Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 08:47 pm BST

PDB ID	:	3NZP
Title	:	Crystal Structure of the Biosynthetic Arginine decarboxylase SpeA from Campylobacter jejuni, Northeast Structural Genomics Consortium Target BR53
Authors	:	Forouhar, F.; Lew, S.; Seetharaman, J.; Sahdev, S.; Xiao, R.; Ciccosanti, C.; Belote, R.L.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2010-07-16
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

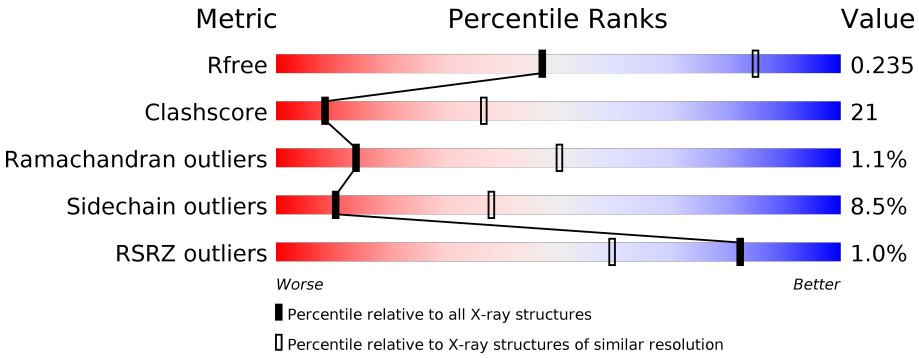
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	619	% 55% 35% · 6%
1	B	619	% 55% 36% 5% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9685 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.

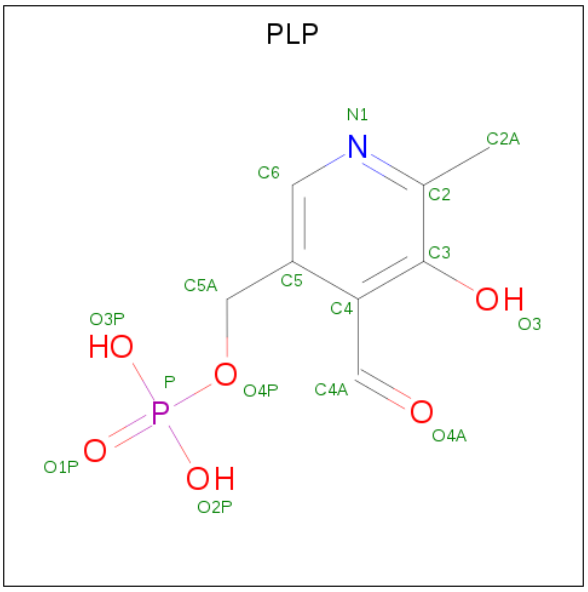
- Molecule 1 is a protein called Arginine decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	Se	0	0	0
			4701	3035	773	881	2	10			
1	B	591	Total	C	N	O	S	Se	0	0	0
			4775	3081	793	889	2	10			

There are 16 discrepancies between the modelled and reference sequences:

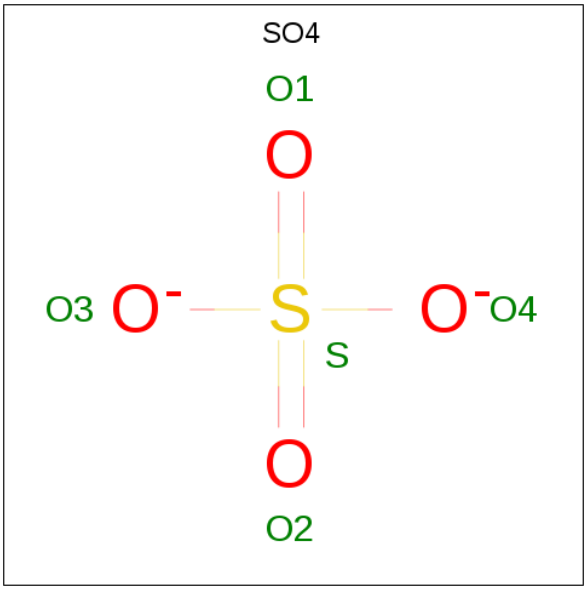
Chain	Residue	Modelled	Actual	Comment	Reference
A	612	LEU	-	expression tag	UNP Q0PAC6
A	613	GLU	-	expression tag	UNP Q0PAC6
A	614	HIS	-	expression tag	UNP Q0PAC6
A	615	HIS	-	expression tag	UNP Q0PAC6
A	616	HIS	-	expression tag	UNP Q0PAC6
A	617	HIS	-	expression tag	UNP Q0PAC6
A	618	HIS	-	expression tag	UNP Q0PAC6
A	619	HIS	-	expression tag	UNP Q0PAC6
B	612	LEU	-	expression tag	UNP Q0PAC6
B	613	GLU	-	expression tag	UNP Q0PAC6
B	614	HIS	-	expression tag	UNP Q0PAC6
B	615	HIS	-	expression tag	UNP Q0PAC6
B	616	HIS	-	expression tag	UNP Q0PAC6
B	617	HIS	-	expression tag	UNP Q0PAC6
B	618	HIS	-	expression tag	UNP Q0PAC6
B	619	HIS	-	expression tag	UNP Q0PAC6

