Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 11:37 PM EDT

PDB ID	:	3K4D
Title	:	Crystal structure of E. coli beta-glucuronidase with the glucaro-d-lactam inhibitor bound
Authors	:	Wallace, B.D.; Redinbo, M.R.
Deposited on	:	2009-10-05
Resolution	:	2.39 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 ⓘ 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 ⓘ) were used in the production of this report:

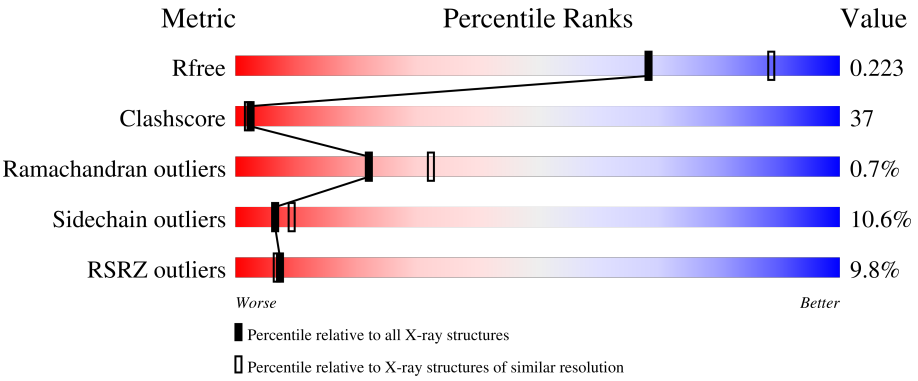
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	605	6% 59% 31% 6%
1	B	605	13% 46% 43% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9933 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.

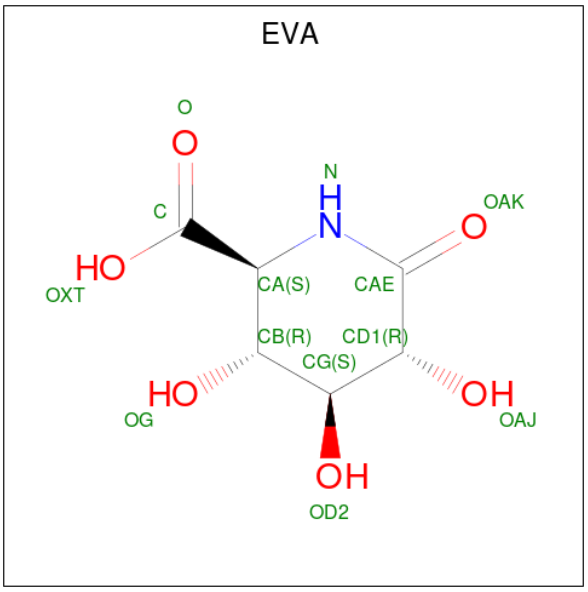
- Molecule 1 is a protein called Beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4776	3032	825	897	22			
1	B	596	Total	C	N	O	S	0	0	0
			4776	3032	825	897	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P05804
A	0	HIS	-	expression tag	UNP P05804
B	-1	SER	-	expression tag	UNP P05804
B	0	HIS	-	expression tag	UNP P05804

- Molecule 2 is (2S,3R,4S,5R)-3,4,5-trihydroxy-6-oxopiperidine-2-carboxylic acid (three-letter code: EVA) (formula: $C_6H_9NO_6$).



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

- Molecule 3 is water.

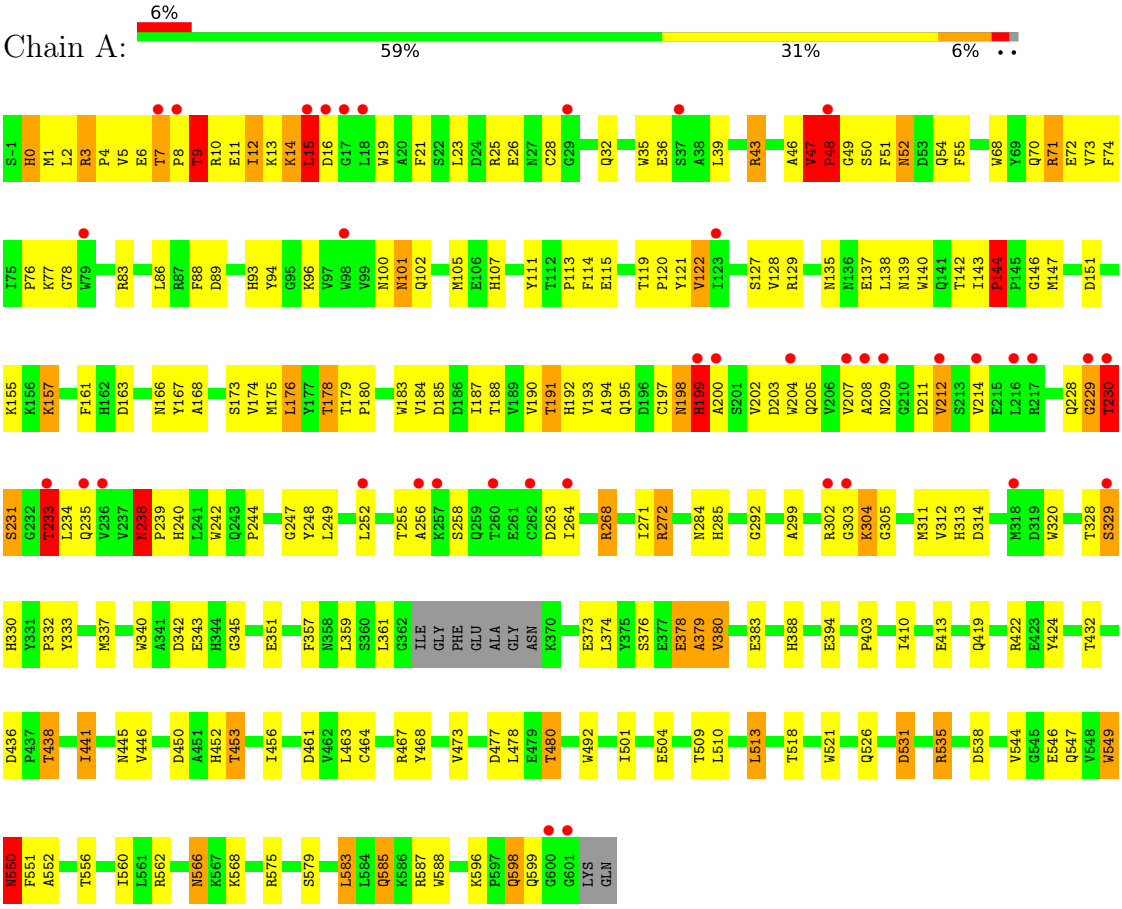
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total	O	0	0
			244	244		
3	B	111	Total	O	0	0
			111	111		

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.

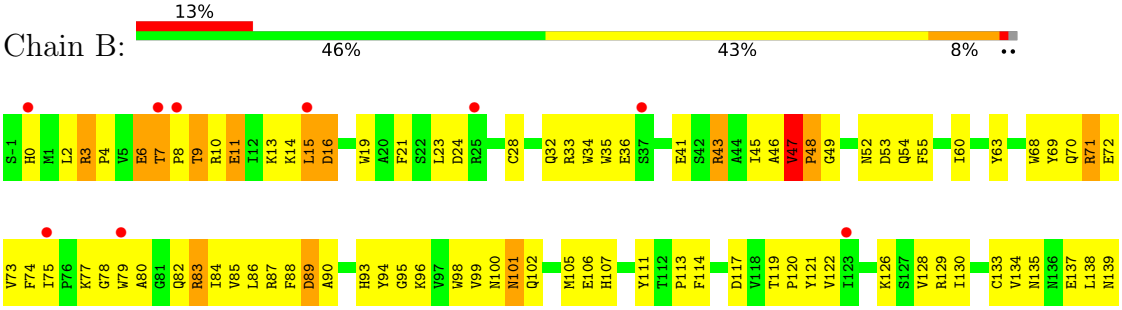
• Molecule 1: Beta-glucuronidase

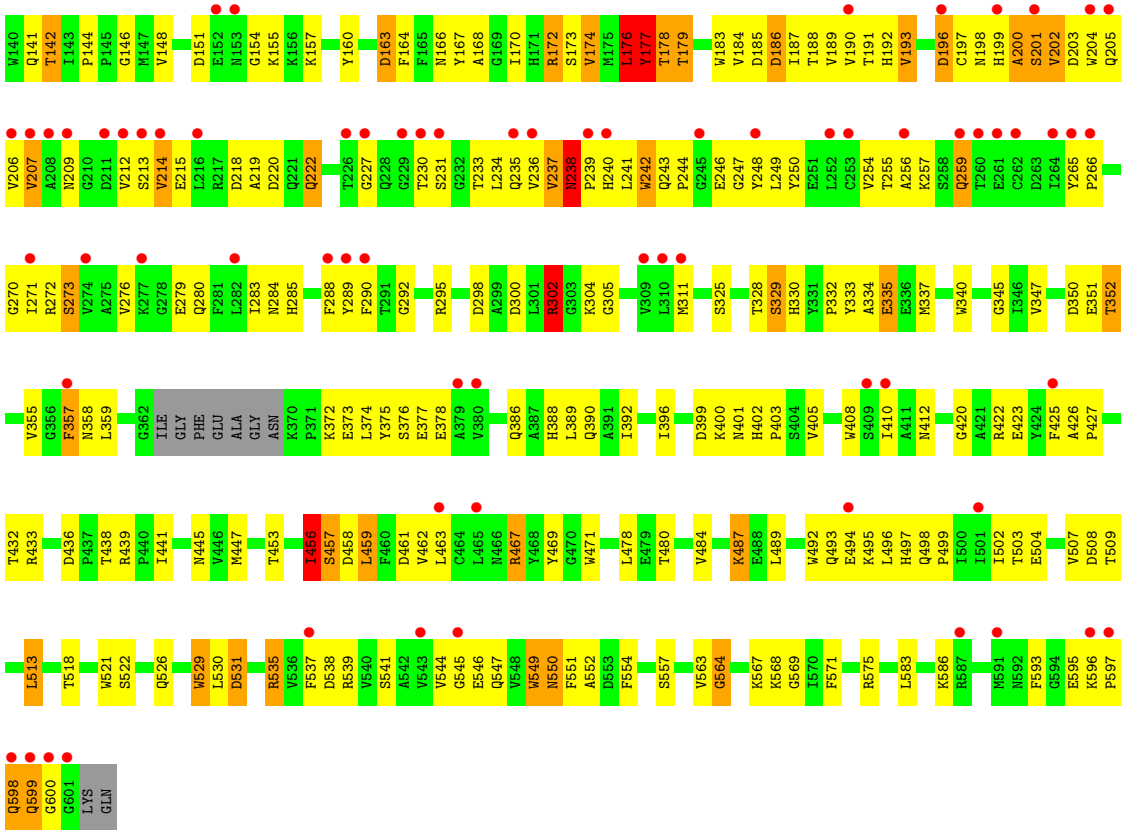
Chain A:



