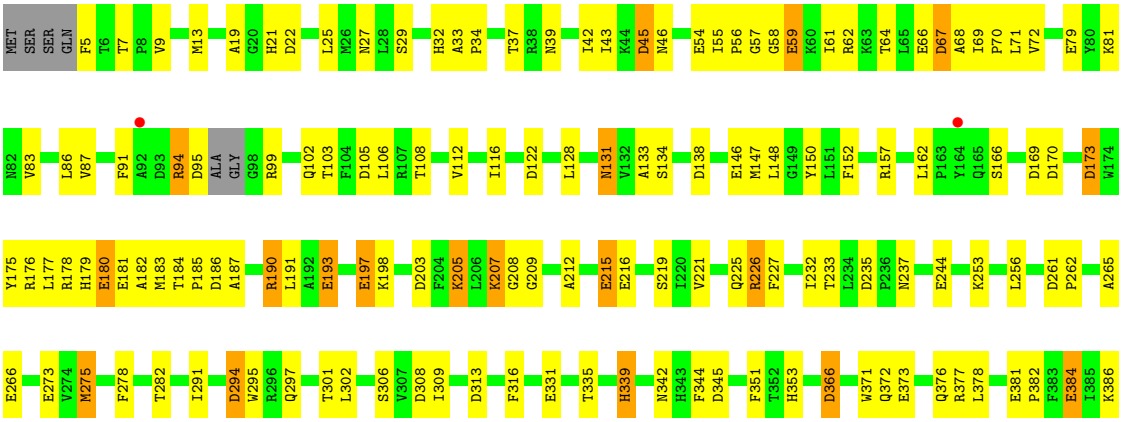
• Molecule 1: GLUCARATE DEHYDRATASE

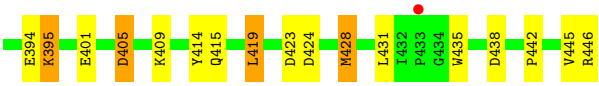
Chain A:



• Molecule 1: GLUCARATE DEHYDRATASE

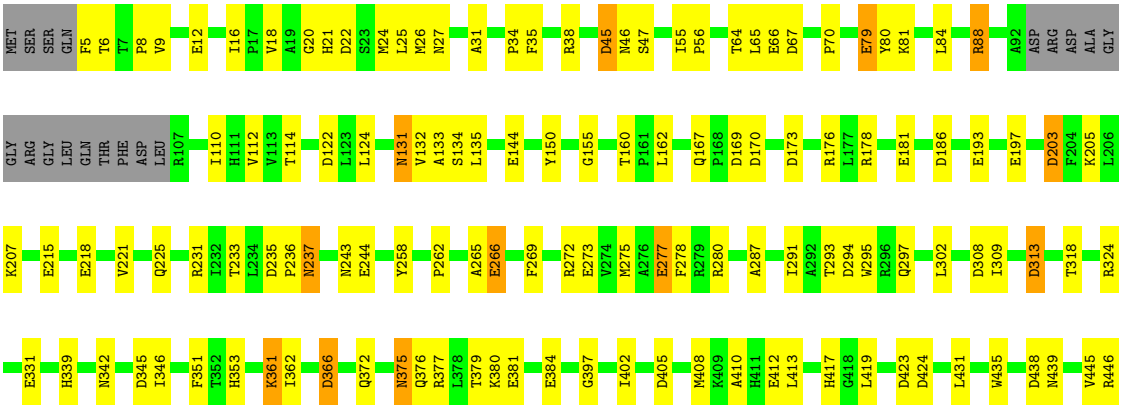
Chain B:





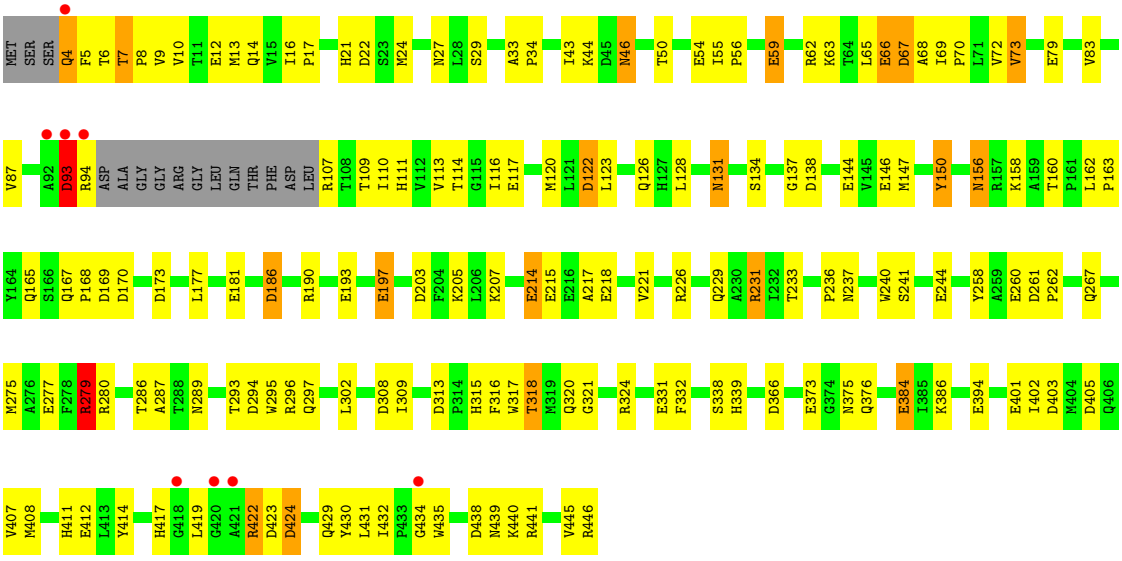
• Molecule 1: GLUCARATE DEHYDRATASE

Chain C:



• Molecule 1: GLUCARATE DEHYDRATASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.25Å 84.55Å 98.92Å 103.30° 94.00° 113.10°	Depositor
Resolution (Å)	30.00 – 1.90 19.86 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-1.90) 87.7 (19.86-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.50 (at 1.70Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.194 , (Not available) 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 84.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14443	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: IPA, MG

