Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 12:38 AM EST

PDB ID	:	1ECQ
Title	:	E. COLI GLUCARATE DEHYDRATASE BOUND TO 4-DEOXYGLUCARATE
Authors	:	Gulick, A.M.; Hubbard, B.K.; Gerlt, J.A.; Rayment, I.
Deposited on	:	2000-01-25
Resolution	:	2.00 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:

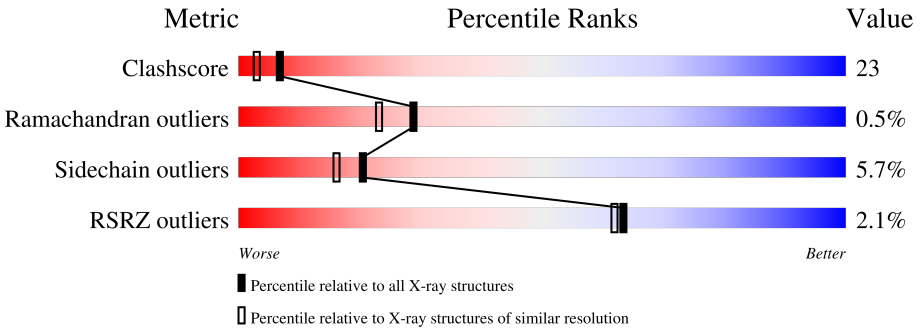
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	2% 57% 37% 5%
1	B	446	3% 49% 42% 8% •
1	C	446	2% 59% 34% 6% •
1	D	446	2% 55% 36% 8% ••

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
2	DXG	D	502	-	-	X	-
4	IPA	C	604	-	-	X	-

2 Entry composition (i)

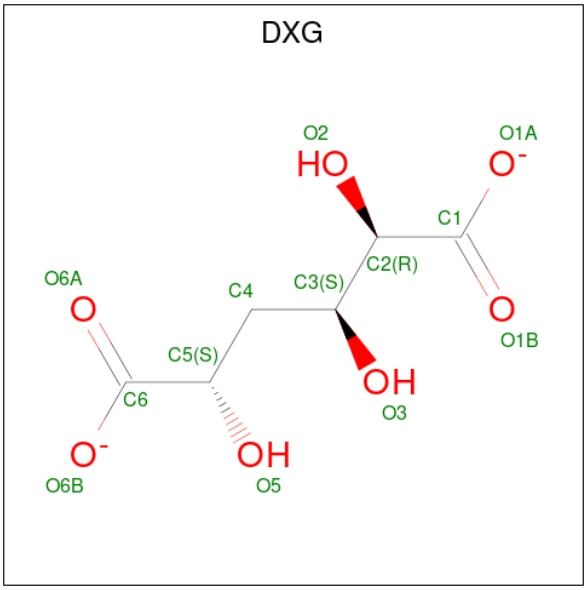
There are 5 unique types of molecules in this entry. The entry contains 14643 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	444	3436	2171	602	642	21	0	0	0
1	B	442	3408	2153	598	636	21	0	0	0
1	C	443	3421	2161	599	640	21	0	1	0
1	D	442	3405	2153	595	636	21	0	0	0

- Molecule 2 is 4-DEOXYGLUCARATE (three-letter code: DXG) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	6	7	0	0
2	B	1	13	6	7	0	0

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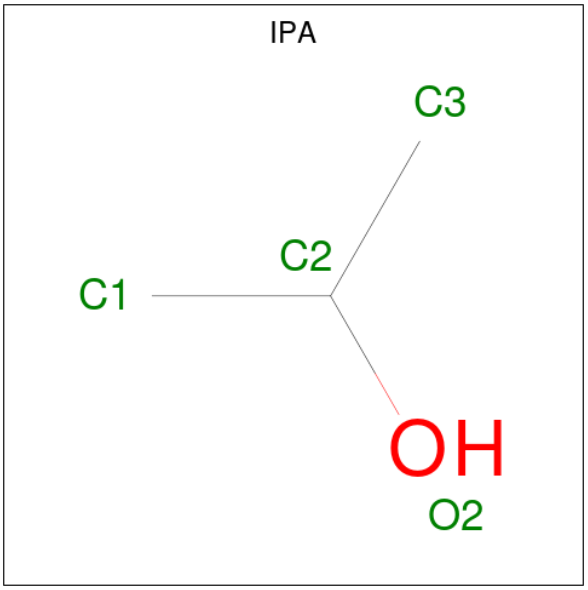
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0

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

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

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



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

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

- Molecule 5 is water.

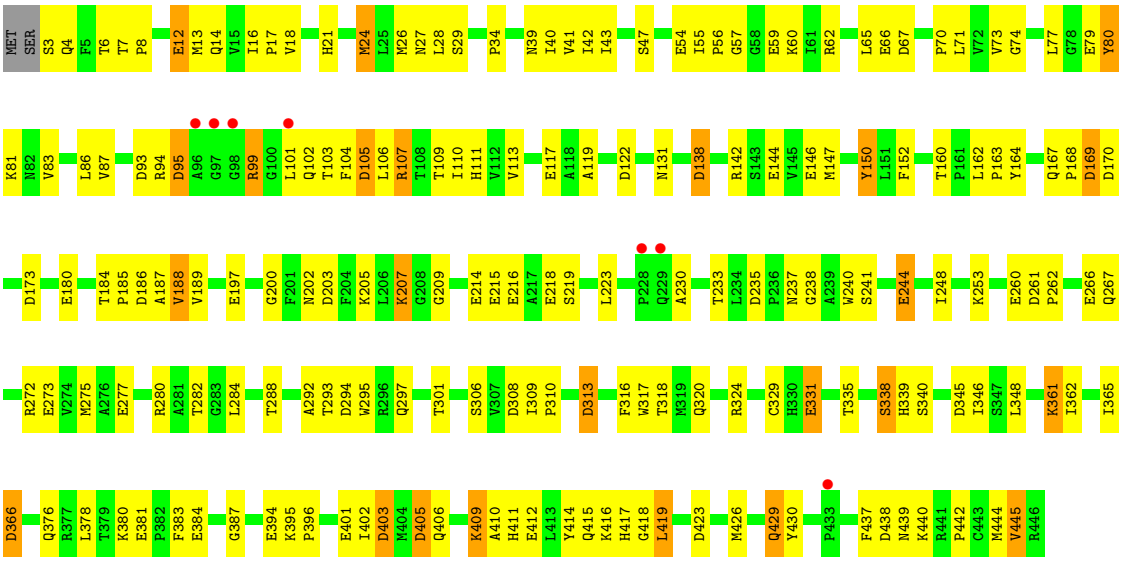
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	229	229	229	0	0
			Total	O		
5	B	168	168	168	0	0
			Total	O		
5	C	276	276	276	0	0
			Total	O		
5	D	228	228	228	0	0

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.