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

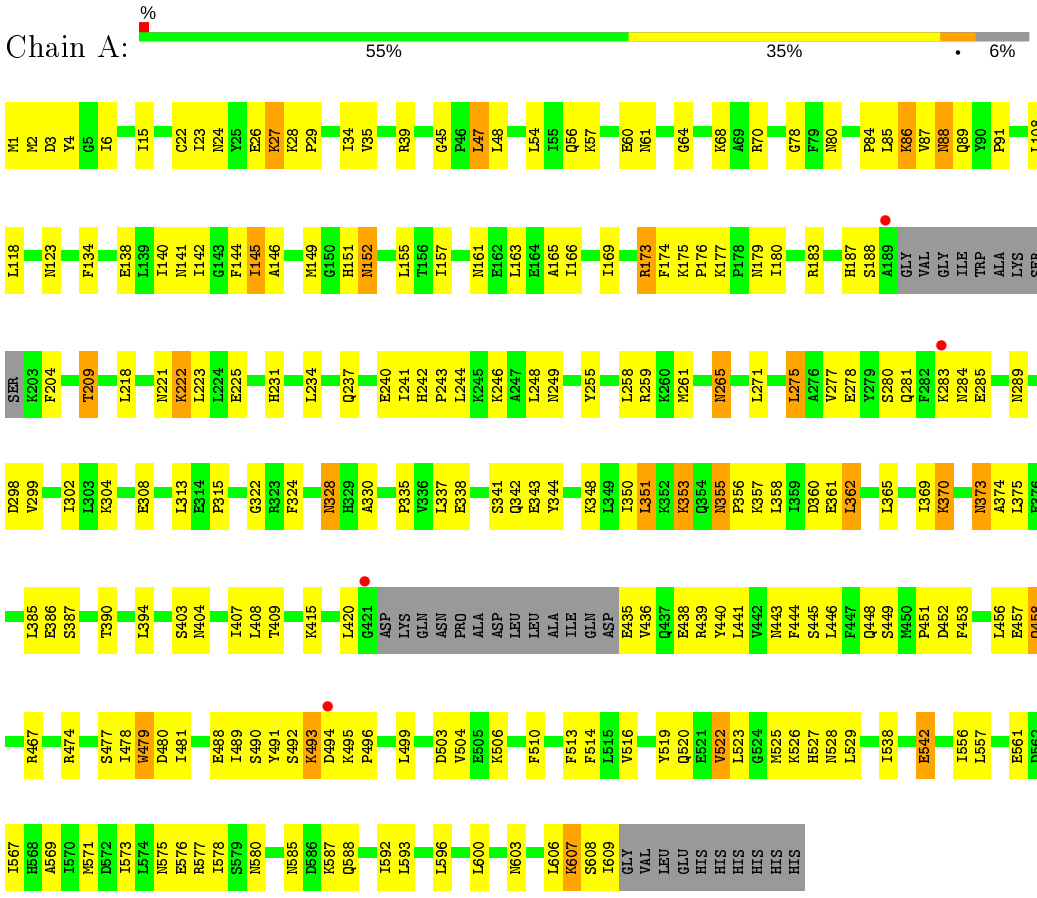
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	93	Total O 93 93	0	0
4	B	71	Total O 71 71	0	0

3 Residue-property plots (i)

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

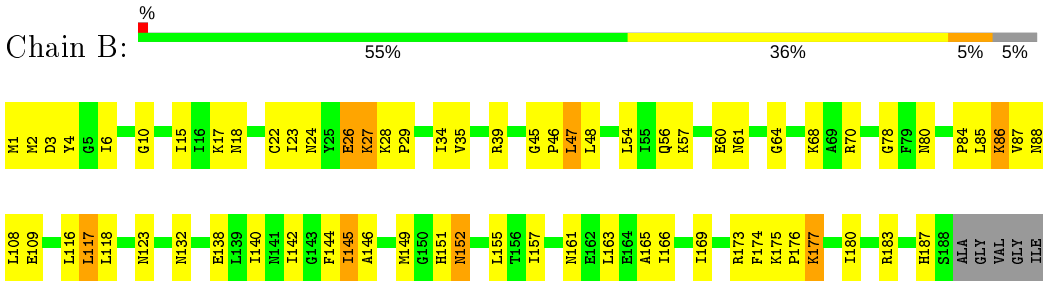
- Molecule 1: Arginine decarboxylase

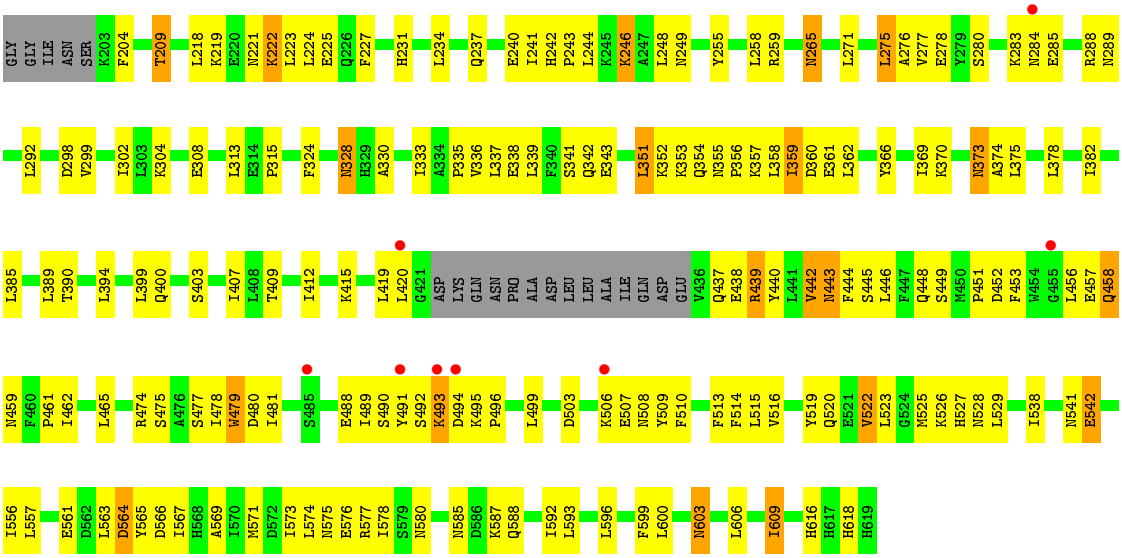
Chain A:



- Molecule 1: Arginine decarboxylase

Chain B:




GLY GLY ILE ASN SER K203 F204 T209 L218 K219 E220 N221 K222 L223 L224 E225 Q226 F227 H231 L234 Q237 E240 I241 H242 P243 L244 K245 K246 A247 L248 N249 Y255 L258 R259 N265 L271 L275 A276 V277 E278 Y279 S280 K283 N284 E285 R288 N289
L292 D298 V299 I302 L303 K304 E308 L313 E314 P315 F324 N328 H329 A330 I333 A334 P335 V336 L337 E338 L339 F340 S341 Q342 E343 L351 K352 K353 Q354 N355 P356 K357 L358 I359 D360 E361 L362 Y366 I369 K370 N373 A374 L375 L378 I382
L385 L389 T390 L394 L399 Q400 S403 I407 L408 T409 I412 K415 L419 L420 G421 ASP LYS GLN ASN PRO ALA ASP LEU LEU ALA ILE GLN ASP GLU V436 Q437 E438 R439 Y440 L441 V442 N443 F444 S445 L446 F447 Q448 S449 N450 P451 D452 F453 W454 G455 L456 E457 Q458
N459 F460 P461 I462 L465 R474 S475 A476 S477 I478 W479 D480 I481 S485 E488 I489 S490 Y491 S492 K493 D494 K495 P496 L499 D503 K506 E507 N508 Y509 F510 F513 F514 L515 V516 Y519 Q520 E521 V522 L523 G524 M525 K526 H527 N528 L529 I538 N541 E542
I556 L557 E561 D562 L563 D564 Y565 D566 I567 H568 A569 I570 M571 D572 I573 L574 N575 E576 R577 I578 S579 N580 N585 D586 K587 Q588 I592 L593 L596 F599 L600 N603 L606 I609 H616 H617 H618 H619

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	203.07Å 203.07Å 101.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 3.00 29.37 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.6 (19.96-3.00) 97.5 (29.37-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.76 (at 3.00Å)	Xtriage
Refinement program	REFMAC, CNS 1.2	Depositor
R, R_{free}	0.180 , 0.219 0.197 , 0.235	Depositor DCC
R_{free} test set	9166 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 64.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9685	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: SO4, PLP

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	0.44	0/4784	0.58	0/6440
1	B	0.44	0/4864	0.58	0/6549
All	All	0.44	0/9648	0.58	0/12989

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4701	0	4734	201	0
1	B	4775	0	4794	214	0
2	A	15	0	7	2	0
2	B	15	0	7	2	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	A	93	0	0	4	0
4	B	71	0	0	3	0
All	All	9685	0	9542	392	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 21.