• Molecule 1: Beta-glucuronidase

Chain B:




W140 Q141 T142 I143 P144 P145 G146 M147 V148 D151 E152 N153 G154 K155 K156 K157 Y160 D163 F164 F165 N166 Y167 A168 G169 I170 H171 R172 S173 V174 M175 L176 Y177 T178 T179 W183 V184 D185 D186 I187 T188 V189 V190 T191 H192 V193 D196 C197 N198 H199 A200 S201 V202 D203 W204 Q205
V206 V207 A208 N209 G210 D211 V212 S213 V214 E215 L216 R217 D218 A219 D220 Q221 Q222 T226 G227 Q228 G229 T230 S231 G232 T233 L234 Q235 V236 V237 N238 P239 H240 L241 W242 Q243 P244 G245 E246 G247 Y248 L249 Y250 E251 L252 C253 V254 T255 A256 K257 S258 Q259 T260 E261 C262 D263 I264 Y265 P266
G270 I271 R272 S273 V274 A275 V276 K277 G278 E279 Q280 F281 L282 I283 N284 H285 F288 Y289 F290 T291 G292 R295 D298 A299 D300 L301 R302 G303 K304 G305 V309 L310 M311 S325 T328 S329 H330 Y331 P332 Y333 A334 E335 E336 M337 W340 G345 I346 V347 D350 E351 T352
V355 G356 F357 N358 L359 G362 ILE GLY PHE GLU ALA GLY ASN K370 P371 K372 E373 L374 Y375 S376 E377 E378 A379 V380 Q386 A387 H388 L389 Q390 A391 I392 I396 D399 K400 N401 H402 P403 S404 V405 W408 S409 I410 A411 N412 G420 A421 R422 E423 Y424 F425 A426 P427
T432 R433 D436 P437 T438 R439 P440 I441 N445 V446 M447 T453 I456 S457 D458 L459 F460 D461 V462 L463 C464 L465 N466 R467 Y468 Y469 G470 W471 L478 E479 T480 V484 K487 E488 L489 W492 Q493 E494 K495 L496 H497 Q498 P499 I500 I501 I502 T503 E504 V507 D508 T509
L513 T518 W521 S522 Q526 W529 L530 D531 R535 V536 F537 D538 R539 V540 S541 A542 V543 V544 G545 E546 Q547 V548 W549 N550 F551 A552 D553 F554 S557 V563 G564 K567 K568 G569 I570 F571 R575 L583 K586 R587 M591 N592 F593 G594 E595 K596 P597
Q598 Q599 G600 G601 LYS GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	167.65Å 76.97Å 125.47Å 90.00° 124.98° 90.00°	Depositor
Resolution (Å)	29.57 – 2.39 47.79 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.57-2.39) 98.2 (47.79-2.39)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.33 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102, PHENIX	Depositor
R, R_{free}	0.205 , 0.237 0.208 , 0.223	Depositor DCC
R_{free} test set	2602 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 56.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9933	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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

5.1 Standard geometry

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

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	0.65	3/4904 (0.1%)	0.91	26/6673 (0.4%)
1	B	0.49	0/4904	0.85	22/6673 (0.3%)
All	All	0.57	3/9808 (0.0%)	0.88	48/13346 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	6
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	TYR	CD2-CE2	-6.67	1.29	1.39
1	A	468	TYR	CD1-CE1	-5.42	1.31	1.39
1	A	468	TYR	CE1-CZ	-5.22	1.31	1.38

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	231	SER	N-CA-CB	-14.31	89.04	110.50
1	B	80	ALA	CB-CA-C	-11.67	92.59	110.10
1	B	599	GLN	N-CA-CB	-10.65	91.43	110.60
1	B	358	ASN	N-CA-CB	-10.25	92.15	110.60
1	A	229	GLY	N-CA-C	-9.35	89.72	113.10
1	A	379	ALA	N-CA-C	8.89	135.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	380	VAL	N-CA-C	-8.57	87.87	111.00
1	A	14	LYS	CB-CA-C	-8.38	93.64	110.40
1	A	231	SER	CB-CA-C	8.00	125.31	110.10
1	A	233	THR	N-CA-CB	7.52	124.58	110.30
1	A	562	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	B	456	ILE	CB-CA-C	-7.08	97.44	111.60
1	A	379	ALA	CB-CA-C	-7.04	99.54	110.10
1	A	230	THR	CB-CA-C	6.96	130.38	111.60
1	A	329	SER	CB-CA-C	6.92	123.25	110.10
1	B	214	VAL	N-CA-C	6.82	129.42	111.00
1	A	329	SER	N-CA-C	-6.75	92.79	111.00
1	A	583	LEU	CA-CB-CG	6.65	130.60	115.30
1	A	233	THR	CB-CA-C	-6.55	93.91	111.60
1	A	15	LEU	N-CA-C	-6.51	93.43	111.00
1	B	16	ASP	N-CA-C	-6.44	93.62	111.00
1	B	302	ARG	N-CA-C	-6.37	93.80	111.00
1	B	583	LEU	CA-CB-CG	6.29	129.77	115.30
1	A	380	VAL	N-CA-CB	6.27	125.30	111.50
1	B	598	GLN	N-CA-C	-6.23	94.18	111.00
1	A	562	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	357	PHE	CB-CA-C	5.79	121.99	110.40
1	B	550	ASN	N-CA-C	5.79	126.64	111.00
1	A	228	GLN	N-CA-C	-5.79	95.38	111.00
1	A	199	HIS	N-CA-C	5.78	126.60	111.00
1	B	522	SER	N-CA-CB	5.76	119.14	110.50
1	A	48	PRO	N-CA-C	-5.71	97.27	112.10
1	B	177	TYR	CA-CB-CG	5.68	124.19	113.40
1	B	80	ALA	N-CA-C	5.61	126.14	111.00
1	A	378	GLU	CB-CA-C	5.60	121.59	110.40
1	B	6	GLU	CB-CA-C	-5.59	99.22	110.40
1	B	215	GLU	N-CA-C	5.51	125.89	111.00
1	B	599	GLN	N-CA-C	-5.51	96.12	111.00
1	A	550	ASN	N-CA-CB	5.44	120.40	110.60
1	B	200	ALA	N-CA-CB	-5.42	102.52	110.10
1	B	329	SER	CB-CA-C	5.39	120.34	110.10
1	B	457	SER	N-CA-CB	5.38	118.57	110.50
1	B	163	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	9	THR	N-CA-CB	-5.27	100.28	110.30
1	B	6	GLU	N-CA-C	5.26	125.21	111.00
1	A	144	PRO	N-CA-C	-5.25	98.46	112.10
1	A	329	SER	N-CA-CB	5.12	118.18	110.50
1	A	208	ALA	CB-CA-C	5.12	117.78	110.10

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ILE	Mainchain,Peptide
1	A	198	ASN	Peptide
1	A	238	ASN	Peptide
1	A	47	VAL	Peptide
1	A	549	TRP	Mainchain,Peptide
1	B	176	LEU	Peptide
1	B	238	ASN	Peptide
1	B	47	VAL	Mainchain,Peptide
1	B	549	TRP	Peptide
1	B	564	GLY	Peptide

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	4776	0	4557	309	0
1	B	4776	0	4558	408	0
2	A	13	0	8	2	0
2	B	13	0	8	3	0
3	A	244	0	0	15	0
3	B	111	0	0	19	0
All	All	9933	0	9131	696	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 37.