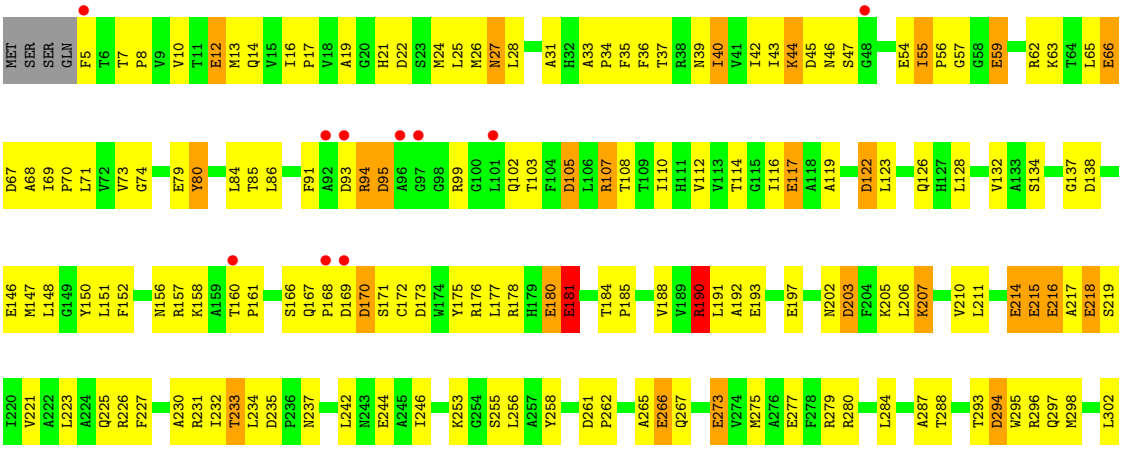
• Molecule 1: GLUCARATE DEHYDRATASE

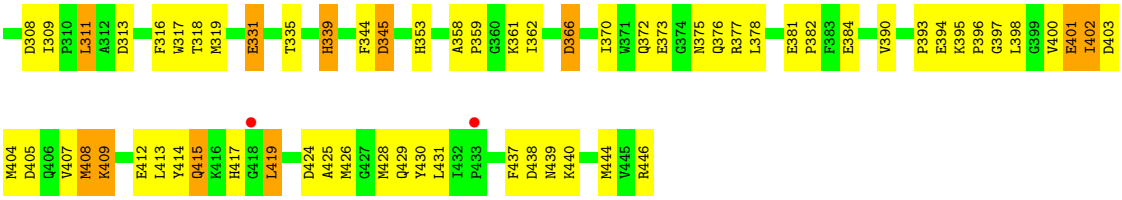
Chain A: 2% 57% 37% 5%



• Molecule 1: GLUCARATE DEHYDRATASE

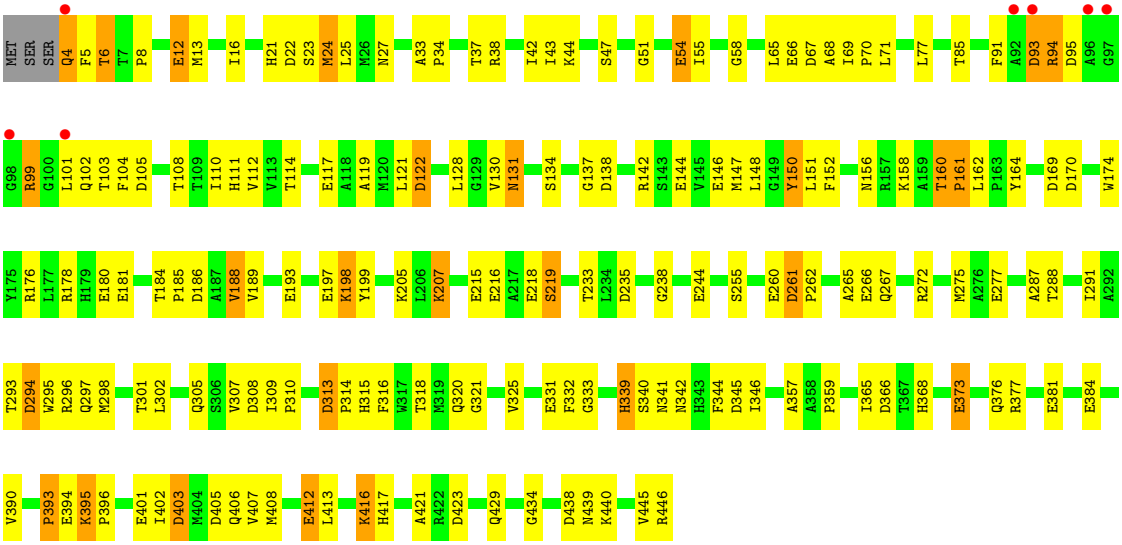
Chain B: 3% 49% 42% 8%





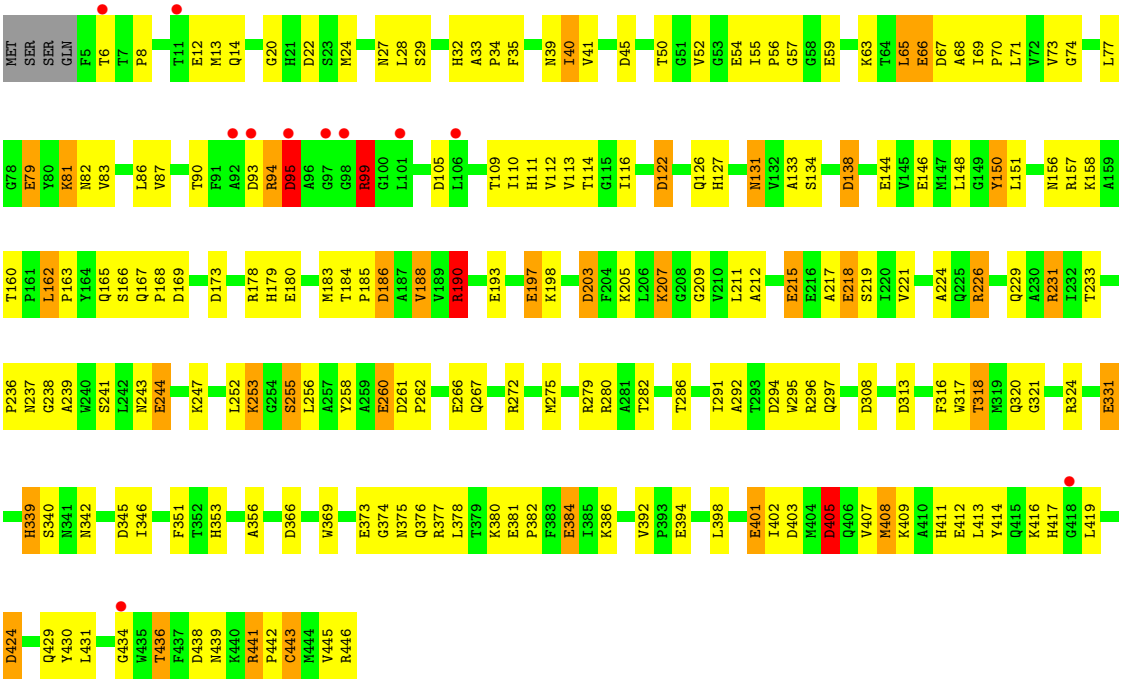
• Molecule 1: GLUCARATE DEHYDRATASE

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	71.11Å 84.60Å 98.78Å 103.46° 93.97° 113.03°	Depositor
Resolution (Å)	30.00 – 2.00 20.03 – 2.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 93.9 (20.03-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.90 (at 2.01Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.209 , 0.305 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 89.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14643	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: DXG, 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	1.03	21/3515 (0.6%)	1.28	39/4763 (0.8%)
1	B	1.00	24/3486 (0.7%)	1.26	39/4725 (0.8%)
1	C	1.04	19/3500 (0.5%)	1.25	34/4746 (0.7%)
1	D	1.04	21/3484 (0.6%)	1.30	45/4724 (1.0%)
All	All	1.03	85/13985 (0.6%)	1.27	157/18958 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	1	0

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	190	ARG	NE-CZ	12.02	1.48	1.33
1	C	412	GLU	CD-OE2	7.37	1.33	1.25
1	C	394	GLU	CD-OE2	7.32	1.33	1.25
1	B	331	GLU	CD-OE2	7.18	1.33	1.25
1	B	193	GLU	CD-OE2	7.15	1.33	1.25
1	C	244	GLU	CD-OE2	7.14	1.33	1.25
1	B	117	GLU	CD-OE2	7.13	1.33	1.25
1	A	394	GLU	CD-OE2	7.08	1.33	1.25
1	B	412	GLU	CD-OE2	6.86	1.33	1.25
1	D	54	GLU	CD-OE2	6.76	1.33	1.25
1	A	79	GLU	CD-OE2	6.62	1.32	1.25
1	C	180	GLU	CD-OE2	6.55	1.32	1.25
1	D	66	GLU	CD-OE2	6.52	1.32	1.25
1	D	384	GLU	CD-OE2	6.49	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	GLU	CD-OE2	6.48	1.32	1.25
1	C	146	GLU	CD-OE2	6.40	1.32	1.25
1	D	412	GLU	CD-OE2	6.40	1.32	1.25
1	B	244	GLU	CD-OE2	6.37	1.32	1.25
1	B	79	GLU	CD-OE2	6.36	1.32	1.25
1	B	180	GLU	CD-OE2	6.34	1.32	1.25
1	B	381	GLU	CD-OE2	6.31	1.32	1.25
1	A	197	GLU	CD-OE2	6.17	1.32	1.25
1	C	384	GLU	CD-OE2	6.15	1.32	1.25
1	D	144	GLU	CD-OE2	6.15	1.32	1.25
1	B	394	GLU	CD-OE2	6.12	1.32	1.25
1	B	215	GLU	CD-OE2	6.11	1.32	1.25
1	A	384	GLU	CD-OE2	6.09	1.32	1.25
1	A	66	GLU	CD-OE2	6.08	1.32	1.25
1	D	12	GLU	CD-OE2	6.05	1.32	1.25
1	D	197	GLU	CD-OE2	6.00	1.32	1.25
1	A	54	GLU	CD-OE2	6.00	1.32	1.25
1	C	197	GLU	CD-OE2	6.00	1.32	1.25
1	A	146	GLU	CD-OE2	5.97	1.32	1.25
1	B	216	GLU	CD-OE2	5.96	1.32	1.25
1	D	215	GLU	CD-OE2	5.96	1.32	1.25
1	D	244	GLU	CD-OE2	5.95	1.32	1.25
1	D	266	GLU	CD-OE2	5.94	1.32	1.25
1	D	260	GLU	CD-OE2	5.93	1.32	1.25
1	C	216	GLU	CD-OE1	-5.86	1.19	1.25
1	A	214	GLU	CD-OE2	5.85	1.32	1.25
1	B	214	GLU	CD-OE2	5.83	1.32	1.25
1	B	59	GLU	CD-OE2	5.82	1.32	1.25
1	C	215	GLU	CD-OE2	5.79	1.32	1.25
1	D	59	GLU	CD-OE2	5.79	1.32	1.25
1	C	381	GLU	CD-OE2	5.78	1.32	1.25
1	C	54	GLU	CD-OE2	5.77	1.31	1.25
1	D	193	GLU	CD-OE2	5.73	1.31	1.25
1	A	180	GLU	CD-OE2	5.71	1.31	1.25
1	D	180	GLU	CD-OE2	5.70	1.31	1.25
1	A	59	GLU	CD-OE2	5.68	1.31	1.25
1	A	218	GLU	CD-OE2	5.67	1.31	1.25
1	B	197	GLU	CD-OE2	5.66	1.31	1.25
1	B	12	GLU	CD-OE2	5.64	1.31	1.25
1	B	401	GLU	CD-OE2	5.64	1.31	1.25
1	A	216	GLU	CD-OE2	5.63	1.31	1.25
1	B	146	GLU	CD-OE2	5.60	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	GLU	CD-OE2	5.55	1.31	1.25
1	D	79	GLU	CD-OE2	5.54	1.31	1.25
1	A	266	GLU	CD-OE2	5.54	1.31	1.25
1	A	12	GLU	CD-OE2	5.50	1.31	1.25
1	C	401	GLU	CD-OE2	5.47	1.31	1.25
1	A	381	GLU	CD-OE2	5.45	1.31	1.25
1	B	273	GLU	CD-OE2	5.39	1.31	1.25
1	D	381	GLU	CD-OE2	5.39	1.31	1.25
1	D	218	GLU	CD-OE2	5.38	1.31	1.25
1	D	146	GLU	CD-OE2	5.37	1.31	1.25
1	A	412	GLU	CD-OE2	5.35	1.31	1.25
1	C	373	GLU	CD-OE2	5.30	1.31	1.25
1	D	401	GLU	CD-OE2	5.28	1.31	1.25
1	B	218	GLU	CD-OE2	5.28	1.31	1.25
1	A	215	GLU	CD-OE2	5.24	1.31	1.25
1	C	193	GLU	CD-OE2	5.24	1.31	1.25
1	A	244	GLU	CD-OE2	5.20	1.31	1.25
1	B	54	GLU	CD-OE2	5.18	1.31	1.25
1	C	277	GLU	CD-OE2	5.18	1.31	1.25
1	C	66	GLU	CD-OE2	5.17	1.31	1.25
1	C	12	GLU	CD-OE2	5.16	1.31	1.25
1	D	331	GLU	CD-OE2	5.16	1.31	1.25
1	A	331	GLU	CD-OE2	5.16	1.31	1.25
1	A	144	GLU	CD-OE2	5.14	1.31	1.25
1	B	373	GLU	CD-OE2	5.12	1.31	1.25
1	A	117	GLU	CD-OE2	5.09	1.31	1.25
1	B	181	GLU	CD-OE2	5.08	1.31	1.25
1	C	218	GLU	CD-OE2	5.07	1.31	1.25
1	C	260	GLU	CD-OE2	5.02	1.31	1.25