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	1.06	16/3377 (0.5%)	1.28	48/4582 (1.0%)
1	B	1.00	18/3476 (0.5%)	1.24	44/4710 (0.9%)
1	C	1.05	15/3386 (0.4%)	1.21	38/4592 (0.8%)
1	D	1.07	20/3391 (0.6%)	1.26	41/4602 (0.9%)
All	All	1.04	69/13630 (0.5%)	1.25	171/18486 (0.9%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	422	ARG	C-N	12.14	1.61	1.34
1	D	218	GLU	CD-OE2	8.67	1.35	1.25
1	A	79	GLU	CD-OE2	8.59	1.35	1.25
1	A	412	GLU	CD-OE2	8.37	1.34	1.25
1	D	144	GLU	CD-OE2	8.12	1.34	1.25
1	C	277	GLU	CD-OE1	-7.38	1.17	1.25
1	C	193	GLU	CD-OE2	7.29	1.33	1.25
1	A	331	GLU	CD-OE2	7.21	1.33	1.25
1	D	412	GLU	CD-OE2	7.04	1.33	1.25
1	D	384	GLU	CD-OE2	6.67	1.32	1.25
1	B	394	GLU	CD-OE2	6.54	1.32	1.25
1	B	59	GLU	CD-OE2	6.50	1.32	1.25
1	C	79	GLU	CD-OE2	6.50	1.32	1.25
1	C	384	GLU	CD-OE2	6.50	1.32	1.25
1	C	197	GLU	CD-OE2	6.44	1.32	1.25
1	D	146	GLU	CD-OE2	6.41	1.32	1.25
1	B	381	GLU	CD-OE2	6.40	1.32	1.25
1	A	214	GLU	CD-OE2	6.36	1.32	1.25
1	A	59	GLU	CD-OE2	6.35	1.32	1.25
1	C	412	GLU	CD-OE2	6.34	1.32	1.25
1	B	79	GLU	CD-OE2	6.32	1.32	1.25
1	B	146	GLU	CD-OE2	6.31	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	12	GLU	CD-OE2	6.24	1.32	1.25
1	C	66	GLU	CD-OE2	6.23	1.32	1.25
1	B	373	GLU	CD-OE2	6.23	1.32	1.25
1	B	215	GLU	CD-OE2	6.23	1.32	1.25
1	B	180	GLU	CD-OE2	6.04	1.32	1.25
1	D	79	GLU	CD-OE2	5.93	1.32	1.25
1	C	381	GLU	CD-OE2	5.88	1.32	1.25
1	A	394	GLU	CD-OE2	5.85	1.32	1.25
1	B	54	GLU	CD-OE2	5.84	1.32	1.25
1	A	54	GLU	CD-OE2	5.82	1.32	1.25
1	A	401	GLU	CD-OE2	5.81	1.32	1.25
1	A	244	GLU	CD-OE2	5.79	1.32	1.25
1	D	59	GLU	CD-OE2	5.77	1.31	1.25
1	D	197	GLU	CD-OE2	5.77	1.31	1.25
1	C	181	GLU	CD-OE2	5.75	1.31	1.25
1	D	394	GLU	CD-OE2	5.74	1.31	1.25
1	B	66	GLU	CD-OE2	5.74	1.31	1.25
1	C	144	GLU	CD-OE1	-5.72	1.19	1.25
1	D	401	GLU	CD-OE2	5.70	1.31	1.25
1	A	381	GLU	CD-OE2	5.68	1.31	1.25
1	D	54	GLU	CD-OE2	5.65	1.31	1.25
1	A	146	GLU	CD-OE2	5.62	1.31	1.25
1	C	12	GLU	CD-OE2	5.60	1.31	1.25
1	B	384	GLU	CD-OE2	5.59	1.31	1.25
1	A	180	GLU	CD-OE2	5.57	1.31	1.25
1	A	216	GLU	CD-OE2	5.52	1.31	1.25
1	D	215	GLU	CD-OE2	5.52	1.31	1.25
1	B	197	GLU	CD-OE2	5.51	1.31	1.25
1	D	181	GLU	CD-OE1	-5.51	1.19	1.25
1	C	266	GLU	CD-OE1	-5.49	1.19	1.25
1	D	214	GLU	CD-OE2	5.45	1.31	1.25
1	A	215	GLU	CD-OE2	5.45	1.31	1.25
1	A	66	GLU	CD-OE2	5.42	1.31	1.25
1	B	401	GLU	CD-OE2	5.42	1.31	1.25
1	B	216	GLU	CD-OE2	5.39	1.31	1.25
1	D	277	GLU	CD-OE1	-5.39	1.19	1.25
1	A	218	GLU	CD-OE2	5.37	1.31	1.25
1	B	193	GLU	CD-OE2	5.34	1.31	1.25
1	C	218	GLU	CD-OE2	5.33	1.31	1.25
1	B	181	GLU	CD-OE2	5.28	1.31	1.25
1	B	244	GLU	CD-OE2	5.21	1.31	1.25
1	D	373	GLU	CD-OE2	5.19	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	193	GLU	CD-OE1	-5.11	1.20	1.25
1	C	215	GLU	CD-OE2	5.09	1.31	1.25
1	D	66	GLU	CD-OE2	5.09	1.31	1.25
1	C	244	GLU	CD-OE2	5.09	1.31	1.25
1	B	273	GLU	CD-OE2	5.04	1.31	1.25

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	294	ASP	CB-CG-OD2	-10.04	109.26	118.30
1	A	366	ASP	CB-CG-OD1	8.84	126.26	118.30
1	A	173	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	A	366	ASP	CB-CG-OD2	-8.48	110.67	118.30
1	B	22	ASP	CB-CG-OD2	-8.37	110.77	118.30
1	D	308	ASP	CB-CG-OD2	-8.34	110.80	118.30
1	B	190	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	D	231	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	B	67	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	A	324	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	B	366	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	A	294	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	A	22	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	B	122	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	C	294	ASP	CB-CG-OD1	7.79	125.31	118.30
1	D	422	ARG	O-C-N	7.69	135.00	122.70
1	A	138	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	B	294	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	B	424	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	D	422	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	294	ASP	CB-CG-OD1	7.53	125.07	118.30
1	D	169	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	B	170	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	294	ASP	CB-CG-OD1	7.40	124.96	118.30
1	D	170	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	B	173	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	D	366	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	B	157	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	B	203	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	A	22	ASP	CB-CG-OD1	7.21	124.79	118.30
1	C	366	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	A	38	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	D	422	ARG	CA-C-N	-7.13	101.52	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	122	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	A	169	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	D	261	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	308	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	B	366	ASP	CB-CG-OD1	6.94	124.54	118.30
1	C	308	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	D	93	ASP	CB-CG-OD1	6.92	124.53	118.30
1	B	186	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	22	ASP	CB-CG-OD1	6.88	124.49	118.30
1	B	67	ASP	CB-CG-OD1	6.88	124.49	118.30
1	D	308	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	423	ASP	CB-CG-OD1	6.86	124.48	118.30
1	B	308	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	C	438	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	122	ASP	CB-CG-OD1	6.83	124.45	118.30
1	C	22	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	423	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	D	280	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	D	138	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	203	ASP	CB-CG-OD1	6.75	124.37	118.30
1	D	338	SER	N-CA-CB	6.74	120.62	110.50
1	D	324	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	D	138	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	D	261	ASP	CB-CG-OD1	6.68	124.32	118.30
1	B	235	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	B	95	ASP	CB-CG-OD1	6.62	124.26	118.30
1	D	423	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	424	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	272	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	A	170	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	D	405	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	308	ASP	CB-CG-OD1	6.42	124.08	118.30
1	C	170	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	A	203	ASP	CB-CG-OD2	-6.32	112.62	118.30
1	A	122	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	C	324	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	294	ASP	CB-CG-OD1	6.30	123.97	118.30
1	B	122	ASP	CB-CG-OD1	6.26	123.94	118.30
1	D	186	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	B	226	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	D	22	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	405	ASP	CB-CG-OD2	-6.22	112.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	438	ASP	CB-CG-OD1	6.22	123.89	118.30
1	C	405[A]	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	C	405[B]	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	C	424	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	D	122	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	B	138	ASP	CB-CG-OD1	6.13	123.81	118.30
1	A	169	ASP	CB-CG-OD1	6.12	123.80	118.30
1	C	366	ASP	CB-CG-OD1	6.08	123.78	118.30
1	A	438	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	138	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	169	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	D	438	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	A	438	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	A	417	HIS	C-N-CA	-6.03	109.64	122.30
1	B	173	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	405	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C	122	ASP	CB-CG-OD1	6.02	123.71	118.30
1	A	173	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	377	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	308	ASP	CB-CG-OD1	5.92	123.63	118.30
1	D	318	THR	N-CA-CB	5.92	121.55	110.30
1	A	324	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	424	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	122	ASP	CB-CG-OD1	5.86	123.58	118.30
1	C	22	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	D	423	ASP	CB-CG-OD1	5.85	123.56	118.30
1	C	38	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	176	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	C	173	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	438	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	446	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	424	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	152	PHE	CB-CA-C	-5.73	98.94	110.40
1	B	438	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	169	ASP	CB-CG-OD2	-5.69	113.17	118.30
1	C	313	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	423	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	C	438	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	B	186	ASP	CB-CG-OD1	5.64	123.37	118.30
1	A	272	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	C	351	PHE	N-CA-CB	5.63	120.73	110.60
1	A	235	ASP	CB-CG-OD2	-5.62	113.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	45	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	279	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	235	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	403	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	446	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	D	93	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	D	424	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	345	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	279	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	C	186	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	67	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	226	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	280	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	367	THR	N-CA-CB	5.46	120.68	110.30
1	D	22	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	D	73	VAL	N-CA-C	5.45	125.72	111.00
1	D	366	ASP	CB-CG-OD1	5.44	123.20	118.30
1	D	405	ASP	CB-CG-OD1	5.44	123.20	118.30
1	D	170	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	170	ASP	CB-CG-OD1	5.44	123.19	118.30
1	C	345	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	138	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	186	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	105	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	B	105	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	170	ASP	CB-CG-OD1	5.25	123.03	118.30
1	D	67	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	424	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	178	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	C	203	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	C	45	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	405	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	C	169	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	176	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	275	MET	CG-SD-CE	5.16	108.45	100.20
1	C	235	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	C	176	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	203	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	45	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	423	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	88	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	423	ASP	CB-CG-OD1	5.11	122.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	170	ASP	CB-CG-OD1	5.09	122.88	118.30
1	D	422	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	C	405[A]	ASP	CB-CG-OD1	5.08	122.88	118.30
1	C	405[B]	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	308	ASP	CB-CG-OD1	5.08	122.87	118.30
1	D	403	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	176	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	345	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	B	424	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	12	GLU	CB-CA-C	-5.02	100.36	110.40
1	D	401	GLU	N-CA-CB	5.01	119.62	110.60
1	A	318	THR	N-CA-CB	5.01	119.81	110.30