All (392) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ASN:HB3	1:B:359:ILE:HD11	1.26	1.10
1:B:370:LYS:H	1:B:373:ASN:HD21	1.01	1.00
1:A:353:LYS:HD3	1:A:353:LYS:H	1.30	0.95
1:A:2:MSE:HE2	1:A:4:TYR:H	1.33	0.94
1:A:1:MSE:HG2	1:A:2:MSE:H	1.33	0.94
1:A:567:ILE:HG22	1:A:571:MSE:HE2	1.52	0.92
1:B:1:MSE:HG2	1:B:2:MSE:H	1.35	0.91
1:B:2:MSE:HE2	1:B:4:TYR:H	1.35	0.91
1:B:567:ILE:HG22	1:B:571:MSE:HE2	1.53	0.91
1:B:26:GLU:HG2	1:B:542:GLU:HA	1.56	0.85
1:B:359:ILE:HD13	1:B:360:ASP:N	1.92	0.85
1:B:370:LYS:N	1:B:373:ASN:HD21	1.75	0.84
1:A:27:LYS:HE2	1:A:542:GLU:O	1.79	0.82
1:A:561:GLU:HB2	1:A:567:ILE:HD11	1.61	0.82
1:B:370:LYS:H	1:B:373:ASN:ND2	1.78	0.82
1:A:26:GLU:HG2	1:A:542:GLU:HA	1.61	0.82
1:B:27:LYS:HE2	1:B:542:GLU:O	1.80	0.81
1:B:561:GLU:HB2	1:B:567:ILE:HD11	1.61	0.81
1:A:237:GLN:HE22	1:A:277:VAL:H	1.31	0.79
1:A:355:ASN:H	1:A:355:ASN:ND2	1.84	0.76
1:A:241:ILE:HD12	1:A:244:LEU:HD12	1.69	0.74
1:B:569:ALA:O	1:B:573:ILE:HG22	1.88	0.74
1:B:355:ASN:HB3	1:B:359:ILE:CD1	2.15	0.73
1:A:569:ALA:O	1:A:573:ILE:HG22	1.90	0.72
1:B:241:ILE:HD12	1:B:244:LEU:HD12	1.72	0.72
1:B:237:GLN:HE22	1:B:277:VAL:H	1.38	0.71
1:A:522:VAL:HG23	1:A:523:LEU:HD13	1.73	0.70
1:B:234:LEU:HD12	1:B:244:LEU:HD23	1.73	0.70
1:B:352:LYS:HB3	1:B:355:ASN:ND2	2.06	0.70
1:A:355:ASN:H	1:A:355:ASN:HD22	1.37	0.70
1:A:234:LEU:HD12	1:A:244:LEU:HD23	1.74	0.70
1:A:493:LYS:HE3	1:A:493:LYS:N	2.06	0.70
1:B:522:VAL:HG23	1:B:523:LEU:HD13	1.72	0.70
1:B:446:LEU:HD21	1:B:489:ILE:HD11	1.74	0.70
1:A:259:ARG:HH12	1:A:313:LEU:HD23	1.56	0.69
1:B:356:PRO:HG2	1:B:359:ILE:HG23	1.75	0.69
1:B:175:LYS:HB3	1:B:176:PRO:HD3	1.75	0.68
1:A:446:LEU:HD21	1:A:489:ILE:HD11	1.73	0.68
1:A:84:PRO:HA	1:A:109:GLU:HB3	1.74	0.68
1:B:259:ARG:HH12	1:B:313:LEU:HD23	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LYS:O	1:A:361:GLU:HG3	1.94	0.67
1:B:529:LEU:HD21	1:B:563:LEU:HD11	1.76	0.67
1:A:338:GLU:HA	1:A:504:VAL:HG11	1.77	0.66
1:A:1:MSE:HG2	1:A:2:MSE:N	2.08	0.66
1:B:84:PRO:HA	1:B:109:GLU:HB3	1.76	0.66
1:B:493:LYS:N	1:B:493:LYS:HE3	2.11	0.66
4:A:650:HOH:O	1:B:599:PHE:HB3	1.95	0.66
1:A:525:MSE:O	1:A:526:LYS:HB3	1.96	0.66
1:B:440:TYR:HB2	1:B:478:ILE:HG22	1.78	0.65
1:A:353:LYS:N	1:A:353:LYS:HD3	2.08	0.65
1:A:175:LYS:HB3	1:A:176:PRO:HD3	1.77	0.65
1:A:445:SER:HB3	1:A:448:GLN:HB3	1.79	0.65
1:A:2:MSE:HE2	1:A:4:TYR:N	2.10	0.65
1:B:462:ILE:HD13	1:B:478:ILE:HD11	1.78	0.64
1:A:240:GLU:HA	1:A:289:ASN:HD21	1.62	0.64
1:B:240:GLU:HA	1:B:289:ASN:HD21	1.60	0.64
1:A:362:LEU:HB3	1:A:408:LEU:HD13	1.80	0.64
1:A:462:ILE:HD13	1:A:478:ILE:HD11	1.78	0.64
1:B:526:LYS:HE3	4:B:688:HOH:O	1.96	0.64
1:A:529:LEU:HD21	1:A:563:LEU:HD11	1.79	0.64
1:B:444:PHE:O	1:B:480:ASP:HB2	1.98	0.64
1:A:440:TYR:HB2	1:A:478:ILE:HG22	1.79	0.64
1:A:525:MSE:HE3	1:B:523:LEU:HG	1.78	0.64
1:B:492:SER:HB3	1:B:495:LYS:HB2	1.80	0.63
1:B:525:MSE:O	1:B:526:LYS:HB3	1.97	0.63
1:B:445:SER:HB3	1:B:448:GLN:HB3	1.79	0.63
1:B:609:ILE:HD13	1:B:609:ILE:N	2.14	0.63
1:B:369:ILE:HG21	1:B:415:LYS:HD3	1.81	0.62
1:B:15:ILE:HB	1:B:24:ASN:HD22	1.64	0.62
1:A:117:LEU:HD23	1:B:556:ILE:HD13	1.80	0.62
1:A:492:SER:HB3	1:A:495:LYS:HB2	1.81	0.62
1:B:452:ASP:HB2	1:B:520:GLN:HE22	1.64	0.62
1:A:222:LYS:HE2	1:A:222:LYS:HA	1.81	0.62
1:A:15:ILE:HB	1:A:24:ASN:HD22	1.65	0.61
1:B:222:LYS:HE2	1:B:222:LYS:HA	1.80	0.61
1:A:369:ILE:HD11	1:A:374:ALA:HA	1.82	0.61
1:A:341:SER:HB3	1:A:438:GLU:HG2	1.81	0.61
1:A:608:SER:O	1:A:609:ILE:HD13	1.99	0.61
1:B:240:GLU:HA	1:B:289:ASN:ND2	2.16	0.61