All (696) 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:A:7:THR:CG2	1:A:8:PRO:HD3	1.44	1.47
1:B:7:THR:HB	1:B:8:PRO:CD	1.29	1.43
1:A:183:TRP:CZ3	1:A:185:ASP:HB3	1.63	1.34
1:B:7:THR:CB	1:B:8:PRO:CD	2.00	1.23
1:B:456:ILE:O	1:B:456:ILE:CG2	1.86	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:THR:CB	1:B:8:PRO:HD3	1.68	1.18
1:B:357:PHE:O	1:B:374:LEU:HD11	1.44	1.17
1:A:3:ARG:HG2	1:A:3:ARG:HH11	1.01	1.14
1:A:7:THR:HB	1:A:8:PRO:CD	1.78	1.14
1:B:212:VAL:HB	1:B:255:THR:O	1.48	1.14
1:A:598:GLN:O	1:A:598:GLN:HG2	1.43	1.13
1:B:436:ASP:OD1	1:B:438:THR:HG22	1.50	1.11
1:A:205:GLN:HE21	1:A:207:VAL:HG23	1.11	1.11
1:A:183:TRP:CZ3	1:A:185:ASP:CB	2.31	1.11
1:B:509:THR:HG21	1:B:526:GLN:HB2	1.35	1.09
1:A:184:VAL:HG13	1:A:205:GLN:HE22	1.16	1.08
1:A:15:LEU:HD12	1:A:173:SER:HA	1.17	1.08
1:B:214:VAL:O	1:B:214:VAL:CG1	2.00	1.08
1:A:212:VAL:HG13	1:A:230:THR:HG23	1.34	1.07
1:A:205:GLN:HE21	1:A:207:VAL:CG2	1.68	1.07
1:B:100:ASN:HA	1:B:129:ARG:NH2	1.69	1.07
1:A:7:THR:CB	1:A:8:PRO:CD	2.30	1.06
1:A:183:TRP:CE3	1:A:185:ASP:HB3	1.90	1.05
1:A:7:THR:CG2	1:A:8:PRO:CD	2.33	1.05
1:B:212:VAL:HG13	1:B:230:THR:OG1	1.55	1.05
1:A:7:THR:HG22	1:A:8:PRO:CD	1.85	1.04
1:A:7:THR:HB	1:A:8:PRO:HD2	1.33	1.04
1:B:193:VAL:O	1:B:285:HIS:NE2	1.90	1.03
1:B:240:HIS:CE1	1:B:248:TYR:CG	2.45	1.03
1:B:564:GLY:HA3	1:B:567:LYS:NZ	1.74	1.02
1:B:456:ILE:O	1:B:456:ILE:HG23	1.23	1.01
1:B:183:TRP:CZ3	1:B:185:ASP:HB3	1.97	1.00
1:B:7:THR:CB	1:B:8:PRO:HD2	1.89	1.00
1:A:77:LYS:NZ	1:B:8:PRO:O	1.95	0.99
1:B:598:GLN:C	1:B:600:GLY:H	1.61	0.99
1:A:203:ASP:OD1	1:A:233:THR:O	1.78	0.99
1:A:7:THR:HG22	1:A:8:PRO:HD3	1.01	0.99
1:B:8:PRO:HB2	3:B:675:HOH:O	1.62	0.99
1:A:203:ASP:OD1	1:A:233:THR:OG1	1.79	0.98
1:B:68:TRP:HZ3	1:B:98:TRP:CZ3	1.80	0.98
1:A:212:VAL:N	1:A:230:THR:OG1	1.95	0.97
1:B:6:GLU:HG2	1:B:11:GLU:OE2	1.63	0.96
1:B:240:HIS:HE1	1:B:248:TYR:CG	1.82	0.96
1:B:9:THR:HG22	1:B:178:THR:O	1.66	0.95
1:B:179:THR:CG2	1:B:183:TRP:CD1	2.50	0.94
1:A:212:VAL:H	1:A:230:THR:CG2	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HG2	1:B:35:TRP:CZ2	2.01	0.94
1:B:214:VAL:O	1:B:214:VAL:HG13	1.67	0.94
1:A:272:ARG:HA	1:A:284:ASN:HD21	1.33	0.94
1:B:7:THR:OG1	1:B:8:PRO:HD2	1.68	0.93
1:A:357:PHE:O	1:A:374:LEU:HD21	1.69	0.93
1:B:218:ASP:OD1	1:B:248:TYR:OH	1.86	0.93
1:A:119:THR:HB	1:A:120:PRO:HD3	1.50	0.93
1:B:85:VAL:O	1:B:177:TYR:HB3	1.69	0.92
1:B:513:LEU:HD13	1:B:521:TRP:O	1.67	0.92
1:A:7:THR:CB	1:A:8:PRO:HD3	1.94	0.92
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.34	0.91
1:A:3:ARG:HH11	1:A:3:ARG:CG	1.82	0.91
1:B:196:ASP:O	1:B:239:PRO:HG3	1.68	0.91
1:A:477:ASP:OD1	1:A:480:THR:HG23	1.71	0.90
1:A:14:LYS:HZ3	1:A:86:LEU:HD13	1.37	0.90
1:B:218:ASP:HB3	1:B:222:GLN:HG3	1.53	0.90
1:B:598:GLN:HB3	1:B:600:GLY:O	1.71	0.90
1:A:292:GLY:O	1:A:547:GLN:HA	1.71	0.89
1:A:191:THR:HG21	1:A:272:ARG:H	1.37	0.89
1:A:139:ASN:O	1:A:142:THR:HG22	1.71	0.89
1:A:183:TRP:HZ3	1:A:185:ASP:CB	1.76	0.89
1:A:513:LEU:HD12	1:A:521:TRP:O	1.74	0.87
1:B:179:THR:HG21	1:B:183:TRP:CD1	2.10	0.87
1:B:71:ARG:HH11	1:B:71:ARG:HG2	1.40	0.87
1:A:192:HIS:O	1:A:199:HIS:HB3	1.73	0.87
1:A:46:ALA:H	1:A:54:GLN:HE22	1.20	0.86
1:A:14:LYS:HD2	1:A:176:LEU:HD22	1.56	0.86
1:A:43:ARG:HD2	1:A:55:PHE:CE1	2.11	0.86
1:A:140:TRP:CE3	1:A:379:ALA:O	2.29	0.86
1:A:598:GLN:O	1:A:598:GLN:CG	2.25	0.85
1:B:212:VAL:HG13	1:B:230:THR:CB	2.07	0.85
1:B:240:HIS:CE1	1:B:248:TYR:CD1	2.65	0.85
1:B:46:ALA:H	1:B:54:GLN:HE22	1.23	0.84
1:B:357:PHE:O	1:B:374:LEU:CD1	2.24	0.84
1:A:15:LEU:CD1	1:A:173:SER:HA	2.04	0.84
1:A:3:ARG:HG2	1:A:3:ARG:NH1	1.82	0.84
1:A:198:ASN:O	1:A:199:HIS:HB2	1.76	0.84
1:B:240:HIS:ND1	1:B:240:HIS:O	2.09	0.84
1:B:200:ALA:HA	1:B:235:GLN:O	1.78	0.83
1:B:122:VAL:HG23	1:B:128:VAL:HG11	1.59	0.83
1:A:599:GLN:O	1:A:599:GLN:HG2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:LEU:CD1	1:B:521:TRP:O	2.26	0.83
1:A:15:LEU:HD13	1:A:173:SER:OG	1.78	0.82
1:A:14:LYS:NZ	1:A:86:LEU:HD13	1.92	0.82
1:A:52:ASN:HD21	1:A:168:ALA:H	1.26	0.82
1:A:105:MET:SD	3:A:844:HOH:O	2.36	0.82
1:A:36:GLU:HA	1:A:101:ASN:ND2	1.95	0.82
1:A:247:GLY:O	1:A:249:LEU:HD12	1.80	0.81
1:B:199:HIS:ND1	1:B:200:ALA:N	2.28	0.81
1:B:214:VAL:O	1:B:214:VAL:HG12	1.78	0.81
1:B:192:HIS:O	1:B:199:HIS:HB3	1.81	0.81
1:B:68:TRP:CZ3	1:B:98:TRP:CZ3	2.69	0.81
1:A:15:LEU:HD12	1:A:173:SER:CA	2.07	0.80
1:B:198:ASN:HB2	1:B:237:VAL:C	2.02	0.80
1:B:598:GLN:C	1:B:600:GLY:N	2.32	0.80
1:A:513:LEU:CD1	1:A:521:TRP:O	2.29	0.80
1:B:7:THR:HB	1:B:8:PRO:HD2	1.48	0.80
1:B:422:ARG:NH2	1:B:458:ASP:OD2	2.15	0.80
1:A:212:VAL:H	1:A:230:THR:CB	1.95	0.79
1:B:179:THR:HG21	1:B:183:TRP:CG	2.18	0.78
1:B:295:ARG:O	1:B:329:SER:HB2	1.84	0.78
1:A:212:VAL:CG1	1:A:230:THR:HG23	2.14	0.78
1:B:550:ASN:HD22	1:B:552:ALA:H	1.29	0.78
1:B:0:HIS:CD2	1:B:186:ASP:OD2	2.37	0.78
1:B:432:THR:HB	1:B:441:ILE:HD11	1.64	0.78
1:A:214:VAL:HG13	1:A:252:LEU:HD11	1.64	0.78
1:A:163:ASP:O	1:A:556:THR:HG22	1.83	0.78
1:A:579:SER:HB3	3:A:766:HOH:O	1.82	0.78
1:A:598:GLN:O	1:A:599:GLN:HB3	1.84	0.78
1:B:212:VAL:CG1	1:B:230:THR:OG1	2.32	0.77
1:A:202:VAL:HG12	1:A:234:LEU:HD21	1.64	0.77
1:B:179:THR:HG22	1:B:183:TRP:CD1	2.20	0.77
1:A:9:THR:HG22	1:A:178:THR:O	1.84	0.77
1:B:75:ILE:HG13	1:B:122:VAL:HG22	1.65	0.77
1:A:142:THR:HG23	1:A:144:PRO:O	1.84	0.77
1:B:335:GLU:H	1:B:335:GLU:CD	1.84	0.77
1:A:93:HIS:HE1	1:A:166:ASN:OD1	1.67	0.77
1:A:191:THR:HG21	1:A:272:ARG:N	1.99	0.77
1:B:564:GLY:HA3	1:B:567:LYS:HZ1	1.48	0.76
1:A:205:GLN:NE2	1:A:207:VAL:HG23	1.96	0.76
1:A:212:VAL:HG13	1:A:230:THR:CG2	2.13	0.76
1:B:172:ARG:NH2	1:B:333:TYR:C	2.39	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PRO:O	3:A:800:HOH:O	2.04	0.76
1:B:68:TRP:CZ3	1:B:98:TRP:CH2	2.74	0.75
1:B:15:LEU:C	1:B:15:LEU:HD23	2.06	0.75
1:A:3:ARG:HD2	1:A:4:PRO:HD2	1.68	0.75
1:A:184:VAL:HG13	1:A:205:GLN:NE2	1.99	0.75
1:A:14:LYS:NZ	1:A:86:LEU:CD1	2.49	0.75
1:A:212:VAL:H	1:A:230:THR:HG21	1.51	0.75
1:B:183:TRP:CZ3	1:B:185:ASP:CB	2.70	0.75
1:B:551:PHE:HE2	1:B:575:ARG:HH11	1.32	0.74
1:B:292:GLY:O	1:B:547:GLN:HA	1.88	0.74
1:A:477:ASP:OD1	1:A:480:THR:CG2	2.36	0.74
1:A:14:LYS:HZ3	1:A:86:LEU:CD1	2.00	0.73
1:B:469:TYR:O	1:B:529:TRP:CZ3	2.41	0.73
1:B:204:TRP:CD1	1:B:231:SER:O	2.41	0.73
1:B:420:GLY:O	1:B:423:GLU:HG3	1.87	0.73
1:A:205:GLN:HG2	1:A:212:VAL:HG21	1.71	0.73
1:B:328:THR:O	1:B:351:GLU:HB3	1.89	0.73
1:B:172:ARG:HH21	1:B:333:TYR:C	1.92	0.72
1:B:71:ARG:HH11	1:B:71:ARG:CG	2.02	0.72
1:B:7:THR:HB	1:B:8:PRO:HD3	0.73	0.72
1:B:467:ARG:HG2	1:B:469:TYR:CE1	2.24	0.72
1:A:311:MET:HE3	1:A:337:MET:HA	1.69	0.72
1:B:205:GLN:HG2	1:B:206:VAL:N	2.03	0.72
1:B:432:THR:HB	1:B:441:ILE:CD1	2.19	0.72
1:B:432:THR:CG2	1:B:441:ILE:HD11	2.18	0.72
1:B:105:MET:HE2	1:B:114:PHE:HD1	1.55	0.72
1:B:220:ASP:HB2	1:B:222:GLN:HG2	1.70	0.72
1:B:179:THR:HG22	1:B:183:TRP:HD1	1.55	0.72
1:B:539:ARG:HA	1:B:599:GLN:HG3	1.70	0.71
1:B:272:ARG:HA	1:B:284:ASN:HD21	1.55	0.71
1:A:8:PRO:HA	1:B:77:LYS:HZ3	1.56	0.71
1:A:107:HIS:HE1	1:A:394:GLU:OE1	1.74	0.71
1:B:247:GLY:O	1:B:249:LEU:HD12	1.91	0.71
1:B:432:THR:CB	1:B:441:ILE:HD11	2.21	0.71
1:B:212:VAL:CB	1:B:255:THR:O	2.34	0.71
1:B:425:PHE:HB2	1:B:456:ILE:HD11	1.71	0.70
1:B:101:ASN:N	1:B:101:ASN:HD22	1.88	0.70
1:B:7:THR:OG1	1:B:8:PRO:CD	2.32	0.70
1:A:14:LYS:HA	1:A:71:ARG:HH21	1.57	0.70
1:B:598:GLN:O	1:B:600:GLY:N	2.25	0.69
1:B:49:GLY:HA2	1:B:305:GLY:HA3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ASP:O	3:B:634:HOH:O	2.09	0.69
1:B:463:LEU:HD21	1:B:492:TRP:CE3	2.27	0.69
1:A:13:LYS:HG2	1:A:15:LEU:HB3	1.73	0.69
1:A:183:TRP:HZ3	1:A:185:ASP:HB2	1.54	0.69
1:A:26:GLU:HB2	1:A:28:CYS:SG	2.32	0.69
1:A:202:VAL:HG12	1:A:234:LEU:CD2	2.21	0.69