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	294	ASP	CB-CG-OD2	-9.85	109.44	118.30
1	B	67	ASP	CB-CG-OD2	-9.58	109.68	118.30
1	B	366	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	B	366	ASP	CB-CG-OD1	9.07	126.46	118.30
1	A	203	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	B	345	ASP	CB-CG-OD1	8.60	126.04	118.30
1	A	122	ASP	CB-CG-OD1	8.60	126.04	118.30
1	B	67	ASP	CB-CG-OD1	8.41	125.87	118.30
1	B	279	ARG	NE-CZ-NH1	8.21	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	324	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	D	441	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	D	122	ASP	CB-CG-OD1	7.80	125.32	118.30
1	C	294	ASP	CB-CG-OD1	7.75	125.27	118.30
1	D	138	ASP	CB-CG-OD1	7.74	125.26	118.30
1	A	324	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	B	122	ASP	CB-CG-OD2	-7.66	111.40	118.30
1	A	203	ASP	CB-CG-OD1	7.66	125.20	118.30
1	D	203	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	A	122	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	B	294	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	A	294	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	C	366	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	D	99	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	C	138	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	D	138	ASP	CB-CG-OD2	-7.34	111.70	118.30
1	A	308	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	C	308	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	D	67	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	A	235	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	B	424	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	D	122	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	B	294	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	294	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	203	ASP	CB-CG-OD2	-6.99	112.00	118.30
1	B	138	ASP	CB-CG-OD2	-6.97	112.02	118.30
1	D	441	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	308	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	D	169	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	138	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	D	345	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	B	138	ASP	CB-CG-OD1	6.81	124.43	118.30
1	D	45	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	167	GLN	C-N-CD	-6.79	105.66	120.60
1	B	95	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	D	294	ASP	CB-CG-OD1	6.74	124.36	118.30
1	D	226	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	D	93	ASP	CB-CG-OD1	6.63	124.27	118.30
1	D	294	ASP	CB-CG-OD2	-6.63	112.34	118.30
1	A	366	ASP	CB-CG-OD1	6.62	124.25	118.30
1	D	203	ASP	CB-CG-OD1	6.59	124.23	118.30
1	D	226	ARG	NE-CZ-NH1	6.57	123.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	345	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	A	95	ASP	CB-CG-OD1	6.55	124.19	118.30
1	B	95	ASP	CB-CG-OD1	6.50	124.15	118.30
1	D	190	ARG	CD-NE-CZ	-6.50	114.51	123.60
1	C	22	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	93	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	170	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	D	405	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	B	122	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	445	VAL	CB-CA-C	6.29	123.35	111.40
1	A	186	ASP	CB-CG-OD1	6.23	123.91	118.30
1	C	94	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	C	345	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	366	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	105	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	173	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	D	313	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	186	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	A	93	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	B	45	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	B	438	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	D	95	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	D	95	ASP	CB-CG-OD1	6.12	123.80	118.30
1	B	438	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	405	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	173	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	C	105	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	A	345	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	C	366	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	405[A]	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	405[B]	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	122	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	B	105	ASP	CB-CG-OD1	6.01	123.71	118.30
1	D	231	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	B	405	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	93	ASP	CB-CG-OD2	-5.98	112.91	118.30
1	C	22	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	B	45	ASP	CB-CG-OD1	5.95	123.65	118.30
1	D	318	THR	N-CA-CB	5.84	121.39	110.30
1	B	446	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	D	173	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	B	93	ASP	CB-CG-OD1	5.80	123.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	93	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	105	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	22	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	C	403	ASP	CB-CG-OD1	5.77	123.49	118.30
1	C	67	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	C	235	ASP	CB-CG-OD1	5.75	123.47	118.30
1	D	403	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	405	ASP	CB-CG-OD1	5.74	123.46	118.30
1	D	345	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	203	ASP	CB-CG-OD1	5.72	123.45	118.30
1	C	421	ALA	N-CA-CB	5.71	118.09	110.10
1	C	170	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	169	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	B	190	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	377	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	C	152	PHE	CB-CA-C	-5.61	99.19	110.40
1	D	366	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	C	186	ASP	CB-CG-OD1	5.55	123.29	118.30
1	C	438	ASP	CB-CG-OD1	5.54	123.29	118.30
1	D	157	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	122	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	313	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	C	186	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	D	94	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	166	SER	N-CA-CB	5.42	118.64	110.50
1	D	22	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	138	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	423	ASP	CB-CG-OD1	5.37	123.14	118.30
1	D	438	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	235	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	170	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	A	170	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	351	PHE	N-CA-CB	5.30	120.15	110.60
1	B	235	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	D	280	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	261	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	186	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	138	ASP	CB-CG-OD1	5.28	123.05	118.30
1	C	93	ASP	CB-CG-OD1	5.26	123.03	118.30
1	D	186	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	105	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	D	105	ASP	CB-CG-OD1	5.24	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	152	PHE	CB-CA-C	-5.23	99.93	110.40
1	A	169	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	308	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	423	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	169	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	C	313	ASP	CB-CG-OD1	5.18	122.97	118.30
1	B	308	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	C	393	PRO	N-CA-CB	5.15	109.48	103.30
1	A	272	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	169	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	280	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	178	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	95	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	D	405	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	94	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	403	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	403	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	B	22	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	176	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	99	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	405	ASP	CB-CG-OD1	5.00	122.81	118.30
1	D	424	ASP	CB-CG-OD1	5.00	122.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	351	PHE	CA

