Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 08:46 PM EST

PDB ID	:	1SJB
Title	:	X-ray structure of o-succinylbenzoate synthase complexed with o-succinylbenzoic acid
Authors	:	Thoden, J.B.; Taylor-Ringia, E.A.; Garrett, J.B.; Gerlt, J.A.; Holden, H.M.; Rayment, I.
Deposited on	:	2004-03-03
Resolution	:	2.20 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:

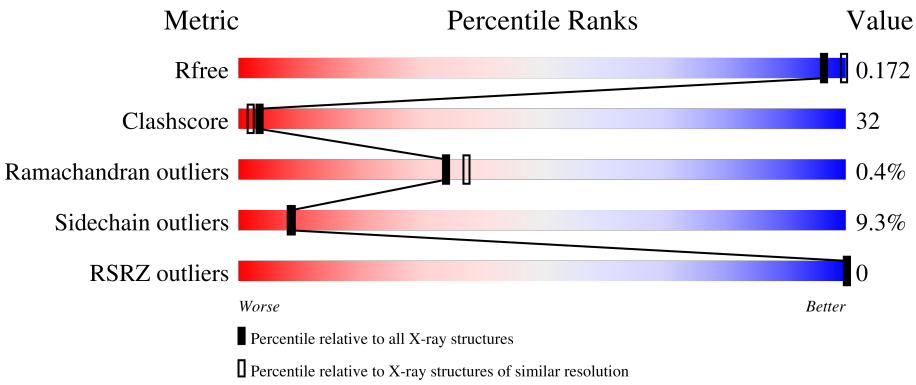
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	368	48% 40% 11% •
1	B	368	55% 33% 11% •
1	C	368	51% 38% 10% •
1	D	368	46% 42% 10% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11955 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.

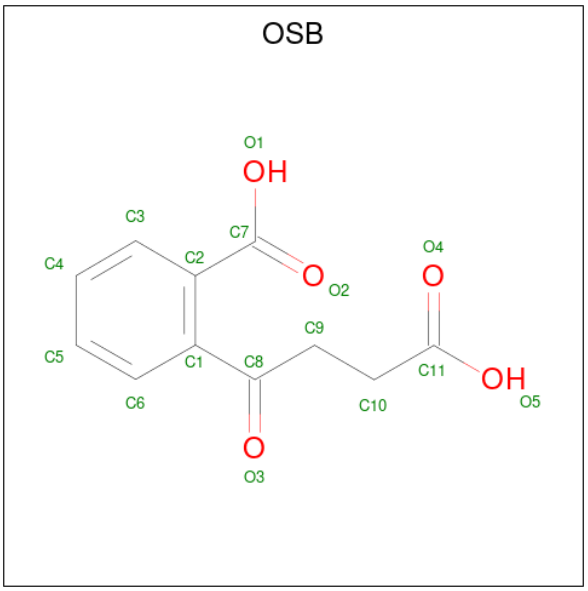
- Molecule 1 is a protein called N-acylamino acid racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	367	2772	1762	483	515	12	0	1	0
1	B	368	2781	1766	481	522	12	0	2	0
1	C	367	2782	1768	483	519	12	0	3	0
1	D	368	2778	1765	484	517	12	0	1	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 2-SUCCINYLBENZOATE (three-letter code: OSB) (formula: $C_{11}H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	16	11	5	0	0
			Total	C	O		
3	B	1	16	11	5	0	0
			Total	C	O		
3	C	1	16	11	5	0	0
			Total	C	O		
3	D	1	16	11	5	0	0

- Molecule 4 is water.

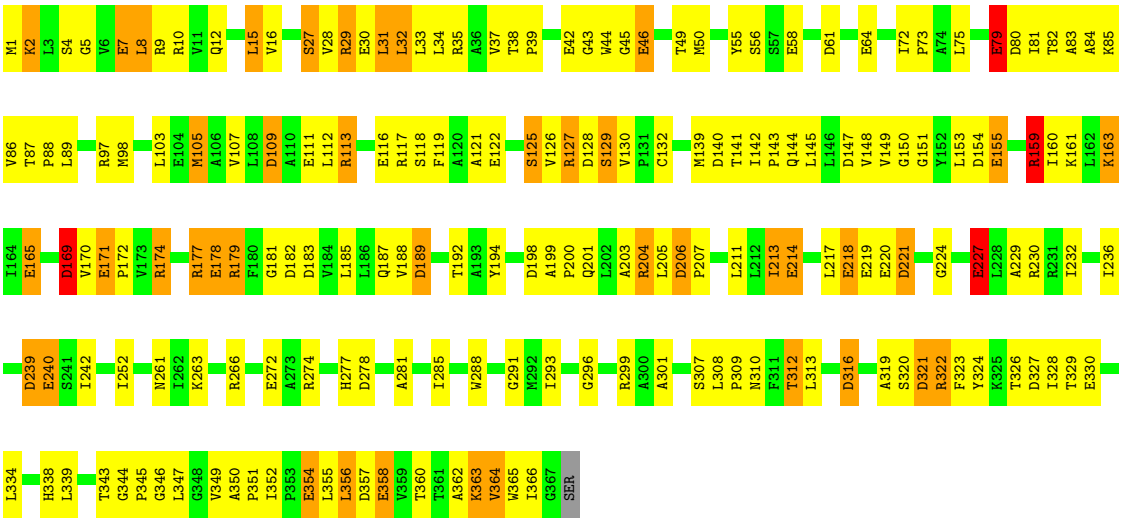
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	180	180	180	0	0
			Total	O		
4	B	249	249	249	0	0
			Total	O		
4	C	196	196	196	0	0
			Total	O		
4	D	149	149	149	0	0

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.

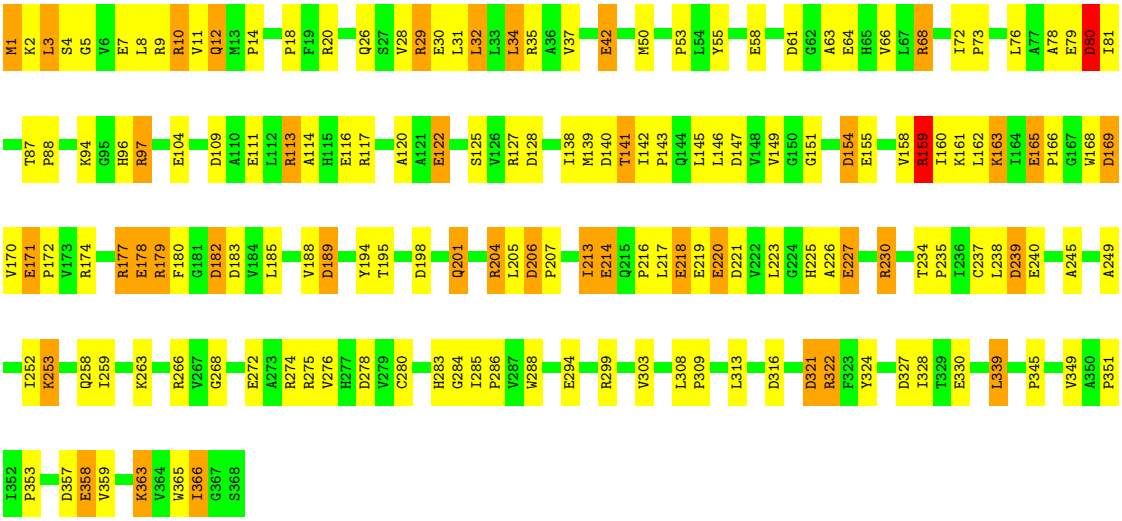
• Molecule 1: N-acylamino acid racemase

Chain A:



• Molecule 1: N-acylamino acid racemase

Chain B:



• Molecule 1: N-acylamino acid racemase

Chain C: 51% 38% 10% •

M1 K2 L3 S4 G5 V6 E7 L8 R9 R10 V11 Q12 M13 P18 F19 R20 T25 Q26 S27 V28 R29 E30 L31 L32 L33 L34 R35 A36 V37 T38 P39 E42 E46 C47 V48 T49 M50 Y55 E58 D61 E64 H65 L71 I72 P73 A74 L75 L76 E79 D80

I81 T82 A83 A84 K85 V86 T87 P88 L89 G95 H96 R97 M98 A99 K100 L103 E104 V107 L108 D109 A110 E111 L112 R113 R117 S118 F119 E122 V126 R127 D128 C132 I138 M139 D140 T141 I142 P143 Q144 L145 L146 D147 V148 G151 D154 E155 V158 R159 I160

K163 I164 E165 W168 D169 V170 E171 P172 V173 R174 R177 E178 D182 D183 V184 L185 D189 A190 N191 T192 A193 Y194 D198 Q201 L202 A203 R204 L205 D206 P207 L211 L212 P216 L217 E218 E219 E220 D221 H225 A226 E227 R230 R231 I232 P235 D239 E240

R246 A247 A248 A249 I252 K253 V257 P264 L271 R274 H277 D278 I285 W288 I293 E294 T295 G296 L297 G298 R299 L305 A306 S307 L308 P309 L313 D316 S320 D321 R322 F323 Y324 D327 I328 T329 E330 L334 G337 H338 L339 T343

V349 A350 P351 I352 P353 E354 L355 L356 D357 E358 V359 A362 W365 I366 G367 SER

• Molecule 1: N-acylamino acid racemase

Chain D: 46% 42% 10% •

M1 K2 L3 S4 E7 L8 R9 Q12 M13 P14 L15 V16 A17 P18 F19 R20 T21 S22 F23 Q26 S27 V28 R29 E30 L31 L32 L33 L34 R35 A36 V37 T38 P39 A40 G41 E42 G43 W44 G45 E46 C47 V48 T49 Y55 E58 Y59 N60 D61 E64 H65 V66 L67 R68

L71 A74 L75 E79 D80 I81 T82 A83 A84 K85 V86 T87 P88 L89 L90 N98 E104 M105 A106 D109 A110 E111 L112 R113 E116 R117 S118 F119 E122 L123 G124 S125 V126 R127 D128 S129 V130 P131 C132 G137 I138 M139 D140 T141 I142 P143 Q144 L145 L146 D147 V148

G151 Y152 L153 D154 E155 V158 R159 I160 K161 L162 K163 I164 E165 P166 G167 W168 D169 V170 E171 P172 V173 R174 A175 V176 R177 E178 D182 D183 V184 L185 L186 Q187 V188 D189 Y194 D198 A199 P200 Q201 L202 A203 R204 L205 D206 P207 L211 L212 I213 E214 Q215 P216 L217 E218 E219 E220

D221 G224 H225 A226 E227 R230 Q233 T234 P235 L238 D239 E240 A248 A249 D250 A251 I252 Q258 N261 P264 R274 H277 D278 I285 G291 M292 I293 E294 T295 G296 L297 G298 R299 N302 L305 A306 S307 L308 P309 D316 D321 R322 F323 Y324

D327 I328 T329 E330 P331 F332 V333 L334 S335 G336 G337 H338 L339 T343 G344 P345 G346 L347 G348 V349 A350 P351 I352 P353 E354 L355 L356 D357 E358 V359 K363 V364 W365 I366 G367 S368

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	216.00Å 216.00Å 261.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-2.20) 95.1 (29.95-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.20Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.204 , 0.272 0.174 , 0.172	Depositor DCC
R_{free} test set	11644 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	13.0	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 121.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.30$, $< L^2 > = 0.14$	Xtriage
Estimated twinning fraction	0.217 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.216 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.208 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11955	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% 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: MG, OSB

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	1.08	22/2832 (0.8%)	1.37	42/3856 (1.1%)
1	B	1.09	21/2845 (0.7%)	1.42	51/3873 (1.3%)
1	C	1.10	23/2850 (0.8%)	1.37	42/3880 (1.1%)
1	D	1.10	24/2838 (0.8%)	1.42	48/3864 (1.2%)
All	All	1.09	90/11365 (0.8%)	1.39	183/15473 (1.2%)