1:A:211:ASP:HA	1:A:230:THR:HG21	1.73	0.69
1:A:538:ASP:HB3	1:A:599:GLN:HA	1.74	0.69
1:B:163:ASP:O	3:B:652:HOH:O	2.10	0.69
1:B:203:ASP:OD1	1:B:233:THR:OG1	2.07	0.69
1:A:328:THR:O	1:A:351:GLU:HB3	1.93	0.69
1:B:6:GLU:CG	1:B:11:GLU:OE2	2.39	0.69
1:A:139:ASN:H	1:A:142:THR:CG2	2.06	0.69
1:A:436:ASP:OD1	1:A:438:THR:CG2	2.41	0.68
1:B:196:ASP:HB3	1:B:241:LEU:HD11	1.73	0.68
1:A:212:VAL:HA	1:A:255:THR:O	1.92	0.68
1:A:15:LEU:HG	1:A:48:PRO:HD3	1.75	0.68
1:A:36:GLU:C	1:A:129:ARG:HH21	1.97	0.68
1:B:15:LEU:HG	1:B:48:PRO:HD3	1.75	0.68
1:A:200:ALA:HA	1:A:235:GLN:O	1.93	0.68
1:A:311:MET:CE	1:A:340:TRP:HB2	2.24	0.68
1:B:19:TRP:CD1	1:B:47:VAL:HG13	2.29	0.68
1:A:378:GLU:O	3:A:619:HOH:O	2.12	0.68
1:B:179:THR:HG23	1:B:183:TRP:HB3	1.75	0.67
1:B:205:GLN:HE22	1:B:212:VAL:HG21	1.59	0.67
1:A:450:ASP:OD2	1:A:453:THR:HG23	1.94	0.67
1:B:447:MET:HG2	1:B:467:ARG:HG3	1.76	0.67
1:B:89:ASP:OD1	1:B:173:SER:O	2.13	0.67
1:B:445:ASN:ND2	1:B:467:ARG:HH22	1.92	0.67
1:A:138:LEU:HA	1:A:142:THR:HG21	1.76	0.66
1:A:205:GLN:NE2	1:A:207:VAL:CG2	2.51	0.66
1:B:242:TRP:CD1	1:B:270:GLY:HA3	2.31	0.66
1:A:240:HIS:HB2	1:A:248:TYR:CD2	2.31	0.66
1:A:477:ASP:CG	1:A:480:THR:HG23	2.15	0.66
1:B:0:HIS:HD2	1:B:186:ASP:OD2	1.77	0.66
1:B:0:HIS:HB3	1:B:186:ASP:OD2	1.95	0.66
1:B:90:ALA:HB3	1:B:172:ARG:HD3	1.77	0.66
1:B:96:LYS:HD3	1:B:98:TRP:CZ2	2.31	0.66
1:B:138:LEU:HD22	1:B:142:THR:HG21	1.76	0.65
1:B:355:VAL:HG23	1:B:412:ASN:HD22	1.60	0.65
1:A:8:PRO:HA	1:B:77:LYS:NZ	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LYS:HA	3:B:704:HOH:O	1.96	0.65
1:B:388:HIS:O	1:B:392:ILE:HG13	1.96	0.65
1:B:564:GLY:HA3	1:B:567:LYS:HZ3	1.57	0.65
1:A:450:ASP:OD2	1:A:453:THR:CG2	2.45	0.65
1:B:101:ASN:ND2	1:B:129:ARG:HH22	1.95	0.65
1:B:392:ILE:HG21	1:B:410:ILE:HD11	1.79	0.65
1:B:75:ILE:HG13	1:B:122:VAL:CG2	2.27	0.65
1:B:179:THR:CG2	1:B:183:TRP:CG	2.79	0.64
1:B:204:TRP:HD1	1:B:231:SER:O	1.79	0.64
1:B:240:HIS:CE1	1:B:248:TYR:CD2	2.84	0.64
1:A:244:PRO:O	1:A:345:GLY:O	2.15	0.64
1:A:94:TYR:HB3	1:A:135:ASN:HB3	1.80	0.63
1:A:35:TRP:HD1	1:A:101:ASN:HA	1.62	0.63
1:A:550:ASN:HD22	1:A:552:ALA:H	1.44	0.63
1:B:509:THR:HG21	1:B:526:GLN:CB	2.22	0.63
1:B:187:ILE:HG22	1:B:188:THR:N	2.14	0.63
1:A:83:ARG:CB	1:A:179:THR:HG22	2.29	0.63
1:B:283:ILE:HG12	1:B:288:PHE:HB2	1.81	0.63
1:B:71:ARG:NH1	1:B:72:GLU:O	2.32	0.62
1:B:14:LYS:HD3	1:B:73:VAL:HG11	1.81	0.62
1:B:311:MET:CE	1:B:340:TRP:HB2	2.28	0.62
1:A:357:PHE:O	1:A:374:LEU:HD11	1.99	0.62
1:B:68:TRP:HZ3	1:B:98:TRP:CH2	2.09	0.62
1:B:240:HIS:HE1	1:B:248:TYR:CB	2.11	0.62
1:A:139:ASN:H	1:A:142:THR:HG22	1.63	0.62
1:B:15:LEU:HD23	1:B:15:LEU:O	2.00	0.62
1:B:52:ASN:HD21	1:B:168:ALA:H	1.47	0.62
1:B:111:TYR:HB2	1:B:332:PRO:HD2	1.81	0.62
1:B:14:LYS:NZ	1:B:130:ILE:HG13	2.15	0.62
1:B:172:ARG:HD2	3:B:627:HOH:O	2.00	0.62
1:A:36:GLU:C	1:A:129:ARG:NH2	2.54	0.61
1:A:357:PHE:O	1:A:374:LEU:CD2	2.47	0.61
1:B:189:VAL:H	1:B:401:ASN:HD21	1.48	0.61
1:B:243:GLN:NE2	1:B:284:ASN:OD1	2.33	0.61
1:B:311:MET:HE3	1:B:337:MET:HA	1.81	0.61
1:B:102:GLN:HG2	1:B:121:TYR:CD1	2.35	0.61
1:B:551:PHE:HE2	1:B:575:ARG:NH1	1.98	0.61
1:A:111:TYR:HB2	1:A:332:PRO:HD2	1.82	0.61
1:B:15:LEU:HD12	1:B:173:SER:CB	2.30	0.61
1:B:93:HIS:HE1	1:B:166:ASN:OD1	1.84	0.61
1:B:101:ASN:ND2	1:B:129:ARG:NH2	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASN:HD21	1:A:137:GLU:HB2	1.65	0.61
1:B:83:ARG:NE	1:B:117:ASP:HB2	2.15	0.61
1:A:207:VAL:CG1	1:A:256:ALA:HB1	2.31	0.60
1:A:26:GLU:OE1	1:A:26:GLU:HA	2.01	0.60
1:A:452:HIS:HE1	3:A:743:HOH:O	1.83	0.60
1:B:405:VAL:HG11	1:B:408:TRP:CZ3	2.37	0.60
1:B:529:TRP:CD1	1:B:529:TRP:C	2.74	0.60
1:A:43:ARG:NH1	3:A:781:HOH:O	2.34	0.60
1:A:52:ASN:H	1:A:52:ASN:HD22	1.48	0.60
1:A:155:LYS:HD3	3:A:835:HOH:O	2.01	0.60
1:A:138:LEU:CA	1:A:142:THR:HG21	2.32	0.60
1:B:163:ASP:HB3	3:B:665:HOH:O	2.00	0.60
1:B:295:ARG:O	1:B:333:TYR:OH	2.19	0.59
1:B:33:ARG:CG	1:B:35:TRP:CZ2	2.82	0.59
1:B:138:LEU:HD22	1:B:142:THR:CG2	2.30	0.59
1:A:105:MET:HE1	1:A:115:GLU:N	2.18	0.59
1:B:568:LYS:NZ	2:B:604:EVA:OXT	2.34	0.59
1:A:122:VAL:HG23	1:A:128:VAL:HG11	1.84	0.59
1:B:151:ASP:OD1	1:B:155:LYS:N	2.35	0.59
1:B:24:ASP:O	1:B:63:TYR:OH	2.21	0.59
1:A:441:ILE:HG22	1:A:461:ASP:OD2	2.03	0.58
1:A:15:LEU:CD1	1:A:173:SER:OG	2.51	0.58
1:A:413:GLU:OE2	2:A:604:EVA:OAK	2.21	0.58
1:B:389:LEU:HA	1:B:392:ILE:HD12	1.86	0.58
1:A:35:TRP:CD1	1:A:101:ASN:HA	2.38	0.58
1:B:240:HIS:HB3	1:B:250:TYR:OH	2.03	0.58
1:A:6:GLU:HG2	1:A:10:ARG:HA	1.86	0.58
1:A:193:VAL:HA	1:A:199:HIS:CB	2.34	0.58
1:B:101:ASN:HD22	1:B:129:ARG:NH2	2.01	0.58
1:B:276:VAL:CG1	1:B:499:PRO:HG3	2.34	0.58
1:B:83:ARG:N	1:B:179:THR:O	2.31	0.57
1:A:83:ARG:HB2	1:A:179:THR:HG22	1.86	0.57
1:B:183:TRP:CH2	1:B:185:ASP:HB3	2.39	0.57
1:B:399:ASP:HA	1:B:402:HIS:HD2	1.69	0.57
1:B:494:GLU:HG2	1:B:495:LYS:H	1.68	0.57
1:B:33:ARG:HB3	1:B:36:GLU:HG3	1.85	0.57
1:B:83:ARG:HE	1:B:117:ASP:HB2	1.69	0.57
1:B:276:VAL:HG13	1:B:499:PRO:HG3	1.85	0.57
1:B:509:THR:CG2	1:B:526:GLN:HB2	2.22	0.57
1:B:111:TYR:CB	1:B:332:PRO:HD2	2.34	0.57
1:B:83:ARG:HH11	1:B:83:ARG:CG	2.09	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:VAL:HG11	1:A:256:ALA:HB1	1.87	0.57
1:B:23:LEU:HD11	1:B:60:ILE:HG12	1.86	0.57
1:B:328:THR:HA	1:B:333:TYR:CZ	2.40	0.57
1:B:438:THR:HG23	1:B:439:ARG:HG3	1.87	0.57
1:A:312:VAL:HG11	1:B:54:GLN:HE21	1.69	0.57
1:B:164:PHE:N	3:B:665:HOH:O	2.38	0.57
1:B:212:VAL:HG13	1:B:230:THR:HB	1.83	0.56
1:B:11:GLU:CD	1:B:11:GLU:N	2.58	0.56
1:A:6:GLU:O	1:A:7:THR:OG1	2.19	0.56
1:B:85:VAL:HB	1:B:177:TYR:CD2	2.41	0.56
1:B:100:ASN:CA	1:B:129:ARG:NH2	2.59	0.56
1:B:462:VAL:HG22	1:B:499:PRO:HG2	1.86	0.56
1:A:436:ASP:OD1	1:A:438:THR:HG23	2.04	0.56
1:B:377:GLU:CD	1:B:377:GLU:H	2.07	0.56
1:B:138:LEU:CD2	1:B:142:THR:HG21	2.35	0.56
1:B:83:ARG:HG2	1:B:83:ARG:NH1	2.12	0.56
1:A:83:ARG:HH11	1:A:179:THR:HG21	1.71	0.56
1:A:7:THR:HG21	1:A:8:PRO:HD3	1.71	0.56
1:B:15:LEU:HD12	1:B:173:SER:HB2	1.88	0.56
1:B:179:THR:CG2	1:B:183:TRP:CB	2.83	0.56
1:B:596:LYS:HG2	1:B:597:PRO:O	2.06	0.56
1:A:140:TRP:CD2	1:A:379:ALA:O	2.58	0.56
1:A:212:VAL:N	1:A:230:THR:CG2	2.61	0.56
1:A:272:ARG:CA	1:A:284:ASN:HD21	2.13	0.56
1:B:144:PRO:HD3	3:B:615:HOH:O	2.06	0.56
1:B:213:SER:O	1:B:227:GLY:O	2.24	0.56
1:B:425:PHE:HB2	1:B:456:ILE:CD1	2.35	0.56
1:A:199:HIS:ND1	1:A:200:ALA:N	2.52	0.55
1:A:205:GLN:HE21	1:A:207:VAL:HG22	1.64	0.55
1:A:550:ASN:ND2	1:A:551:PHE:N	2.55	0.55
1:B:151:ASP:OD1	1:B:154:GLY:N	2.39	0.55
1:A:101:ASN:HD21	1:A:129:ARG:NH2	2.05	0.55
1:B:550:ASN:O	1:B:569:GLY:HA2	2.06	0.55
1:B:330:HIS:N	1:B:330:HIS:CD2	2.73	0.55
1:B:122:VAL:HG23	1:B:128:VAL:CG1	2.34	0.55
1:B:88:PHE:O	1:B:113:PRO:HA	2.07	0.55
1:B:207:VAL:CG1	1:B:256:ALA:HB1	2.37	0.55
1:A:107:HIS:CE1	1:A:394:GLU:OE1	2.57	0.54
1:B:247:GLY:O	1:B:249:LEU:CD1	2.55	0.54
1:A:193:VAL:HA	1:A:199:HIS:HB2	1.89	0.54
1:B:179:THR:HG23	1:B:183:TRP:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:HB2	3:A:814:HOH:O	2.08	0.54
1:A:445:ASN:HD21	1:A:467:ARG:HH22	1.55	0.54
1:B:14:LYS:HZ1	1:B:130:ILE:HG13	1.73	0.54
1:B:207:VAL:HG13	1:B:256:ALA:HB1	1.90	0.54
1:B:357:PHE:O	1:B:374:LEU:HD21	2.07	0.54
1:A:14:LYS:O	1:A:174:VAL:HG22	2.07	0.54
1:A:28:CYS:HB3	1:A:32:GLN:NE2	2.21	0.54
1:A:180:PRO:HG2	1:A:263:ASP:HB2	1.88	0.54
1:A:272:ARG:HA	1:A:284:ASN:ND2	2.14	0.54
1:B:192:HIS:HE1	1:B:202:VAL:HG13	1.72	0.54
1:B:432:THR:HG21	1:B:441:ILE:HD11	1.88	0.54
1:B:563:VAL:HG23	1:B:564:GLY:N	2.22	0.54
1:A:566:ASN:HD22	1:A:568:LYS:H	1.54	0.54
1:A:0:HIS:N	1:A:0:HIS:CD2	2.76	0.54
1:B:493:GLN:O	1:B:496:LEU:O	2.26	0.54
1:A:50:SER:HB2	1:A:303:GLY:H	1.73	0.54
1:A:78:GLY:HA3	1:B:78:GLY:HA3	1.89	0.54
1:B:494:GLU:HG2	1:B:495:LYS:N	2.23	0.54
1:A:191:THR:HG21	1:A:271:ILE:HA	1.90	0.53