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	3300	0	3214	105	0
1	B	3398	0	3325	118	0
1	C	3309	0	3235	90	0
1	D	3314	0	3219	142	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	8	1	0
3	C	4	0	8	1	0
3	D	8	0	16	5	0
4	A	312	0	0	14	1
4	B	232	0	0	7	0
4	C	304	0	0	5	1
4	D	254	0	0	9	0
All	All	14443	0	13025	442	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 17.

All (442) 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:D:429:GLN:NE2	1:D:435:TRP:H	1.43	1.15
1:D:21:HIS:H	1:D:376:GLN:HE22	1.05	0.96
1:B:414:TYR:HA	1:B:419:LEU:HD12	1.51	0.92
1:C:26:MET:HE2	1:C:31:ALA:HA	1.51	0.92
1:B:414:TYR:HA	1:B:419:LEU:CD1	2.00	0.91
1:A:428:MET:CE	1:A:444:MET:HE2	2.01	0.90
1:D:293:THR:H	1:D:297:GLN:NE2	1.70	0.89
1:D:293:THR:H	1:D:297:GLN:HE21	1.18	0.88
1:D:43:ILE:HG21	1:D:120:MET:HE3	1.54	0.87
1:D:429:GLN:HE22	1:D:435:TRP:H	1.15	0.87
1:B:147:MET:HE1	1:B:351:PHE:HE2	1.41	0.86
1:D:384:GLU:HB2	1:D:386:LYS:HE3	1.55	0.86
1:D:429:GLN:HE22	1:D:435:TRP:N	1.74	0.85
1:D:4:GLN:NE2	1:D:5:PHE:H	1.75	0.85
1:D:120:MET:HE1	1:D:123:LEU:HD12	1.58	0.85
1:D:313:ASP:H	1:D:339:HIS:CE1	1.96	0.84
1:D:429:GLN:NE2	1:D:435:TRP:N	2.23	0.83
1:B:7:THR:HG21	1:D:128:LEU:HA	1.59	0.83
1:D:408:MET:HE3	1:D:408:MET:HA	1.61	0.82
1:D:43:ILE:HD13	1:D:120:MET:HE3	1.61	0.82
1:C:293:THR:H	1:C:297:GLN:HE21	1.26	0.82
1:C:293:THR:H	1:C:297:GLN:NE2	1.77	0.82
1:B:187:ALA:O	1:B:190:ARG:HG3	1.80	0.81
1:A:375:ASN:HD22	1:A:375:ASN:H	1.28	0.81
1:A:238:GLY:O	1:A:440:LYS:HE2	1.80	0.81
1:A:293:THR:H	1:A:297:GLN:NE2	1.81	0.79
1:C:35:PHE:CE1	1:C:413:LEU:HD21	2.17	0.79
1:D:417:HIS:CB	1:D:419:LEU:HG	2.14	0.78
1:C:24:MET:HE3	1:C:431:LEU:HD11	1.63	0.77
1:B:21:HIS:H	1:B:376:GLN:HE22	1.30	0.77
1:D:236:PRO:HG2	1:D:262:PRO:HA	1.66	0.77
1:D:21:HIS:H	1:D:376:GLN:NE2	1.80	0.76
1:B:221:VAL:O	1:B:225:GLN:HG3	1.87	0.75
1:C:25:LEU:C	1:C:26:MET:HE3	2.07	0.75
1:A:428:MET:HE3	1:A:444:MET:HE2	1.68	0.74
1:C:21:HIS:H	1:C:376:GLN:HE22	1.36	0.73
1:B:384:GLU:HB2	1:B:386:LYS:HE3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LEU:HB3	1:D:163:PRO:HD2	1.71	0.73
1:C:167:GLN:HE22	1:C:178:ARG:HH21	1.33	0.72
1:A:428:MET:HE1	1:A:444:MET:HE2	1.69	0.71
1:C:26:MET:HE3	1:C:26:MET:N	2.04	0.71
1:C:24:MET:CE	1:C:155:GLY:HA3	2.20	0.71
1:C:26:MET:HE2	1:C:26:MET:HA	1.73	0.71
1:B:58:GLY:HA3	4:B:1518:HOH:O	1.89	0.71
1:D:122:ASP:O	1:D:126:GLN:HG3	1.90	0.70
1:C:55:ILE:HD11	1:C:65:LEU:HD11	1.73	0.70
1:A:262:PRO:HD2	1:A:275:MET:SD	2.30	0.70
1:A:272:ARG:NH1	1:A:297:GLN:HG2	2.05	0.70
1:C:16:ILE:HD13	1:C:408:MET:CE	2.22	0.70
1:A:420:GLY:HA2	4:A:2001:HOH:O	1.90	0.70
1:D:43:ILE:CD1	1:D:120:MET:HE3	2.21	0.70
1:D:408:MET:HA	1:D:408:MET:CE	2.20	0.70
1:D:422:ARG:HD3	4:D:1432:HOH:O	1.91	0.70
1:A:293:THR:H	1:A:297:GLN:HE21	1.40	0.70
1:A:375:ASN:HD22	1:A:375:ASN:N	1.83	0.70
1:B:302:LEU:HD22	3:D:602:IPA:H33	1.74	0.69
1:C:361:LYS:HE2	1:C:362:ILE:O	1.91	0.69
1:D:384:GLU:HB2	1:D:386:LYS:CE	2.23	0.69
1:A:375:ASN:H	1:A:375:ASN:ND2	1.90	0.69
1:D:402:ILE:HD11	1:D:407:VAL:HG21	1.74	0.69
1:C:26:MET:HA	1:C:26:MET:CE	2.23	0.69
1:C:233:THR:HG21	1:C:258:TYR:CZ	2.27	0.69
1:B:13:MET:HB2	1:B:43:ILE:HG12	1.73	0.69
1:C:243:ASN:ND2	4:C:1574:HOH:O	2.23	0.69
1:A:21:HIS:H	1:A:376:GLN:HE22	1.40	0.69
1:B:198:LYS:O	1:B:198:LYS:HG3	1.91	0.69
1:A:63:LYS:NZ	4:A:1693:HOH:O	2.26	0.69
1:B:81:LYS:HE2	1:D:137:GLY:O	1.93	0.69
1:C:375:ASN:H	1:C:375:ASN:HD22	1.39	0.69
1:D:21:HIS:N	1:D:376:GLN:HE22	1.85	0.68
1:D:93:ASP:OD1	1:D:94:ARG:N	2.25	0.68
1:B:428:MET:HG2	1:B:435:TRP:CD2	2.28	0.68
1:B:187:ALA:C	1:B:190:ARG:HG3	2.13	0.68
1:D:429:GLN:HE22	1:D:434:GLY:N	1.91	0.68
1:D:150:TYR:OH	1:D:205:LYS:NZ	2.25	0.68
1:C:366:ASP:OD2	4:C:1420:HOH:O	2.12	0.68
1:D:10:VAL:O	1:D:73:VAL:O	2.12	0.68
1:D:107:ARG:O	1:D:110:ILE:HG22	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ASP:O	1:B:409:LYS:HG3	1.93	0.67
1:D:422:ARG:HD2	1:D:424:ASP:OD2	1.94	0.67
1:D:231:ARG:NH2	4:D:1665:HOH:O	2.26	0.67
1:C:380:LYS:NZ	4:C:1332:HOH:O	2.28	0.67
1:A:55:ILE:HD11	1:A:65:LEU:HD11	1.76	0.67
1:D:417:HIS:HB3	1:D:419:LEU:HG	1.76	0.66
1:A:416:LYS:HG2	1:A:417:HIS:CD2	2.30	0.66
1:A:55:ILE:HB	1:A:56:PRO:HD2	1.77	0.66
1:D:241:SER:OG	1:D:244:GLU:HG3	1.95	0.65
1:C:35:PHE:CD1	1:C:413:LEU:HD21	2.31	0.65
4:A:2019:HOH:O	3:C:601:IPA:H13	1.96	0.65
1:C:203:ASP:OD1	1:C:231:ARG:HB2	1.97	0.65
1:D:165:GLN:HE22	1:D:375:ASN:HD21	1.45	0.65
1:D:43:ILE:HG21	1:D:120:MET:CE	2.25	0.65
1:D:156:ASN:ND2	1:D:158:LYS:H	1.94	0.65
1:A:417:HIS:ND1	4:A:1745:HOH:O	2.30	0.65
1:B:39:ASN:ND2	1:B:57:GLY:HA2	2.11	0.65
1:D:9:VAL:N	1:D:46:ASN:OD1	2.30	0.64
1:D:4:GLN:CD	1:D:5:PHE:H	2.02	0.64
1:D:214:GLU:CD	1:D:214:GLU:H	2.01	0.63
1:B:187:ALA:HA	1:B:190:ARG:HG3	1.80	0.63
1:A:6:THR:O	1:C:5:PHE:HA	1.98	0.63
1:A:439:ASN:C	1:A:439:ASN:HD22	2.02	0.63
1:B:91:PHE:HB3	1:B:94:ARG:HD3	1.80	0.62
1:B:187:ALA:HA	1:B:190:ARG:CG	2.29	0.62
1:C:377:ARG:HD2	1:C:379:THR:O	1.99	0.62