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	122	GLU	CD-OE2	8.16	1.34	1.25
1	A	171	GLU	CD-OE2	8.10	1.34	1.25
1	C	155	GLU	CD-OE2	7.55	1.33	1.25
1	B	358	GLU	CD-OE2	7.50	1.33	1.25
1	D	354	GLU	CD-OE2	7.49	1.33	1.25
1	A	30	GLU	CD-OE2	7.43	1.33	1.25
1	C	178	GLU	CD-OE2	7.34	1.33	1.25
1	B	30	GLU	CD-OE2	7.33	1.33	1.25
1	D	155	GLU	CD-OE2	7.23	1.33	1.25
1	A	358	GLU	CD-OE2	7.13	1.33	1.25
1	D	358	GLU	CD-OE2	7.11	1.33	1.25
1	D	46	GLU	CD-OE2	6.98	1.33	1.25
1	D	42	GLU	CD-OE2	6.90	1.33	1.25
1	D	330	GLU	CD-OE2	6.85	1.33	1.25
1	C	330	GLU	CD-OE2	6.84	1.33	1.25
1	A	178	GLU	CD-OE2	6.82	1.33	1.25
1	A	46	GLU	CD-OE2	6.82	1.33	1.25
1	D	79	GLU	CD-OE2	6.74	1.33	1.25
1	B	79	GLU	CD-OE2	6.70	1.33	1.25
1	D	116	GLU	CD-OE2	6.69	1.33	1.25
1	B	227	GLU	CD-OE2	6.68	1.33	1.25
1	A	116	GLU	CD-OE2	6.65	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	294	GLU	CD-OE2	6.65	1.32	1.25
1	D	227	GLU	CD-OE2	6.62	1.32	1.25
1	B	111	GLU	CD-OE2	6.59	1.32	1.25
1	C	354	GLU	CD-OE2	6.59	1.32	1.25
1	A	79	GLU	CD-OE2	6.54	1.32	1.25
1	C	227	GLU	CD-OE2	6.54	1.32	1.25
1	A	122	GLU	CD-OE2	6.53	1.32	1.25
1	B	220[A]	GLU	CD-OE2	6.51	1.32	1.25
1	B	220[B]	GLU	CD-OE2	6.51	1.32	1.25
1	A	354	GLU	CD-OE2	6.49	1.32	1.25
1	C	30	GLU	CD-OE2	6.49	1.32	1.25
1	B	155	GLU	CD-OE2	6.46	1.32	1.25
1	C	219	GLU	CD-OE2	6.42	1.32	1.25
1	D	171	GLU	CD-OE2	6.42	1.32	1.25
1	D	30	GLU	CD-OE2	6.41	1.32	1.25
1	A	240	GLU	CD-OE2	6.41	1.32	1.25
1	A	218	GLU	CD-OE2	6.34	1.32	1.25
1	A	42	GLU	CD-OE2	6.31	1.32	1.25
1	A	272	GLU	CD-OE2	6.28	1.32	1.25
1	B	165	GLU	CD-OE2	6.18	1.32	1.25
1	C	46	GLU	CD-OE2	6.18	1.32	1.25
1	B	219	GLU	CD-OE2	6.16	1.32	1.25
1	C	220[A]	GLU	CD-OE2	6.15	1.32	1.25
1	C	220[B]	GLU	CD-OE2	6.15	1.32	1.25
1	D	122	GLU	CD-OE2	6.15	1.32	1.25
1	A	214	GLU	CD-OE2	6.06	1.32	1.25
1	A	220	GLU	CD-OE2	6.02	1.32	1.25
1	B	178	GLU	CD-OE2	6.00	1.32	1.25
1	A	330	GLU	CD-OE2	5.96	1.32	1.25
1	D	104	GLU	CD-OE2	5.91	1.32	1.25
1	C	7	GLU	CD-OE2	5.90	1.32	1.25
1	D	58	GLU	CD-OE2	5.88	1.32	1.25
1	A	7	GLU	CD-OE2	5.86	1.32	1.25
1	B	122	GLU	CD-OE2	5.86	1.32	1.25
1	B	171	GLU	CD-OE2	5.76	1.31	1.25
1	B	240	GLU	CD-OE2	5.76	1.31	1.25
1	D	111	GLU	CD-OE2	5.74	1.31	1.25
1	A	155	GLU	CD-OE2	5.73	1.31	1.25
1	A	227	GLU	CD-OE2	5.67	1.31	1.25
1	D	218	GLU	CD-OE2	5.66	1.31	1.25
1	C	42	GLU	CD-OE2	5.61	1.31	1.25
1	D	240	GLU	CD-OE2	5.60	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	GLU	CD-OE2	5.58	1.31	1.25
1	D	220	GLU	CD-OE2	5.58	1.31	1.25
1	C	79[A]	GLU	CD-OE2	5.58	1.31	1.25
1	C	79[B]	GLU	CD-OE2	5.58	1.31	1.25
1	B	104	GLU	CD-OE2	5.56	1.31	1.25
1	C	64	GLU	CD-OE2	5.55	1.31	1.25
1	D	178	GLU	CD-OE2	5.55	1.31	1.25
1	C	165	GLU	CD-OE2	5.54	1.31	1.25
1	B	58	GLU	CD-OE1	-5.54	1.19	1.25
1	A	64	GLU	CD-OE2	5.54	1.31	1.25
1	C	104	GLU	CD-OE2	5.52	1.31	1.25
1	C	171	GLU	CD-OE2	5.50	1.31	1.25
1	D	7	GLU	CD-OE2	5.49	1.31	1.25
1	D	165	GLU	CD-OE2	5.43	1.31	1.25
1	B	218	GLU	CD-OE2	5.40	1.31	1.25
1	D	219	GLU	CD-OE2	5.38	1.31	1.25
1	B	272	GLU	CD-OE2	5.38	1.31	1.25
1	C	358	GLU	CD-OE2	5.38	1.31	1.25
1	A	219	GLU	CD-OE2	5.30	1.31	1.25
1	B	42	GLU	CD-OE2	5.27	1.31	1.25
1	B	214	GLU	CD-OE2	5.21	1.31	1.25
1	D	214	GLU	CD-OE2	5.19	1.31	1.25
1	C	218	GLU	CD-OE2	5.15	1.31	1.25
1	B	330	GLU	CD-OE2	5.05	1.31	1.25
1	C	111	GLU	CD-OE2	5.03	1.31	1.25
1	C	240	GLU	CD-OE2	5.02	1.31	1.25

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	159	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	B	221	ASP	CB-CG-OD2	-9.47	109.78	118.30
1	D	68[A]	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	D	68[B]	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A	322	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	B	274	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	221	ASP	CB-CG-OD1	8.16	125.65	118.30
1	B	109	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	C	189	ASP	CB-CG-OD1	8.13	125.62	118.30
1	B	206	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	B	169	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	A	183	ASP	CB-CG-OD2	-7.88	111.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	113	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	D	113	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	97	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	C	299	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	C	109	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	A	321	ASP	CB-CG-OD1	7.66	125.20	118.30
1	C	183	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	D	128	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	A	316	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	A	206	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	B	10	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	D	80	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	B	159	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	B	140	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	C	169	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	B	239	ASP	CB-CG-OD1	7.32	124.89	118.30
1	D	159	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	D	182	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	A	321	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	D	128	ASP	CB-CG-OD1	7.23	124.81	118.30
1	B	80	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	183	ASP	CB-CG-OD1	7.12	124.71	118.30
1	B	147	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	C	204	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	169	ASP	CB-CG-OD1	7.08	124.67	118.30
1	C	327	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	D	169	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	B	127	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	327	ASP	CB-CG-OD1	6.97	124.58	118.30
1	A	182	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	C	189	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	C	182	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	C	140	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	189	ASP	CB-CG-OD1	6.92	124.53	118.30
1	D	154	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	D	182	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	239	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	B	97	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	B	127	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	327	ASP	CB-CG-OD1	6.72	124.35	118.30
1	B	128	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	140	ASP	CB-CG-OD2	-6.67	112.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	327	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	B	154	ASP	CB-CG-OD2	-6.66	112.30	118.30
1	A	109	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	B	321	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	C	321	ASP	CB-CG-OD1	6.62	124.26	118.30
1	B	189	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	B	128	ASP	CB-CG-OD1	6.60	124.24	118.30
1	C	321	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	B	183[A]	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	B	183[B]	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	D	239	ASP	CB-CG-OD1	6.54	124.18	118.30
1	D	250	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	B	322	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	B	357	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	198	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	97	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	357	ASP	CB-CG-OD1	6.45	124.11	118.30
1	D	327	ASP	CB-CG-OD1	6.45	124.10	118.30
1	C	169	ASP	CB-CG-OD1	6.42	124.08	118.30
1	D	221	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	C	113	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	147	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	D	127	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	182	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	182	ASP	CB-CG-OD1	6.33	123.99	118.30
1	A	128	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	D	183	ASP	CB-CG-OD1	6.32	123.99	118.30
1	D	61	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	154	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	113	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	C	206	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	B	182	ASP	CB-CG-OD2	-6.27	112.65	118.30
1	C	357	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	C	246	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	D	221	ASP	CB-CG-OD1	6.26	123.94	118.30
1	C	127	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	169	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	159	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	B	113	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	D	189	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	D	204	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	D	327	ASP	CB-CG-OD2	-6.18	112.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	109	ASP	CB-CG-OD1	6.17	123.85	118.30
1	C	80	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	B	316	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	61	ASP	CB-CG-OD1	6.14	123.82	118.30
1	D	357	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	A	154	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	C	128	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	D	198	ASP	CB-CG-OD1	6.04	123.73	118.30
1	D	147	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	239	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	D	147	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	C	183	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	154	ASP	CB-CG-OD1	5.95	123.66	118.30
1	D	321	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	189	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	A	299	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	97	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	230	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	221	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	B	80	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	316	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	D	80	ASP	CB-CG-OD1	5.85	123.56	118.30
1	D	159	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	147	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	128	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	147	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	154	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	C	221	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	105	MET	CG-SD-CE	5.77	109.43	100.20
1	D	198	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	C	128	ASP	CB-CG-OD1	5.75	123.47	118.30
1	B	147	ASP	CB-CG-OD1	5.75	123.47	118.30
1	B	61	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	C	278	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	B	183[A]	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	183[B]	ASP	CB-CG-OD1	5.73	123.46	118.30
1	D	322	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	198	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	D	239	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	C	140	ASP	CB-CG-OD1	5.70	123.42	118.30
1	B	165	GLU	N-CA-CB	-5.68	100.37	110.60
1	D	61	ASP	CB-CG-OD1	5.67	123.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	278	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	B	321	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	127	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	B	278	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	A	61	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	B	61	ASP	CB-CG-OD1	5.59	123.33	118.30
1	D	35	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	C	61	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	C	147	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	253	LYS	N-CA-CB	5.54	120.56	110.60
1	B	353	PRO	N-CA-CB	5.53	109.94	103.30
1	C	117	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	140	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	230	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	204[A]	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	204[B]	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	154	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	327	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	D	183	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	D	206	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	A	140	ASP	CB-CG-OD1	5.39	123.16	118.30
1	A	239	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	169	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	169	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	316	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	299	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	322	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	80	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	198	ASP	CB-CG-OD1	5.27	123.04	118.30
1	C	182	ASP	CB-CG-OD1	5.27	123.04	118.30
1	C	206	ASP	CB-CG-OD1	5.27	123.04	118.30
1	C	127	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	D	9	ARG	CB-CA-C	-5.22	99.95	110.40
1	A	322	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	140	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	C	117	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	189	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	321	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	221	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	D	204	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	D	154	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	20	ARG	NE-CZ-NH1	5.07	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	358	GLU	N-CA-CB	5.05	119.70	110.60
1	A	174	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	312	THR	CA-CB-CG2	-5.00	105.39	112.40

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	2772	0	2814	199	1
1	B	2781	0	2812	135	0
1	C	2782	0	2818	178	0
1	D	2778	0	2819	214	1
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	16	0	8	4	0
3	B	16	0	8	2	0
3	C	16	0	8	0	0
3	D	16	0	8	3	0
4	A	180	0	0	2	0
4	B	249	0	0	6	0
4	C	196	0	0	13	0
4	D	149	0	0	7	0
All	All	11955	0	11295	724	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 32.