1:B:193:VAL:HG11	1:B:284:ASN:HD21	1.73	0.53
1:B:191:THR:HG21	1:B:272:ARG:H	1.73	0.53
1:A:513:LEU:HD13	1:A:521:TRP:O	2.08	0.53
1:B:191:THR:HG21	1:B:271:ILE:HA	1.90	0.53
1:B:218:ASP:CB	1:B:222:GLN:HE21	2.21	0.53
1:A:52:ASN:H	1:A:52:ASN:ND2	2.07	0.53
1:B:85:VAL:HB	1:B:177:TYR:CG	2.44	0.53
1:A:445:ASN:ND2	1:A:467:ARG:HH12	2.05	0.53
1:B:425:PHE:CB	1:B:456:ILE:HD11	2.37	0.53
1:B:10:ARG:CZ	1:B:79:TRP:HE1	2.22	0.53
1:B:480:THR:O	1:B:484:VAL:HG23	2.08	0.53
1:A:13:LYS:HB3	1:B:13:LYS:HZ1	1.74	0.53
1:B:163:ASP:CB	3:B:665:HOH:O	2.57	0.53
1:A:13:LYS:HZ2	1:B:15:LEU:HD22	1.74	0.53
1:B:83:ARG:NH2	1:B:117:ASP:HB2	2.23	0.53
1:B:494:GLU:CG	1:B:495:LYS:N	2.71	0.53
1:B:96:LYS:HD3	1:B:98:TRP:HZ2	1.73	0.53
1:A:238:ASN:N	3:A:810:HOH:O	2.42	0.52
1:A:135:ASN:ND2	1:A:137:GLU:H	2.07	0.52
1:A:376:SER:O	1:A:380:VAL:O	2.27	0.52
1:A:6:GLU:HG3	1:A:11:GLU:OE2	2.09	0.52
1:A:233:THR:O	1:A:233:THR:OG1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ARG:HA	1:B:284:ASN:ND2	2.22	0.52
1:A:212:VAL:N	1:A:230:THR:HG21	2.22	0.52
1:B:496:LEU:HB3	3:B:690:HOH:O	2.08	0.52
1:A:193:VAL:HG22	1:A:285:HIS:NE2	2.25	0.52
1:A:214:VAL:HG13	1:A:252:LEU:CD1	2.37	0.52
1:B:426:ALA:HA	1:B:459:LEU:CD1	2.39	0.52
1:B:28:CYS:O	1:B:32:GLN:HG3	2.10	0.52
1:B:408:TRP:HE1	1:B:436:ASP:HB3	1.74	0.52
1:A:198:ASN:O	1:A:199:HIS:CB	2.54	0.52
1:A:566:ASN:ND2	1:A:568:LYS:H	2.08	0.52
1:B:10:ARG:NH1	1:B:79:TRP:HE1	2.07	0.52
1:B:433:ARG:NH1	1:B:461:ASP:OD1	2.43	0.52
1:B:10:ARG:H	1:B:178:THR:HG22	1.75	0.51
1:B:119:THR:HB	1:B:120:PRO:HD3	1.92	0.51
1:A:311:MET:HE1	1:A:340:TRP:HB2	1.90	0.51
1:A:538:ASP:OD2	1:A:587:ARG:NH2	2.41	0.51
1:B:183:TRP:HE3	1:B:183:TRP:C	2.14	0.51
1:B:504:GLU:OE1	2:B:604:EVA:CAE	2.59	0.51
1:A:10:ARG:HH21	1:B:77:LYS:HD2	1.76	0.51
1:A:184:VAL:HG22	1:A:207:VAL:HG22	1.93	0.51
1:A:212:VAL:HG22	1:A:230:THR:HA	1.92	0.51
1:B:43:ARG:HD2	1:B:55:PHE:CE1	2.45	0.51
1:A:195:GLN:N	1:A:195:GLN:OE1	2.44	0.51
1:B:325:SER:HA	1:B:347:VAL:O	2.10	0.51
1:B:83:ARG:CZ	1:B:117:ASP:HB2	2.41	0.51
1:A:14:LYS:HZ1	1:A:86:LEU:HD11	1.75	0.51
1:A:36:GLU:O	1:A:129:ARG:NH2	2.44	0.51
1:B:163:ASP:C	3:B:665:HOH:O	2.49	0.51
1:A:122:VAL:CG2	1:A:128:VAL:HG11	2.40	0.51
1:A:147:MET:HE3	1:A:161:PHE:CZ	2.45	0.51
1:B:3:ARG:NH1	1:B:335:GLU:HG2	2.26	0.51
1:B:445:ASN:ND2	1:B:467:ARG:NH2	2.58	0.51
1:A:73:VAL:O	1:A:127:SER:HA	2.11	0.50
1:A:83:ARG:HB3	1:A:179:THR:HG22	1.93	0.50
1:B:68:TRP:CH2	1:B:98:TRP:CH2	2.99	0.50
1:B:95:GLY:HA2	1:B:133:CYS:O	2.10	0.50
1:B:311:MET:HE1	1:B:340:TRP:HB2	1.93	0.50
1:B:144:PRO:HG3	3:B:615:HOH:O	2.11	0.50
1:B:373:GLU:O	1:B:376:SER:HB3	2.10	0.50
1:B:289:TYR:HA	1:B:544:VAL:O	2.10	0.50
1:A:36:GLU:HA	1:A:101:ASN:HD21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:HD13	1:B:176:LEU:HD13	1.93	0.50
1:A:314:ASP:OD1	1:A:575:ARG:HD2	2.12	0.50
1:A:74:PHE:CE2	1:B:6:GLU:O	2.64	0.50
1:A:83:ARG:NH1	1:A:183:TRP:CD2	2.79	0.50
1:B:10:ARG:NH1	1:B:79:TRP:NE1	2.59	0.50
1:B:554:PHE:HE2	3:B:665:HOH:O	1.93	0.50
1:A:203:ASP:OD2	1:A:233:THR:HG23	2.11	0.49
1:A:535:ARG:HH11	1:A:535:ARG:HG2	1.77	0.49
1:A:167:TYR:CD1	1:A:303:GLY:HA3	2.47	0.49
1:A:299:ALA:O	1:A:302:ARG:O	2.30	0.49
1:A:445:ASN:HD22	1:A:467:ARG:HH12	1.58	0.49
1:B:183:TRP:C	1:B:183:TRP:CE3	2.85	0.49
1:B:212:VAL:HG21	1:B:214:VAL:HG23	1.94	0.49
1:A:3:ARG:CG	1:A:3:ARG:NH1	2.52	0.49
1:A:13:LYS:NZ	1:B:15:LEU:CD2	2.75	0.49
1:A:207:VAL:CG1	1:A:256:ALA:CB	2.90	0.49
1:A:303:GLY:O	1:A:304:LYS:HG2	2.12	0.49
1:B:101:ASN:N	1:B:101:ASN:ND2	2.59	0.49
1:B:191:THR:HG21	1:B:272:ARG:N	2.27	0.49
1:A:83:ARG:HD3	1:A:179:THR:CG2	2.43	0.49
1:A:546:GLU:OE1	1:A:587:ARG:HD3	2.12	0.49
1:B:83:ARG:CG	1:B:83:ARG:NH1	2.72	0.49
1:B:467:ARG:HD3	1:B:469:TYR:HE1	1.77	0.49
1:A:203:ASP:OD1	1:A:233:THR:CB	2.59	0.49
1:A:214:VAL:CG1	1:A:252:LEU:HD11	2.37	0.49
1:B:279:GLU:OE2	1:B:493:GLN:HG3	2.13	0.49
1:A:8:PRO:HG2	1:A:264:ILE:HB	1.95	0.49
1:A:179:THR:HG23	1:A:180:PRO:O	2.13	0.49
1:A:13:LYS:NZ	1:B:15:LEU:HD22	2.28	0.49
1:A:139:ASN:HA	1:A:146:GLY:O	2.13	0.49
1:B:71:ARG:CG	1:B:71:ARG:NH1	2.68	0.49
1:B:351:GLU:HG2	1:B:352:THR:O	2.12	0.49
1:A:531:ASP:OD1	1:A:583:LEU:HD21	2.13	0.49
1:B:15:LEU:C	1:B:15:LEU:CD2	2.78	0.49
1:B:283:ILE:HG12	1:B:288:PHE:CB	2.43	0.49
1:A:101:ASN:HD21	1:A:129:ARG:HH22	1.61	0.48
1:B:4:PRO:HG3	1:B:177:TYR:CE2	2.48	0.48
1:B:292:GLY:HA3	1:B:325:SER:O	2.12	0.48
1:B:469:TYR:O	1:B:529:TRP:CH2	2.65	0.48
1:B:551:PHE:CE2	1:B:575:ARG:NH1	2.77	0.48
1:B:189:VAL:N	1:B:401:ASN:HD21	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HG13	1:B:273:SER:HB3	1.96	0.48
1:A:93:HIS:HD2	3:A:708:HOH:O	1.96	0.48
1:B:240:HIS:HE1	1:B:248:TYR:CD1	2.18	0.48
1:B:218:ASP:OD2	1:B:222:GLN:NE2	2.46	0.48
1:B:242:TRP:HD1	1:B:270:GLY:HA3	1.76	0.48
1:B:160:TYR:OH	1:B:557:SER:HB3	2.14	0.48
1:B:244:PRO:HG2	1:B:593:PHE:HE1	1.78	0.48
1:B:538:ASP:HA	3:B:671:HOH:O	2.13	0.48
1:A:49:GLY:HA2	1:A:305:GLY:HA3	1.94	0.48
1:A:410:ILE:HD11	1:A:432:THR:HG21	1.96	0.48
1:B:155:LYS:NZ	3:B:702:HOH:O	2.39	0.48
1:B:187:ILE:CG2	1:B:188:THR:N	2.77	0.48
1:B:564:GLY:CA	1:B:567:LYS:HZ3	2.26	0.48
1:A:183:TRP:CZ3	1:A:185:ASP:CG	2.85	0.48
1:A:187:ILE:HG12	1:A:205:GLN:OE1	2.14	0.48
1:A:330:HIS:HD2	1:A:351:GLU:OE1	1.96	0.48
1:A:207:VAL:HG11	1:A:256:ALA:CB	2.44	0.47
1:A:585:GLN:HG2	3:A:830:HOH:O	2.13	0.47
1:B:179:THR:CG2	1:B:183:TRP:HB3	2.40	0.47
1:B:33:ARG:HA	1:B:35:TRP:CZ3	2.49	0.47
1:B:139:ASN:HA	1:B:146:GLY:O	2.14	0.47
1:B:172:ARG:NH2	1:B:334:ALA:N	2.62	0.47
1:B:212:VAL:CG2	1:B:214:VAL:HG23	2.43	0.47
1:B:100:ASN:HA	1:B:129:ARG:HH22	1.70	0.47
1:A:268:ARG:HH22	1:A:343:GLU:HB2	1.78	0.47
1:A:256:ALA:HB3	1:A:263:ASP:HB3	1.97	0.47
1:B:350:ASP:OD2	1:B:399:ASP:OD2	2.33	0.47
1:B:502:ILE:N	1:B:502:ILE:HD12	2.29	0.47
1:A:12:ILE:HG22	1:A:14:LYS:HG3	1.96	0.47
1:A:19:TRP:CD1	1:A:47:VAL:HG13	2.49	0.47
1:A:138:LEU:HB3	1:A:142:THR:HG21	1.97	0.47
1:A:205:GLN:NE2	1:A:207:VAL:HG22	2.27	0.47
1:A:320:TRP:CE2	1:A:585:GLN:NE2	2.83	0.47
1:B:19:TRP:CE2	1:B:71:ARG:HD2	2.50	0.47
1:B:34:TRP:CE3	1:B:68:TRP:CD1	3.03	0.47
1:B:198:ASN:OD1	1:B:198:ASN:O	2.32	0.47
1:B:471:TRP:CZ2	1:B:508:ASP:HB2	2.49	0.47
1:B:538:ASP:HB3	1:B:599:GLN:HA	1.97	0.47
1:B:105:MET:CE	1:B:114:PHE:HD1	2.24	0.47
1:B:498:GLN:HG2	1:B:499:PRO:HD2	1.97	0.47
1:B:396:ILE:O	1:B:400:LYS:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:VAL:C	1:B:568:LYS:HG2	2.34	0.47
1:A:100:ASN:ND2	1:A:129:ARG:HB3	2.29	0.47
1:A:163:ASP:O	1:A:556:THR:CG2	2.60	0.47
1:B:21:PHE:HB2	1:B:45:ILE:CG2	2.44	0.47
1:B:89:ASP:HB2	1:B:172:ARG:HB3	1.97	0.47
1:B:183:TRP:CZ3	1:B:185:ASP:CG	2.88	0.47
1:A:7:THR:HA	1:B:74:PHE:CE1	2.51	0.46
1:A:599:GLN:O	1:A:599:GLN:CG	2.52	0.46
1:B:242:TRP:CZ2	1:B:345:GLY:HA2	2.50	0.46
1:A:6:GLU:CG	1:A:11:GLU:OE2	2.63	0.46
1:A:6:GLU:HA	1:A:9:THR:O	2.15	0.46
1:B:513:LEU:HD12	1:B:521:TRP:O	2.10	0.46
1:A:202:VAL:HG12	1:A:234:LEU:CG	2.44	0.46
1:A:328:THR:HB	1:A:333:TYR:CD2	2.51	0.46
1:B:14:LYS:HB2	1:B:174:VAL:HG22	1.98	0.46
1:B:205:GLN:CG	1:B:206:VAL:N	2.74	0.46
1:B:456:ILE:HD13	1:B:459:LEU:HG	1.97	0.46
1:B:487:LYS:O	1:B:487:LYS:HD3	2.15	0.46
1:A:190:VAL:HB	1:A:202:VAL:HG22	1.96	0.46
1:A:509:THR:OG1	1:A:526:GLN:HB2	2.16	0.46
1:B:84:ILE:HA	1:B:177:TYR:O	2.14	0.46
1:A:249:LEU:HD11	1:A:342:ASP:O	2.15	0.46
1:A:330:HIS:HE1	2:A:604:EVA:OD2	1.98	0.46
1:B:11:GLU:CD	1:B:11:GLU:H	2.19	0.46
1:A:7:THR:HG23	1:B:74:PHE:CZ	2.51	0.46
1:B:70:GLN:NE2	1:B:129:ARG:HD2	2.30	0.46
1:B:563:VAL:CG2	1:B:564:GLY:N	2.78	0.46
1:A:83:ARG:HB2	1:A:179:THR:CG2	2.45	0.46
1:A:188:THR:HB	1:A:204:TRP:HE3	1.81	0.46
1:B:167:TYR:HB2	1:B:304:LYS:HD2	1.97	0.46
1:B:192:HIS:HE1	1:B:202:VAL:CG1	2.28	0.46
1:B:198:ASN:HB3	1:B:238:ASN:HA	1.98	0.46