1:B:414:TYR:CA	1:B:419:LEU:HD12	2.28	0.62
1:C:262:PRO:HD2	1:C:275:MET:SD	2.39	0.62
1:B:68:ALA:C	1:B:70:PRO:HD2	2.19	0.62
1:A:346:ILE:HD11	1:A:402:ILE:HD12	1.81	0.62
1:C:16:ILE:HD13	1:C:408:MET:HE1	1.82	0.62
1:B:147:MET:HE1	1:B:351:PHE:CE2	2.28	0.62
1:C:24:MET:HE2	1:C:155:GLY:HA3	1.81	0.62
1:B:180:GLU:O	1:B:190:ARG:NH2	2.30	0.61
1:D:59:GLU:OE1	1:D:62:ARG:NH2	2.27	0.61
1:D:197:GLU:HG2	4:D:1864:HOH:O	1.98	0.61
1:D:24:MET:CE	1:D:431:LEU:HD11	2.31	0.61
1:D:214:GLU:OE2	1:D:214:GLU:N	2.33	0.61
1:D:267:GLN:NE2	4:D:1455:HOH:O	2.25	0.61
1:D:13:MET:HG3	1:D:43:ILE:HG12	1.82	0.61
1:B:233:THR:HA	1:B:256:LEU:HD22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ASN:HB2	1:D:339:HIS:CD2	2.36	0.61
1:D:55:ILE:HD11	1:D:65:LEU:HD11	1.82	0.60
1:B:428:MET:HA	1:B:431:LEU:HD13	1.84	0.60
1:C:313:ASP:HB2	1:C:339:HIS:CD2	2.36	0.60
1:B:21:HIS:H	1:B:376:GLN:NE2	1.99	0.60
1:C:21:HIS:H	1:C:376:GLN:NE2	1.99	0.60
1:A:55:ILE:HB	1:A:56:PRO:CD	2.32	0.60
1:A:143:SER:HB2	4:A:1942:HOH:O	2.01	0.60
1:B:175:TYR:OH	1:B:198:LYS:HE2	2.02	0.60
1:C:236:PRO:HG2	1:C:262:PRO:HA	1.84	0.60
1:B:344:PHE:CD1	1:B:378:LEU:HD11	2.37	0.59
1:A:273:GLU:O	1:A:277:GLU:HG3	2.01	0.59
1:A:324:ARG:NH2	1:C:331:GLU:OE1	2.33	0.59
1:D:55:ILE:HB	1:D:56:PRO:CD	2.32	0.59
1:D:55:ILE:HB	1:D:56:PRO:HD2	1.85	0.59
1:D:384:GLU:CB	1:D:386:LYS:HE3	2.31	0.59
1:C:26:MET:CE	1:C:26:MET:CA	2.81	0.59
1:D:332:PHE:CD2	3:D:604:IPA:H11	2.38	0.59
1:D:411:HIS:O	1:D:414:TYR:HB3	2.03	0.59
1:A:26:MET:CE	1:A:444:MET:CE	2.81	0.58
1:B:182:ALA:C	1:B:183:MET:HG2	2.22	0.58
1:B:193:GLU:OE1	1:B:226:ARG:NE	2.35	0.58
1:D:302:LEU:HD22	3:D:604:IPA:H12	1.86	0.58
1:B:226:ARG:HG3	1:B:227:PHE:CD1	2.39	0.58
1:A:174:TRP:HZ3	1:A:191:LEU:HD22	1.69	0.58
1:A:34:PRO:HG3	1:A:162:LEU:HB3	1.86	0.58
1:B:33:ALA:HB1	1:B:34:PRO:HD2	1.86	0.57
1:D:13:MET:HB3	1:D:69:ILE:HG23	1.86	0.57
1:B:177:LEU:O	1:B:190:ARG:NH1	2.37	0.57
1:A:67:ASP:O	1:A:70:PRO:HD2	2.05	0.57
1:D:24:MET:HE1	1:D:431:LEU:HD11	1.85	0.57
1:D:63:LYS:O	1:D:66:GLU:HB3	2.05	0.57
1:A:156:ASN:ND2	1:A:158:LYS:H	2.04	0.56
1:C:34:PRO:HG3	1:C:162:LEU:HB3	1.88	0.56
1:C:346:ILE:HD11	1:C:402:ILE:HD12	1.87	0.56
1:D:205:LYS:HD2	4:D:1235:HOH:O	2.05	0.56
1:D:67:ASP:O	1:D:70:PRO:HD2	2.05	0.56
1:B:187:ALA:CA	1:B:190:ARG:HG3	2.36	0.56
1:A:267:GLN:OE1	4:A:1927:HOH:O	2.17	0.56
1:A:26:MET:CE	1:A:444:MET:HE3	2.35	0.56
1:D:432:ILE:O	1:D:435:TRP:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:VAL:O	1:C:225:GLN:HG3	2.04	0.56
1:A:6:THR:HG22	1:C:5:PHE:CE2	2.41	0.56
1:B:262:PRO:HD2	1:B:275:MET:SD	2.46	0.56
1:D:4:GLN:NE2	1:D:6:THR:HG23	2.21	0.55
1:D:110:ILE:CG2	1:D:111:HIS:N	2.68	0.55
1:D:8:PRO:HA	1:D:46:ASN:HD21	1.71	0.55
1:D:279:ARG:HG3	1:D:286:THR:HG23	1.87	0.55
1:B:5:PHE:CZ	1:D:46:ASN:ND2	2.75	0.55
1:A:320:GLN:HG2	4:A:1339:HOH:O	2.07	0.54
1:C:133:ALA:H	1:C:353:HIS:HD2	1.53	0.54
1:D:44:LYS:HE2	1:D:50:THR:OG1	2.07	0.54
1:B:128:LEU:HA	1:D:7:THR:HG21	1.89	0.54
1:C:24:MET:HE1	1:C:155:GLY:HA3	1.90	0.54
1:D:27:ASN:OD1	1:D:29:SER:OG	2.22	0.54
1:B:55:ILE:HD12	1:B:61:ILE:HG21	1.90	0.54
1:B:131:ASN:HD22	1:B:131:ASN:C	2.09	0.54
1:D:445:VAL:O	1:D:446:ARG:HD3	2.08	0.54
1:C:207:LYS:NZ	1:C:237:ASN:HD21	2.06	0.54
1:D:417:HIS:HB3	1:D:419:LEU:CG	2.37	0.54
1:A:174:TRP:CZ3	1:A:191:LEU:HD22	2.43	0.54
1:D:417:HIS:HB2	1:D:419:LEU:HG	1.89	0.54
1:D:445:VAL:C	1:D:446:ARG:HG2	2.28	0.54
1:B:344:PHE:CG	1:B:378:LEU:HD11	2.43	0.54
1:D:226:ARG:HG3	1:D:226:ARG:O	2.06	0.53
1:B:233:THR:HA	1:B:256:LEU:CD2	2.38	0.53
1:D:186:ASP:O	1:D:190:ARG:HG3	2.08	0.53
1:D:313:ASP:N	1:D:339:HIS:CE1	2.72	0.53
1:A:133:ALA:H	1:A:353:HIS:HD2	1.57	0.53
1:B:207:LYS:HG3	1:B:208:GLY:N	2.24	0.53
1:C:24:MET:CE	1:C:431:LEU:HD11	2.37	0.53
1:D:69:ILE:N	1:D:70:PRO:CD	2.72	0.53
1:B:81:LYS:NZ	4:B:1075:HOH:O	2.30	0.53
1:C:64:THR:HB	1:C:112:VAL:HG21	1.90	0.53
1:B:209:GLY:O	1:B:442:PRO:HA	2.08	0.53
1:A:197:GLU:O	1:A:197:GLU:HG2	2.07	0.52
1:B:253:LYS:HE2	1:B:282:THR:O	2.09	0.52
1:A:428:MET:CE	1:A:444:MET:CE	2.83	0.52
1:A:148:LEU:HD12	1:A:148:LEU:C	2.30	0.52
1:B:71:LEU:HD22	1:B:86:LEU:HD21	1.92	0.52
1:D:417:HIS:CB	1:D:419:LEU:CG	2.87	0.52
1:A:80:TYR:OH	1:A:81:LYS:HE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:THR:HA	4:A:1902:HOH:O	2.09	0.52
1:C:25:LEU:C	1:C:26:MET:CE	2.78	0.52
1:A:414:TYR:OH	4:A:2001:HOH:O	2.18	0.52
1:D:402:ILE:O	1:D:402:ILE:HG23	2.08	0.52
1:B:377:ARG:HG3	1:B:377:ARG:HH11	1.74	0.52
1:B:414:TYR:O	1:B:419:LEU:HD12	2.09	0.52
1:D:233:THR:HG21	1:D:258:TYR:CZ	2.43	0.52
1:A:233:THR:HG21	1:A:258:TYR:CZ	2.45	0.52
1:B:25:LEU:HB3	1:B:152:PHE:CD1	2.46	0.51
1:B:366:ASP:OD2	4:B:1540:HOH:O	2.19	0.51
1:C:88:ARG:NH2	1:C:110:ILE:HD11	2.25	0.51
1:D:68:ALA:C	1:D:70:PRO:HD2	2.30	0.51
1:B:265:ALA:O	1:B:266:GLU:HB3	2.10	0.51
1:B:205:LYS:HB2	1:B:233:THR:HG22	1.93	0.51
1:C:67:ASP:O	1:C:70:PRO:HD2	2.10	0.51
1:C:342:ASN:HD22	1:C:372:GLN:HE22	1.59	0.51