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	3436	0	3368	162	0
1	B	3408	0	3332	191	0
1	C	3421	0	3333	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3405	0	3318	165	0
2	A	13	0	8	5	0
2	B	13	0	8	3	0
2	C	13	0	8	4	0
2	D	13	0	8	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	8	0	0
4	B	4	0	8	0	0
4	C	4	0	8	5	0
4	D	4	0	8	1	0
5	A	229	0	0	10	0
5	B	168	0	0	11	0
5	C	276	0	0	12	0
5	D	228	0	0	11	0
All	All	14643	0	13415	632	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (632) 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:C:339:HIS:NE2	2:C:501:DXG:H51	1.66	1.11
1:B:287:ALA:HB1	1:B:311:LEU:HD21	1.29	1.10
1:A:339:HIS:NE2	2:A:499:DXG:H51	1.70	1.07
1:B:24:MET:HG2	1:B:26:MET:HE3	1.40	1.03
1:B:339:HIS:NE2	2:B:500:DXG:H51	1.76	0.99
1:B:55:ILE:HB	1:B:56:PRO:HD2	1.45	0.98
1:A:414:TYR:HA	1:A:419:LEU:HD12	1.45	0.97
1:B:293:THR:H	1:B:297:GLN:NE2	1.66	0.94
1:B:293:THR:H	1:B:297:GLN:HE21	1.01	0.93
1:A:240:TRP:HB3	1:A:244:GLU:HG3	1.51	0.91
1:D:122:ASP:O	1:D:126:GLN:HG3	1.70	0.90
1:A:293:THR:H	1:A:297:GLN:HE21	1.21	0.87
1:B:156:ASN:HB2	1:B:181:GLU:OE2	1.74	0.86
1:D:66:GLU:O	1:D:69:ILE:HG13	1.76	0.86
1:B:24:MET:HG2	1:B:26:MET:CE	2.05	0.86
1:A:417:HIS:HB2	1:A:419:LEU:HD11	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:NZ	1:A:94:ARG:HD3	1.91	0.85
1:C:150:TYR:CZ	1:C:205:LYS:HE2	2.11	0.84
1:A:60:LYS:HZ2	1:A:94:ARG:HD3	1.43	0.84
1:A:293:THR:H	1:A:297:GLN:NE2	1.75	0.83
1:B:151:LEU:CD1	1:B:223:LEU:HD21	2.08	0.83
1:B:339:HIS:CD2	2:B:500:DXG:H51	2.14	0.81
1:D:253:LYS:HE2	1:D:282:THR:O	1.80	0.81
1:A:267:GLN:NE2	5:A:1498:HOH:O	2.12	0.81
1:C:293:THR:H	1:C:297:GLN:NE2	1.78	0.81
1:D:65:LEU:HD23	1:D:116:ILE:HD11	1.63	0.81
1:B:294:ASP:OD1	1:B:297:GLN:HG3	1.81	0.81
1:D:339:HIS:HE2	2:D:502:DXG:H51	1.46	0.80
1:A:55:ILE:HB	1:A:56:PRO:HD2	1.64	0.80
1:B:188:VAL:O	1:B:191:LEU:HB2	1.81	0.80
5:A:1815:HOH:O	1:C:85:THR:HG22	1.80	0.80
1:A:8:PRO:HG3	1:A:47:SER:HB3	1.63	0.79
1:A:147:MET:HG2	1:A:365:ILE:HG13	1.65	0.79
1:D:339:HIS:NE2	2:D:502:DXG:H51	1.97	0.79
1:D:185:PRO:HA	1:D:188:VAL:CG2	2.12	0.79
1:B:415:GLN:NE2	1:B:415:GLN:HA	1.99	0.77
1:A:346:ILE:HD11	1:A:402:ILE:HD13	1.66	0.77
1:C:205:LYS:HG3	1:C:233:THR:HG23	1.67	0.77
1:B:313:ASP:HB3	1:B:316:PHE:CE1	2.20	0.76
1:C:205:LYS:HG3	1:C:233:THR:CG2	2.16	0.76
1:B:14:GLN:OE1	1:B:16:ILE:HD11	1.87	0.75
1:B:221:VAL:O	1:B:225:GLN:HG3	1.87	0.75
1:B:24:MET:HE2	1:B:431:LEU:HD11	1.67	0.75
1:B:33:ALA:HB1	1:B:34:PRO:HD2	1.69	0.75
1:B:218:GLU:HB3	5:B:1454:HOH:O	1.85	0.75
1:B:409:LYS:HD3	1:B:409:LYS:N	2.00	0.74
1:C:313:ASP:HB3	1:C:316:PHE:CE1	2.22	0.74
1:C:339:HIS:CD2	2:C:501:DXG:H51	2.22	0.74
1:A:21:HIS:H	1:A:376:GLN:HE22	1.35	0.74
1:B:401:GLU:HG2	5:B:1750:HOH:O	1.86	0.74
1:D:186:ASP:O	1:D:190:ARG:HD3	1.87	0.74
1:A:67:ASP:O	1:A:70:PRO:HD2	1.88	0.73
1:A:147:MET:HG2	1:A:365:ILE:CG1	2.17	0.73
1:C:4:GLN:HB2	5:C:1892:HOH:O	1.87	0.73
1:B:404:MET:HA	1:B:407:VAL:CG2	2.19	0.73
1:C:313:ASP:HB3	1:C:316:PHE:CD1	2.24	0.72
1:D:417:HIS:HB2	1:D:419:LEU:CD1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:THR:H	1:C:297:GLN:HE21	1.35	0.72
1:A:99:ARG:HG3	1:A:105:ASP:OD2	1.89	0.71
1:A:4:GLN:HA	1:C:4:GLN:N	2.05	0.71
1:A:416:LYS:HD3	1:A:417:HIS:CE1	2.25	0.71
1:D:405:ASP:O	1:D:409:LYS:HG3	1.91	0.71
1:A:162:LEU:HD11	1:A:430:TYR:CE1	2.25	0.71
1:B:262:PRO:HD2	1:B:275:MET:SD	2.31	0.71
1:C:267:GLN:NE2	5:C:1401:HOH:O	2.24	0.71
1:A:142:ARG:NH1	1:A:362:ILE:HG12	2.06	0.70
1:A:142:ARG:HH12	1:A:362:ILE:HG12	1.56	0.70
1:D:95:ASP:N	1:D:95:ASP:OD2	2.24	0.70
1:C:185:PRO:HA	1:C:188:VAL:CG1	2.20	0.69
1:A:21:HIS:ND1	5:A:1810:HOH:O	2.25	0.69
1:B:55:ILE:HB	1:B:56:PRO:CD	2.21	0.69
1:B:226:ARG:HD2	1:B:226:ARG:O	1.92	0.69
1:A:313:ASP:HB3	1:A:316:PHE:CE1	2.27	0.69
1:A:380:LYS:HD2	1:A:401:GLU:HB3	1.74	0.69
1:A:7:THR:HG21	1:C:128:LEU:HD23	1.74	0.69
1:A:168:PRO:HD2	5:A:1356:HOH:O	1.93	0.69
1:A:348:LEU:CD2	1:A:383:PHE:HB2	2.23	0.69
1:B:39:ASN:ND2	1:B:57:GLY:HA2	2.08	0.68
1:B:59:GLU:OE2	1:B:62:ARG:NE	2.25	0.68
1:A:7:THR:HG21	1:C:128:LEU:HA	1.75	0.68
1:A:71:LEU:HD22	1:A:86:LEU:HD21	1.75	0.68
1:A:205:LYS:NZ	1:A:366:ASP:OD2	2.22	0.68
1:B:68:ALA:C	1:B:70:PRO:HD2	2.14	0.68
1:D:203:ASP:OD1	1:D:231:ARG:HB2	1.94	0.68
1:D:384:GLU:HB2	1:D:386:LYS:HE2	1.76	0.68
1:A:103:THR:O	2:A:499:DXG:H42	1.93	0.68
1:C:294:ASP:OD1	1:C:297:GLN:HG3	1.94	0.68
1:D:55:ILE:HB	1:D:56:PRO:CD	2.24	0.68
1:D:417:HIS:CB	1:D:419:LEU:HG	2.24	0.68
1:B:311:LEU:N	1:B:311:LEU:HD22	2.08	0.68
1:B:265:ALA:O	1:B:266:GLU:HB3	1.94	0.68
1:C:185:PRO:HA	1:C:188:VAL:HG12	1.76	0.67
1:D:346:ILE:HD11	1:D:402:ILE:HD13	1.75	0.67
1:A:262:PRO:HD2	1:A:275:MET:SD	2.34	0.67
1:A:415:GLN:O	1:A:418:GLY:N	2.22	0.67
1:A:241:SER:H	1:A:244:GLU:CG	2.07	0.67
1:C:21:HIS:H	1:C:376:GLN:HE22	1.40	0.67
1:A:207:LYS:HE2	1:A:237:ASN:OD1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:MET:CE	1:B:431:LEU:HD11	2.24	0.67
1:B:71:LEU:HD13	1:B:86:LEU:HG	1.75	0.67
1:A:55:ILE:HD11	1:A:65:LEU:HD11	1.75	0.66
1:A:310:PRO:HG2	1:A:329:CYS:SG	2.36	0.66
1:B:344:PHE:CG	1:B:378:LEU:HD11	2.30	0.66
1:D:133:ALA:H	1:D:353:HIS:HD2	1.40	0.66
1:B:415:GLN:HA	1:B:415:GLN:HE21	1.60	0.66
1:B:404:MET:HA	1:B:407:VAL:HG22	1.77	0.66
1:A:378:LEU:O	1:A:402:ILE:HD12	1.96	0.66
1:C:188:VAL:HG11	1:C:219:SER:OG	1.95	0.66
1:A:241:SER:H	1:A:244:GLU:HG2	1.60	0.65
1:A:105:ASP:OD1	1:A:107:ARG:HB2	1.97	0.65
1:B:99:ARG:HG3	1:B:105:ASP:OD2	1.97	0.65
1:D:339:HIS:CD2	2:D:502:DXG:H51	2.31	0.65
1:B:28:LEU:HG	1:B:437:PHE:HE2	1.60	0.65
1:B:122:ASP:OD2	1:B:398:LEU:HD12	1.96	0.65
1:D:243:ASN:ND2	5:D:1883:HOH:O	2.29	0.65
1:B:167:GLN:O	1:B:176:ARG:HB2	1.97	0.65
1:B:107:ARG:NH2	5:B:1085:HOH:O	2.15	0.64
1:A:205:LYS:HD2	5:A:1727:HOH:O	1.96	0.64
1:A:209:GLY:O	1:A:442:PRO:HA	1.97	0.64
1:B:293:THR:N	1:B:297:GLN:HE21	1.85	0.64
1:A:414:TYR:CA	1:A:419:LEU:HD12	2.25	0.64
1:D:378:LEU:O	1:D:402:ILE:HD12	1.97	0.64
1:D:33:ALA:HB1	1:D:34:PRO:HD2	1.78	0.64
1:B:226:ARG:HG3	1:B:227:PHE:CD1	2.32	0.64
1:B:108:THR:O	1:B:112:VAL:HG23	1.98	0.64
1:B:344:PHE:CD1	1:B:378:LEU:HD11	2.31	0.64
1:D:27:ASN:OD1	1:D:29:SER:N	2.30	0.63
1:C:340:SER:HB2	5:C:1573:HOH:O	1.97	0.63
1:B:157:ARG:NH2	1:B:180:GLU:OE1	2.25	0.63
1:D:185:PRO:HA	1:D:188:VAL:HG22	1.80	0.63
1:A:21:HIS:H	1:A:376:GLN:NE2	1.97	0.63
1:A:429:GLN:OE1	1:A:429:GLN:HA	1.97	0.63
1:B:59:GLU:OE1	1:B:62:ARG:NH2	2.27	0.62
1:C:12:GLU:HG3	1:C:44:LYS:HB2	1.81	0.62
1:D:205:LYS:HE3	1:D:260:GLU:OE1	1.99	0.62
1:B:172:CYS:HB3	1:B:175:TYR:HB2	1.81	0.62
1:A:34:PRO:HD3	1:A:164:TYR:CZ	2.34	0.62
1:B:417:HIS:HB2	1:B:419:LEU:HD11	1.80	0.62
1:B:417:HIS:HB2	1:B:419:LEU:CD1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:MET:HE3	1:B:390:VAL:HG21	1.82	0.62
1:A:109:THR:O	1:A:113:VAL:HG23	2.00	0.62
1:A:338:SER:HB3	5:A:1372:HOH:O	2.00	0.62
1:A:405:ASP:O	1:A:409:LYS:HD3	2.00	0.62
1:A:219:SER:O	1:A:223:LEU:HD12	2.00	0.61
1:A:104:PHE:CE1	1:A:106:LEU:HD21	2.36	0.61
1:B:210:VAL:O	1:B:444:MET:HB2	2.00	0.61
1:C:416:LYS:HG2	1:C:417:HIS:CD2	2.34	0.61
1:D:68:ALA:C	1:D:70:PRO:HD2	2.21	0.61
1:D:156:ASN:OD1	1:D:158:LYS:HE3	1.99	0.61
1:D:55:ILE:HB	1:D:56:PRO:HD2	1.83	0.61
1:B:151:LEU:HD12	1:B:223:LEU:HD21	1.83	0.61
1:D:316:PHE:HD2	5:D:1377:HOH:O	1.84	0.61
1:B:425:ALA:O	1:B:428:MET:HB2	2.01	0.61
1:B:8:PRO:HB3	1:B:47:SER:HB3	1.82	0.60
1:B:26:MET:HE1	1:B:31:ALA:CB	2.31	0.60
1:D:69:ILE:N	1:D:70:PRO:HD2	2.16	0.60
1:C:293:THR:OG1	1:C:297:GLN:NE2	2.34	0.60
1:D:39:ASN:ND2	1:D:57:GLY:HA2	2.16	0.60
1:D:241:SER:N	1:D:244:GLU:OE1	2.27	0.60
1:B:168:PRO:HD2	5:B:1451:HOH:O	2.01	0.60
1:C:8:PRO:HB3	1:C:47:SER:HB3	1.82	0.60
1:C:156:ASN:HB2	1:C:181:GLU:OE1	2.02	0.60
1:C:58:GLY:HA3	5:C:1097:HOH:O	2.00	0.60
1:B:287:ALA:HB1	1:B:311:LEU:CD2	2.19	0.60
1:A:14:GLN:HB3	5:A:1609:HOH:O	2.01	0.60
1:A:150:TYR:OH	1:A:205:LYS:HE2	2.02	0.60
1:B:161:PRO:HG2	1:B:430:TYR:CE2	2.37	0.60
1:B:288:THR:H	1:B:311:LEU:HD23	1.67	0.60
1:A:26:MET:HE2	1:A:444:MET:HE2	1.83	0.59
1:B:233:THR:HA	1:B:256:LEU:HD22	1.82	0.59
1:C:160:THR:HB	1:C:161:PRO:HD2	1.83	0.59
1:A:440:LYS:HE3	5:A:1628:HOH:O	2.01	0.59
1:C:68:ALA:C	1:C:70:PRO:HD2	2.23	0.59
1:B:226:ARG:HG3	1:B:227:PHE:CE1	2.38	0.59
1:D:8:PRO:HD3	1:D:127:HIS:CE1	2.38	0.59
1:D:408:MET:O	1:D:411:HIS:HB3	2.03	0.59
1:C:205:LYS:HD2	5:C:1001:HOH:O	2.02	0.59
1:B:55:ILE:CB	1:B:56:PRO:HD2	2.28	0.58
1:C:117:GLU:OE1	1:C:320:GLN:HG3	2.02	0.58
1:B:26:MET:HE1	1:B:31:ALA:HB1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PRO:HD2	1:A:169:ASP:H	1.67	0.58
1:B:267:GLN:OE1	5:B:1833:HOH:O	2.17	0.58
1:A:348:LEU:HD23	1:A:383:PHE:HB2	1.84	0.58
1:C:408:MET:O	1:C:412:GLU:HG3	2.04	0.58
1:A:184:THR:O	1:A:187:ALA:HB3	2.03	0.58
1:C:287:ALA:HA	1:C:309:ILE:O	2.04	0.58
1:A:13:MET:HA	1:A:42:ILE:O	2.04	0.58
1:B:33:ALA:HB1	1:B:34:PRO:CD	2.33	0.58
1:A:184:THR:O	1:A:188:VAL:N	2.29	0.58
1:A:365:ILE:HA	5:A:1503:HOH:O	2.03	0.58
1:C:34:PRO:HG3	1:C:162:LEU:HB3	1.85	0.58
1:D:411:HIS:O	1:D:414:TYR:HB3	2.03	0.58
1:D:436:THR:HG22	5:D:1708:HOH:O	2.03	0.58
1:D:158:LYS:NZ	5:D:1517:HOH:O	2.36	0.58
1:A:241:SER:N	1:A:244:GLU:HG2	2.19	0.57
1:D:162:LEU:HD11	1:D:430:TYR:CE2	2.39	0.57
1:D:217:ALA:O	1:D:221:VAL:HG23	2.04	0.57
1:B:205:LYS:HG3	1:B:233:THR:CG2	2.35	0.57
1:A:55:ILE:HB	1:A:56:PRO:CD	2.32	0.57
1:B:27:ASN:HD22	1:B:27:ASN:N	2.03	0.57
1:B:122:ASP:CG	1:B:398:LEU:HD12	2.25	0.57
1:B:288:THR:N	1:B:311:LEU:HD23	2.20	0.57
1:C:65:LEU:HG	1:C:112:VAL:HG13	1.87	0.57
1:C:150:TYR:OH	1:C:205:LYS:HE2	2.03	0.57
1:D:247:LYS:NZ	5:D:1782:HOH:O	2.37	0.57