1:B:207:VAL:CG2	1:B:230:THR:OG1	2.64	0.46
1:B:504:GLU:HG2	1:B:549:TRP:CE3	2.51	0.46
1:A:7:THR:HA	1:B:74:PHE:CZ	2.50	0.46
1:B:167:TYR:HB2	1:B:304:LYS:CD	2.46	0.46
1:A:342:ASP:CG	1:A:403:PRO:HD2	2.36	0.45
1:B:107:HIS:HD2	3:B:668:HOH:O	1.97	0.45
1:B:192:HIS:CE1	1:B:202:VAL:HG13	2.50	0.45
1:B:193:VAL:HG11	1:B:284:ASN:ND2	2.31	0.45
1:B:10:ARG:HB2	1:B:79:TRP:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:O	1:B:16:ASP:C	2.54	0.45
1:A:191:THR:HG23	1:A:271:ILE:HG23	1.98	0.45
1:A:249:LEU:HD22	1:A:268:ARG:NH2	2.30	0.45
1:B:94:TYR:O	1:B:134:VAL:HA	2.16	0.45
1:B:183:TRP:CE3	1:B:183:TRP:O	2.69	0.45
1:B:467:ARG:HG2	1:B:469:TYR:CD1	2.51	0.45
1:B:529:TRP:CD1	1:B:530:LEU:N	2.85	0.45
1:B:355:VAL:CG2	1:B:412:ASN:HD22	2.27	0.45
1:A:16:ASP:OD2	1:B:13:LYS:NZ	2.47	0.45
1:A:151:ASP:CG	3:A:835:HOH:O	2.55	0.45
1:B:172:ARG:HH21	1:B:334:ALA:N	2.14	0.45
1:B:183:TRP:HZ3	1:B:185:ASP:CG	2.20	0.45
1:B:75:ILE:HD11	1:B:128:VAL:HG22	1.98	0.45
1:B:117:ASP:OD2	1:B:119:THR:OG1	2.22	0.45
1:B:96:LYS:HE3	1:B:106:GLU:OE2	2.16	0.45
1:A:73:VAL:HG22	1:A:74:PHE:N	2.32	0.45
1:B:396:ILE:HD11	1:B:432:THR:HG23	1.99	0.45
1:B:489:LEU:O	1:B:492:TRP:HB2	2.17	0.45
1:A:8:PRO:O	1:B:77:LYS:NZ	2.50	0.45
1:B:34:TRP:CZ3	1:B:68:TRP:CD1	3.05	0.45
1:A:242:TRP:CZ2	1:A:345:GLY:HA2	2.52	0.44
1:B:376:SER:OG	1:B:378:GLU:HG2	2.16	0.44
1:A:86:LEU:HD12	1:A:175:MET:O	2.17	0.44
1:A:102:GLN:HG2	1:A:121:TYR:CD1	2.52	0.44
1:A:36:GLU:CA	1:A:129:ARG:HH21	2.30	0.44
1:A:50:SER:OG	1:A:303:GLY:HA3	2.17	0.44
1:A:463:LEU:HD21	1:A:492:TRP:CD2	2.53	0.44
1:B:433:ARG:NH2	1:B:461:ASP:OD1	2.50	0.44
1:A:119:THR:HB	1:A:120:PRO:CD	2.33	0.44
1:A:167:TYR:CZ	1:A:303:GLY:HA2	2.52	0.44
1:B:142:THR:HG22	1:B:144:PRO:O	2.17	0.44
1:B:184:VAL:HG21	1:B:254:VAL:HG12	2.00	0.44
1:B:374:LEU:HD23	1:B:375:TYR:CE2	2.53	0.44
1:A:596:LYS:HE3	3:A:782:HOH:O	2.16	0.44
1:A:504:GLU:HG2	1:A:549:TRP:CE3	2.53	0.44
1:B:0:HIS:CG	1:B:186:ASP:OD2	2.70	0.44
1:A:14:LYS:HZ1	1:A:86:LEU:CD1	2.25	0.44
1:A:212:VAL:HG13	1:A:230:THR:CB	2.47	0.44
1:A:373:GLU:O	1:A:376:SER:HB2	2.17	0.44
1:A:445:ASN:ND2	1:A:467:ARG:HH22	2.14	0.44
1:B:69:TYR:CD1	1:B:170:ILE:HD12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:HH21	1:B:117:ASP:HB2	1.81	0.44
1:B:205:GLN:NE2	1:B:212:VAL:HG21	2.29	0.44
1:A:43:ARG:HD2	1:A:55:PHE:CD1	2.52	0.44
1:A:138:LEU:CB	1:A:142:THR:HG21	2.47	0.44
1:A:88:PHE:O	1:A:113:PRO:HA	2.18	0.43
1:B:52:ASN:ND2	1:B:168:ALA:H	2.14	0.43
1:B:242:TRP:CE3	1:B:242:TRP:C	2.91	0.43
1:B:288:PHE:HE2	1:B:290:PHE:HA	1.82	0.43
1:B:302:ARG:CZ	1:B:302:ARG:HB3	2.47	0.43
1:A:13:LYS:HE3	1:A:15:LEU:HD22	2.00	0.43
1:B:236:VAL:O	1:B:237:VAL:HG23	2.19	0.43
1:A:77:LYS:H	1:B:10:ARG:HE	1.66	0.43
1:B:198:ASN:CB	1:B:237:VAL:C	2.80	0.43
1:A:111:TYR:CB	1:A:332:PRO:HD2	2.46	0.43
1:A:464:CYS:HA	1:A:501:ILE:O	2.18	0.43
1:B:2:LEU:O	1:B:87:ARG:NH1	2.52	0.43
1:B:276:VAL:HG13	1:B:280:GLN:O	2.18	0.43
1:B:537:PHE:CD1	1:B:546:GLU:HG2	2.54	0.43
1:A:422:ARG:HA	1:A:456:ILE:CD1	2.49	0.43
1:B:85:VAL:O	1:B:177:TYR:CB	2.54	0.43
1:B:422:ARG:HH22	1:B:458:ASP:CG	2.16	0.43
1:A:76:PRO:HA	1:B:10:ARG:CD	2.49	0.43
1:A:193:VAL:HG22	1:A:285:HIS:HE2	1.83	0.43
1:A:229:GLY:O	1:A:231:SER:N	2.52	0.43
1:B:218:ASP:OD1	1:B:219:ALA:N	2.47	0.43
1:B:328:THR:HA	1:B:333:TYR:CE1	2.54	0.43
1:A:13:LYS:O	1:A:174:VAL:O	2.37	0.43
1:A:147:MET:HE3	1:A:161:PHE:HZ	1.84	0.43
1:A:188:THR:HB	1:A:204:TRP:CE3	2.54	0.43
1:A:238:ASN:HB2	3:A:810:HOH:O	2.19	0.43
1:A:361:LEU:HD23	1:A:361:LEU:HA	1.79	0.43
1:B:213:SER:HB3	1:B:255:THR:OG1	2.19	0.43
1:B:426:ALA:HA	1:B:459:LEU:HD13	2.01	0.43
1:A:15:LEU:CD1	1:A:173:SER:CA	2.82	0.43
1:A:77:LYS:CE	1:B:8:PRO:O	2.67	0.43
1:A:204:TRP:HA	1:A:231:SER:O	2.19	0.43
1:B:207:VAL:HG13	1:B:256:ALA:CB	2.49	0.43
1:B:531:ASP:O	1:B:535:ARG:HD3	2.17	0.43
1:B:193:VAL:O	1:B:193:VAL:HG22	2.18	0.42
1:B:290:PHE:HB2	1:B:545:GLY:HA3	1.99	0.42
1:B:99:VAL:HG22	1:B:130:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HD12	1:A:25:ARG:NH1	2.34	0.42
1:A:357:PHE:O	1:A:374:LEU:CD1	2.66	0.42
1:B:33:ARG:HA	1:B:35:TRP:CE3	2.55	0.42
1:A:14:LYS:HD2	1:A:176:LEU:CD2	2.38	0.42
1:A:200:ALA:HB1	1:A:234:LEU:CD2	2.50	0.42
1:A:388:HIS:HD2	1:A:424:TYR:OH	2.02	0.42
1:B:595:GLU:HB3	3:B:676:HOH:O	2.19	0.42
1:B:426:ALA:HB3	1:B:427:PRO:HD3	2.00	0.42
1:A:240:HIS:HB2	1:A:248:TYR:CE2	2.54	0.42
1:B:83:ARG:HB3	1:B:179:THR:HG22	2.02	0.42
1:B:529:TRP:HD1	1:B:530:LEU:N	2.18	0.42
1:A:14:LYS:NZ	1:A:86:LEU:HD11	2.28	0.42
1:A:566:ASN:HD21	1:A:568:LYS:HB2	1.84	0.42
1:B:240:HIS:ND1	1:B:240:HIS:C	2.73	0.42
1:B:447:MET:CG	1:B:467:ARG:HG3	2.48	0.42
1:B:552:ALA:HA	1:B:571:PHE:O	2.19	0.42
1:B:0:HIS:CB	1:B:186:ASP:OD2	2.63	0.41
1:B:242:TRP:O	1:B:242:TRP:HE3	2.03	0.41
1:A:51:PHE:CD1	1:A:51:PHE:C	2.93	0.41
1:A:77:LYS:H	1:B:10:ARG:NE	2.18	0.41
1:B:14:LYS:O	1:B:16:ASP:O	2.37	0.41
1:B:43:ARG:HD3	3:B:616:HOH:O	2.20	0.41
1:B:272:ARG:HH21	1:B:403:PRO:HA	1.85	0.41
1:B:279:GLU:OE2	1:B:493:GLN:CG	2.67	0.41
1:B:467:ARG:HD3	1:B:469:TYR:CE1	2.55	0.41
1:A:199:HIS:CG	1:A:200:ALA:H	2.33	0.41
1:A:207:VAL:HG13	1:A:256:ALA:HB1	2.02	0.41
1:B:21:PHE:HB2	1:B:45:ILE:HG21	2.02	0.41
1:A:93:HIS:CE1	1:A:166:ASN:OD1	2.58	0.41
1:A:193:VAL:C	1:A:199:HIS:HD2	2.23	0.41
1:B:35:TRP:CE3	1:B:98:TRP:CZ2	3.08	0.41
1:A:13:LYS:O	1:A:14:LYS:HB2	2.19	0.41
1:B:11:GLU:OE2	1:B:11:GLU:N	2.54	0.41
1:B:15:LEU:CD1	1:B:173:SER:OG	2.68	0.41
1:B:135:ASN:HD21	1:B:137:GLU:HB2	1.85	0.41
1:B:190:VAL:O	1:B:201:SER:HA	2.21	0.41
1:B:200:ALA:CA	1:B:235:GLN:O	2.59	0.41
1:A:89:ASP:OD2	1:A:173:SER:HB2	2.20	0.41
1:A:192:HIS:HE1	1:A:202:VAL:HG13	1.86	0.41
1:A:21:PHE:HA	1:A:68:TRP:O	2.20	0.41
1:A:194:ALA:HB2	1:A:199:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ASN:HD22	1:A:551:PHE:N	2.19	0.41
1:B:10:ARG:CZ	1:B:79:TRP:NE1	2.83	0.41
1:B:94:TYR:HB3	1:B:135:ASN:HB3	2.02	0.41
1:B:497:HIS:N	3:B:690:HOH:O	2.53	0.41
1:A:39:LEU:N	1:A:70:GLN:OE1	2.50	0.41
1:B:35:TRP:CD1	1:B:101:ASN:HA	2.55	0.41
1:B:237:VAL:CG1	1:B:238:ASN:N	2.83	0.41
1:B:386:GLN:O	1:B:390:GLN:N	2.43	0.41
1:A:2:LEU:HD23	1:A:2:LEU:HA	1.85	0.41
1:A:303:GLY:O	1:A:304:LYS:CG	2.68	0.41
1:A:313:HIS:HD2	1:B:53:ASP:O	2.04	0.41
1:A:566:ASN:HD22	1:A:566:ASN:C	2.24	0.41
1:B:3:ARG:O	1:B:265:TYR:OH	2.29	0.41
1:B:7:THR:HG1	1:B:8:PRO:CD	2.31	0.41
1:B:10:ARG:HB2	1:B:79:TRP:NE1	2.36	0.41
1:B:242:TRP:C	1:B:242:TRP:HE3	2.25	0.41
1:B:259:GLN:H	1:B:259:GLN:HG3	1.58	0.41
1:B:568:LYS:CE	2:B:604:EVA:OXT	2.69	0.41
1:A:105:MET:HE2	1:A:105:MET:HB2	1.68	0.41
1:A:330:HIS:CD2	1:A:330:HIS:N	2.85	0.41
1:A:361:LEU:HD21	1:A:446:VAL:HG21	2.03	0.41
1:A:550:ASN:ND2	1:A:552:ALA:H	2.15	0.41
1:A:587:ARG:HG2	1:A:588:TRP:CD1	2.55	0.41
1:B:7:THR:HG1	1:B:8:PRO:N	2.19	0.40
1:B:183:TRP:HZ3	1:B:185:ASP:CB	2.30	0.40
1:A:73:VAL:HG22	1:A:74:PHE:H	1.86	0.40
1:A:151:ASP:OD2	3:A:835:HOH:O	2.22	0.40
1:A:247:GLY:O	1:A:249:LEU:CD1	2.62	0.40
1:A:105:MET:HE2	1:A:114:PHE:HD1	1.86	0.40
1:B:35:TRP:HD1	1:B:101:ASN:HA	1.85	0.40
1:B:83:ARG:O	1:B:179:THR:N	2.51	0.40
1:B:422:ARG:HA	1:B:456:ILE:HG12	2.03	0.40
1:A:72:GLU:HA	1:A:128:VAL:O	2.22	0.40
1:A:94:TYR:OH	1:A:96:LYS:HE3	2.21	0.40
1:B:35:TRP:HB3	1:B:98:TRP:CE3	2.56	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	592/605 (98%)	568 (96%)	19 (3%)	5 (1%)	19 29
1	B	592/605 (98%)	566 (96%)	23 (4%)	3 (0%)	29 41
All	All	1184/1210 (98%)	1134 (96%)	42 (4%)	8 (1%)	22 32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	B	7	THR
1	B	48	PRO
1	A	304	LYS
1	A	48	PRO
1	A	144	PRO
1	A	238	ASN
1	B	266	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	506/513 (99%)	459 (91%)	47 (9%)	9 13
1	B	506/513 (99%)	446 (88%)	60 (12%)	5 6
All	All	1012/1026 (99%)	905 (89%)	107 (11%)	6 9