1:D:69:ILE:N	1:D:70:PRO:HD2	2.26	0.51
1:D:203:ASP:OD2	1:D:231:ARG:HB2	2.10	0.51
1:A:26:MET:HE1	1:A:444:MET:HE1	1.93	0.50
1:B:59:GLU:OE1	1:B:62:ARG:NE	2.34	0.50
1:D:236:PRO:HD2	1:D:260:GLU:O	2.11	0.50
1:A:429:GLN:OE1	1:A:429:GLN:HA	2.12	0.50
1:D:229:GLN:OE1	1:D:229:GLN:HA	2.11	0.50
1:D:233:THR:HG21	1:D:258:TYR:CE1	2.46	0.50
1:D:408:MET:HE3	1:D:411:HIS:HB3	1.93	0.50
1:B:99:ARG:O	1:B:99:ARG:HG2	2.11	0.50
1:B:184:THR:HG23	1:B:185:PRO:HD2	1.94	0.50
1:D:417:HIS:HB2	1:D:419:LEU:CD1	2.42	0.50
1:A:133:ALA:H	1:A:353:HIS:CD2	2.29	0.50
1:A:292:ALA:HA	1:A:297:GLN:HB3	1.93	0.50
1:C:293:THR:N	1:C:297:GLN:HE21	2.04	0.50
1:A:71:LEU:HD22	1:A:86:LEU:HD21	1.94	0.50
1:D:120:MET:HE1	1:D:123:LEU:CD1	2.37	0.50
1:A:233:THR:HG21	1:A:258:TYR:CE1	2.47	0.50
1:B:83:VAL:O	1:B:87:VAL:HG23	2.11	0.50
1:C:445:VAL:O	1:C:446:ARG:HD3	2.11	0.50
1:D:429:GLN:NE2	1:D:434:GLY:N	2.59	0.50
1:C:26:MET:N	1:C:26:MET:CE	2.74	0.50
1:A:26:MET:CE	1:A:444:MET:HE1	2.42	0.49
1:A:114:THR:OG1	1:A:318:THR:HA	2.13	0.49
1:B:69:ILE:N	1:B:70:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLN:NE2	1:B:415:GLN:HA	2.27	0.49
1:C:272:ARG:HA	1:C:291:ILE:HD12	1.95	0.49
1:B:27:ASN:OD1	1:B:29:SER:HB2	2.13	0.49
1:B:55:ILE:HB	1:B:56:PRO:HD2	1.94	0.49
1:B:133:ALA:HB2	1:B:353:HIS:HD2	1.77	0.49
1:D:150:TYR:CZ	1:D:205:LYS:NZ	2.78	0.49
1:D:332:PHE:CD2	3:D:604:IPA:C1	2.96	0.49
1:C:16:ILE:HD13	1:C:408:MET:HE3	1.93	0.49
1:D:293:THR:N	1:D:297:GLN:HE21	1.98	0.49
1:A:190:ARG:HD3	4:A:1715:HOH:O	2.13	0.48
1:B:232:ILE:CG2	1:B:233:THR:N	2.76	0.48
1:D:156:ASN:HD21	1:D:158:LYS:HB2	1.78	0.48
1:D:339:HIS:HB2	4:D:2073:HOH:O	2.13	0.48
1:B:103:THR:HG22	1:B:237:ASN:CG	2.33	0.48
1:C:24:MET:O	1:C:26:MET:HE3	2.13	0.48
1:D:431:LEU:C	1:D:432:ILE:HG13	2.34	0.48
1:A:160:THR:HB	1:A:161:PRO:HD2	1.96	0.48
1:A:261:ASP:N	1:A:262:PRO:CD	2.76	0.48
1:D:43:ILE:CD1	1:D:120:MET:CE	2.91	0.48
1:D:217:ALA:O	1:D:221:VAL:HG23	2.13	0.48
1:A:6:THR:HG22	1:C:5:PHE:CD2	2.49	0.48
1:A:432:ILE:HG22	1:A:432:ILE:O	2.13	0.48
1:D:167:GLN:N	1:D:168:PRO:HD3	2.29	0.48
1:A:375:ASN:N	1:A:375:ASN:ND2	2.48	0.48
1:A:439:ASN:HD22	1:A:440:LYS:N	2.12	0.48
1:B:187:ALA:O	1:B:190:ARG:CG	2.59	0.48
1:B:190:ARG:HH11	1:B:191:LEU:CD2	2.27	0.48
1:C:79:GLU:OE2	4:C:1526:HOH:O	2.20	0.48
1:B:29:SER:OG	1:B:102:GLN:NE2	2.47	0.48
1:D:4:GLN:HE21	1:D:6:THR:HG23	1.78	0.48
1:B:445:VAL:O	1:B:445:VAL:HG12	2.14	0.47
1:D:93:ASP:CG	1:D:94:ARG:H	2.16	0.47
1:D:114:THR:OG1	1:D:318:THR:HA	2.15	0.47
1:D:240:TRP:HB3	1:D:244:GLU:HB2	1.96	0.47
1:D:109:THR:O	1:D:113:VAL:HG23	2.15	0.47
1:A:21:HIS:H	1:A:376:GLN:NE2	2.11	0.47
1:B:9:VAL:HG12	1:B:46:ASN:ND2	2.29	0.47
1:B:190:ARG:NH1	1:B:191:LEU:HD21	2.30	0.47
1:B:344:PHE:CG	1:B:378:LEU:CD1	2.98	0.47
4:B:1656:HOH:O	3:D:602:IPA:H31	2.14	0.47
1:D:17:PRO:O	1:D:411:HIS:HD2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:VAL:HG21	1:D:116:ILE:HD13	1.96	0.47
1:D:408:MET:HE3	1:D:411:HIS:CB	2.44	0.47
1:B:173:ASP:HB2	4:B:1761:HOH:O	2.14	0.47
1:C:133:ALA:H	1:C:353:HIS:CD2	2.32	0.47
1:D:46:ASN:C	1:D:46:ASN:HD22	2.18	0.47
1:D:110:ILE:HD12	1:D:110:ILE:HA	1.59	0.47
1:A:239:ALA:O	1:A:440:LYS:HD3	2.14	0.47
1:A:313:ASP:OD2	1:A:314:PRO:HD2	2.14	0.47
1:B:175:TYR:CZ	1:B:198:LYS:HE2	2.50	0.47
1:B:184:THR:CG2	1:B:185:PRO:HD2	2.45	0.47
1:C:233:THR:HG21	1:C:258:TYR:CE1	2.49	0.47
1:B:108:THR:O	1:B:112:VAL:HG23	2.14	0.47
1:B:13:MET:HA	1:B:42:ILE:O	2.15	0.46
1:A:414:TYR:HA	1:A:419:LEU:HD12	1.96	0.46
1:A:395:LYS:HB2	1:A:396:PRO:HD2	1.97	0.46
1:C:114:THR:OG1	1:C:318:THR:HA	2.15	0.46
1:A:137:GLY:O	1:C:81:LYS:NZ	2.27	0.46
1:A:331:GLU:HB3	1:C:295:TRP:HB3	1.98	0.46
1:B:294:ASP:OD1	1:B:297:GLN:HG3	2.16	0.46
1:D:33:ALA:HB1	1:D:34:PRO:HD2	1.98	0.46
1:B:275:MET:HG3	1:B:291:ILE:HD13	1.98	0.46
1:D:131:ASN:ND2	1:D:134:SER:H	2.13	0.46
1:A:224:ALA:HA	1:A:232:ILE:HD12	1.98	0.46
1:B:59:GLU:CD	1:B:62:ARG:HE	2.16	0.46
1:B:431:LEU:N	1:B:431:LEU:HD12	2.30	0.46
1:B:212:ALA:O	1:B:215:GLU:HB2	2.15	0.46
1:B:34:PRO:HG3	1:B:162:LEU:HB3	1.97	0.45
1:C:124:LEU:HD23	1:C:135:LEU:HD13	1.97	0.45
1:C:417:HIS:HE1	4:C:1599:HOH:O	1.99	0.45
1:D:402:ILE:HG22	4:D:1464:HOH:O	2.16	0.45
1:C:361:LYS:C	1:C:361:LYS:HD3	2.37	0.45
1:C:375:ASN:H	1:C:375:ASN:ND2	2.10	0.45
1:D:83:VAL:O	1:D:87:VAL:HG23	2.16	0.45
1:D:431:LEU:O	1:D:432:ILE:HG13	2.16	0.45
3:A:603:IPA:H33	1:C:302:LEU:HB3	1.99	0.45
1:C:375:ASN:HD22	1:C:375:ASN:N	2.05	0.45
1:D:156:ASN:C	1:D:156:ASN:HD22	2.19	0.45
1:B:377:ARG:HB2	1:B:382:PRO:HG3	1.98	0.45
1:C:88:ARG:CZ	1:C:110:ILE:HD11	2.46	0.45
1:A:286:THR:OG1	1:A:307:VAL:HA	2.17	0.45
1:B:166:SER:HA	1:B:179:HIS:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:PRO:HB3	1:B:219:SER:HA	1.97	0.45
1:A:261:ASP:N	1:A:262:PRO:HD3	2.31	0.45
1:C:80:TYR:O	1:C:84:LEU:HG	2.17	0.45
1:D:317:TRP:O	1:D:321:GLY:HA3	2.16	0.45
1:A:73:VAL:HG12	1:A:74:GLY:N	2.32	0.45
1:A:88:ARG:HD2	4:A:1563:HOH:O	2.17	0.45
1:B:226:ARG:HG3	1:B:227:PHE:CE1	2.51	0.45