1:A:163:LEU:HD11	1:A:218:LEU:HD21	1.83	0.61
1:A:145:ILE:HD11	1:B:596:LEU:HD13	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MSE:HG2	1:B:2:MSE:N	2.10	0.60
1:A:108:LEU:HD12	1:A:123:ASN:HB2	1.83	0.60
1:A:225:GLU:HA	1:A:265:ASN:HD22	1.66	0.60
1:A:596:LEU:HD13	1:B:145:ILE:HD11	1.83	0.60
1:B:2:MSE:HE2	1:B:4:TYR:N	2.12	0.60
1:B:373:ASN:C	1:B:373:ASN:HD22	2.04	0.60
1:A:585:ASN:OD1	1:A:588:GLN:HG3	2.01	0.60
1:B:479:TRP:HB3	1:B:488:GLU:HB2	1.83	0.60
1:A:278:GLU:OE2	1:A:280:SER:HB3	2.02	0.60
1:A:452:ASP:HB2	1:A:520:GLN:HE22	1.65	0.60
1:A:355:ASN:ND2	1:A:355:ASN:N	2.45	0.60
1:B:298:ASP:O	1:B:302:ILE:HG12	2.01	0.60
1:A:444:PHE:O	1:A:480:ASP:HB2	2.02	0.59
1:A:259:ARG:NH1	1:A:313:LEU:HD23	2.17	0.59
1:B:585:ASN:OD1	1:B:588:GLN:HG3	2.02	0.59
1:A:479:TRP:HB3	1:A:488:GLU:HB2	1.83	0.59
1:B:437:GLN:HG3	1:B:475:SER:H	1.67	0.59
1:A:503:ASP:HB3	1:A:506:LYS:HB3	1.85	0.58
1:A:240:GLU:HA	1:A:289:ASN:ND2	2.18	0.58
1:A:563:LEU:O	1:A:564:ASP:HB2	2.04	0.58
1:B:442:VAL:HB	1:B:444:PHE:CD1	2.39	0.58
1:B:578:ILE:HD11	1:B:596:LEU:HD22	1.86	0.58
1:B:259:ARG:NH1	1:B:313:LEU:HD23	2.18	0.58
1:B:341:SER:HB2	1:B:438:GLU:HG2	1.85	0.58
1:B:336:VAL:HG23	1:B:509:TYR:O	2.03	0.58
1:B:503:ASP:HB3	1:B:506:LYS:HB3	1.86	0.58
1:A:556:ILE:HD13	1:B:117:LEU:HD23	1.86	0.57
1:B:117:LEU:HD13	1:B:142:ILE:HD11	1.85	0.57
1:A:382:ILE:O	1:A:386:GLU:HG2	2.04	0.57
1:A:146:ALA:O	1:A:151:HIS:HB2	2.05	0.57
1:A:403:SER:OG	1:B:209:THR:HB	2.04	0.57
1:B:225:GLU:HA	1:B:265:ASN:HD22	1.68	0.57
4:A:697:HOH:O	1:B:523:LEU:HD21	2.04	0.57
1:B:22:CYS:HB3	1:B:29:PRO:O	2.04	0.56
1:B:163:LEU:HD11	1:B:218:LEU:HD21	1.87	0.56
1:A:373:ASN:C	1:A:373:ASN:HD22	2.09	0.56
1:A:174:PHE:HE2	1:B:592:ILE:HD11	1.71	0.56
1:A:157:ILE:HD11	1:A:166:ILE:HD12	1.86	0.56
1:A:525:MSE:CE	1:B:523:LEU:HG	2.35	0.56
1:B:108:LEU:HD12	1:B:123:ASN:HB2	1.88	0.56
1:B:481:ILE:HD12	1:B:606:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ILE:HD11	1:A:596:LEU:HD22	1.86	0.56
1:B:390:THR:O	1:B:394:LEU:HD13	2.06	0.56
1:B:157:ILE:HD11	1:B:166:ILE:HD12	1.88	0.56
1:B:609:ILE:HD13	1:B:609:ILE:H	1.69	0.56
1:A:248:LEU:CD2	1:A:299:VAL:HA	2.35	0.55
1:A:342:GLN:HB3	1:A:344:TYR:CD2	2.41	0.55
1:B:146:ALA:O	1:B:151:HIS:HB2	2.06	0.55
1:A:452:ASP:O	1:A:458:GLN:HB3	2.07	0.55
1:A:375:LEU:HD13	1:A:375:LEU:O	2.07	0.55
1:B:563:LEU:O	1:B:564:ASP:HB2	2.06	0.55
1:B:248:LEU:CD2	1:B:299:VAL:HA	2.35	0.55
1:A:523:LEU:HG	1:B:525:MSE:HE3	1.88	0.55
1:B:616:HIS:O	1:B:618:HIS:HD2	1.90	0.55
1:A:344:TYR:HD1	1:A:407:ILE:HD13	1.71	0.55
1:B:278:GLU:OE2	1:B:280:SER:HB3	2.07	0.55
1:A:149:MSE:HE2	1:B:578:ILE:HG12	1.89	0.55
1:A:209:THR:HB	1:B:403:SER:OG	2.07	0.55
1:B:452:ASP:O	1:B:458:GLN:HB3	2.07	0.54
1:B:26:GLU:CG	1:B:542:GLU:HA	2.34	0.54
1:A:298:ASP:O	1:A:302:ILE:HG12	2.06	0.54
1:A:370:LYS:N	1:A:373:ASN:HD21	2.05	0.54
1:A:477:SER:HB2	1:A:490:SER:HA	1.90	0.54
1:A:603:ASN:H	1:A:603:ASN:HD22	1.56	0.54
1:B:56:GLN:O	1:B:60:GLU:HG2	2.08	0.54
1:A:355:ASN:HD22	1:A:355:ASN:N	2.01	0.54
1:B:369:ILE:HD11	1:B:374:ALA:HA	1.89	0.54
1:B:403:SER:O	1:B:407:ILE:HG13	2.08	0.54
1:A:86:LYS:HE3	1:B:528:ASN:HD21	1.71	0.54
1:A:608:SER:C	1:A:609:ILE:HD13	2.29	0.54
1:A:117:LEU:HD13	1:A:142:ILE:HD11	1.91	0.53
1:A:378:LEU:O	1:A:382:ILE:HG12	2.09	0.53
1:B:144:PHE:CD2	1:B:169:ILE:HD11	2.44	0.53
1:B:140:ILE:HG22	1:B:169:ILE:HD11	1.90	0.53
1:A:144:PHE:CD2	1:A:169:ILE:HD11	2.44	0.53
1:A:526:LYS:O	1:A:526:LYS:HG2	2.09	0.53
1:B:359:ILE:HD13	1:B:360:ASP:H	1.68	0.53