All (724) 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:38:THR:HB	1:D:39:PRO:HD2	1.20	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:VAL:HG13	1:A:160:ILE:HD13	1.25	1.11
1:D:352:ILE:O	1:D:355:LEU:HB2	1.51	1.10
1:D:49:THR:HG22	1:D:98:MET:HE3	1.27	1.07
1:A:58:GLU:HB2	1:A:98:MET:CE	1.84	1.06
1:A:29:ARG:HD3	1:A:31:LEU:CD2	1.85	1.05
1:A:352:ILE:CG2	1:A:355:LEU:HD12	1.88	1.04
1:A:144:GLN:O	1:A:148:VAL:HG23	1.58	1.04
1:D:15:LEU:HD23	1:D:324:TYR:HE2	1.23	1.04
1:D:68[A]:ARG:HH11	1:D:68[A]:ARG:HG2	1.22	1.03
1:D:171:GLU:OE1	1:D:174:ARG:NH1	1.91	1.03
1:C:141:THR:CG2	1:C:143:PRO:HD2	1.89	1.03
1:D:125:SER:HB2	1:D:307:SER:OG	1.59	1.01
1:A:149:VAL:HG13	1:A:160:ILE:CD1	1.90	1.01
1:B:159:ARG:HB2	1:B:185:LEU:CB	1.90	1.00
1:C:205:LEU:C	1:C:207:PRO:HD2	1.83	0.99
1:D:21:THR:HG22	1:D:23:PHE:H	1.25	0.98
1:D:7:GLU:OE1	1:D:9:ARG:NH1	1.96	0.98
1:C:141:THR:HG22	1:C:143:PRO:CD	1.93	0.97
1:D:68[A]:ARG:HG3	1:D:366:ILE:CD1	1.93	0.96
1:A:4:SER:HB2	1:A:37:VAL:HG12	1.47	0.95
1:A:352:ILE:HB	1:A:355:LEU:HD12	1.47	0.95
1:C:33:LEU:C	1:C:34:LEU:HD23	1.87	0.95
1:A:29:ARG:HD3	1:A:31:LEU:HD21	1.42	0.94
1:C:49:THR:HG22	1:C:98:MET:HE1	1.46	0.94
1:C:141:THR:HG22	1:C:143:PRO:HD2	1.49	0.94
1:C:159:ARG:NH2	1:C:316:ASP:OD1	2.00	0.94
1:C:58:GLU:HB2	1:C:98:MET:CE	1.98	0.93
1:C:38:THR:HB	1:C:39:PRO:HD2	1.49	0.93
1:C:201:GLN:O	1:C:204:ARG:HB2	1.69	0.93
1:A:352:ILE:CB	1:A:355:LEU:HD12	1.99	0.92
1:D:68[B]:ARG:HG2	1:D:366:ILE:HD11	1.52	0.92
1:B:78:ALA:HB3	1:B:81:ILE:HD11	1.50	0.92
1:C:10[B]:ARG:HD3	1:C:362:ALA:HB3	1.52	0.91
1:A:35:ARG:HG3	1:A:44:TRP:CZ2	2.06	0.91
1:D:38:THR:HB	1:D:39:PRO:CD	2.01	0.89
1:D:206:ASP:N	1:D:207:PRO:HD2	1.86	0.89
1:B:142:ILE:N	1:B:143:PRO:HD2	1.88	0.89
1:B:159:ARG:HB2	1:B:185:LEU:HB2	1.56	0.88
1:A:15:LEU:HB2	1:A:27:SER:O	1.74	0.88
1:D:15:LEU:CD2	1:D:324:TYR:HE2	1.87	0.88
1:D:68[A]:ARG:HG3	1:D:366:ILE:HD11	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:VAL:HG23	1:A:213:ILE:HD12	1.57	0.85
1:C:352:ILE:HB	1:C:355:LEU:HD12	1.57	0.85
1:D:141:THR:HG22	1:D:143:PRO:HD2	1.56	0.85
1:B:366:ILE:N	1:B:366:ILE:HD12	1.92	0.85
1:A:338:HIS:O	1:A:339:LEU:HD12	1.77	0.84
1:D:348:GLY:HA2	4:D:1438:HOH:O	1.78	0.84
1:D:169:ASP:OD1	1:D:194:TYR:OH	1.94	0.84
1:D:328:ILE:O	1:D:351:PRO:HA	1.78	0.84
1:A:58:GLU:HB2	1:A:98:MET:HE3	1.59	0.84
1:C:58:GLU:HB2	1:C:98:MET:HE2	1.57	0.84
1:C:141:THR:CG2	1:C:143:PRO:CD	2.51	0.84
1:A:169:ASP:OD1	1:A:194:TYR:OH	1.96	0.83
1:D:353:PRO:HA	1:D:356:LEU:CB	2.07	0.83
1:A:354:GLU:O	1:A:358:GLU:HG3	1.79	0.83
1:D:35:ARG:HG2	1:D:35:ARG:HH11	1.43	0.83
1:B:8:LEU:CD2	1:B:34:LEU:HD22	2.09	0.83
1:C:169:ASP:OD1	1:C:194:TYR:OH	1.96	0.82
1:B:159:ARG:HB2	1:B:185:LEU:HB3	1.59	0.82
1:C:49:THR:HG22	1:C:98:MET:CE	2.09	0.82
1:D:141:THR:CG2	1:D:143:PRO:HD2	2.08	0.82
1:D:353:PRO:HA	1:D:356:LEU:HB3	1.60	0.82
1:A:125:SER:HB2	1:A:307:SER:OG	1.80	0.82
1:C:139:MET:HB2	1:C:168:TRP:CZ2	2.15	0.82
1:C:141:THR:HG23	1:C:143:PRO:HD2	1.60	0.82
1:D:68[A]:ARG:HG2	1:D:68[A]:ARG:NH1	1.91	0.82
1:C:87:THR:HB	1:C:88:PRO:HD3	1.61	0.82
1:A:58:GLU:HB2	1:A:98:MET:HE2	1.62	0.82
1:A:58:GLU:CB	1:A:98:MET:HE3	2.10	0.82
1:D:21:THR:HG21	1:D:23:PHE:CE1	2.15	0.82
1:A:199:ALA:HB3	1:A:200:PRO:HD3	1.60	0.82
1:C:81:ILE:HD11	4:C:1296:HOH:O	1.79	0.82
1:D:159:ARG:O	1:D:160:ILE:HD13	1.80	0.81
1:D:1:MET:SD	1:D:38:THR:HG21	2.20	0.81
1:D:151:GLY:HA3	4:D:1448:HOH:O	1.80	0.81
1:D:87:THR:HB	1:D:88:PRO:HD3	1.62	0.80
1:C:248:ALA:O	1:C:252:ILE:HG13	1.80	0.80
1:D:351:PRO:HB2	1:D:356:LEU:HD22	1.61	0.80
1:D:353:PRO:O	1:D:357:ASP:N	2.13	0.80
1:C:75:LEU:HD11	1:C:103:LEU:HD13	1.64	0.80
1:D:68[A]:ARG:HG3	1:D:366:ILE:HD13	1.62	0.80
1:C:127:ARG:HH11	1:C:307:SER:HA	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ALA:O	1:B:253:LYS:HG3	1.81	0.79
1:D:233:GLN:HG2	4:D:1446:HOH:O	1.82	0.79
1:D:33:LEU:O	1:D:34:LEU:HD23	1.83	0.79
1:D:206:ASP:N	1:D:207:PRO:CD	2.45	0.79
1:B:218:GLU:HG3	1:B:220[B]:GLU:OE1	1.82	0.78
1:C:87:THR:HB	1:C:88:PRO:CD	2.13	0.78
1:A:149:VAL:CG1	1:A:160:ILE:HD13	2.11	0.78
1:A:29:ARG:HD3	1:A:31:LEU:HD23	1.66	0.78
1:A:7:GLU:CD	1:A:35:ARG:HH21	1.87	0.77
1:A:364:VAL:HG13	1:A:366:ILE:HD11	1.65	0.77
1:A:87:THR:HB	1:A:88:PRO:HD3	1.65	0.77
1:B:142:ILE:N	1:B:143:PRO:CD	2.48	0.77
1:B:201:GLN:O	1:B:204:ARG:HB2	1.85	0.77
1:C:75:LEU:CD1	1:C:103:LEU:HD13	2.15	0.77
1:B:365:TRP:C	1:B:366:ILE:HD12	2.05	0.77
1:A:201:GLN:O	1:A:204[A]:ARG:HB2	1.83	0.77
1:D:132:CYS:O	1:D:158:VAL:HG22	1.85	0.77
1:A:329:THR:HG22	1:A:350:ALA:O	1.85	0.76
1:C:65:HIS:HB2	4:C:1291:HOH:O	1.84	0.76
1:C:206:ASP:N	1:C:207:PRO:CD	2.48	0.76
1:A:201:GLN:O	1:A:204[B]:ARG:HB2	1.84	0.76
1:A:334:LEU:HD12	1:A:339:LEU:HD13	1.68	0.76
1:C:95:GLY:O	1:C:100:LYS:HE3	1.85	0.76
1:A:2:LYS:HE2	1:A:39:PRO:HG3	1.66	0.75
1:A:159:ARG:HG2	1:A:160:ILE:N	1.99	0.75
1:C:139:MET:CE	1:C:148:VAL:HG21	2.16	0.75
1:C:13:MET:HG3	1:C:31:LEU:HD11	1.68	0.75
1:D:293:ILE:HG23	1:D:323:PHE:CD1	2.22	0.75
1:D:38:THR:CB	1:D:39:PRO:HD2	2.08	0.74
1:A:352:ILE:HG21	1:A:355:LEU:HD12	1.68	0.74
1:D:15:LEU:HD23	1:D:324:TYR:CE2	2.16	0.74
1:A:29:ARG:CD	1:A:31:LEU:CD2	2.64	0.74
1:A:139:MET:HG3	1:A:145:LEU:HA	1.69	0.74
1:C:65:HIS:N	4:C:1291:HOH:O	1.99	0.74
1:A:293:ILE:HG22	1:A:293:ILE:O	1.86	0.73
1:D:352:ILE:HB	1:D:355:LEU:HD22	1.69	0.73
1:D:68[B]:ARG:HG2	1:D:366:ILE:CD1	2.19	0.73
1:C:334:LEU:HD21	1:C:337:GLY:HA2	1.69	0.72
1:D:58:GLU:OE1	1:D:98:MET:HG3	1.89	0.72
1:B:138:ILE:HG23	1:B:168:TRP:CD1	2.25	0.72
1:D:159:ARG:NH2	1:D:316:ASP:OD1	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ARG:HD2	4:B:1300:HOH:O	1.89	0.71
1:A:364:VAL:CG1	1:A:366:ILE:HD11	2.21	0.71
1:B:169:ASP:OD1	1:B:194:TYR:OH	2.09	0.71
1:C:141:THR:CG2	1:C:143:PRO:HG2	2.21	0.71
1:D:21:THR:HG21	1:D:23:PHE:CD1	2.26	0.71
1:A:206:ASP:N	1:A:207:PRO:CD	2.53	0.71
1:A:349:VAL:CG1	1:A:350:ALA:N	2.52	0.71
1:C:141:THR:CG2	1:C:143:PRO:CG	2.69	0.71
1:A:49:THR:HG22	1:A:98:MET:HE3	1.72	0.71
1:B:217:LEU:HB2	1:B:225:HIS:CE1	2.25	0.71
1:B:358:GLU:O	1:B:358:GLU:HG2	1.91	0.70
1:A:29:ARG:CD	1:A:31:LEU:HD23	2.21	0.70
1:B:8:LEU:HD23	1:B:34:LEU:HD22	1.73	0.70
1:A:1:MET:HE3	1:A:38:THR:HG21	1.74	0.70
1:D:35:ARG:HD3	1:D:44:TRP:CH2	2.27	0.70
1:C:10[B]:ARG:HG2	1:C:10[B]:ARG:HH11	1.54	0.70
1:C:31:LEU:HD22	1:C:295:THR:HG23	1.73	0.70
1:C:205:LEU:C	1:C:207:PRO:CD	2.58	0.70