1:B:21:HIS:N	1:B:376:GLN:HE22	2.06	0.45
1:B:25:LEU:HB2	1:B:32:HIS:CG	2.52	0.45
1:B:187:ALA:HA	1:B:190:ARG:HG2	1.98	0.45
1:B:371:TRP:HB2	1:B:372:GLN:HE22	1.81	0.44
1:A:25:LEU:HB3	1:A:152:PHE:CD1	2.53	0.44
1:D:110:ILE:HG23	1:D:111:HIS:N	2.32	0.44
1:C:21:HIS:N	1:C:376:GLN:HE22	2.09	0.44
1:A:438:ASP:OD2	1:A:438:ASP:C	2.56	0.44
1:B:67:ASP:O	1:B:70:PRO:HD2	2.17	0.44
1:D:111:HIS:HD2	1:D:315:HIS:O	2.01	0.44
1:D:111:HIS:NE2	1:D:316:PHE:CE1	2.84	0.44
1:A:5:PHE:HA	1:C:6:THR:O	2.17	0.44
1:B:64:THR:HB	1:B:112:VAL:HG21	2.00	0.44
1:B:344:PHE:CB	1:B:378:LEU:HD12	2.47	0.44
1:B:395:LYS:H	1:B:395:LYS:HG2	1.60	0.44
1:B:45:ASP:OD2	1:B:45:ASP:C	2.56	0.44
1:A:184:THR:HB	1:A:185:PRO:HD2	2.00	0.44
1:C:9:VAL:HG12	1:C:46:ASN:CG	2.38	0.44
1:C:313:ASP:HB2	1:C:339:HIS:NE2	2.32	0.44
1:A:376:GLN:O	1:A:377:ARG:HB3	2.17	0.43
1:D:408:MET:O	1:D:411:HIS:HB3	2.18	0.43
1:D:429:GLN:NE2	1:D:429:GLN:HA	2.33	0.43
1:C:265:ALA:O	1:C:266:GLU:HB3	2.17	0.43
1:C:45:ASP:OD2	1:C:45:ASP:C	2.57	0.43
1:A:185:PRO:HB3	1:A:219:SER:HA	2.00	0.43
1:B:19:ALA:HB2	1:B:37:THR:HG22	2.00	0.43
1:C:24:MET:HG2	1:C:26:MET:HE1	2.00	0.43
1:C:131:ASN:ND2	1:C:134:SER:OG	2.50	0.43
1:D:24:MET:HE2	1:D:431:LEU:HD11	1.98	0.43
1:D:262:PRO:HD2	1:D:275:MET:SD	2.59	0.43
1:A:17:PRO:HG3	1:A:62:ARG:HD3	2.01	0.43
1:A:339:HIS:CD2	4:A:1489:HOH:O	2.71	0.43
1:C:20:GLY:O	1:C:35:PHE:HA	2.19	0.43
1:A:9:VAL:HG22	1:A:76:THR:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ASP:N	1:B:262:PRO:HD3	2.34	0.43
1:C:269:PHE:CZ	1:D:296:ARG:HD3	2.53	0.43
1:C:8:PRO:HB3	1:C:47:SER:HB3	2.01	0.43
1:A:91:PHE:O	1:A:109:THR:OG1	2.25	0.43
1:A:29:SER:O	1:A:424:ASP:HB2	2.19	0.42
1:A:202:ASN:O	1:A:230:ALA:HB1	2.19	0.42
1:C:18:VAL:HB	1:C:410:ALA:HB1	2.00	0.42
1:C:342:ASN:HD22	1:C:372:GLN:NE2	2.16	0.42
1:B:301:THR:HG23	1:B:306:SER:HB2	2.01	0.42
1:C:55:ILE:HB	1:C:56:PRO:CD	2.49	0.42
1:D:440:LYS:HB3	4:D:1331:HOH:O	2.17	0.42
1:B:313:ASP:HB3	1:B:316:PHE:CE1	2.54	0.42
1:B:442:PRO:HG3	4:B:1781:HOH:O	2.19	0.42
1:C:205:LYS:HG3	1:C:233:THR:OG1	2.19	0.42
1:D:117:GLU:OE1	1:D:320:GLN:HG3	2.19	0.42
1:A:76:THR:O	1:A:79:GLU:HB2	2.19	0.42
1:D:287:ALA:HA	1:D:309:ILE:O	2.20	0.42
1:D:417:HIS:C	1:D:419:LEU:H	2.22	0.42
1:B:342:ASN:HD22	1:B:372:GLN:NE2	2.17	0.42
1:D:162:LEU:HD11	1:D:430:TYR:CE1	2.54	0.42
1:D:417:HIS:CB	1:D:419:LEU:CD1	2.97	0.42
1:B:384:GLU:CB	1:B:386:LYS:HE3	2.46	0.42
1:C:309:ILE:O	1:C:309:ILE:HG22	2.18	0.42
1:A:184:THR:O	1:A:187:ALA:HB3	2.19	0.42
1:A:415:GLN:O	1:A:417:HIS:O	2.37	0.42
1:B:148:LEU:C	1:B:148:LEU:HD12	2.40	0.42
1:B:309:ILE:HA	1:B:335:THR:O	2.20	0.42
1:B:69:ILE:N	1:B:70:PRO:HD2	2.35	0.42
1:A:221:VAL:O	1:A:225:GLN:HG3	2.20	0.42
1:A:342:ASN:HD22	1:A:372:GLN:NE2	2.18	0.42
1:B:261:ASP:OD2	4:B:1365:HOH:O	2.21	0.42
1:B:295:TRP:HB3	1:D:331:GLU:HB3	2.01	0.42
1:D:173:ASP:O	1:D:177:LEU:HD12	2.20	0.42
1:C:55:ILE:HD11	1:C:65:LEU:CD1	2.47	0.42
1:D:214:GLU:CD	1:D:214:GLU:N	2.71	0.42
1:A:408:MET:O	1:A:412:GLU:HG3	2.20	0.41
1:D:7:THR:HA	1:D:8:PRO:HD3	1.83	0.41
1:D:384:GLU:OE1	1:D:386:LYS:HE2	2.20	0.41
1:A:376:GLN:NE2	4:A:1507:HOH:O	2.23	0.41
1:C:273:GLU:O	1:C:277:GLU:HG3	2.20	0.41
1:D:162:LEU:HA	1:D:163:PRO:HD3	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:HIS:N	1:A:376:GLN:HE22	2.15	0.41
1:A:156:ASN:C	1:A:156:ASN:HD22	2.24	0.41
1:A:345:ASP:OD1	1:A:379:THR:OG1	2.26	0.41
1:B:37:THR:HG22	1:B:414:TYR:HD2	1.86	0.41
1:B:342:ASN:HD22	1:B:372:GLN:HE22	1.67	0.41
1:A:295:TRP:HB3	1:C:331:GLU:HB3	2.01	0.41
1:B:331:GLU:HB3	1:D:295:TRP:CB	2.51	0.41
1:C:287:ALA:HA	1:C:309:ILE:O	2.20	0.41
1:A:110:ILE:HD13	1:A:110:ILE:HA	1.95	0.41
1:A:201:PHE:HB2	1:A:204:PHE:CZ	2.55	0.41
1:A:224:ALA:HA	1:A:232:ILE:CD1	2.51	0.41
1:A:342:ASN:HD22	1:A:372:GLN:HE22	1.69	0.41
1:B:72:VAL:HG21	1:B:116:ILE:HD13	2.02	0.41
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.88	0.41
1:B:131:ASN:ND2	1:B:134:SER:H	2.18	0.41
1:A:395:LYS:HD2	4:A:1357:HOH:O	2.21	0.41
1:A:404:MET:O	1:A:408:MET:HG2	2.21	0.41
1:B:278:PHE:CD1	1:B:278:PHE:C	2.95	0.41
1:C:132:VAL:HG23	1:C:397:GLY:C	2.40	0.41
1:D:156:ASN:HD22	1:D:158:LYS:H	1.66	0.41
1:D:167:GLN:N	1:D:168:PRO:CD	2.83	0.41
1:A:289:ASN:CG	1:A:339:HIS:CD2	2.94	0.41
1:B:190:ARG:HD2	1:B:191:LEU:HG	2.02	0.41
1:B:313:ASP:OD1	1:B:339:HIS:HD2	2.04	0.41
1:B:377:ARG:HH11	1:B:377:ARG:CG	2.33	0.40
1:A:324:ARG:HG2	1:A:324:ARG:HH11	1.85	0.40
1:C:55:ILE:HB	1:C:56:PRO:HD2	2.04	0.40
1:B:148:LEU:HD12	1:B:148:LEU:O	2.20	0.40
1:C:278:PHE:CD1	1:C:278:PHE:C	2.93	0.40
1:D:237:ASN:OD1	4:D:1869:HOH:O	2.22	0.40
1:A:204:PHE:O	1:A:232:ILE:HA	2.21	0.40
1:C:417:HIS:HB2	1:C:419:LEU:HG	2.04	0.40
1:A:8:PRO:HG3	1:A:47:SER:HB3	2.03	0.40
1:A:27:ASN:N	1:A:27:ASN:HD22	2.20	0.40
1:A:184:THR:O	1:A:188:VAL:HG23	2.22	0.40
1:D:14:GLN:HG2	1:D:16:ILE:HG13	2.03	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)
4:A:2002:HOH:O	4:C:2036:HOH:O[1_455]	0.88	1.32