1:A:370:LYS:H	1:A:373:ASN:HD21	1.57	0.53
1:B:242:HIS:N	1:B:243:PRO:HD2	2.24	0.53
1:A:255:TYR:CZ	1:A:315:PRO:HB3	2.44	0.53
1:A:351:LEU:HD22	1:A:351:LEU:H	1.74	0.53
1:A:578:ILE:HG12	1:B:149:MSE:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:SER:HB2	1:B:490:SER:HA	1.91	0.53
1:B:603:ASN:HD22	1:B:603:ASN:H	1.57	0.53
1:A:157:ILE:HD13	1:A:180:ILE:HG23	1.91	0.52
1:A:461:PRO:HG2	1:A:514:PHE:HB2	1.92	0.52
1:A:242:HIS:N	1:A:243:PRO:HD2	2.25	0.52
1:A:35:VAL:O	1:A:39:ARG:HG3	2.08	0.52
1:B:23:ILE:O	1:B:28:LYS:HA	2.09	0.52
1:A:34:ILE:HD13	1:A:538:ILE:HG21	1.92	0.52
1:B:138:GLU:O	1:B:142:ILE:HG22	2.10	0.52
1:A:435:GLU:HG2	1:A:436:VAL:H	1.74	0.52
1:B:453:PHE:CE2	1:B:489:ILE:HG12	2.44	0.52
1:A:481:ILE:HG21	1:A:606:LEU:HD22	1.91	0.52
1:B:157:ILE:HD13	1:B:180:ILE:HG23	1.92	0.52
1:B:341:SER:CB	1:B:438:GLU:HG2	2.40	0.52
1:A:259:ARG:HH12	1:A:313:LEU:CD2	2.23	0.52
1:A:56:GLN:O	1:A:60:GLU:HG2	2.10	0.52
1:B:35:VAL:O	1:B:39:ARG:HG3	2.10	0.52
1:B:259:ARG:HH12	1:B:313:LEU:CD2	2.23	0.51
1:A:261:MSE:HE1	1:B:399:LEU:HD23	1.92	0.51
1:A:134:PHE:O	1:B:606:LEU:HD21	2.10	0.51
1:A:390:THR:O	1:A:394:LEU:HD13	2.09	0.51
1:B:442:VAL:HB	1:B:444:PHE:CE1	2.46	0.51
1:B:333:ILE:HG12	1:B:465:LEU:HD21	1.93	0.51
1:B:461:PRO:HG2	1:B:514:PHE:HB2	1.91	0.51
1:B:491:TYR:CE1	1:B:496:PRO:HA	2.46	0.51
1:A:22:CYS:HB3	1:A:29:PRO:O	2.11	0.51
1:A:528:ASN:HD21	1:B:86:LYS:HE3	1.76	0.51
1:A:140:ILE:HG22	1:A:169:ILE:HD11	1.93	0.51
1:B:439:ARG:HG2	1:B:479:TRP:CZ3	2.46	0.50
1:B:54:LEU:HD23	1:B:328:ASN:O	2.10	0.50
1:B:557:LEU:HD13	1:B:600:LEU:HG	1.92	0.50
1:A:403:SER:O	1:A:407:ILE:HG12	2.12	0.50
1:B:255:TYR:CZ	1:B:315:PRO:HB3	2.45	0.50
1:A:283:LYS:HG2	1:A:284:ASN:OD1	2.12	0.50
1:A:23:ILE:O	1:A:28:LYS:HA	2.12	0.50
1:B:449:SER:O	1:B:520:GLN:HB3	2.11	0.50
1:A:335:PRO:HB3	1:A:510:PHE:CE2	2.46	0.50
1:B:609:ILE:CD1	1:B:609:ILE:H	2.20	0.50
1:A:237:GLN:NE2	1:A:277:VAL:H	2.06	0.50
1:A:557:LEU:HD13	1:A:600:LEU:HG	1.93	0.50
1:B:357:LYS:O	1:B:361:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:LYS:O	1:B:419:LEU:HD13	2.12	0.50
1:B:516:VAL:HG23	1:B:520:GLN:HG3	1.94	0.50
1:A:491:TYR:CE1	1:A:496:PRO:HA	2.47	0.50
1:A:565:TYR:CE1	1:B:91:PRO:HB3	2.47	0.49
1:A:138:GLU:O	1:A:142:ILE:HG22	2.12	0.49
1:A:54:LEU:HD23	1:A:328:ASN:O	2.11	0.49
1:B:452:ASP:HB2	1:B:520:GLN:NE2	2.27	0.49
1:A:566:ASP:HB3	1:A:569:ALA:HB3	1.93	0.49
1:A:357:LYS:HA	1:A:360:ASP:HB2	1.94	0.49
1:B:375:LEU:HD13	1:B:375:LEU:O	2.11	0.49
1:A:523:LEU:HG	1:B:525:MSE:CE	2.43	0.49
1:B:588:GLN:O	1:B:592:ILE:HG12	2.12	0.49
1:A:449:SER:O	1:A:520:GLN:HB3	2.13	0.49
1:A:453:PHE:CE2	1:A:489:ILE:HG12	2.47	0.49
1:A:561:GLU:HG3	4:A:680:HOH:O	2.13	0.49
1:B:448:GLN:HE21	1:B:526:LYS:HA	1.78	0.49
1:A:448:GLN:HE21	1:A:526:LYS:HA	1.78	0.49
1:B:335:PRO:HB3	1:B:510:PHE:CE2	2.48	0.49
1:B:526:LYS:O	1:B:526:LYS:HG2	2.12	0.49
1:A:183:ARG:NH2	1:A:204:PHE:HB2	2.28	0.49
1:A:355:ASN:HB2	1:A:356:PRO:HD2	1.95	0.49
1:A:353:LYS:CD	1:A:353:LYS:H	2.14	0.48
1:A:526:LYS:HE2	1:A:526:LYS:HB3	1.62	0.48
1:B:222:LYS:NZ	1:B:225:GLU:HG2	2.28	0.48
1:B:481:ILE:HG13	1:B:481:ILE:O	2.14	0.48
1:A:343:GLU:HB2	1:A:348:LYS:HE3	1.94	0.48
1:A:481:ILE:O	1:A:481:ILE:HG13	2.12	0.48
1:B:359:ILE:HD13	1:B:359:ILE:C	2.33	0.48
1:A:592:ILE:HD11	1:B:174:PHE:HE2	1.78	0.48
1:A:87:VAL:HG12	1:A:519:TYR:CZ	2.49	0.48
1:B:575:ASN:OD1	1:B:593:LEU:HD21	2.14	0.48
1:B:474:ARG:HB2	1:B:499:LEU:O	2.13	0.48
1:A:573:ILE:HD11	1:A:577:ARG:NE	2.28	0.48
1:B:275:LEU:HD13	1:B:324:PHE:CG	2.49	0.48