1:A:238:GLY:N	1:A:261:ASP:O	2.35	0.57
1:C:445:VAL:O	1:C:446:ARG:HD3	2.04	0.57
1:C:332:PHE:CD2	4:C:604:IPA:H12	2.40	0.57
1:D:339:HIS:HD2	2:D:502:DXG:O6B	1.87	0.57
1:D:417:HIS:HB2	1:D:419:LEU:HD11	1.85	0.57
1:A:339:HIS:NE2	2:A:499:DXG:C5	2.57	0.56
1:C:373:GLU:OE2	5:C:1868:HOH:O	2.18	0.56
1:A:442:PRO:HG2	1:A:445:VAL:HG11	1.86	0.56
1:C:267:GLN:NE2	1:D:296:ARG:HH12	2.03	0.56
1:C:429:GLN:OE1	1:C:434:GLY:N	2.37	0.56
1:B:65:LEU:CD2	1:B:116:ILE:HD11	2.35	0.56
1:B:288:THR:H	1:B:311:LEU:CD2	2.17	0.56
1:C:151:LEU:N	1:C:205:LYS:O	2.35	0.56
1:B:344:PHE:CB	1:B:378:LEU:HD12	2.36	0.56
1:A:101:LEU:HD13	1:A:439:ASN:ND2	2.20	0.56
1:A:267:GLN:NE2	1:B:296:ARG:HH12	2.02	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:GLU:OE2	1:D:218:GLU:HA	2.06	0.55
1:D:394:GLU:OE2	1:D:394:GLU:HA	2.05	0.55
1:B:273:GLU:O	1:B:277:GLU:HG3	2.06	0.55
1:C:144:GLU:O	5:C:1663:HOH:O	2.17	0.55
1:A:21:HIS:N	1:A:376:GLN:HE22	2.04	0.55
1:A:99:ARG:CG	1:A:105:ASP:OD2	2.55	0.55
1:A:162:LEU:HD11	1:A:430:TYR:HE1	1.72	0.55
1:D:207:LYS:HE2	1:D:237:ASN:ND2	2.22	0.55
1:A:409:LYS:HD2	1:A:409:LYS:N	2.22	0.55
1:D:185:PRO:O	1:D:188:VAL:HG23	2.06	0.55
1:A:150:TYR:CZ	1:A:205:LYS:HE2	2.41	0.55
1:B:85:THR:CG2	1:D:138:ASP:HB3	2.36	0.55
1:A:348:LEU:HD21	1:A:383:PHE:HB2	1.88	0.55
1:B:185:PRO:O	1:B:188:VAL:N	2.40	0.55
1:A:365:ILE:HG13	1:A:365:ILE:O	2.06	0.55
1:C:238:GLY:N	1:C:261:ASP:O	2.37	0.55
1:C:294:ASP:HB2	5:C:1434:HOH:O	2.06	0.55
1:B:184:THR:O	1:B:188:VAL:HG23	2.07	0.54
1:B:331:GLU:HB3	1:D:295:TRP:HB3	1.89	0.54
1:C:307:VAL:HG12	1:C:310:PRO:HD3	1.88	0.54
1:D:69:ILE:N	1:D:70:PRO:CD	2.70	0.54
1:A:26:MET:HE1	1:A:444:MET:HE1	1.88	0.54
1:C:403:ASP:HB3	1:C:406:GLN:HB2	1.88	0.54
1:D:166:SER:HA	1:D:179:HIS:CG	2.42	0.54
1:A:253:LYS:HE2	1:A:282:THR:O	2.07	0.54
4:C:604:IPA:H11	5:C:1572:HOH:O	2.06	0.54
1:A:205:LYS:HG3	1:A:233:THR:HG23	1.90	0.54
1:D:162:LEU:HB3	1:D:163:PRO:HD2	1.89	0.54
1:A:200:GLY:HA3	1:A:387:GLY:HA2	1.90	0.54
1:D:384:GLU:HB2	1:D:386:LYS:CE	2.37	0.54
1:D:207:LYS:HE2	1:D:237:ASN:HD21	1.73	0.53
1:B:178:ARG:NH1	1:B:370:ILE:O	2.41	0.53
1:B:344:PHE:HB3	1:B:378:LEU:HD12	1.90	0.53
1:C:91:PHE:HD1	1:C:94:ARG:CZ	2.21	0.53
1:D:272:ARG:HA	1:D:291:ILE:HD12	1.89	0.53
1:B:122:ASP:O	1:B:126:GLN:HG3	2.09	0.53
1:B:344:PHE:CG	1:B:378:LEU:CD1	2.91	0.53
1:D:79:GLU:O	1:D:83:VAL:HG23	2.08	0.53
1:B:192:ALA:HB2	1:B:223:LEU:HD11	1.89	0.53
1:C:114:THR:HG21	1:C:315:HIS:HA	1.90	0.53
1:A:411:HIS:O	1:A:414:TYR:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:VAL:O	1:D:52:VAL:HA	2.09	0.53
1:C:346:ILE:HD11	1:C:402:ILE:CD1	2.39	0.53
1:D:65:LEU:HD23	1:D:116:ILE:CD1	2.36	0.53
1:B:317:TRP:O	1:B:318:THR:OG1	2.26	0.53
1:B:377:ARG:HB2	1:B:382:PRO:HG3	1.90	0.53
1:B:24:MET:O	1:B:26:MET:HE3	2.09	0.53
1:A:414:TYR:HA	1:A:419:LEU:CD1	2.30	0.52
1:B:147:MET:CE	1:B:390:VAL:HG21	2.38	0.52
1:A:41:VAL:C	1:A:42:ILE:HG13	2.29	0.52
1:A:202:ASN:O	1:A:230:ALA:HB1	2.10	0.52
1:B:86:LEU:O	1:B:86:LEU:HD12	2.09	0.52
1:B:95:ASP:OD2	1:B:107:ARG:HB3	2.09	0.52
1:C:131:ASN:ND2	1:C:134:SER:OG	2.42	0.52
1:D:233:THR:HA	1:D:256:LEU:HD22	1.91	0.52
1:D:238:GLY:N	1:D:261:ASP:O	2.40	0.52
1:A:437:PHE:CE2	1:A:439:ASN:HB3	2.44	0.52
1:D:63:LYS:O	1:D:66:GLU:HB3	2.10	0.52
1:D:162:LEU:HD11	1:D:430:TYR:HE2	1.75	0.52
1:D:417:HIS:HB2	1:D:419:LEU:HG	1.91	0.52
1:A:261:ASP:N	1:A:262:PRO:HD3	2.25	0.52
1:C:267:GLN:HE22	1:D:296:ARG:HH12	1.56	0.52
1:D:111:HIS:CE1	1:D:316:PHE:HB3	2.45	0.52
1:D:35:PHE:CD1	1:D:413:LEU:HD21	2.45	0.52
1:A:403:ASP:HB3	1:A:406:GLN:HB2	1.91	0.52
1:C:207:LYS:HE3	1:C:207:LYS:HA	1.91	0.52
1:D:236:PRO:HG2	1:D:262:PRO:HA	1.91	0.52
1:B:12:GLU:HB2	1:B:44:LYS:HG3	1.92	0.52
1:A:24:MET:HG3	1:A:164:TYR:CZ	2.45	0.51
1:D:375:ASN:OD1	1:D:376:GLN:HG3	2.11	0.51
1:B:43:ILE:HD12	1:B:119:ALA:HB3	1.92	0.51
1:B:398:LEU:HB2	1:B:400:VAL:HG22	1.93	0.51
1:D:110:ILE:CG2	1:D:111:HIS:N	2.73	0.51
1:B:293:THR:OG1	1:B:297:GLN:NE2	2.43	0.51
1:B:376:GLN:OE1	5:B:1443:HOH:O	2.19	0.51
1:C:429:GLN:OE1	1:C:429:GLN:HA	2.11	0.51
1:D:133:ALA:H	1:D:353:HIS:CD2	2.26	0.51
1:A:17:PRO:HG3	1:A:62:ARG:HD3	1.93	0.51
1:B:402:ILE:HG13	1:B:403:ASP:N	2.24	0.51
1:D:236:PRO:HD2	1:D:260:GLU:O	2.10	0.51
1:A:105:ASP:OD2	1:A:107:ARG:NH2	2.44	0.51
1:C:162:LEU:HB2	1:C:164:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:GLN:OE1	1:D:434:GLY:N	2.40	0.51
1:A:29:SER:OG	1:A:102:GLN:NE2	2.43	0.51
1:A:83:VAL:O	1:A:87:VAL:HG23	2.11	0.51
1:A:105:ASP:OD1	1:A:107:ARG:N	2.43	0.51
1:A:27:ASN:OD1	1:A:29:SER:HB2	2.11	0.51
1:A:292:ALA:HA	1:A:297:GLN:HB3	1.92	0.50
1:B:35:PHE:CD1	1:B:413:LEU:HD21	2.46	0.50
1:B:242:LEU:HD11	1:B:246:ILE:HD11	1.91	0.50
1:B:287:ALA:HA	1:B:309:ILE:O	2.10	0.50
1:B:17:PRO:HB2	1:B:414:TYR:CD1	2.47	0.50
1:D:184:THR:O	1:D:188:VAL:HG22	2.11	0.50
1:A:4:GLN:CA	1:C:4:GLN:N	2.72	0.50
1:A:417:HIS:HB2	1:A:419:LEU:CD1	2.38	0.50
1:C:110:ILE:CG2	1:C:111:HIS:N	2.74	0.50
1:B:91:PHE:O	1:B:94:ARG:HG3	2.12	0.50
1:C:21:HIS:H	1:C:376:GLN:NE2	2.07	0.50
1:A:309:ILE:HA	1:A:335:THR:O	2.12	0.50
1:B:24:MET:CG	1:B:26:MET:CE	2.86	0.50
1:C:111:HIS:HD2	1:C:315:HIS:O	1.94	0.50
1:A:273:GLU:O	1:A:277:GLU:HG3	2.11	0.50
1:A:8:PRO:HD3	1:C:5:PHE:HD2	1.77	0.49
1:B:17:PRO:HB2	1:B:414:TYR:CE1	2.47	0.49
1:D:73:VAL:HG12	1:D:74:GLY:N	2.26	0.49
1:D:203:ASP:CG	1:D:231:ARG:HB2	2.32	0.49
1:B:73:VAL:HG12	1:B:74:GLY:N	2.27	0.49
1:C:321:GLY:O	1:C:325:VAL:HG23	2.12	0.49
1:C:346:ILE:HD11	1:C:402:ILE:HD13	1.95	0.49
1:D:417:HIS:HB2	1:D:419:LEU:CG	2.41	0.49
1:A:184:THR:O	1:A:188:VAL:HG12	2.13	0.49
1:B:261:ASP:N	1:B:262:PRO:HD3	2.26	0.49
1:A:7:THR:CG2	1:C:128:LEU:HD23	2.41	0.49
1:B:214:GLU:O	1:B:217:ALA:HB3	2.12	0.49
1:C:302:LEU:HB3	4:C:604:IPA:H32	1.93	0.49
1:A:103:THR:HG22	1:A:237:ASN:CG	2.32	0.49
1:B:407:VAL:HG23	1:B:408:MET:N	2.27	0.49
1:C:69:ILE:N	1:C:70:PRO:CD	2.75	0.49
1:A:437:PHE:CZ	1:A:439:ASN:HB3	2.48	0.49
1:B:26:MET:CE	1:B:31:ALA:CB	2.91	0.49
1:B:309:ILE:HA	1:B:335:THR:O	2.12	0.49
1:D:73:VAL:CG1	1:D:74:GLY:N	2.75	0.49
1:A:43:ILE:HD12	1:A:119:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ILE:N	1:B:70:PRO:CD	2.76	0.49
1:D:71:LEU:HD13	1:D:86:LEU:HD22	1.94	0.49
1:D:86:LEU:C	1:D:86:LEU:HD23	2.33	0.49
1:A:185:PRO:HA	1:A:188:VAL:CG1	2.42	0.49
1:C:68:ALA:O	1:C:71:LEU:HB2	2.13	0.49
1:A:261:ASP:N	1:A:262:PRO:CD	2.76	0.48
1:D:8:PRO:CD	1:D:127:HIS:ND1	2.76	0.48
1:C:198:LYS:O	1:C:198:LYS:HG3	2.11	0.48
1:D:262:PRO:HD2	1:D:275:MET:SD	2.54	0.48
1:D:292:ALA:HA	1:D:297:GLN:HB3	1.95	0.48
1:B:80:TYR:O	1:B:84:LEU:HG	2.13	0.48
1:C:275:MET:HG3	1:C:291:ILE:HD13	1.95	0.48
1:D:445:VAL:O	1:D:446:ARG:HD3	2.14	0.48
1:C:99:ARG:HD2	1:C:293:THR:HG21	1.95	0.48
1:C:93:ASP:OD1	1:C:94:ARG:HG3	2.14	0.48
1:D:110:ILE:HG23	1:D:111:HIS:N	2.28	0.48
1:D:205:LYS:HD2	5:D:1012:HOH:O	2.14	0.48
1:C:23:SER:O	1:C:25:LEU:HG	2.14	0.48
1:C:332:PHE:CD2	4:C:604:IPA:C1	2.96	0.48
1:D:65:LEU:HG	1:D:112:VAL:HG13	1.94	0.48
1:D:109:THR:O	1:D:113:VAL:HG23	2.13	0.48
1:A:110:ILE:HD12	1:A:110:ILE:HA	1.75	0.48
1:A:168:PRO:CD	1:A:169:ASP:H	2.26	0.48
1:D:20:GLY:O	1:D:35:PHE:HA	2.14	0.48
1:D:218:GLU:HB3	5:D:1783:HOH:O	2.13	0.48
1:C:174:TRP:O	1:C:178:ARG:HG2	2.14	0.48
1:D:148:LEU:HD12	1:D:148:LEU:C	2.34	0.48
1:D:417:HIS:CB	1:D:419:LEU:CG	2.90	0.48
1:B:185:PRO:HB3	1:B:219:SER:HA	1.96	0.48
1:A:317:TRP:O	1:A:318:THR:OG1	2.29	0.47
1:B:13:MET:CE	1:B:116:ILE:HD11	2.43	0.47
1:B:114:THR:OG1	1:B:318:THR:HA	2.14	0.47
1:C:185:PRO:O	1:C:189:VAL:HG23	2.14	0.47
1:C:198:LYS:HG2	1:C:199:TYR:CE1	2.50	0.47
1:D:131:ASN:C	1:D:131:ASN:HD22	2.18	0.47
1:D:190:ARG:HD3	1:D:190:ARG:N	2.29	0.47
1:B:311:LEU:N	1:B:311:LEU:CD2	2.76	0.47
1:C:357:ALA:O	1:C:359:PRO:HD3	2.14	0.47
1:D:377:ARG:HB2	1:D:382:PRO:HG3	1.95	0.47
1:D:445:VAL:C	1:D:446:ARG:HG2	2.34	0.47
1:A:60:LYS:NZ	1:A:94:ARG:CD	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:LYS:HE3	5:C:1428:HOH:O	2.15	0.47
1:D:167:GLN:N	1:D:168:PRO:HD3	2.29	0.47
1:D:212:ALA:O	1:D:215:GLU:HB3	2.15	0.47
1:B:295:TRP:HB3	1:D:331:GLU:HB3	1.95	0.47
1:C:160:THR:CB	1:C:161:PRO:CD	2.92	0.47
1:B:148:LEU:C	1:B:148:LEU:HD12	2.35	0.47
1:D:28:LEU:CD1	1:D:442:PRO:HA	2.44	0.47
1:D:111:HIS:HE1	1:D:316:PHE:HB3	1.78	0.47
1:A:313:ASP:CB	1:A:316:PHE:CE1	2.96	0.47
1:B:19:ALA:HA	1:B:36:PHE:O	2.13	0.47
1:B:85:THR:HG21	1:D:138:ASP:HB3	1.95	0.47
1:B:190:ARG:HA	1:B:190:ARG:HD3	1.61	0.47
1:C:160:THR:HB	1:C:161:PRO:CD	2.45	0.47
1:C:265:ALA:O	1:C:266:GLU:HB3	2.15	0.47
1:D:407:VAL:HG12	1:D:408:MET:HE1	1.97	0.47
1:D:24:MET:HE1	1:D:431:LEU:HD11	1.97	0.47
1:B:37:THR:HG22	1:B:414:TYR:HD2	1.79	0.47
1:B:170:ASP:OD1	1:B:172:CYS:N	2.35	0.47
1:C:16:ILE:HD13	1:C:408:MET:HE1	1.97	0.47
1:B:298:MET:O	1:B:302:LEU:HG	2.14	0.47
1:D:353:HIS:HE1	1:D:398:LEU:O	1.97	0.47
1:A:320:GLN:HG2	5:A:1013:HOH:O	2.13	0.46
1:B:211:LEU:HD13	1:B:215:GLU:OE1	2.15	0.46
1:C:102:GLN:HG3	1:C:104:PHE:CZ	2.50	0.46
1:D:39:ASN:C	1:D:40:ILE:HD13	2.34	0.46
1:D:275:MET:HG3	1:D:291:ILE:HD13	1.97	0.46
1:A:73:VAL:HG12	1:A:74:GLY:N	2.31	0.46
1:B:207:LYS:HE3	1:B:207:LYS:HA	1.97	0.46
1:B:404:MET:CA	1:B:407:VAL:HG22	2.43	0.46
1:C:339:HIS:CD2	2:C:501:DXG:C5	2.96	0.46
1:A:138:ASP:O	1:C:85:THR:HG21	2.15	0.46
1:D:320:GLN:HG2	5:D:1054:HOH:O	2.15	0.46
1:A:162:LEU:HA	1:A:163:PRO:HD3	1.84	0.46
1:D:8:PRO:CD	1:D:127:HIS:CE1	2.98	0.46
1:D:99:ARG:HD3	5:D:1897:HOH:O	2.15	0.46
1:D:198:LYS:HD2	1:D:198:LYS:O	2.16	0.46
1:A:104:PHE:CE1	1:A:106:LEU:CD2	2.98	0.46
1:B:361:LYS:HE2	1:B:362:ILE:O	2.16	0.46
1:B:21:HIS:N	1:B:21:HIS:CD2	2.84	0.46
1:B:288:THR:O	1:B:311:LEU:HD23	2.14	0.46