1:A:352:ILE:CG2	1:A:355:LEU:CD1	2.66	0.69
1:D:171:GLU:CD	1:D:174:ARG:HH12	1.94	0.69
1:D:215:GLN:HG3	1:D:240:GLU:OE1	1.93	0.69
1:B:20:ARG:HG2	1:B:138:ILE:HD12	1.75	0.69
1:C:20:ARG:HD3	1:C:138:ILE:CG2	2.23	0.69
1:C:34:LEU:HD23	1:C:34:LEU:N	2.05	0.69
1:C:174:ARG:O	1:C:178:GLU:HB2	1.91	0.69
1:B:12:GLN:NE2	1:B:28:VAL:HG11	2.08	0.68
1:A:29:ARG:NE	1:A:31:LEU:HD23	2.09	0.68
1:C:127:ARG:NH1	1:C:307:SER:HA	2.08	0.68
1:A:82:THR:HG22	1:A:84:ALA:H	1.58	0.68
1:B:288:TRP:HB3	1:B:313:LEU:HB2	1.76	0.68
1:D:49:THR:HG22	1:D:98:MET:CE	2.14	0.68
1:A:291:GLY:O	3:A:1000:OSB:H92	1.93	0.67
1:C:10[A]:ARG:HD2	1:C:32:LEU:HD12	1.74	0.67
1:D:49:THR:CG2	1:D:98:MET:HE3	2.14	0.67
1:B:8:LEU:HD21	1:B:34:LEU:HD22	1.77	0.67
1:D:15:LEU:CD2	1:D:324:TYR:CE2	2.74	0.67
1:D:205:LEU:C	1:D:207:PRO:HD2	2.14	0.67
1:A:1:MET:CE	1:A:38:THR:HG21	2.24	0.67
1:A:334:LEU:HD12	1:A:339:LEU:CD1	2.24	0.67
1:B:206:ASP:HB2	1:B:207:PRO:HD3	1.75	0.67
1:A:58:GLU:CB	1:A:98:MET:CE	2.65	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:VAL:HG13	1:A:366:ILE:CD1	2.25	0.67
1:B:206:ASP:N	1:B:207:PRO:CD	2.58	0.67
1:D:49:THR:HA	1:D:98:MET:HE1	1.77	0.67
1:B:72:ILE:HB	1:B:73:PRO:HD3	1.77	0.66
1:B:213:ILE:HG12	1:B:216:PRO:HG3	1.75	0.66
1:B:366:ILE:N	1:B:366:ILE:CD1	2.58	0.66
1:D:21:THR:CG2	1:D:22:SER:N	2.58	0.66
1:C:65:HIS:CB	4:C:1291:HOH:O	2.40	0.66
1:D:87:THR:N	1:D:88:PRO:HD2	2.10	0.66
1:D:352:ILE:HB	1:D:355:LEU:CD2	2.25	0.66
1:A:163:LYS:NZ	3:A:1000:OSB:O3	2.29	0.66
1:B:205:LEU:C	1:B:207:PRO:HD2	2.15	0.66
1:D:29:ARG:NH1	1:D:49:THR:O	2.27	0.66
1:A:188:VAL:CG2	1:A:213:ILE:HD12	2.25	0.66
1:B:206:ASP:N	1:B:207:PRO:HD2	2.11	0.66
1:C:169:ASP:HB2	1:C:170:VAL:HG23	1.77	0.66
1:D:353:PRO:HA	1:D:356:LEU:HB2	1.78	0.66
1:A:352:ILE:HG21	1:A:355:LEU:CD1	2.25	0.65
1:D:159:ARG:HG2	1:D:160:ILE:N	2.10	0.65
1:D:334:LEU:HD12	1:D:339:LEU:HD13	1.78	0.65
1:A:87:THR:N	1:A:88:PRO:HD2	2.10	0.65
1:D:75:LEU:HB3	1:D:81:ILE:CD1	2.25	0.65
1:B:159:ARG:HG2	1:B:160:ILE:N	2.11	0.65
1:C:127:ARG:NH1	1:C:306:ALA:O	2.29	0.65
1:D:201:GLN:O	1:D:204:ARG:HB2	1.97	0.65
1:C:334:LEU:HD11	1:C:337:GLY:C	2.18	0.65
1:D:291:GLY:O	3:D:1300:OSB:H91	1.96	0.65
1:C:35:ARG:HE	1:C:42:GLU:CD	2.00	0.64
1:A:7:GLU:OE1	1:A:35:ARG:NH2	2.27	0.64
1:D:71:LEU:O	1:D:74:ALA:HB3	1.97	0.64
1:C:142:ILE:O	1:C:145:LEU:HB3	1.97	0.64
1:C:20:ARG:HD3	1:C:138:ILE:HG22	1.79	0.64
1:C:127:ARG:NH2	1:C:308:LEU:O	2.30	0.64
1:A:75:LEU:HD12	1:A:103:LEU:HD21	1.78	0.64
1:D:82:THR:HG22	1:D:84:ALA:H	1.62	0.64
1:A:29:ARG:NH2	1:A:49:THR:O	2.30	0.64
1:B:227:GLU:OE1	1:B:230:ARG:NH1	2.30	0.63
1:D:7:GLU:CD	1:D:9:ARG:NH1	2.50	0.63
1:D:68[B]:ARG:CZ	1:D:364:VAL:HG11	2.27	0.63
1:D:352:ILE:O	1:D:355:LEU:CB	2.38	0.63
1:C:85:LYS:NZ	4:C:1389:HOH:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:VAL:CG1	1:A:160:ILE:CD1	2.72	0.63
1:C:58:GLU:CB	1:C:98:MET:CE	2.75	0.63
1:B:139:MET:HG3	1:B:145:LEU:HA	1.81	0.63
1:D:67:LEU:HD23	1:D:71:LEU:HB2	1.81	0.63
1:C:10[B]:ARG:CD	1:C:362:ALA:HB3	2.26	0.63
1:A:33:LEU:HD23	1:A:46:GLU:HA	1.81	0.63
1:A:338:HIS:O	1:A:339:LEU:CD1	2.46	0.63
1:C:366:ILE:HA	4:C:1375:HOH:O	1.99	0.63
1:A:35:ARG:HG3	1:A:44:TRP:CE2	2.34	0.62
1:A:8:LEU:CD2	1:A:32:LEU:CD2	2.76	0.62
1:D:206:ASP:CG	1:D:233:GLN:HB2	2.19	0.62
1:D:141:THR:HG22	1:D:143:PRO:CD	2.29	0.62
1:C:211:LEU:O	1:C:235:PRO:HG2	2.00	0.62
1:A:329:THR:HG21	1:A:349:VAL:CG1	2.29	0.62
1:C:142:ILE:N	1:C:143:PRO:HD2	2.14	0.62
1:A:87:THR:CB	1:A:88:PRO:HD3	2.30	0.62
1:A:171:GLU:N	1:A:172:PRO:HD2	2.15	0.62
1:A:356:LEU:HD22	1:A:360:THR:OG1	2.00	0.62
1:C:139:MET:HB2	1:C:168:TRP:HZ2	1.64	0.62
1:C:194:TYR:CE2	1:C:202:LEU:HD21	2.34	0.62
1:D:159:ARG:C	1:D:160:ILE:HD13	2.19	0.62
1:A:349:VAL:HG12	1:A:350:ALA:N	2.15	0.62
1:A:352:ILE:O	1:A:355:LEU:HB2	1.99	0.61
1:D:48:VAL:HG22	4:D:1347:HOH:O	2.00	0.61
1:D:75:LEU:O	1:D:81:ILE:HD11	2.00	0.61
1:A:112:LEU:HB3	1:A:117:ARG:O	2.00	0.61
1:A:144:GLN:O	1:A:148:VAL:CG2	2.43	0.61
1:D:2:LYS:HD2	1:D:3:LEU:N	2.15	0.61
1:A:321:ASP:HA	1:A:324:TYR:O	2.00	0.61
1:C:308:LEU:HB3	1:C:309:PRO:HD2	1.83	0.61
1:D:159:ARG:HD2	4:D:1432:HOH:O	2.00	0.61
1:D:68[A]:ARG:HH11	1:D:68[A]:ARG:CG	2.08	0.61
1:C:87:THR:CB	1:C:88:PRO:CD	2.77	0.61
1:C:293:ILE:O	1:C:293:ILE:HG22	2.00	0.61
1:A:159:ARG:NH2	1:A:316:ASP:OD1	2.21	0.61
1:A:329:THR:CG2	1:A:349:VAL:CG1	2.78	0.61
1:A:203:ALA:HA	1:A:232:ILE:HG22	1.82	0.61
1:A:352:ILE:O	1:A:355:LEU:N	2.34	0.61
1:C:141:THR:HG22	1:C:143:PRO:N	2.16	0.60
1:C:109:ASP:O	1:C:113:ARG:HG3	2.01	0.60
1:A:8:LEU:CD2	1:A:32:LEU:HD22	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:HD2	1:A:362:ALA:HB3	1.84	0.60
1:C:33:LEU:O	1:C:34:LEU:HD23	2.01	0.60
1:D:199:ALA:HB3	1:D:200:PRO:HD3	1.83	0.60
1:C:87:THR:CB	1:C:88:PRO:HD3	2.32	0.60
1:D:44:TRP:O	1:D:106:ALA:HA	2.02	0.60
1:A:1:MET:HE3	1:A:38:THR:CG2	2.31	0.60
1:D:32:LEU:C	1:D:32:LEU:HD23	2.22	0.59
1:D:248:ALA:O	1:D:252:ILE:HG13	2.01	0.59
1:A:129:SER:OG	1:A:338:HIS:HB3	2.01	0.59
1:B:29:ARG:HD2	1:B:31:LEU:HG	1.84	0.59
1:A:206:ASP:N	1:A:207:PRO:HD2	2.16	0.59
1:C:163:LYS:HE3	1:C:189:ASP:HB3	1.85	0.59
1:A:82:THR:O	1:A:83:ALA:C	2.38	0.59
1:A:239:ASP:OD1	1:A:266:ARG:NH1	2.35	0.59
1:C:96:HIS:O	1:C:100:LYS:HG3	2.03	0.59
1:C:10[B]:ARG:HG2	1:C:10[B]:ARG:NH1	2.15	0.59
1:A:177:ARG:HD2	1:A:181:GLY:O	2.03	0.59
1:B:4:SER:HB2	1:B:37:VAL:HG12	1.84	0.59
1:D:68[B]:ARG:NH2	1:D:364:VAL:HG21	2.18	0.58
1:A:205:LEU:C	1:A:207:PRO:HD2	2.23	0.58
1:D:297:LEU:HD23	1:D:329:THR:HG21	1.85	0.58
1:C:10[A]:ARG:HD2	1:C:32:LEU:CD1	2.33	0.58
1:B:252:ILE:HG12	1:B:285:ILE:HG13	1.84	0.58
1:C:3:LEU:HB2	1:C:81:ILE:HD13	1.85	0.58
1:D:87:THR:HB	1:D:88:PRO:CD	2.32	0.58
1:B:171:GLU:HB2	1:B:172:PRO:HD3	1.85	0.58
1:D:55:TYR:OH	1:D:239:ASP:OD1	2.19	0.58
1:A:263:LYS:HB2	1:A:266:ARG:NH1	2.18	0.58
1:A:329:THR:HG21	1:A:349:VAL:HG11	1.86	0.58
1:A:16:VAL:HG23	1:A:323:PHE:O	2.04	0.58
1:B:283:HIS:ND1	1:C:253:LYS:HE2	2.18	0.58
1:B:294:GLU:O	1:B:299:ARG:NH1	2.37	0.58
1:D:206:ASP:HB2	1:D:207:PRO:HD3	1.84	0.58
1:A:139:MET:HG3	1:A:145:LEU:CA	2.32	0.57
1:D:38:THR:OG1	1:D:41:GLY:O	2.17	0.57
1:D:227:GLU:O	1:D:230:ARG:HB2	2.04	0.57
1:B:87:THR:N	1:B:88:PRO:HD2	2.20	0.57
1:C:328:ILE:O	1:C:351:PRO:HA	2.05	0.57
1:D:351:PRO:CB	1:D:356:LEU:HD22	2.35	0.57
1:D:18:PRO:HA	1:D:26:GLN:O	2.04	0.57