1:B:26:GLU:HG2	1:B:541:ASN:O	2.13	0.48
1:B:87:VAL:HG12	1:B:519:TYR:CZ	2.48	0.48
1:A:248:LEU:HD21	1:A:299:VAL:HA	1.96	0.48
1:A:453:PHE:CZ	1:A:489:ILE:HG23	2.49	0.48
1:A:45:GLY:O	1:A:47:LEU:HD23	2.14	0.47
1:A:474:ARG:HB2	1:A:499:LEU:O	2.14	0.47
1:B:378:LEU:O	1:B:382:ILE:HG12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:NZ	1:A:225:GLU:HG2	2.29	0.47
1:A:275:LEU:HD13	1:A:324:PHE:CG	2.48	0.47
1:A:358:LEU:HD11	1:A:387:SER:HB3	1.96	0.47
1:A:452:ASP:HB2	1:A:520:GLN:NE2	2.28	0.47
1:B:352:LYS:HB3	1:B:355:ASN:CG	2.35	0.47
1:A:344:TYR:CD1	1:A:407:ILE:HD13	2.50	0.47
1:B:283:LYS:HG2	1:B:284:ASN:OD1	2.13	0.47
1:B:70:ARG:NH2	1:B:78:GLY:HA2	2.30	0.47
1:A:607:LYS:HB2	1:A:607:LYS:NZ	2.30	0.47
1:B:452:ASP:CB	1:B:520:GLN:HE22	2.28	0.47
1:A:149:MSE:HE2	1:B:578:ILE:CG1	2.45	0.47
1:B:448:GLN:NE2	1:B:526:LYS:HA	2.29	0.47
1:B:84:PRO:HG3	2:B:701:PLP:H5A2	1.95	0.47
1:A:446:LEU:HD11	1:A:489:ILE:HG13	1.97	0.47
1:B:373:ASN:HD22	1:B:374:ALA:N	2.12	0.47
1:B:453:PHE:CZ	1:B:489:ILE:HG23	2.50	0.46
1:B:566:ASP:HB3	1:B:569:ALA:HB3	1.98	0.46
1:B:516:VAL:CG2	1:B:520:GLN:HG3	2.45	0.46
1:A:435:GLU:HG2	1:A:436:VAL:N	2.29	0.46
1:B:132:ASN:ND2	2:B:701:PLP:H2A3	2.30	0.46
1:B:437:GLN:CG	1:B:475:SER:H	2.28	0.46
1:A:519:TYR:HA	1:A:522:VAL:CG2	2.46	0.46
1:A:370:LYS:HG2	1:A:373:ASN:ND2	2.31	0.46
1:A:448:GLN:NE2	1:A:526:LYS:HA	2.30	0.46
1:B:248:LEU:HD13	1:B:271:LEU:CD2	2.45	0.46
1:B:259:ARG:NH1	1:B:313:LEU:HB3	2.31	0.46
1:A:152:ASN:HD22	1:A:152:ASN:C	2.19	0.46
1:B:519:TYR:HA	1:B:522:VAL:CG2	2.46	0.46
1:B:3:ASP:HB2	1:B:6:ILE:HG22	1.97	0.46
1:A:441:LEU:HD11	1:A:481:ILE:HG22	1.98	0.46
1:A:70:ARG:NH2	1:A:78:GLY:HA2	2.30	0.46
1:B:446:LEU:HD11	1:B:489:ILE:HG13	1.98	0.46
1:A:451:PRO:HD2	1:A:520:GLN:OE1	2.17	0.45
1:B:304:LYS:O	1:B:308:GLU:HG3	2.16	0.45
1:A:452:ASP:CB	1:A:520:GLN:HE22	2.29	0.45
1:A:588:GLN:O	1:A:592:ILE:HG12	2.16	0.45
1:B:354:GLN:NE2	1:B:354:GLN:HA	2.32	0.45
1:A:84:PRO:HG3	2:A:701:PLP:H5A2	1.98	0.45
1:B:165:ALA:O	1:B:169:ILE:HG23	2.17	0.45
1:B:15:ILE:CB	1:B:24:ASN:HD22	2.30	0.45
1:B:385:LEU:HD22	1:B:409:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASN:HD22	1:A:374:ALA:N	2.14	0.45
1:A:304:LYS:O	1:A:308:GLU:HG3	2.16	0.45
1:A:3:ASP:HB2	1:A:6:ILE:HG22	1.98	0.45
1:B:462:ILE:HG12	1:B:513:PHE:CD1	2.52	0.45
1:B:573:ILE:HD11	1:B:577:ARG:NE	2.31	0.45
1:A:578:ILE:CG1	1:B:149:MSE:HE2	2.46	0.45
1:B:276:ALA:HB3	1:B:288:ARG:HD3	1.99	0.44
1:A:48:LEU:HD11	1:A:330:ALA:HB1	2.00	0.44
1:A:91:PRO:HB3	1:B:565:TYR:CE1	2.53	0.44
1:B:351:LEU:H	1:B:351:LEU:HD12	1.82	0.44
1:B:338:GLU:HG3	1:B:609:ILE:HD11	1.99	0.44
1:A:222:LYS:HE2	1:A:222:LYS:CA	2.45	0.44
1:A:576:GLU:HG2	1:A:580:ASN:ND2	2.32	0.44
1:B:152:ASN:HD22	1:B:152:ASN:C	2.20	0.44
1:A:350:ILE:H	1:A:404:ASN:HD21	1.65	0.44
1:A:557:LEU:HA	1:A:557:LEU:HD12	1.80	0.44
1:B:526:LYS:HB3	1:B:526:LYS:HE2	1.62	0.44
1:B:354:GLN:HE21	1:B:354:GLN:HA	1.83	0.44
1:B:616:HIS:O	1:B:618:HIS:CD2	2.71	0.44
1:B:34:ILE:HD13	1:B:538:ILE:HG21	1.99	0.44
1:B:2:MSE:HA	1:B:2:MSE:HE3	1.98	0.44
1:A:503:ASP:OD1	1:A:506:LYS:HB2	2.18	0.43
1:A:179:ASN:HD22	1:A:179:ASN:HA	1.60	0.43
1:B:45:GLY:O	1:B:47:LEU:HD23	2.17	0.43
1:A:2:MSE:HA	1:A:2:MSE:HE3	2.00	0.43
1:B:385:LEU:O	1:B:389:LEU:HG	2.17	0.43
1:A:248:LEU:HD13	1:A:271:LEU:CD2	2.48	0.43
1:B:222:LYS:CA	1:B:222:LYS:HE2	2.46	0.43
1:A:462:ILE:HG12	1:A:513:PHE:CD1	2.54	0.43
1:A:87:VAL:O	1:A:88:ASN:HB2	2.17	0.43
1:B:479:TRP:HB3	1:B:488:GLU:CB	2.49	0.43