1:C:110:ILE:HD12	1:C:110:ILE:HA	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:THR:O	1:C:188:VAL:HG12	2.15	0.46
1:D:148:LEU:HD12	1:D:148:LEU:O	2.16	0.46
1:D:224:ALA:HB2	1:D:255:SER:HB3	1.97	0.46
1:B:331:GLU:HG2	5:B:1599:HOH:O	2.16	0.46
1:C:130:VAL:O	1:C:396:PRO:HA	2.16	0.46
1:D:339:HIS:HD2	2:D:502:DXG:C6	2.29	0.46
1:D:86:LEU:C	1:D:86:LEU:CD2	2.84	0.46
1:D:86:LEU:HD23	1:D:86:LEU:O	2.15	0.46
1:B:137:GLY:HA2	5:B:1330:HOH:O	2.16	0.46
1:B:232:ILE:CG2	1:B:233:THR:N	2.79	0.46
1:D:339:HIS:CD2	2:D:502:DXG:C6	2.99	0.46
1:D:353:HIS:O	1:D:356:ALA:HB3	2.16	0.46
1:A:313:ASP:HB3	1:A:316:PHE:CD1	2.51	0.45
1:A:34:PRO:HG3	1:A:162:LEU:HB3	1.98	0.45
1:A:293:THR:N	1:A:297:GLN:HE21	2.02	0.45
1:C:43:ILE:HD12	1:C:119:ALA:HB3	1.99	0.45
1:C:101:LEU:HD23	1:C:101:LEU:HA	1.77	0.45
1:C:261:ASP:N	1:C:262:PRO:CD	2.79	0.45
1:C:262:PRO:HD2	1:C:275:MET:SD	2.56	0.45
1:B:375:ASN:OD1	1:B:376:GLN:HG3	2.16	0.45
1:B:404:MET:HA	1:B:407:VAL:HG21	1.97	0.45
1:D:83:VAL:O	1:D:87:VAL:HG23	2.16	0.45
1:B:66:GLU:O	1:B:69:ILE:HG13	2.15	0.45
1:C:131:ASN:ND2	1:C:134:SER:H	2.13	0.45
1:C:147:MET:CE	1:C:390:VAL:HG21	2.46	0.45
1:A:110:ILE:CG2	1:A:111:HIS:N	2.79	0.45
1:B:395:LYS:HB2	1:B:396:PRO:HD2	1.99	0.45
1:A:188:VAL:HG11	1:A:219:SER:HB3	1.98	0.45
1:B:205:LYS:HG3	1:B:233:THR:HG22	1.99	0.45
1:C:288:THR:HG22	1:C:307:VAL:HG21	1.99	0.45
1:D:185:PRO:HB3	1:D:219:SER:HA	1.99	0.45
1:A:415:GLN:O	1:A:416:LYS:C	2.55	0.45
1:B:117:GLU:CD	1:B:319:MET:HB2	2.38	0.45
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.75	0.45
1:C:332:PHE:CG	4:C:604:IPA:H12	2.52	0.45
1:A:147:MET:HG2	1:A:365:ILE:HG12	1.99	0.45
1:A:295:TRP:HB3	1:C:331:GLU:HB3	1.99	0.45
1:B:103:THR:HG22	1:B:237:ASN:CG	2.37	0.45
1:D:29:SER:O	1:D:424:ASP:HB2	2.17	0.45
1:D:190:ARG:N	1:D:190:ARG:CD	2.80	0.45
1:C:341:ASN:O	1:C:342:ASN:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:TYR:CZ	1:D:205:LYS:NZ	2.78	0.44
1:D:392:VAL:O	5:D:1147:HOH:O	2.21	0.44
1:C:365:ILE:HD12	1:C:365:ILE:HG23	1.78	0.44
1:D:86:LEU:HD23	1:D:90:THR:OG1	2.18	0.44
1:C:185:PRO:CA	1:C:188:VAL:HG12	2.46	0.44
1:D:86:LEU:CD2	1:D:90:THR:OG1	2.65	0.44
1:A:442:PRO:HG2	1:A:445:VAL:CG1	2.46	0.44
1:C:108:THR:O	1:C:112:VAL:HG23	2.17	0.44
1:D:185:PRO:CA	1:D:188:VAL:HG22	2.48	0.44
1:C:296:ARG:HH12	1:D:267:GLN:NE2	2.16	0.44
1:D:131:ASN:ND2	1:D:134:SER:H	2.16	0.44
1:D:165:GLN:HG3	1:D:179:HIS:CE1	2.53	0.44
1:A:142:ARG:NH1	1:A:362:ILE:CG1	2.80	0.44
1:A:426:MET:O	1:A:429:GLN:HB2	2.17	0.44
1:B:211:LEU:HB2	1:B:216:GLU:CG	2.47	0.44
1:B:345:ASP:OD2	1:B:345:ASP:N	2.48	0.44
1:C:33:ALA:HB1	1:C:34:PRO:HD2	1.99	0.44
1:C:54:GLU:OE1	1:C:344:PHE:HB2	2.18	0.44
1:A:39:ASN:ND2	1:A:57:GLY:HA2	2.33	0.44
1:A:77:LEU:O	1:A:80:TYR:HB3	2.16	0.44
1:A:361:LYS:HE2	1:A:362:ILE:O	2.18	0.44
1:A:202:ASN:O	1:A:230:ALA:CB	2.65	0.44
1:A:260:GLU:C	1:A:262:PRO:HD3	2.39	0.44
1:C:103:THR:O	2:C:501:DXG:H42	2.18	0.44
1:D:114:THR:OG1	1:D:318:THR:HA	2.18	0.44
1:A:339:HIS:CG	1:A:340:SER:N	2.86	0.43
1:D:197:GLU:OE1	1:D:197:GLU:HA	2.16	0.43
1:D:233:THR:HG21	1:D:258:TYR:CE2	2.53	0.43
1:D:416:LYS:O	1:D:416:LYS:CG	2.66	0.43
1:C:413:LEU:O	1:C:417:HIS:HD2	2.01	0.43
1:A:331:GLU:HB3	1:C:295:TRP:HB3	2.00	0.43
1:B:26:MET:CE	1:B:31:ALA:HB1	2.48	0.43
1:B:110:ILE:HA	1:B:110:ILE:HD12	1.69	0.43
1:B:114:THR:O	1:B:117:GLU:HB3	2.18	0.43
1:B:233:THR:HA	1:B:256:LEU:CD2	2.47	0.43
1:B:366:ASP:OD2	5:B:1335:HOH:O	2.21	0.43
1:A:185:PRO:O	1:A:189:VAL:HG23	2.19	0.43
1:B:398:LEU:CB	1:B:400:VAL:HG22	2.48	0.43
1:C:298:MET:O	1:C:301:THR:HB	2.18	0.43
1:A:18:VAL:HB	1:A:410:ALA:HB1	1.99	0.43
1:B:27:ASN:N	1:B:27:ASN:ND2	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:HD3	1:C:137:GLY:O	2.18	0.43
1:A:260:GLU:O	1:A:261:ASP:C	2.57	0.43
1:B:26:MET:HE1	1:B:31:ALA:HB2	2.00	0.43
1:C:288:THR:CG2	1:C:307:VAL:HG21	2.49	0.43
1:D:183:MET:HE3	1:D:211:LEU:HD21	2.00	0.43
1:A:244:GLU:O	1:A:248:ILE:HG13	2.18	0.43
1:B:232:ILE:HG22	1:B:233:THR:N	2.33	0.43
1:C:272:ARG:HA	1:C:291:ILE:HD12	2.01	0.43
1:D:27:ASN:OD1	1:D:29:SER:HB2	2.19	0.43
1:A:39:ASN:C	1:A:40:ILE:HD13	2.39	0.43
1:B:13:MET:HE2	1:B:69:ILE:HG12	2.00	0.43
1:B:134:SER:OG	1:D:82:ASN:ND2	2.48	0.43
1:B:8:PRO:HA	1:B:46:ASN:OD1	2.18	0.43
1:B:280:ARG:NH2	1:C:305:GLN:OE1	2.52	0.43
1:B:404:MET:SD	1:B:407:VAL:HG21	2.59	0.43
1:A:346:ILE:HD11	1:A:402:ILE:CD1	2.43	0.42
1:C:51:GLY:HA2	1:C:122:ASP:OD2	2.19	0.42
1:D:13:MET:HB3	1:D:69:ILE:HG23	2.00	0.42
1:A:28:LEU:HD12	1:A:442:PRO:HA	2.01	0.42
1:A:339:HIS:HD2	2:A:499:DXG:O6B	2.02	0.42
1:A:438:ASP:OD2	1:A:438:ASP:C	2.58	0.42
1:B:103:THR:O	2:B:500:DXG:H42	2.19	0.42
1:D:226:ARG:O	1:D:226:ARG:HG3	2.19	0.42
1:D:407:VAL:HG12	1:D:408:MET:CE	2.48	0.42
1:B:156:ASN:OD1	1:B:158:LYS:HB2	2.19	0.42
1:B:375:ASN:OD1	1:B:375:ASN:N	2.52	0.42
1:C:114:THR:O	1:C:117:GLU:HB3	2.19	0.42
1:C:307:VAL:CG1	1:C:310:PRO:HD3	2.49	0.42
1:C:313:ASP:HA	1:C:314:PRO:HD2	1.89	0.42
1:D:50:THR:O	1:D:126:GLN:NE2	2.52	0.42
1:B:13:MET:HA	1:B:42:ILE:O	2.19	0.42
1:B:203:ASP:OD1	1:B:231:ARG:HB2	2.18	0.42
1:D:6:THR:O	1:D:127:HIS:HE1	2.02	0.42
1:D:151:LEU:N	1:D:205:LYS:O	2.48	0.42
1:D:429:GLN:OE1	1:D:429:GLN:HA	2.17	0.42
1:B:13:MET:HE1	1:B:116:ILE:HD11	2.00	0.42
1:C:102:GLN:NE2	1:C:102:GLN:HA	2.34	0.42
1:D:28:LEU:HD22	1:D:239:ALA:HB2	2.02	0.42
1:A:80:TYR:OH	1:A:81:LYS:HE2	2.19	0.42
1:B:403:ASP:O	1:B:407:VAL:HG22	2.20	0.42
1:C:23:SER:O	1:C:25:LEU:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:MET:HE3	1:D:183:MET:HB3	1.95	0.42
1:D:373:GLU:HG2	1:D:374:GLY:H	1.84	0.42
1:D:373:GLU:CG	1:D:374:GLY:N	2.83	0.42
1:A:26:MET:CE	1:A:444:MET:CE	2.97	0.42
1:A:110:ILE:HG23	1:A:111:HIS:N	2.35	0.42
1:B:69:ILE:N	1:B:70:PRO:HD2	2.34	0.42
1:D:158:LYS:HD2	5:D:1517:HOH:O	2.19	0.42
1:A:138:ASP:HB3	1:C:85:THR:CG2	2.49	0.42
1:B:148:LEU:HD12	1:B:148:LEU:O	2.19	0.42
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.82	0.42
1:B:233:THR:OG1	1:B:258:TYR:O	2.34	0.42
1:C:156:ASN:OD1	1:C:158:LYS:HB2	2.20	0.42
1:D:417:HIS:CB	1:D:419:LEU:HD11	2.50	0.42
1:A:395:LYS:HA	1:A:396:PRO:HD3	1.80	0.42
1:B:86:LEU:HD12	1:B:86:LEU:C	2.40	0.42
1:B:206:LEU:O	1:B:234:LEU:HD12	2.20	0.42
1:C:142:ARG:HH11	1:C:142:ARG:HD3	1.72	0.42
1:C:148:LEU:C	1:C:148:LEU:HD12	2.40	0.42
1:A:310:PRO:HD2	1:A:335:THR:O	2.20	0.42
1:A:411:HIS:O	1:A:414:TYR:N	2.52	0.42
1:A:442:PRO:HB2	1:A:445:VAL:HG12	2.02	0.42
1:B:284:LEU:HA	1:B:284:LEU:HD23	1.87	0.42
1:B:287:ALA:HB2	1:B:309:ILE:HB	2.02	0.42
1:B:128:LEU:HA	1:B:128:LEU:HD23	1.64	0.41
1:B:440:LYS:HE3	5:B:1074:HOH:O	2.20	0.41
1:C:333:GLY:HA2	5:C:1686:HOH:O	2.19	0.41
1:B:404:MET:C	1:B:407:VAL:HG22	2.41	0.41
1:C:13:MET:HA	1:C:42:ILE:O	2.20	0.41
1:A:142:ARG:NH1	1:A:362:ILE:CD1	2.83	0.41
1:B:5:PHE:HA	1:D:6:THR:O	2.20	0.41
1:B:7:THR:HA	1:B:8:PRO:HD3	1.96	0.41
1:B:358:ALA:HA	1:B:359:PRO:HD3	1.80	0.41
1:C:121:LEU:HD23	1:C:121:LEU:HA	1.79	0.41
1:D:162:LEU:HA	1:D:163:PRO:HD3	1.92	0.41
1:B:192:ALA:CB	1:B:223:LEU:HD11	2.48	0.41
1:C:77:LEU:N	1:C:77:LEU:HD23	2.34	0.41
1:B:202:ASN:O	1:B:230:ALA:CB	2.68	0.41
1:B:256:LEU:HA	1:B:256:LEU:HD23	1.68	0.41
1:C:24:MET:HG3	1:C:164:TYR:CZ	2.55	0.41
1:C:395:LYS:HA	1:C:396:PRO:HD3	1.80	0.41
1:B:25:LEU:HB3	1:B:152:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:GLN:HA	1:B:376:GLN:NE2	2.36	0.41
1:C:114:THR:OG1	1:C:318:THR:HA	2.20	0.41
1:D:32:HIS:CE1	1:D:342:ASN:OD1	2.73	0.41
1:D:40:ILE:HD13	1:D:40:ILE:N	2.36	0.41
1:B:10:VAL:CG1	1:B:73:VAL:HA	2.50	0.41
1:C:37:THR:C	1:C:38:ARG:HG2	2.41	0.41
1:D:77:LEU:HD23	1:D:77:LEU:HA	1.89	0.41
1:A:4:GLN:O	1:C:6:THR:OG1	2.29	0.41
1:A:282:THR:OG1	1:A:284:LEU:HB2	2.21	0.41
1:A:331:GLU:HB3	1:C:295:TRP:CB	2.50	0.41
1:B:117:GLU:OE1	1:B:319:MET:HB2	2.21	0.41
1:B:137:GLY:O	1:D:81:LYS:NZ	2.40	0.41
1:C:342:ASN:HA	1:C:368:HIS:CB	2.51	0.41
1:C:395:LYS:CB	1:C:396:PRO:HD2	2.50	0.41
1:C:407:VAL:HG12	1:C:408:MET:HE1	2.01	0.41
1:D:27:ASN:O	1:D:443:CYS:HB3	2.21	0.41
1:D:256:LEU:HD23	1:D:256:LEU:HA	1.86	0.41
1:D:279:ARG:HG3	1:D:286:THR:HG23	2.03	0.41
1:B:33:ALA:CB	1:B:34:PRO:CD	2.98	0.41
1:B:429:GLN:C	1:B:431:LEU:N	2.74	0.41
1:C:440:LYS:NZ	5:C:1565:HOH:O	2.54	0.41
1:D:441:ARG:HG3	1:D:442:PRO:HD2	2.03	0.41
1:A:261:ASP:OD1	1:A:288:THR:OG1	2.35	0.40
1:A:301:THR:HG23	1:A:306:SER:HB2	2.02	0.40
1:B:43:ILE:HG22	1:B:123:LEU:HD11	2.01	0.40
1:B:302:LEU:HB3	4:D:601:IPA:H33	2.03	0.40
1:A:162:LEU:HD11	1:A:430:TYR:CD1	2.56	0.40
1:B:353:HIS:CE1	5:B:1119:HOH:O	2.73	0.40
1:D:28:LEU:HD12	1:D:442:PRO:HA	2.03	0.40
1:D:209:GLY:O	1:D:442:PRO:HA	2.21	0.40
1:D:252:LEU:O	1:D:253:LYS:C	2.55	0.40
1:D:380:LYS:HG3	1:D:401:GLU:HB3	2.02	0.40
1:C:16:ILE:HD13	1:C:408:MET:CE	2.51	0.40
1:C:21:HIS:N	1:C:376:GLN:HE22	2.14	0.40
1:D:110:ILE:HD12	1:D:110:ILE:HA	1.78	0.40
1:D:317:TRP:O	1:D:321:GLY:HA3	2.21	0.40
1:B:39:ASN:C	1:B:40:ILE:HD13	2.42	0.40
1:B:132:VAL:HG23	1:B:397:GLY:C	2.42	0.40
1:D:369:TRP:NE1	1:D:373:GLU:HG3	2.36	0.40
1:A:16:ILE:HD13	1:A:16:ILE:HG21	1.83	0.40
1:A:339:HIS:CD2	2:A:499:DXG:O6B	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ILE:HD11	1:C:65:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/446 (99%)	414 (94%)	28 (6%)	0	100	100
1	B	440/446 (99%)	405 (92%)	30 (7%)	5 (1%)	14	8
1	C	442/446 (99%)	412 (93%)	28 (6%)	2 (0%)	29	23
1	D	440/446 (99%)	409 (93%)	30 (7%)	1 (0%)	47	44
All	All	1764/1784 (99%)	1640 (93%)	116 (7%)	8 (0%)	29	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	107	ARG
1	B	102	GLN
1	B	80	TYR
1	C	24	MET
1	D	443	CYS
1	B	181	GLU
1	B	266	GLU
1	C	161	PRO