1:D:112:LEU:HD12	1:D:119:PHE:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:VAL:HG12	1:D:152:TYR:CE1	2.40	0.57
1:A:7:GLU:CD	1:A:35:ARG:NH2	2.58	0.57
1:C:10[A]:ARG:NH1	1:C:61:ASP:OD1	2.36	0.57
1:D:142:ILE:HB	1:D:143:PRO:HD3	1.86	0.57
1:D:274:ARG:O	1:D:277:HIS:HB3	2.04	0.57
1:C:58:GLU:HB2	1:C:98:MET:HE1	1.86	0.57
1:A:38:THR:HB	1:A:39:PRO:HD2	1.86	0.57
1:A:328:ILE:O	1:A:351:PRO:HA	2.05	0.57
1:D:199:ALA:N	1:D:200:PRO:HD2	2.19	0.56
1:B:239:ASP:OD2	1:B:263:LYS:NZ	2.31	0.56
1:C:35:ARG:NE	1:C:42:GLU:OE2	2.34	0.56
1:C:72:ILE:HB	1:C:73:PRO:HD3	1.87	0.56
1:A:206:ASP:HB2	1:A:207:PRO:HD3	1.87	0.56
1:A:49:THR:HG22	1:A:98:MET:CE	2.35	0.56
1:B:1:MET:HE1	1:B:114:ALA:CB	2.35	0.56
1:B:11:VAL:HG13	1:B:359:VAL:HG23	1.88	0.56
1:C:82:THR:HG23	1:C:85:LYS:HD2	1.87	0.56
1:D:30:GLU:O	1:D:60:ASN:ND2	2.35	0.56
1:D:252:ILE:HD13	1:D:285:ILE:HG13	1.87	0.56
1:B:3:LEU:HD22	1:B:5:GLY:H	1.71	0.56
1:B:141:THR:CB	1:B:143:PRO:HD2	2.36	0.56
1:A:192:THR:HB	1:A:218:GLU:HA	1.86	0.55
1:C:329:THR:HG21	1:C:349:VAL:CG1	2.36	0.55
1:D:350:ALA:HB1	1:D:351:PRO:CD	2.36	0.55
1:A:10:ARG:CD	1:A:362:ALA:HB3	2.37	0.55
1:B:201:GLN:OE1	1:B:201:GLN:HA	2.06	0.55
1:C:139:MET:HE3	1:C:148:VAL:HG21	1.88	0.55
1:D:328:ILE:HD12	1:D:351:PRO:HB3	1.88	0.55
1:C:55:TYR:OH	1:C:239:ASP:OD1	2.25	0.55
1:C:206:ASP:N	1:C:207:PRO:HD2	2.17	0.55
1:D:75:LEU:HB3	1:D:81:ILE:HD13	1.88	0.55
1:D:142:ILE:O	1:D:145:LEU:N	2.40	0.55
1:B:139:MET:HG3	1:B:145:LEU:CA	2.37	0.55
1:A:301:ALA:HB2	1:A:347:LEU:CD2	2.36	0.55
1:A:263:LYS:NZ	3:A:1000:OSB:C7	2.70	0.55
1:B:283:HIS:CE1	1:C:253:LYS:HE2	2.42	0.55
1:A:58:GLU:HB3	1:A:98:MET:HE3	1.87	0.54
1:B:237:CYS:HA	1:B:259:ILE:O	2.07	0.54
1:D:21:THR:HG22	1:D:22:SER:N	2.21	0.54
1:A:5:GLY:HA3	1:A:365:TRP:CZ2	2.43	0.54
1:D:166:PRO:HD3	1:D:194:TYR:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:CB	1:A:88:PRO:CD	2.85	0.54
1:A:127:ARG:NH1	1:A:308:LEU:O	2.36	0.54
1:B:141:THR:C	1:B:143:PRO:HD2	2.27	0.54
1:D:352:ILE:CB	1:D:355:LEU:HD22	2.38	0.54
1:D:171:GLU:HB2	1:D:172:PRO:HD3	1.89	0.54
1:A:87:THR:N	1:A:88:PRO:CD	2.70	0.54
1:B:94:LYS:HE2	4:B:1235:HOH:O	2.07	0.54
1:C:18:PRO:HA	1:C:26:GLN:O	2.07	0.54
1:C:171:GLU:N	1:C:172:PRO:HD2	2.23	0.54
1:D:159:ARG:HB2	1:D:185:LEU:HB3	1.90	0.54
1:A:82:THR:CG2	1:A:84:ALA:HB3	2.37	0.54
1:C:10[A]:ARG:NH2	4:C:1219:HOH:O	2.40	0.54
1:D:305:LEU:O	1:D:307:SER:N	2.40	0.54
1:C:12:GLN:NE2	4:C:1212:HOH:O	2.40	0.53
1:D:87:THR:N	1:D:88:PRO:CD	2.71	0.53
1:D:113:ARG:HA	1:D:345:PRO:HB2	1.89	0.53
1:B:141:THR:OG1	1:B:143:PRO:HD2	2.08	0.53
1:D:350:ALA:HB1	1:D:351:PRO:HD2	1.90	0.53
1:C:20:ARG:HD3	1:C:138:ILE:CB	2.37	0.53
1:B:141:THR:OG1	1:B:143:PRO:HG2	2.07	0.53
1:B:159:ARG:CB	1:B:185:LEU:HB2	2.33	0.53
1:C:49:THR:CG2	1:C:98:MET:CE	2.85	0.53
1:A:171:GLU:HB2	1:A:172:PRO:HD3	1.91	0.53
1:C:20:ARG:HD3	1:C:138:ILE:HB	1.90	0.53
1:C:141:THR:HB	1:C:144:GLN:HB3	1.91	0.53
1:A:82:THR:HG22	1:A:84:ALA:N	2.23	0.53
1:B:80:ASP:C	1:B:81:ILE:HG12	2.30	0.52
1:B:171:GLU:N	1:B:172:PRO:HD2	2.23	0.52
1:D:171:GLU:CD	1:D:174:ARG:NH1	2.58	0.52
1:D:354:GLU:HG3	1:D:355:LEU:N	2.24	0.52
1:A:201:GLN:HE22	1:A:204[B]:ARG:NH1	2.07	0.52
1:C:352:ILE:HD12	1:C:355:LEU:HD12	1.90	0.52
1:D:199:ALA:N	1:D:200:PRO:CD	2.72	0.52
1:A:174:ARG:O	1:A:178:GLU:HB2	2.09	0.52
1:A:263:LYS:HZ3	3:A:1000:OSB:C7	2.22	0.52
1:A:199:ALA:N	1:A:200:PRO:HD2	2.24	0.52
1:C:184:VAL:HG12	1:C:185:LEU:N	2.24	0.52
1:A:8:LEU:HG	1:A:34:LEU:CD2	2.40	0.52
1:D:58:GLU:CD	1:D:98:MET:HG3	2.30	0.52
1:A:8:LEU:CD2	1:A:32:LEU:HD21	2.40	0.52
1:B:8:LEU:CD2	1:B:34:LEU:CD2	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:VAL:CG1	1:D:152:TYR:CE1	2.93	0.52
1:D:185:LEU:CD1	1:D:185:LEU:N	2.71	0.52
1:D:296:GLY:HA3	1:D:329:THR:OG1	2.09	0.52
1:B:72:ILE:N	1:B:73:PRO:HD2	2.25	0.51
1:D:132:CYS:O	1:D:158:VAL:CG2	2.57	0.51
1:B:179:ARG:HG2	1:B:180:PHE:CE1	2.45	0.51
1:B:275:ARG:NH2	4:B:1233:HOH:O	2.43	0.51
1:C:112:LEU:HD12	1:C:119:PHE:CD1	2.45	0.51
1:A:113:ARG:HA	1:A:345:PRO:HB2	1.91	0.51
1:B:158:VAL:O	1:B:185:LEU:HD22	2.10	0.51
1:C:185:LEU:HA	4:C:1323:HOH:O	2.09	0.51
1:A:85:LYS:HA	1:A:88:PRO:HG2	1.91	0.51
1:D:159:ARG:HH21	1:D:161:LYS:HB3	1.76	0.51
1:D:225:HIS:CD2	1:D:238:LEU:HD21	2.46	0.51
1:B:72:ILE:N	1:B:73:PRO:CD	2.73	0.51
1:B:117:ARG:NH1	1:B:122:GLU:OE1	2.42	0.51
1:C:190:ALA:HB3	1:C:216:PRO:HA	1.92	0.51
1:C:192:THR:HB	1:C:218:GLU:HA	1.91	0.51
1:A:199:ALA:HB3	1:A:200:PRO:CD	2.36	0.51
1:C:206:ASP:N	1:C:207:PRO:HD3	2.25	0.51
1:A:242:ILE:O	1:A:266:ARG:NE	2.39	0.51
1:B:20:ARG:HD3	1:B:138:ILE:HB	1.93	0.51
1:B:29:ARG:NH1	1:B:50:MET:HG2	2.26	0.51
1:C:29:ARG:NH1	1:C:50:MET:HG2	2.26	0.51
1:C:71:LEU:O	1:C:74:ALA:HB3	2.11	0.51
1:D:348:GLY:O	1:D:349:VAL:HG13	2.11	0.51
1:A:239:ASP:OD2	1:A:263:LYS:HE3	2.12	0.50
1:D:4:SER:HB2	1:D:37:VAL:HG12	1.93	0.50
1:D:235:PRO:HB3	1:D:258:GLN:NE2	2.26	0.50
1:D:329:THR:O	1:D:331:PRO:HD3	2.11	0.50
1:A:83:ALA:O	1:A:86:VAL:HB	2.12	0.50
1:A:163:LYS:HE3	1:A:189:ASP:OD2	2.11	0.50
1:C:142:ILE:N	1:C:143:PRO:CD	2.74	0.50
1:D:87:THR:CB	1:D:88:PRO:CD	2.89	0.50
1:D:353:PRO:O	1:D:357:ASP:OD2	2.30	0.50
1:B:159:ARG:CB	1:B:185:LEU:HB3	2.37	0.50
1:C:252:ILE:HD13	1:C:285:ILE:HG13	1.93	0.50
1:A:141:THR:OG1	1:A:144:GLN:HB2	2.12	0.50
1:C:33:LEU:HD22	1:C:297:LEU:HD12	1.94	0.50
1:C:38:THR:HB	1:C:39:PRO:CD	2.32	0.50
1:C:75:LEU:HD12	1:C:103:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:LEU:HA	1:D:71:LEU:HB2	1.93	0.50
1:A:296:GLY:HA3	1:A:329:THR:OG1	2.12	0.50
1:D:87:THR:CB	1:D:88:PRO:HD3	2.38	0.50
1:C:12:GLN:HG2	1:C:30:GLU:HG2	1.94	0.50
1:D:35:ARG:HG2	1:D:35:ARG:NH1	2.19	0.50
1:B:195:THR:O	1:B:198:ASP:HB2	2.12	0.49
1:C:11:VAL:HG12	1:C:31:LEU:HD12	1.94	0.49
1:D:33:LEU:C	1:D:34:LEU:HD23	2.32	0.49
1:A:329:THR:HG22	1:A:350:ALA:C	2.33	0.49
1:B:63:ALA:O	1:B:66:VAL:HG12	2.12	0.49
1:C:321:ASP:HA	1:C:324:TYR:O	2.12	0.49
1:B:162:LEU:HB2	1:B:188:VAL:HG12	1.94	0.49
1:B:321:ASP:HA	1:B:324:TYR:O	2.12	0.49
1:C:48:VAL:HG22	4:C:1277:HOH:O	2.12	0.49
1:D:64:GLU:O	1:D:68[A]:ARG:HB2	2.12	0.49
1:A:72:ILE:N	1:A:73:PRO:CD	2.76	0.49
1:A:129:SER:OG	1:A:338:HIS:ND1	2.45	0.49
1:B:223:LEU:O	4:B:1280:HOH:O	2.19	0.49
1:C:13:MET:HG3	1:C:31:LEU:CD1	2.38	0.49
1:C:132:CYS:SG	1:C:339:LEU:HB2	2.53	0.49
1:A:199:ALA:N	1:A:200:PRO:CD	2.75	0.49
1:B:8:LEU:HD23	1:B:34:LEU:CD2	2.39	0.49
1:B:171:GLU:N	1:B:172:PRO:CD	2.75	0.49