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	425/446 (95%)	409 (96%)	16 (4%)	0	100	100
1	B	436/446 (98%)	410 (94%)	25 (6%)	1 (0%)	47	38
1	C	425/446 (95%)	410 (96%)	14 (3%)	1 (0%)	47	38
1	D	427/446 (96%)	409 (96%)	17 (4%)	1 (0%)	47	38
All	All	1713/1784 (96%)	1638 (96%)	72 (4%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	ARG
1	C	435	TRP
1	D	93	ASP

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	343/362 (95%)	331 (96%)	12 (4%)	36	27
1	B	353/362 (98%)	343 (97%)	10 (3%)	43	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	345/362 (95%)	336 (97%)	9 (3%)	46	39
1	D	343/362 (95%)	331 (96%)	12 (4%)	36	27
All	All	1384/1448 (96%)	1341 (97%)	43 (3%)	40	32

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	150	TYR
1	A	156	ASN
1	A	160	THR
1	A	324	ARG
1	A	361	LYS
1	A	375	ASN
1	A	395	LYS
1	A	419	LEU
1	A	426	MET
1	A	436	THR
1	A	439	ASN
1	B	106	LEU
1	B	131	ASN
1	B	150	TYR
1	B	197	GLU
1	B	205	LYS
1	B	207	LYS
1	B	339	HIS
1	B	395	LYS
1	B	419	LEU
1	B	428	MET
1	C	27	ASN
1	C	88	ARG
1	C	131	ASN
1	C	150	TYR
1	C	160	THR
1	C	237	ASN
1	C	361	LYS
1	C	375	ASN
1	C	439	ASN
1	D	4	GLN
1	D	7	THR
1	D	46	ASN