1:B:508:ASN:HD22	1:B:508:ASN:HA	1.61	0.43
1:A:343:GLU:O	1:A:348:LYS:HE3	2.18	0.43
1:A:322:GLY:N	2:A:701:PLP:O3P	2.41	0.43
1:A:85:LEU:O	1:A:89:GLN:HG3	2.18	0.43
1:B:237:GLN:NE2	1:B:277:VAL:H	2.09	0.43
1:A:479:TRP:HB3	1:A:488:GLU:CB	2.49	0.43
1:B:451:PRO:HD2	1:B:520:GLN:OE1	2.18	0.43
1:A:385:LEU:HD22	1:A:409:THR:HG21	2.00	0.43
1:A:369:ILE:HG21	1:A:415:LYS:HD3	2.00	0.43
1:B:248:LEU:HD21	1:B:299:VAL:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:LEU:HA	1:B:574:LEU:HD23	1.91	0.43
1:B:85:LEU:O	1:B:89:GLN:HG3	2.19	0.43
1:A:281:GLN:HE22	1:A:462:ILE:H	1.66	0.42
1:B:221:ASN:O	1:B:222:LYS:C	2.57	0.42
1:A:26:GLU:HB3	1:A:27:LYS:H	1.52	0.42
1:A:467:ARG:HD3	4:A:672:HOH:O	2.19	0.42
1:B:495:LYS:NZ	4:B:641:HOH:O	2.51	0.42
1:A:259:ARG:HE	1:A:259:ARG:HB3	1.63	0.42
1:B:183:ARG:HA	1:B:231:HIS:O	2.18	0.42
1:A:165:ALA:O	1:A:169:ILE:HG23	2.19	0.42
1:B:357:LYS:O	1:B:360:ASP:HB2	2.20	0.42
1:B:373:ASN:C	1:B:373:ASN:ND2	2.72	0.42
1:A:15:ILE:CB	1:A:24:ASN:HD22	2.30	0.42
1:A:561:GLU:HB2	1:A:567:ILE:CD1	2.41	0.42
1:A:259:ARG:NH1	1:A:313:LEU:HB3	2.35	0.42
1:B:142:ILE:HA	1:B:145:ILE:HG23	2.01	0.42
1:A:479:TRP:HD1	1:A:479:TRP:O	2.02	0.42
1:B:6:ILE:O	1:B:10:GLY:HA3	2.20	0.42
1:B:337:LEU:HD21	1:B:443:ASN:HB2	2.02	0.42
1:B:503:ASP:OD1	1:B:506:LYS:HB2	2.19	0.42
1:A:221:ASN:O	1:A:222:LYS:C	2.58	0.42
1:A:575:ASN:OD1	1:A:593:LEU:HD21	2.20	0.42
1:A:337:LEU:HG	1:A:443:ASN:HB2	2.02	0.41
1:B:183:ARG:NH2	1:B:204:PHE:HB2	2.35	0.41
1:A:295:TYR:O	1:A:299:VAL:HG23	2.20	0.41
1:A:355:ASN:CB	1:A:356:PRO:HD2	2.50	0.41
1:A:169:ILE:O	1:A:173:ARG:HG2	2.20	0.41
1:A:141:ASN:OD1	1:A:173:ARG:HD3	2.20	0.41
1:A:183:ARG:HA	1:A:231:HIS:O	2.20	0.41
1:A:375:LEU:HD13	1:A:375:LEU:C	2.40	0.41
1:B:17:LYS:HB3	1:B:18:ASN:H	1.57	0.41
1:B:358:LEU:HA	1:B:358:LEU:HD23	1.88	0.41
1:B:362:LEU:O	1:B:412:ILE:HD11	2.20	0.41
1:A:460:PHE:O	1:A:462:ILE:HG13	2.20	0.41
1:A:516:VAL:HG23	1:A:520:GLN:HG3	2.03	0.41
1:A:64:GLY:O	1:A:68:LYS:HG3	2.21	0.41
1:B:175:LYS:O	1:B:177:LYS:HG2	2.20	0.41
1:B:343:GLU:HG3	4:B:676:HOH:O	2.19	0.41
1:B:561:GLU:HB2	1:B:567:ILE:CD1	2.42	0.41
1:B:64:GLY:O	1:B:68:LYS:HG3	2.20	0.41
1:A:261:MSE:HB2	1:A:261:MSE:HE3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LEU:HG	1:B:89:GLN:OE1	2.21	0.41
1:B:514:PHE:O	1:B:515:LEU:HB2	2.20	0.41
1:B:576:GLU:HG2	1:B:580:ASN:ND2	2.35	0.41
1:B:48:LEU:HD11	1:B:330:ALA:HB1	2.03	0.41
1:B:359:ILE:HA	1:B:362:LEU:HD12	2.01	0.41
1:B:437:GLN:HG3	1:B:474:ARG:HA	2.02	0.41
1:B:246:LYS:HB3	1:B:246:LYS:HE2	1.97	0.41
1:B:26:GLU:HG2	1:B:542:GLU:CA	2.39	0.41
1:B:57:LYS:O	1:B:61:ASN:HB2	2.21	0.41
1:A:596:LEU:O	1:A:600:LEU:HD13	2.21	0.40
1:B:145:ILE:HG22	1:B:173:ARG:NH2	2.36	0.40
1:A:57:LYS:O	1:A:61:ASN:HB2	2.21	0.40
1:A:607:LYS:HB2	1:A:607:LYS:HZ2	1.86	0.40
1:B:219:LYS:HE2	1:B:224:LEU:HD11	2.03	0.40
1:B:17:LYS:HB2	1:B:22:CYS:SG	2.61	0.40
1:B:46:PRO:HB3	1:B:443:ASN:O	2.21	0.40
1:A:27:LYS:CE	1:A:542:GLU:O	2.61	0.40
1:B:366:TYR:O	1:B:369:ILE:HG22	2.21	0.40
1:B:557:LEU:HD12	1:B:557:LEU:HA	1.78	0.40
1:A:365:LEU:HD12	1:A:377:TYR:CE2	2.57	0.40
1:A:514:PHE:N	1:A:514:PHE:CD1	2.90	0.40
1:B:356:PRO:O	1:B:359:ILE:CD1	2.70	0.40
1:B:169:ILE:O	1:B:173:ARG:HG2	2.21	0.40
1:B:452:ASP:HB3	1:B:458:GLN:HB3	2.04	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	577/619 (93%)	527 (91%)	43 (8%)	7 (1%)	13 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	585/619 (94%)	527 (90%)	52 (9%)	6 (1%)	15 53
All	All	1162/1238 (94%)	1054 (91%)	95 (8%)	13 (1%)	14 50