1:D:21:THR:HG22	1:D:23:PHE:N	2.10	0.49
1:D:21:THR:HG23	1:D:22:SER:H	1.77	0.49
1:D:308:LEU:HB3	1:D:309:PRO:HD2	1.95	0.49
1:A:132:CYS:HB2	1:A:334:LEU:HD11	1.95	0.49
1:A:171:GLU:O	1:A:172:PRO:C	2.51	0.49
1:A:201:GLN:HE22	1:A:204[B]:ARG:HH11	1.59	0.49
1:D:116:GLU:HA	1:D:345:PRO:HB3	1.95	0.49
1:C:25:THR:CG2	1:C:26:GLN:N	2.75	0.48
1:D:302:ASN:O	1:D:305:LEU:HB3	2.13	0.48
1:B:87:THR:HB	1:B:88:PRO:HD3	1.93	0.48
1:D:58:GLU:OE1	1:D:98:MET:CG	2.59	0.48
1:A:159:ARG:HD2	4:A:1143:HOH:O	2.12	0.48
1:D:291:GLY:O	3:D:1300:OSB:C9	2.61	0.48
1:C:4:SER:HB2	1:C:37:VAL:HG12	1.94	0.48
1:B:284:GLY:O	1:B:286:PRO:HD3	2.13	0.48
1:C:239:ASP:HB3	1:C:240:GLU:OE1	2.13	0.48
1:D:4:SER:HB2	1:D:37:VAL:O	2.14	0.48
1:B:11:VAL:HG13	1:B:359:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:THR:CG2	1:D:23:PHE:CD1	2.95	0.48
1:D:261:ASN:C	1:D:261:ASN:OD1	2.51	0.48
1:B:308:LEU:HB3	1:B:309:PRO:HD2	1.95	0.48
1:B:328:ILE:O	1:B:351:PRO:HA	2.13	0.48
1:C:103:LEU:O	1:C:107:VAL:HG23	2.14	0.48
1:D:44:TRP:C	1:D:106:ALA:HA	2.34	0.48
1:D:221:ASP:OD2	1:D:224:GLY:HA3	2.14	0.48
1:C:12:GLN:O	1:C:359:VAL:HB	2.12	0.48
1:D:15:LEU:HD21	1:D:29:ARG:HB2	1.95	0.48
1:B:138:ILE:HG23	1:B:168:TRP:CG	2.48	0.48
1:D:144:GLN:O	1:D:148:VAL:HG23	2.14	0.48
1:A:8:LEU:HD21	1:A:32:LEU:HD22	1.95	0.47
1:A:229:ALA:HB2	1:A:236:ILE:HG13	1.95	0.47
1:C:19:PHE:N	1:C:26:GLN:O	2.39	0.47
1:C:274:ARG:O	1:C:277:HIS:HB3	2.14	0.47
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.69	0.47
1:D:174:ARG:O	1:D:178:GLU:HB2	2.14	0.47
1:C:118:SER:HB2	4:C:1374:HOH:O	2.13	0.47
1:A:239:ASP:CG	1:A:263:LYS:HE3	2.34	0.47
1:D:171:GLU:N	1:D:172:PRO:HD2	2.29	0.47
1:A:87:THR:HB	1:A:88:PRO:CD	2.38	0.47
1:A:310:ASN:O	1:A:312:THR:N	2.47	0.47
1:C:3:LEU:HD12	1:C:3:LEU:HA	1.74	0.47
1:C:108:LEU:HD23	1:C:119:PHE:CZ	2.49	0.47
1:A:151:GLY:O	1:A:155:GLU:HG3	2.15	0.47
1:B:113:ARG:HG2	1:B:345:PRO:HB2	1.96	0.47
1:C:221:ASP:O	1:C:225:HIS:ND1	2.47	0.47
1:D:79:GLU:CD	1:D:79:GLU:H	2.18	0.47
1:D:148:VAL:CG1	1:D:152:TYR:HE1	2.28	0.47
1:A:355:LEU:O	1:A:358:GLU:HB2	2.15	0.47
1:D:163:LYS:NZ	3:D:1300:OSB:O3	2.47	0.47
1:A:329:THR:HB	1:A:349:VAL:CG1	2.45	0.47
1:B:10:ARG:NE	1:B:64:GLU:OE1	2.44	0.47
1:B:159:ARG:HA	1:B:185:LEU:HB2	1.95	0.47
1:C:308:LEU:CB	1:C:309:PRO:HD2	2.45	0.47
1:D:86:VAL:O	1:D:90:LEU:HG	2.15	0.47
1:A:29:ARG:NH2	1:A:50:MET:HG2	2.30	0.47
1:C:72:ILE:N	1:C:73:PRO:HD2	2.30	0.46
1:D:354:GLU:O	1:D:358:GLU:HB2	2.16	0.46
1:C:10[B]:ARG:HH11	1:C:10[B]:ARG:CG	2.26	0.46
1:D:109:ASP:OD1	1:D:346:GLY:HA3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ASP:CB	1:D:207:PRO:HD3	2.43	0.46
1:A:28:VAL:HG12	1:A:29:ARG:N	2.29	0.46
1:C:11:VAL:CG1	1:C:12:GLN:N	2.78	0.46
1:D:185:LEU:HA	1:D:185:LEU:HD12	1.65	0.46
1:A:203:ALA:CA	1:A:232:ILE:HG22	2.45	0.46
1:B:280:CYS:HB3	1:B:285:ILE:O	2.15	0.46
1:D:67:LEU:HD23	1:D:67:LEU:HA	1.73	0.46
1:D:356:LEU:O	1:D:359:VAL:HG22	2.16	0.46
1:A:28:VAL:CG1	1:A:29:ARG:N	2.78	0.46
1:C:75:LEU:HD12	1:C:103:LEU:CD1	2.45	0.46
1:B:363:LYS:HB3	1:B:363:LYS:HE2	1.46	0.46
1:A:169:ASP:O	1:A:172:PRO:HG2	2.15	0.46
1:B:206:ASP:CB	1:B:207:PRO:HD3	2.40	0.46
1:A:349:VAL:HG13	1:A:350:ALA:H	1.81	0.46
1:C:3:LEU:HD12	1:C:38:THR:HG22	1.98	0.46
1:C:6:VAL:HG12	1:C:7:GLU:N	2.31	0.46
1:C:205:LEU:O	1:C:207:PRO:HD2	2.12	0.46
1:A:9:ARG:NH2	1:A:357:ASP:OD1	2.49	0.45
1:C:139:MET:HB2	1:C:168:TRP:CH2	2.49	0.45
1:D:21:THR:CG2	1:D:22:SER:H	2.29	0.45
1:D:85:LYS:C	1:D:88:PRO:HD2	2.37	0.45
1:B:174:ARG:O	1:B:178:GLU:HB2	2.17	0.45
1:C:2:LYS:O	1:C:39:PRO:HD3	2.16	0.45
1:C:38:THR:CB	1:C:39:PRO:CD	2.93	0.45
1:C:46:GLU:OE1	1:C:297:LEU:HB2	2.15	0.45
1:C:98:MET:HB2	1:C:98:MET:HE3	1.51	0.45
1:C:127:ARG:NH1	1:C:307:SER:CA	2.77	0.45
1:C:204:ARG:NH1	1:C:204:ARG:HG2	2.31	0.45
1:D:299:ARG:HG2	1:D:332:PHE:CD1	2.52	0.45
1:A:326:THR:HG22	1:A:355:LEU:HD22	1.97	0.45
1:D:142:ILE:HB	1:D:143:PRO:CD	2.47	0.45
1:D:176:VAL:O	1:D:176:VAL:CG1	2.63	0.45
1:A:118:SER:HB3	1:A:344:GLY:O	2.16	0.45
1:A:185:LEU:HD22	1:A:211:LEU:HD21	1.98	0.45
1:A:227:GLU:HA	1:A:230:ARG:HH11	1.81	0.45
1:D:3:LEU:HB3	4:D:1365:HOH:O	2.16	0.45
1:C:103:LEU:HD23	1:C:103:LEU:HA	1.67	0.45
1:C:184:VAL:CG1	1:C:185:LEU:N	2.79	0.45
1:D:85:LYS:O	1:D:88:PRO:HD2	2.16	0.45
1:A:159:ARG:HH21	1:A:161:LYS:HB3	1.82	0.45
1:B:9:ARG:O	1:B:32:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ALA:HA	1:B:276:VAL:HG22	1.99	0.45
1:C:190:ALA:O	1:C:191:ASN:C	2.53	0.45
1:D:159:ARG:HD2	1:D:187:GLN:OE1	2.16	0.45
1:D:252:ILE:CD1	1:D:285:ILE:HG13	2.47	0.45
1:A:179:ARG:O	1:A:179:ARG:HG3	2.14	0.45
1:A:352:ILE:O	1:A:352:ILE:HG22	2.16	0.45
1:C:89:LEU:HA	1:C:89:LEU:HD23	1.73	0.45
1:C:163:LYS:HD2	1:C:163:LYS:HA	1.53	0.45
1:C:352:ILE:CB	1:C:355:LEU:HD12	2.39	0.45
1:C:151:GLY:HA3	4:C:1232:HOH:O	2.16	0.45
1:C:271:LEU:HD23	1:C:271:LEU:HA	1.80	0.45
1:D:363:LYS:HB3	1:D:363:LYS:HE2	1.55	0.45
1:B:161:LYS:HE3	1:B:189:ASP:HB2	1.99	0.45
1:C:29:ARG:HD2	1:C:31:LEU:HG	1.99	0.44
1:D:35:ARG:NH1	1:D:42:GLU:OE2	2.50	0.44
1:D:82:THR:O	1:D:86:VAL:HG23	2.17	0.44
1:B:145:LEU:O	1:B:149:VAL:HG23	2.17	0.44
1:B:159:ARG:CB	1:B:185:LEU:CB	2.78	0.44
1:C:249:ALA:O	1:C:253:LYS:HG3	2.18	0.44
1:D:48:VAL:HG23	1:D:98:MET:SD	2.57	0.44
1:A:125:SER:OG	1:A:126:VAL:N	2.50	0.44
1:C:308:LEU:CB	1:C:309:PRO:CD	2.96	0.44
1:D:353:PRO:O	1:D:356:LEU:HB3	2.17	0.44
1:B:87:THR:HB	1:B:88:PRO:CD	2.47	0.44
1:C:158:VAL:O	1:C:185:LEU:HD12	2.18	0.44
1:D:139:MET:CE	1:D:148:VAL:HG21	2.47	0.44
1:D:293:ILE:HG23	1:D:323:PHE:CG	2.51	0.44
1:D:339:LEU:HD12	1:D:339:LEU:HA	1.69	0.44
1:A:145:LEU:O	1:A:148:VAL:HB	2.17	0.44
1:C:204:ARG:HG2	1:C:204:ARG:HH11	1.82	0.44
1:C:227:GLU:O	1:C:230:ARG:HB2	2.18	0.44
1:D:308:LEU:CB	1:D:309:PRO:HD2	2.48	0.44
1:A:165:GLU:O	1:A:194:TYR:OH	2.35	0.44
1:A:329:THR:HB	1:A:349:VAL:HG13	2.00	0.44
1:B:185:LEU:N	1:B:185:LEU:CD1	2.81	0.44
1:C:159:ARG:HG2	1:C:160:ILE:N	2.32	0.44
1:D:35:ARG:CD	1:D:44:TRP:CH2	2.99	0.44
1:A:72:ILE:N	1:A:73:PRO:HD2	2.33	0.44
1:A:142:ILE:O	1:A:143:PRO:C	2.53	0.44
1:B:120:ALA:HB1	1:B:125:SER:CB	2.48	0.44
1:C:329:THR:HG21	1:C:349:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LEU:O	1:D:363:LYS:HA	2.18	0.44
1:A:103:LEU:O	1:A:107:VAL:HG23	2.17	0.44
1:A:139:MET:CE	1:A:148:VAL:HG11	2.47	0.44
1:C:264:PRO:HG3	1:C:305:LEU:CD2	2.47	0.44
1:A:261:ASN:OD1	1:A:261:ASN:C	2.56	0.44