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	359/362 (99%)	341 (95%)	18 (5%)	24	20
1	B	354/362 (98%)	331 (94%)	23 (6%)	17	12
1	C	355/362 (98%)	338 (95%)	17 (5%)	25	22
1	D	353/362 (98%)	330 (94%)	23 (6%)	17	12
All	All	1421/1448 (98%)	1340 (94%)	81 (6%)	20	16

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	6	THR
1	A	12	GLU
1	A	24	MET
1	A	80	TYR
1	A	95	ASP
1	A	99	ARG
1	A	107	ARG
1	A	131	ASN
1	A	150	TYR
1	A	160	THR
1	A	188	VAL
1	A	207	LYS
1	A	338	SER
1	A	361	LYS
1	A	409	LYS
1	A	419	LEU
1	A	429	GLN
1	B	27	ASN
1	B	40	ILE
1	B	44	LYS
1	B	55	ILE
1	B	63	LYS
1	B	150	TYR
1	B	160	THR
1	B	171	SER
1	B	190	ARG
1	B	207	LYS
1	B	233	THR
1	B	253	LYS

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Mol	Chain	Res	Type
1	B	255	SER
1	B	311	LEU
1	B	339	HIS
1	B	393	PRO
1	B	402	ILE
1	B	408	MET
1	B	409	LYS
1	B	415	GLN
1	B	419	LEU
1	B	426	MET
1	B	439	ASN
1	C	4	GLN
1	C	6	THR
1	C	27	ASN
1	C	99	ARG
1	C	131	ASN
1	C	150	TYR
1	C	160	THR
1	C	188	VAL
1	C	198	LYS
1	C	207	LYS
1	C	219	SER
1	C	255	SER
1	C	339	HIS
1	C	393	PRO
1	C	395	LYS
1	C	416	LYS
1	C	439	ASN
1	D	14	GLN
1	D	40	ILE
1	D	65	LEU
1	D	81	LYS
1	D	94	ARG
1	D	95	ASP
1	D	99	ARG
1	D	131	ASN
1	D	150	TYR
1	D	160	THR
1	D	162	LEU
1	D	188	VAL
1	D	190	ARG
1	D	207	LYS