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	1	MET
1	A	3	ARG
1	A	5	VAL
1	A	9	THR
1	A	12	ILE
1	A	15	LEU
1	A	43	ARG
1	A	47	VAL
1	A	52	ASN
1	A	71	ARG
1	A	101	ASN
1	A	122	VAL
1	A	157	LYS
1	A	176	LEU
1	A	178	THR
1	A	191	THR
1	A	197	CYS
1	A	199	HIS
1	A	209	ASN
1	A	212	VAL
1	A	230	THR
1	A	233	THR
1	A	258	SER
1	A	268	ARG
1	A	272	ARG
1	A	329	SER
1	A	359	LEU
1	A	383	GLU
1	A	419	GLN
1	A	438	THR
1	A	441	ILE
1	A	453	THR
1	A	473	VAL
1	A	478	LEU
1	A	480	THR
1	A	510	LEU
1	A	513	LEU
1	A	518	THR
1	A	531	ASP
1	A	535	ARG
1	A	544	VAL
1	A	550	ASN

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Mol	Chain	Res	Type
1	A	560	ILE
1	A	566	ASN
1	A	585	GLN
1	A	598	GLN
1	B	3	ARG
1	B	9	THR
1	B	11	GLU
1	B	15	LEU
1	B	41	GLU
1	B	43	ARG
1	B	47	VAL
1	B	71	ARG
1	B	82	GLN
1	B	83	ARG
1	B	89	ASP
1	B	101	ASN
1	B	141	GLN
1	B	142	THR
1	B	148	VAL
1	B	157	LYS
1	B	172	ARG
1	B	174	VAL
1	B	176	LEU
1	B	177	TYR
1	B	178	THR
1	B	179	THR
1	B	186	ASP
1	B	193	VAL
1	B	196	ASP
1	B	197	CYS
1	B	201	SER
1	B	202	VAL
1	B	207	VAL
1	B	209	ASN
1	B	222	GLN
1	B	234	LEU
1	B	237	VAL
1	B	238	ASN
1	B	242	TRP
1	B	246	GLU
1	B	257	LYS
1	B	259	GLN