1:A:308:LEU:HA	1:A:309:PRO:HD3	1.77	0.44
1:B:14:PRO:HA	1:B:28:VAL:HG22	1.99	0.44
1:C:212:LEU:C	1:C:212:LEU:HD12	2.38	0.44
1:C:320:SER:OG	1:C:327:ASP:OD2	2.34	0.44
1:D:177:ARG:HA	1:D:177:ARG:HD3	1.68	0.44
1:B:226:ALA:HB3	4:B:1280:HOH:O	2.16	0.43
1:D:143:PRO:O	1:D:144:GLN:C	2.56	0.43
1:A:274:ARG:O	1:A:277:HIS:HB3	2.18	0.43
1:B:151:GLY:O	1:B:154:ASP:HB2	2.18	0.43
1:B:339:LEU:HA	1:B:339:LEU:HD12	1.69	0.43
1:D:16:VAL:HG23	1:D:323:PHE:O	2.18	0.43
1:D:159:ARG:HB2	1:D:185:LEU:CB	2.47	0.43
1:A:45:GLY:HA2	1:A:105:MET:SD	2.59	0.43
1:A:130:VAL:O	1:A:338:HIS:HA	2.18	0.43
1:B:177:ARG:HD2	1:B:182:ASP:HA	1.99	0.43
1:B:179:ARG:O	1:B:179:ARG:HG3	2.09	0.43
1:C:76:LEU:HA	1:C:76:LEU:HD23	1.77	0.43
1:C:87:THR:N	1:C:88:PRO:HD2	2.33	0.43
1:B:165:GLU:O	1:B:166:PRO:C	2.57	0.43
1:B:169:ASP:O	1:B:172:PRO:HD2	2.18	0.43
1:B:169:ASP:HB2	1:B:170:VAL:H	1.19	0.43
1:D:14:PRO:HA	1:D:28:VAL:HG13	2.00	0.43
1:D:64:GLU:O	1:D:68[B]:ARG:HB2	2.19	0.43
1:D:164:ILE:HB	1:D:168:TRP:O	2.18	0.43
1:B:177:ARG:HA	1:B:177:ARG:HD3	1.74	0.43
1:D:334:LEU:HD21	1:D:337:GLY:HA2	2.00	0.43
1:C:8:LEU:HD22	1:C:64:GLU:HG3	2.00	0.43
1:B:141:THR:OG1	1:B:143:PRO:CD	2.67	0.43
1:D:145:LEU:O	1:D:146:LEU:C	2.54	0.43
1:A:278:ASP:O	1:A:281:ALA:HB3	2.19	0.43
1:B:214:GLU:HA	1:B:237:CYS:O	2.19	0.43
1:C:159:ARG:HD2	4:C:1367:HOH:O	2.19	0.43
1:D:356:LEU:HA	1:D:356:LEU:HD12	1.68	0.43
1:B:78:ALA:HB3	1:B:81:ILE:CD1	2.36	0.42
1:B:163:LYS:HE3	1:B:189:ASP:HB3	2.00	0.42
1:D:139:MET:HG3	1:D:145:LEU:HA	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:VAL:O	1:D:176:VAL:HG12	2.19	0.42
1:D:26:GLN:NE2	4:D:1346:HOH:O	2.52	0.42
1:D:356:LEU:O	1:D:359:VAL:CG2	2.68	0.42
1:A:139:MET:HE3	1:A:148:VAL:HG11	2.00	0.42
1:A:163:LYS:HA	1:A:163:LYS:HD2	1.76	0.42
1:A:171:GLU:N	1:A:172:PRO:CD	2.81	0.42
1:B:68:ARG:HH11	1:B:68:ARG:HD3	1.65	0.42
1:C:365:TRP:CD1	1:C:365:TRP:C	2.89	0.42
1:D:308:LEU:N	1:D:308:LEU:HD12	2.34	0.42
1:A:35:ARG:HA	1:A:43:GLY:O	2.20	0.42
1:A:189:ASP:HB2	1:A:214:GLU:OE1	2.19	0.42
1:A:109:ASP:OD1	1:A:346:GLY:HA3	2.19	0.42
1:D:7:GLU:HB2	1:D:365:TRP:HE3	1.84	0.42
1:B:218:GLU:CG	1:B:220[B]:GLU:OE1	2.60	0.42
1:B:234:THR:HG23	1:B:235:PRO:HD2	2.01	0.42
1:D:153:LEU:HD23	1:D:153:LEU:HA	1.88	0.42
1:A:8:LEU:HD23	1:A:32:LEU:HD22	2.02	0.42
1:B:169:ASP:HB2	1:B:170:VAL:HG23	2.02	0.42
1:D:187:GLN:HG2	1:D:211:LEU:HD12	2.00	0.42
1:A:55:TYR:CE2	1:A:240:GLU:HG3	2.55	0.42
3:B:1100:OSB:O5	4:B:1146:HOH:O	2.22	0.42
1:D:123:LEU:O	1:D:308:LEU:HD21	2.19	0.42
1:D:199:ALA:O	1:D:203:ALA:N	2.50	0.42
1:D:355:LEU:O	1:D:359:VAL:HG22	2.20	0.42
1:D:7:GLU:CD	1:D:9:ARG:HH12	2.19	0.42
1:A:169:ASP:HB2	1:A:170:VAL:H	1.43	0.42
1:C:83:ALA:O	1:C:86:VAL:HB	2.20	0.42
1:D:137:GLY:HA2	1:D:163:LYS:HB2	2.02	0.42
1:A:75:LEU:HD11	1:A:103:LEU:HD23	2.00	0.41
1:A:319:ALA:O	1:A:320:SER:C	2.59	0.41
1:B:299:ARG:O	1:B:303:VAL:HG23	2.20	0.41
1:D:35:ARG:HD2	1:D:44:TRP:CZ2	2.54	0.41
1:D:333:VAL:O	1:D:333:VAL:HG12	2.19	0.41
1:D:352:ILE:CG2	1:D:355:LEU:HD22	2.49	0.41
1:A:8:LEU:HD21	1:A:32:LEU:CD2	2.48	0.41
1:A:85:LYS:C	1:A:88:PRO:HD2	2.41	0.41
1:C:349:VAL:HG13	1:C:350:ALA:N	2.35	0.41
1:D:328:ILE:HG13	1:D:329:THR:HG23	2.01	0.41
1:A:39:PRO:HA	4:A:1003:HOH:O	2.20	0.41
1:A:149:VAL:O	1:A:150:GLY:C	2.58	0.41
1:B:3:LEU:HB3	1:B:76:LEU:HD23	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ASN:C	1:C:192:THR:HG23	2.40	0.41
1:D:141:THR:O	1:D:144:GLN:HB3	2.20	0.41
1:D:264:PRO:HG3	1:D:305:LEU:CD2	2.50	0.41
1:A:159:ARG:HD2	1:A:187:GLN:OE1	2.20	0.41
1:B:55:TYR:OH	1:B:239:ASP:OD1	2.33	0.41
1:B:234:THR:HA	1:B:235:PRO:HD3	1.83	0.41
1:C:49:THR:CG2	1:C:98:MET:HE3	2.50	0.41
1:D:139:MET:HG3	1:D:145:LEU:CA	2.51	0.41
1:A:227:GLU:HA	1:A:230:ARG:NH1	2.36	0.41
1:A:352:ILE:HG22	1:A:355:LEU:HD12	1.92	0.41
1:C:217:LEU:HB2	1:C:225:HIS:CE1	2.56	0.41
1:C:288:TRP:HB3	1:C:313:LEU:HB2	2.01	0.41
1:B:87:THR:CB	1:B:88:PRO:CD	2.98	0.41
1:B:263:LYS:HB2	1:B:266:ARG:NH1	2.35	0.41
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.61	0.41
1:A:199:ALA:CB	1:A:200:PRO:CD	2.98	0.41
1:A:329:THR:CG2	1:A:349:VAL:HG11	2.47	0.41
1:B:72:ILE:CB	1:B:73:PRO:HD3	2.48	0.41
1:B:163:LYS:HE3	1:B:189:ASP:OD2	2.21	0.41
1:D:308:LEU:CB	1:D:309:PRO:CD	2.97	0.41
1:A:7:GLU:OE1	1:A:363:LYS:HD3	2.21	0.41
1:A:153:LEU:HG	1:A:160:ILE:HD11	2.03	0.41
1:B:146:LEU:HA	1:B:146:LEU:HD23	1.83	0.41
1:A:75:LEU:HD12	1:A:103:LEU:CD2	2.50	0.41
1:A:117:ARG:HE	1:A:121:ALA:HB1	1.85	0.41
1:A:252:ILE:CD1	1:A:285:ILE:HG13	2.50	0.41
1:A:352:ILE:HG22	1:A:355:LEU:CG	2.51	0.41
1:B:55:TYR:OH	1:B:266:ARG:HD3	2.21	0.41
1:B:117:ARG:NH1	1:C:122:GLU:OE1	2.54	0.41
1:C:7:GLU:OE2	1:C:35:ARG:NH1	2.54	0.41
1:C:20:ARG:CZ	1:C:138:ILE:HG21	2.51	0.41
1:C:141:THR:HG23	1:C:143:PRO:HG2	2.01	0.41
1:C:171:GLU:N	1:C:172:PRO:CD	2.83	0.41
1:A:56:SER:C	1:B:94:LYS:HB2	2.41	0.41
1:A:288:TRP:HB3	1:A:313:LEU:HB2	2.03	0.41
1:B:7:GLU:CD	1:B:35:ARG:NH1	2.74	0.41
1:B:18:PRO:HA	1:B:26:GLN:O	2.20	0.41
1:D:198:ASP:C	1:D:200:PRO:HD2	2.41	0.41
1:D:305:LEU:C	1:D:307:SER:N	2.74	0.41
1:D:328:ILE:O	1:D:351:PRO:CA	2.61	0.41
1:D:352:ILE:HD12	1:D:355:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:THR:HG22	1:A:84:ALA:HB3	2.03	0.40
1:A:89:LEU:HA	1:A:89:LEU:HD23	1.78	0.40
1:B:223:LEU:HD23	1:B:223:LEU:HA	1.91	0.40
1:C:257:VAL:O	1:C:257:VAL:HG13	2.21	0.40
1:A:55:TYR:OH	1:A:266:ARG:HD3	2.22	0.40
1:B:8:LEU:O	1:B:363:LYS:HA	2.21	0.40
1:B:116:GLU:HA	1:B:345:PRO:HB3	2.02	0.40
1:B:169:ASP:C	1:B:172:PRO:HD2	2.41	0.40
1:B:225:HIS:CD2	1:B:238:LEU:HD21	2.56	0.40
3:B:1100:OSB:O1	3:B:1100:OSB:C8	2.69	0.40
1:C:20:ARG:NH1	1:C:138:ILE:HG22	2.36	0.40
1:C:82:THR:CG2	1:C:85:LYS:HD2	2.50	0.40
1:B:32:LEU:HD23	1:B:32:LEU:HA	1.53	0.40
1:B:185:LEU:N	1:B:185:LEU:HD12	2.35	0.40
1:A:221:ASP:OD2	1:A:224:GLY:HA3	2.21	0.40
1:B:94:LYS:O	1:B:96:HIS:HD2	2.05	0.40
1:B:97:ARG:O	1:B:268:GLY:HA2	2.21	0.40
1:A:130:VAL:O	1:A:130:VAL:HG23	2.22	0.40
1:C:31:LEU:HD22	1:C:295:THR:CG2	2.47	0.40
1:C:72:ILE:N	1:C:73:PRO:CD	2.84	0.40
1:C:339:LEU:HD12	1:C:339:LEU:HA	1.76	0.40
1:C:352:ILE:CD1	1:C:355:LEU:HD12	2.50	0.40
1:D:48:VAL:CG1	1:D:292:MET:HB2	2.50	0.40
1:D:130:VAL:O	1:D:338:HIS:HA	2.22	0.40
1:D:216:PRO:C	1:D:217:LEU:HD23	2.42	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)
1:A:111:GLU:OE2	1:D:117:ARG:NH2[17_555]	1.82	0.38