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Mol	Chain	Res	Type
1	D	229	GLN
1	D	253	LYS
1	D	255	SER
1	D	339	HIS
1	D	340	SER
1	D	405	ASP
1	D	408	MET
1	D	436	THR
1	D	439	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	131	ASN
1	A	243	ASN
1	A	267	GLN
1	A	297	GLN
1	A	320	GLN
1	A	376	GLN
1	A	415	GLN
1	A	439	ASN
1	B	21	HIS
1	B	49	HIS
1	B	297	GLN
1	B	353	HIS
1	B	372	GLN
1	B	415	GLN
1	C	4	GLN
1	C	102	GLN
1	C	111	HIS
1	C	131	ASN
1	C	140	GLN
1	C	141	GLN
1	C	225	GLN
1	C	243	ASN
1	C	267	GLN
1	C	297	GLN
1	C	376	GLN
1	C	417	HIS
1	C	439	ASN
1	D	102	GLN

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Mol	Chain	Res	Type
1	D	131	ASN
1	D	140	GLN
1	D	229	GLN
1	D	237	ASN
1	D	243	ASN
1	D	267	GLN
1	D	339	HIS
1	D	353	HIS
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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	DXG	A	499	3	11,12,12	1.41	2 (18%)	12,16,16	1.90	4 (33%)
2	DXG	D	502	3	11,12,12	1.16	1 (9%)	12,16,16	1.98	6 (50%)
2	DXG	B	500	3	11,12,12	1.54	2 (18%)	12,16,16	1.59	3 (25%)
4	IPA	C	604	-	3,3,3	0.55	0	3,3,3	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	IPA	D	601	-	3,3,3	0.70	0	3,3,3	0.30	0
4	IPA	B	603	-	3,3,3	0.22	0	3,3,3	0.57	0
2	DXG	C	501	3	11,12,12	1.51	2 (18%)	12,16,16	1.92	5 (41%)
4	IPA	A	602	-	3,3,3	0.68	0	3,3,3	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DXG	A	499	3	-	5/16/16/16	-
2	DXG	C	501	3	-	7/16/16/16	-
2	DXG	B	500	3	-	7/16/16/16	-
2	DXG	D	502	3	-	8/16/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	DXG	C5-C6	-3.21	1.47	1.52
2	C	501	DXG	C2-C1	-2.64	1.49	1.52
2	B	500	DXG	C2-C1	-2.53	1.49	1.52
2	A	499	DXG	O1B-C1	2.49	1.29	1.22
2	A	499	DXG	C2-C1	-2.46	1.49	1.52
2	C	501	DXG	C5-C6	-2.37	1.48	1.52
2	D	502	DXG	C2-C1	-2.03	1.49	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	499	DXG	O5-C5-C4	3.71	118.20	108.69
2	C	501	DXG	O6B-C6-C5	3.61	120.65	112.72
2	D	502	DXG	O6B-C6-C5	3.49	120.39	112.72
2	D	502	DXG	O1A-C1-C2	3.16	121.82	113.27
2	C	501	DXG	O5-C5-C4	2.90	116.14	108.69
2	A	499	DXG	O6B-C6-C5	2.85	118.97	112.72
2	B	500	DXG	O6B-C6-C5	2.78	118.82	112.72
2	A	499	DXG	C4-C5-C6	2.73	117.46	110.67
2	A	499	DXG	O5-C5-C6	2.50	117.02	110.36
2	B	500	DXG	O3-C3-C4	2.46	114.05	109.11
2	C	501	DXG	O5-C5-C6	2.43	116.82	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	DXG	O5-C5-C4	2.30	114.60	108.69
2	D	502	DXG	O3-C3-C4	2.26	113.64	109.11
2	D	502	DXG	O1B-C1-C2	-2.22	115.79	121.63
2	C	501	DXG	O6A-C6-C5	-2.19	118.26	122.54
2	D	502	DXG	O6A-C6-C5	-2.18	118.29	122.54
2	C	501	DXG	O1A-C1-C2	2.05	118.81	113.27
2	D	502	DXG	O5-C5-C4	2.02	113.87	108.69

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	499	DXG	C3-C4-C5-O5
2	B	500	DXG	C3-C4-C5-O5
2	B	500	DXG	C3-C4-C5-C6
2	C	501	DXG	C3-C4-C5-O5
2	D	502	DXG	C3-C4-C5-O5
2	D	502	DXG	O5-C5-C6-O6A
2	B	500	DXG	O3-C3-C4-C5
2	C	501	DXG	O3-C3-C4-C5
2	D	502	DXG	O5-C5-C6-O6B
2	A	499	DXG	C4-C5-C6-O6A
2	A	499	DXG	C4-C5-C6-O6B
2	B	500	DXG	C4-C5-C6-O6A
2	B	500	DXG	C4-C5-C6-O6B
2	D	502	DXG	C4-C5-C6-O6A
2	D	502	DXG	C4-C5-C6-O6B
2	A	499	DXG	C3-C4-C5-C6
2	C	501	DXG	C3-C4-C5-C6
2	D	502	DXG	C3-C4-C5-C6
2	A	499	DXG	O3-C3-C4-C5
2	B	500	DXG	O5-C5-C6-O6A
2	B	500	DXG	O5-C5-C6-O6B
2	C	501	DXG	O5-C5-C6-O6B
2	D	502	DXG	O3-C3-C4-C5
2	C	501	DXG	C4-C5-C6-O6A
2	C	501	DXG	C4-C5-C6-O6B
2	C	501	DXG	C2-C3-C4-C5
2	D	502	DXG	C2-C3-C4-C5

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	499	DXG	5	0
2	D	502	DXG	6	0
2	B	500	DXG	3	0
4	C	604	IPA	5	0
4	D	601	IPA	1	0
2	C	501	DXG	4	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(Å^2)	Q<0.9
1	A	444/446 (99%)	-0.16	7 (1%)	72	70	14, 33, 66, 100	1 (0%)
1	B	442/446 (99%)	0.03	12 (2%)	54	53	17, 43, 72, 100	0
1	C	443/446 (99%)	-0.26	7 (1%)	72	70	13, 31, 59, 100	0
1	D	442/446 (99%)	-0.09	11 (2%)	57	56	18, 35, 70, 99	0
All	All	1771/1784 (99%)	-0.12	37 (2%)	63	62	13, 35, 68, 100	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	97	GLY	4.9
1	A	101	LEU	4.4
1	C	93	ASP	4.1
1	C	101	LEU	3.9
1	C	97	GLY	3.9
1	D	97	GLY	3.7
1	A	228	PRO	3.6
1	D	418	GLY	3.6
1	D	106	LEU	3.4
1	D	93	ASP	3.4
1	D	6	THR	3.3
1	B	96	ALA	3.3
1	B	92	ALA	3.2
1	B	101	LEU	3.1
1	D	92	ALA	3.1
1	D	98	GLY	2.9
1	B	97	GLY	2.9
1	C	96	ALA	2.9
1	A	98	GLY	2.9
1	B	169	ASP	2.8
1	A	96	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	5	PHE	2.7
1	B	433	PRO	2.6
1	B	418	GLY	2.6
1	D	11	THR	2.6
1	B	93	ASP	2.5
1	C	4	GLN	2.4
1	B	168	PRO	2.4
1	B	48	GLY	2.4
1	C	98	GLY	2.4
1	A	229	GLN	2.3
1	D	101	LEU	2.2
1	D	95	ASP	2.2
1	D	434	GLY	2.2
1	B	160	THR	2.1
1	A	433	PRO	2.1
1	C	92	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
4	IPA	B	603	4/4	0.90	0.18	22,26,26,96	0
2	DXG	D	502	13/13	0.93	0.11	30,42,97,100	0
2	DXG	B	500	13/13	0.94	0.10	30,46,67,68	0
4	IPA	D	601	4/4	0.94	0.16	23,37,44,56	0
2	DXG	C	501	13/13	0.95	0.10	25,35,70,100	0
4	IPA	A	602	4/4	0.95	0.16	17,33,41,54	0
2	DXG	A	499	13/13	0.96	0.09	19,38,62,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	IPA	C	604	4/4	0.97	0.19	19,46,67,100	0
3	MG	A	498	1/1	0.97	0.05	28,28,28,28	0
3	MG	C	498	1/1	0.99	0.04	29,29,29,29	0
3	MG	D	498	1/1	0.99	0.04	34,34,34,34	0
3	MG	B	498	1/1	0.99	0.05	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.