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	HIS
1	B	527	HIS
1	A	188	SER
1	B	351	LEU
1	A	88	ASN
1	A	285	GLU
1	A	351	LEU
1	A	458	GLN
1	B	88	ASN
1	B	458	GLN
1	B	227	PHE
1	B	285	GLU
1	A	173	ARG

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	511/529 (97%)	470 (92%)	41 (8%)	12 40
1	B	519/529 (98%)	472 (91%)	47 (9%)	9 34
All	All	1030/1058 (97%)	942 (92%)	88 (8%)	10 38

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	47	LEU
1	A	80	ASN

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Mol	Chain	Res	Type
1	A	86	LYS
1	A	116	LEU
1	A	117	LEU
1	A	118	LEU
1	A	145	ILE
1	A	152	ASN
1	A	155	LEU
1	A	161	ASN
1	A	177	LYS
1	A	187	HIS
1	A	209	THR
1	A	222	LYS
1	A	223	LEU
1	A	246	LYS
1	A	249	ASN
1	A	258	LEU
1	A	265	ASN
1	A	275	LEU
1	A	292	LEU
1	A	328	ASN
1	A	353	LYS
1	A	355	ASN
1	A	362	LEU
1	A	370	LYS
1	A	373	ASN
1	A	420	LEU
1	A	439	ARG
1	A	456	LEU
1	A	457	GLU
1	A	459	ASN
1	A	479	TRP
1	A	493	LYS
1	A	494	ASP
1	A	522	VAL
1	A	542	GLU
1	A	564	ASP
1	A	587	LYS
1	A	607	LYS
1	B	26	GLU
1	B	27	LYS
1	B	47	LEU
1	B	80	ASN

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Mol	Chain	Res	Type
1	B	86	LYS
1	B	116	LEU
1	B	117	LEU
1	B	118	LEU
1	B	145	ILE
1	B	152	ASN
1	B	155	LEU
1	B	161	ASN
1	B	177	LYS
1	B	187	HIS
1	B	209	THR
1	B	222	LYS
1	B	223	LEU
1	B	246	LYS
1	B	249	ASN
1	B	258	LEU
1	B	265	ASN
1	B	275	LEU
1	B	292	LEU
1	B	328	ASN
1	B	339	LEU
1	B	342	GLN
1	B	353	LYS
1	B	359	ILE
1	B	373	ASN
1	B	400	GLN
1	B	420	LEU
1	B	439	ARG
1	B	442	VAL
1	B	443	ASN
1	B	456	LEU
1	B	457	GLU
1	B	459	ASN
1	B	479	TRP
1	B	493	LYS
1	B	494	ASP
1	B	507	GLU
1	B	522	VAL
1	B	542	GLU
1	B	564	ASP
1	B	587	LYS
1	B	603	ASN

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Mol	Chain	Res	Type
1	B	609	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	24	ASN
1	A	65	ASN
1	A	105	ASN
1	A	123	ASN
1	A	151	HIS
1	A	152	ASN
1	A	179	ASN
1	A	231	HIS
1	A	237	GLN
1	A	265	ASN
1	A	281	GLN
1	A	289	ASN
1	A	328	ASN
1	A	355	ASN
1	A	373	ASN
1	A	404	ASN
1	A	448	GLN
1	A	508	ASN
1	A	528	ASN
1	A	603	ASN
1	B	24	ASN
1	B	65	ASN
1	B	105	ASN
1	B	123	ASN
1	B	132	ASN
1	B	151	HIS
1	B	152	ASN
1	B	179	ASN
1	B	231	HIS
1	B	237	GLN
1	B	265	ASN
1	B	281	GLN
1	B	289	ASN
1	B	328	ASN
1	B	354	GLN
1	B	355	ASN

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Mol	Chain	Res	Type
1	B	373	ASN
1	B	443	ASN
1	B	448	GLN
1	B	508	ASN
1	B	528	ASN
1	B	568	HIS
1	B	603	ASN
1	B	615	HIS
1	B	618	HIS
1	B	619	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

5 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	PLP	B	701	-	15,15,16	1.73	3 (20%)	20,22,23	1.03	1 (5%)
2	PLP	A	701	-	15,15,16	1.71	3 (20%)	20,22,23	1.03	1 (5%)
3	SO4	A	702	-	4,4,4	0.33	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	B	702	-	4,4,4	0.32	0	6,6,6	0.15	0
3	SO4	B	703	-	4,4,4	0.31	0	6,6,6	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	B	701	-	-	0/6/6/8	0/1/1/1
2	PLP	A	701	-	-	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PLP	C5-C4	4.45	1.45	1.40
2	B	701	PLP	C5-C4	4.30	1.45	1.40
2	B	701	PLP	C3-C4	3.08	1.46	1.40
2	A	701	PLP	C3-C4	2.60	1.45	1.40
2	A	701	PLP	C3-C2	2.25	1.43	1.40
2	B	701	PLP	C3-C2	2.23	1.43	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	PLP	C6-N1-C2	2.41	123.63	119.17
2	A	701	PLP	C6-N1-C2	2.29	123.42	119.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	PLP	2	0
2	A	701	PLP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	573/619 (92%)	-0.51	4 (0%)	87	69	22, 44, 82, 119	0
1	B	581/619 (93%)	-0.41	8 (1%)	75	49	25, 46, 87, 121	0
All	All	1154/1238 (93%)	-0.46	12 (1%)	82	59	22, 45, 86, 121	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	494	ASP	3.5
1	B	455	GLY	3.4
1	A	494	ASP	3.4
1	B	491	TYR	3.2
1	B	506	LYS	2.9
1	A	189	ALA	2.8
1	A	421	GLY	2.8
1	B	420	LEU	2.4
1	B	284	ASN	2.3
1	B	485	SER	2.2
1	A	283	LYS	2.2
1	B	493	LYS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
3	SO4	A	702	5/5	0.88	0.22	96,96,101,104	0
3	SO4	B	702	5/5	0.90	0.16	77,85,91,94	0
3	SO4	B	703	5/5	0.91	0.23	88,91,94,100	0
2	PLP	A	701	15/16	0.94	0.24	36,72,88,100	0
2	PLP	B	701	15/16	0.95	0.18	35,59,76,79	0

6.5 Other polymers

There are no such residues in this entry.