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	366/368 (100%)	338 (92%)	27 (7%)	1 (0%)	41	46
1	B	368/368 (100%)	352 (96%)	15 (4%)	1 (0%)	41	46
1	C	368/368 (100%)	346 (94%)	22 (6%)	0	100	100
1	D	367/368 (100%)	337 (92%)	26 (7%)	4 (1%)	14	12
All	All	1469/1472 (100%)	1373 (94%)	90 (6%)	6 (0%)	34	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	40	ALA
1	D	306	ALA
1	D	321	ASP
1	B	53	PRO
1	A	79	GLU
1	D	293	ILE

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	291/291 (100%)	265 (91%)	26 (9%)	9	9
1	B	293/291 (101%)	269 (92%)	24 (8%)	11	11
1	C	293/291 (101%)	265 (90%)	28 (10%)	8	8
1	D	292/291 (100%)	261 (89%)	31 (11%)	6	6
All	All	1169/1164 (100%)	1060 (91%)	109 (9%)	9	8

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

Mol	Chain	Res	Type
1	A	2	LYS
1	A	8	LEU

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Mol	Chain	Res	Type
1	A	12	GLN
1	A	15	LEU
1	A	27	SER
1	A	29	ARG
1	A	31	LEU
1	A	32	LEU
1	A	79	GLU
1	A	81	ILE
1	A	119	PHE
1	A	125	SER
1	A	129	SER
1	A	159	ARG
1	A	163	LYS
1	A	169	ASP
1	A	177	ARG
1	A	179	ARG
1	A	213	ILE
1	A	217	LEU
1	A	227	GLU
1	A	322	ARG
1	A	343	THR
1	A	356	LEU
1	A	363	LYS
1	A	364	VAL
1	B	1	MET
1	B	2	LYS
1	B	3	LEU
1	B	12	GLN
1	B	29	ARG
1	B	32	LEU
1	B	34	LEU
1	B	42	GLU
1	B	68	ARG
1	B	80	ASP
1	B	141	THR
1	B	159	ARG
1	B	163	LYS
1	B	177	ARG
1	B	179	ARG
1	B	201	GLN
1	B	204	ARG
1	B	213	ILE

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Mol	Chain	Res	Type
1	B	258	GLN
1	B	322	ARG
1	B	339	LEU
1	B	349	VAL
1	B	363	LYS
1	B	366	ILE
1	C	1	MET
1	C	8	LEU
1	C	12	GLN
1	C	13	MET
1	C	27	SER
1	C	29	ARG
1	C	31	LEU
1	C	32	LEU
1	C	34	LEU
1	C	80	ASP
1	C	103	LEU
1	C	119	PHE
1	C	126	VAL
1	C	139	MET
1	C	140	ASP
1	C	144	GLN
1	C	159	ARG
1	C	163	LYS
1	C	169	ASP
1	C	177	ARG
1	C	204	ARG
1	C	227	GLU
1	C	232	ILE
1	C	320	SER
1	C	322	ARG
1	C	339	LEU
1	C	343	THR
1	C	356	LEU
1	D	1	MET
1	D	2	LYS
1	D	12	GLN
1	D	27	SER
1	D	29	ARG
1	D	31	LEU
1	D	35	ARG
1	D	42	GLU

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Mol	Chain	Res	Type
1	D	64	GLU
1	D	66	VAL
1	D	68[A]	ARG
1	D	68[B]	ARG
1	D	79	GLU
1	D	98	MET
1	D	116	GLU
1	D	119	PHE
1	D	125	SER
1	D	142	ILE
1	D	155	GLU
1	D	159	ARG
1	D	169	ASP
1	D	177	ARG
1	D	187	GLN
1	D	213	ILE
1	D	217	LEU
1	D	322	ARG
1	D	335	SER
1	D	339	LEU
1	D	343	THR
1	D	355	LEU
1	D	363	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	65	HIS
1	A	69	HIS
1	A	201	GLN
1	A	258	GLN
1	A	283	HIS
1	B	12	GLN
1	B	65	HIS
1	B	69	HIS
1	B	233	GLN
1	C	12	GLN
1	C	258	GLN
1	C	338	HIS
1	D	26	GLN
1	D	69	HIS

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Mol	Chain	Res	Type
1	D	258	GLN

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	OSB	A	1000	2	16,16,16	1.49	3 (18%)	20,21,21	3.52	7 (35%)
3	OSB	C	1200	2	16,16,16	1.32	1 (6%)	20,21,21	2.73	5 (25%)
3	OSB	D	1300	2	16,16,16	1.26	1 (6%)	20,21,21	2.28	4 (20%)
3	OSB	B	1100	2	16,16,16	1.32	2 (12%)	20,21,21	2.57	4 (20%)

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
3	OSB	A	1000	2	-	9/13/13/13	0/1/1/1
3	OSB	C	1200	2	-	2/13/13/13	0/1/1/1
3	OSB	D	1300	2	-	5/13/13/13	0/1/1/1
3	OSB	B	1100	2	-	4/13/13/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	OSB	C9-C8	3.40	1.56	1.51
3	C	1200	OSB	C9-C8	2.56	1.54	1.51
3	D	1300	OSB	C9-C8	2.28	1.54	1.51
3	A	1000	OSB	C2-C7	-2.25	1.44	1.49
3	B	1100	OSB	C2-C7	-2.18	1.45	1.49
3	B	1100	OSB	C9-C8	2.08	1.54	1.51
3	A	1000	OSB	C10-C11	2.07	1.55	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1000	OSB	C10-C9-C8	12.11	127.41	112.76
3	C	1200	OSB	C10-C9-C8	10.54	125.51	112.76
3	B	1100	OSB	C10-C9-C8	10.10	124.98	112.76
3	D	1300	OSB	C10-C9-C8	8.05	122.51	112.76
3	A	1000	OSB	C9-C10-C11	5.74	125.97	113.60
3	A	1000	OSB	C6-C1-C2	-4.11	114.69	119.26
3	A	1000	OSB	O3-C8-C9	-3.56	114.30	120.38
3	C	1200	OSB	C9-C8-C1	-3.18	114.47	119.79
3	A	1000	OSB	C3-C2-C1	3.18	122.80	119.26
3	B	1100	OSB	C9-C8-C1	-3.01	114.75	119.79
3	D	1300	OSB	C9-C10-C11	2.91	119.86	113.60
3	A	1000	OSB	C9-C8-C1	2.68	124.28	119.79
3	D	1300	OSB	C9-C8-C1	-2.50	115.60	119.79
3	D	1300	OSB	O1-C7-C2	2.41	122.24	115.31
3	C	1200	OSB	O2-C7-C2	-2.37	116.18	121.94
3	B	1100	OSB	C9-C10-C11	2.27	118.50	113.60
3	C	1200	OSB	O1-C7-C2	2.19	121.62	115.31
3	C	1200	OSB	O5-C11-C10	2.17	121.01	114.03
3	A	1000	OSB	O5-C11-C10	2.07	120.69	114.03
3	B	1100	OSB	O2-C7-C2	-2.03	117.00	121.94

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	OSB	O3-C8-C9-C10
3	A	1000	OSB	C1-C8-C9-C10
3	B	1100	OSB	C6-C1-C8-O3
3	D	1300	OSB	C6-C1-C8-O3
3	A	1000	OSB	C6-C1-C8-O3
3	A	1000	OSB	C6-C1-C8-C9
3	B	1100	OSB	C2-C1-C8-O3
3	D	1300	OSB	C2-C1-C8-C9
3	D	1300	OSB	C2-C1-C8-O3
3	C	1200	OSB	C6-C1-C8-O3
3	D	1300	OSB	C6-C1-C8-C9
3	A	1000	OSB	C9-C10-C11-O5
3	A	1000	OSB	C9-C10-C11-O4
3	B	1100	OSB	C6-C1-C8-C9
3	D	1300	OSB	C1-C8-C9-C10
3	A	1000	OSB	C2-C1-C8-C9
3	A	1000	OSB	C2-C1-C8-O3
3	B	1100	OSB	C2-C1-C8-C9
3	C	1200	OSB	C3-C2-C7-O1
3	A	1000	OSB	C3-C2-C7-O1

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	OSB	4	0
3	D	1300	OSB	3	0
3	B	1100	OSB	2	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	367/368 (99%)	-1.30	0	100	100	22, 51, 85, 99	0
1	B	368/368 (100%)	-1.46	0	100	100	22, 37, 66, 94	0
1	C	367/368 (99%)	-1.35	0	100	100	25, 47, 80, 100	0
1	D	368/368 (100%)	-1.22	0	100	100	24, 53, 88, 100	0
All	All	1470/1472 (99%)	-1.33	0	100	100	22, 47, 82, 100	0

There are no RSRZ outliers to report.

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	OSB	D	1300	16/16	0.94	0.12	50,72,100,100	0
3	OSB	A	1000	16/16	0.97	0.08	41,61,100,100	0
3	OSB	B	1100	16/16	0.98	0.06	20,49,66,71	0
3	OSB	C	1200	16/16	0.98	0.10	16,48,81,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	C	1201	1/1	0.98	0.06	67,67,67,67	0
2	MG	A	1001	1/1	0.99	0.03	49,49,49,49	0
2	MG	D	1301	1/1	0.99	0.16	69,69,69,69	0
2	MG	B	1101	1/1	1.00	0.03	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.