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Mol	Chain	Res	Type
1	B	273	SER
1	B	298	ASP
1	B	302	ARG
1	B	335	GLU
1	B	352	THR
1	B	359	LEU
1	B	372	LYS
1	B	453	THR
1	B	456	ILE
1	B	457	SER
1	B	459	LEU
1	B	467	ARG
1	B	478	LEU
1	B	487	LYS
1	B	503	THR
1	B	513	LEU
1	B	518	THR
1	B	529	TRP
1	B	531	ASP
1	B	535	ARG
1	B	541	SER
1	B	586	LYS

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

Mol	Chain	Res	Type
1	A	0	HIS
1	A	52	ASN
1	A	54	GLN
1	A	66	ASN
1	A	93	HIS
1	A	100	ASN
1	A	101	ASN
1	A	102	GLN
1	A	107	HIS
1	A	135	ASN
1	A	192	HIS
1	A	205	GLN
1	A	235	GLN
1	A	243	GLN
1	A	280	GLN
1	A	284	ASN

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Mol	Chain	Res	Type
1	A	313	HIS
1	A	330	HIS
1	A	388	HIS
1	A	401	ASN
1	A	445	ASN
1	A	550	ASN
1	A	566	ASN
1	A	599	GLN
1	B	0	HIS
1	B	52	ASN
1	B	54	GLN
1	B	66	ASN
1	B	93	HIS
1	B	101	ASN
1	B	107	HIS
1	B	135	ASN
1	B	181	ASN
1	B	192	HIS
1	B	195	GLN
1	B	205	GLN
1	B	209	ASN
1	B	222	GLN
1	B	235	GLN
1	B	238	ASN
1	B	243	GLN
1	B	284	ASN
1	B	313	HIS
1	B	330	HIS
1	B	385	GLN
1	B	401	ASN
1	B	412	ASN
1	B	445	ASN
1	B	498	GLN
1	B	534	HIS
1	B	550	ASN
1	B	585	GLN
1	B	598	GLN

5.3.3 RNA

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)

2 ligands are modelled in this entry.

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	EVA	A	604	-	13,13,13	0.88	1 (7%)	13,19,19	1.45	1 (7%)
2	EVA	B	604	-	13,13,13	2.01	2 (15%)	13,19,19	1.73	4 (30%)

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	EVA	A	604	-	-	2/3/24/24	0/1/1/1
2	EVA	B	604	-	-	1/3/24/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	604	EVA	CAE-N	6.13	1.43	1.33
2	A	604	EVA	OXT-C	-2.51	1.22	1.30
2	B	604	EVA	CA-N	2.07	1.48	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	604	EVA	OAK-CAE-N	-3.85	117.51	122.69
2	A	604	EVA	OAK-CAE-N	-3.52	117.96	122.69
2	B	604	EVA	OD2-CG-CD1	-2.45	105.01	109.68
2	B	604	EVA	CD1-CAE-N	2.34	123.53	117.93
2	B	604	EVA	OAJ-CD1-CG	-2.12	106.15	110.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	604	EVA	O-C-CA-N
2	B	604	EVA	O-C-CA-N
2	A	604	EVA	OXT-C-CA-CB

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	EVA	2	0
2	B	604	EVA	3	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	596/605 (98%)	0.32	39 (6%) 18 17	19, 46, 107, 127	0
1	B	596/605 (98%)	0.83	78 (13%) 3 3	26, 87, 178, 207	0
All	All	1192/1210 (98%)	0.58	117 (9%) 7 7	19, 67, 152, 207	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	VAL	10.5
1	A	207	VAL	8.7
1	A	303	GLY	8.5
1	B	601	GLY	7.9
1	B	230	THR	7.5
1	B	204	TRP	7.5
1	B	545	GLY	6.9
1	B	8	PRO	6.8
1	B	600	GLY	6.6
1	B	282	LEU	6.4
1	B	213	SER	6.2
1	A	199	HIS	6.1
1	B	425	PHE	5.6
1	B	229	GLY	5.3
1	B	208	ALA	5.2
1	B	212	VAL	5.0
1	A	208	ALA	4.4
1	A	209	ASN	4.3
1	A	230	THR	4.3
1	A	204	TRP	4.2
1	B	357	PHE	4.2
1	A	256	ALA	4.1
1	A	15	LEU	4.0
1	B	205	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	214	VAL	3.9
1	B	196	ASP	3.7
1	B	409	SER	3.7
1	B	239	PRO	3.7
1	B	209	ASN	3.7
1	B	7	THR	3.6
1	B	190	VAL	3.6
1	B	252	LEU	3.5
1	A	8	PRO	3.5
1	A	302	ARG	3.5
1	B	216	LEU	3.4
1	B	265	TYR	3.4
1	B	260	THR	3.4
1	B	271	ILE	3.4
1	B	79	TRP	3.3
1	A	260	THR	3.3
1	B	289	TYR	3.2
1	A	7	THR	3.2
1	B	231	SER	3.2
1	B	262	CYS	3.1
1	B	311	MET	3.1
1	B	463	LEU	3.1
1	A	18	LEU	3.1
1	B	235	GLN	3.0
1	B	598	GLN	3.0
1	B	199	HIS	3.0
1	B	288	PHE	3.0
1	A	37	SER	2.9
1	A	229	GLY	2.9
1	B	410	ILE	2.9
1	B	537	PHE	2.9
1	B	465	LEU	2.9
1	A	235	GLN	2.8
1	A	17	GLY	2.8
1	B	152	GLU	2.8
1	B	277	LYS	2.8
1	B	597	PRO	2.8
1	B	261	GLU	2.8
1	A	212	VAL	2.8
1	B	153	ASN	2.8
1	A	98	TRP	2.7
1	A	29	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	379	ALA	2.6
1	B	587	ARG	2.6
1	A	214	VAL	2.6
1	B	211	ASP	2.5
1	B	309	VAL	2.5
1	A	16	ASP	2.5
1	A	123	ILE	2.5
1	A	236	VAL	2.4
1	B	380	VAL	2.4
1	B	266	PRO	2.4
1	B	0	HIS	2.4
1	B	264	ILE	2.4
1	B	259	GLN	2.4
1	B	274	VAL	2.4
1	B	240	HIS	2.4
1	A	233	THR	2.4
1	B	290	PHE	2.4
1	B	75	ILE	2.3
1	A	257	LYS	2.3
1	A	252	LEU	2.3
1	B	591	MET	2.3
1	B	253	CYS	2.3
1	A	329	SER	2.3
1	A	217	ARG	2.3
1	B	123	ILE	2.3
1	B	599	GLN	2.2
1	B	494	GLU	2.2
1	A	216	LEU	2.2
1	B	201	SER	2.2
1	B	226	THR	2.2
1	A	264	ILE	2.2
1	B	25	ARG	2.2
1	B	248	TYR	2.1
1	B	501	ILE	2.1
1	A	262	CYS	2.1
1	A	600	GLY	2.1
1	B	236	VAL	2.1
1	B	543	VAL	2.1
1	A	601	GLY	2.1
1	B	37	SER	2.1
1	B	245	GLY	2.1
1	B	596	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	200	ALA	2.1
1	A	48	PRO	2.1
1	B	206	VAL	2.1
1	B	227	GLY	2.1
1	B	310	LEU	2.0
1	A	318	MET	2.0
1	A	79	TRP	2.0
1	B	256	ALA	2.0
1	B	15	LEU	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, 95^{th} 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
2	EVA	B	604	13/13	0.89	0.16	22,23,29,30	0
2	EVA	A	604	13/13	0.95	0.15	20,21,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.