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Mol	Chain	Res	Type
1	D	131	ASN
1	D	147	MET
1	D	150	TYR
1	D	156	ASN
1	D	160	THR
1	D	207	LYS
1	D	279	ARG
1	D	439	ASN
1	D	441	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	39	ASN
1	A	111	HIS
1	A	141	GLN
1	A	156	ASN
1	A	297	GLN
1	A	353	HIS
1	A	372	GLN
1	A	375	ASN
1	A	376	GLN
1	A	391	GLN
1	A	415	GLN
1	A	417	HIS
1	A	439	ASN
1	B	102	GLN
1	B	131	ASN
1	B	140	GLN
1	B	156	ASN
1	B	237	ASN
1	B	353	HIS
1	B	372	GLN
1	B	376	GLN
1	B	415	GLN
1	C	27	ASN
1	C	131	ASN
1	C	140	GLN
1	C	165	GLN
1	C	167	GLN
1	C	237	ASN

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Mol	Chain	Res	Type
1	C	243	ASN
1	C	297	GLN
1	C	353	HIS
1	C	372	GLN
1	C	375	ASN
1	C	376	GLN
1	C	415	GLN
1	C	439	ASN
1	D	4	GLN
1	D	21	HIS
1	D	131	ASN
1	D	140	GLN
1	D	141	GLN
1	D	156	ASN
1	D	165	GLN
1	D	243	ASN
1	D	297	GLN
1	D	305	GLN
1	D	339	HIS
1	D	376	GLN
1	D	391	GLN
1	D	415	GLN
1	D	429	GLN
1	D	439	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	IPA	D	602	-	3,3,3	0.50	0	3,3,3	0.30	0
3	IPA	D	604	-	3,3,3	0.50	0	3,3,3	0.38	0
3	IPA	A	603	-	3,3,3	0.68	0	3,3,3	0.18	0
3	IPA	C	601	-	3,3,3	0.55	0	3,3,3	0.27	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	IPA	2	0
3	D	604	IPA	3	0
3	A	603	IPA	1	0
3	C	601	IPA	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	422:ARG	C	423:ASP	N	1.62

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(Å^2)	Q<0.9
1	A	429/446 (96%)	-0.45	4 (0%) 84 85	11, 23, 47, 88	0
1	B	440/446 (98%)	-0.31	3 (0%) 87 88	10, 30, 57, 81	0
1	C	428/446 (95%)	-0.56	0 100 100	10, 21, 45, 85	0
1	D	431/446 (96%)	-0.38	8 (1%) 66 69	11, 23, 57, 95	0
All	All	1728/1784 (96%)	-0.42	15 (0%) 84 85	10, 24, 53, 95	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	LEU	5.0
1	D	92	ALA	4.7
1	A	228	PRO	3.5
1	D	418	GLY	3.2
1	D	420	GLY	3.1
1	D	434	GLY	3.0
1	D	93	ASP	3.0
1	B	92	ALA	2.8
1	A	107	ARG	2.8
1	D	4	GLN	2.7
1	D	94	ARG	2.4
1	B	433	PRO	2.4
1	B	164	TYR	2.2
1	A	433	PRO	2.1
1	D	421	ALA	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	IPA	C	601	4/4	0.91	0.12	23,26,30,35	0
3	IPA	D	604	4/4	0.91	0.12	21,29,30,41	0
3	IPA	A	603	4/4	0.92	0.14	17,21,53,54	0
3	IPA	D	602	4/4	0.93	0.12	16,30,40,44	0
2	MG	B	498	1/1	0.95	0.05	25,25,25,25	0
2	MG	C	498	1/1	0.96	0.07	24,24,24,24	0
2	MG	A	498	1/1	0.97	0.07	17,17,17,17	0
2	MG	D	498	1/1	0.97	0.05	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.