



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:19 PM UTC

PDB ID : 3NZP / pdb_00003nzp
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.; Ciccocanti, 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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

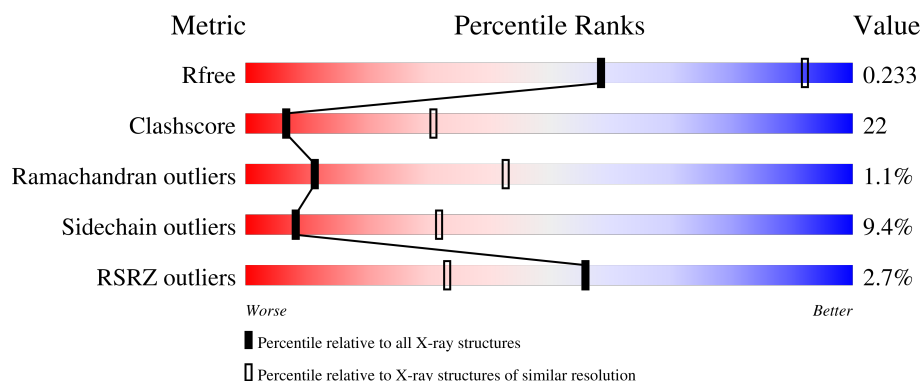
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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 $\leq 5\%$. 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	
1	B	619	

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.

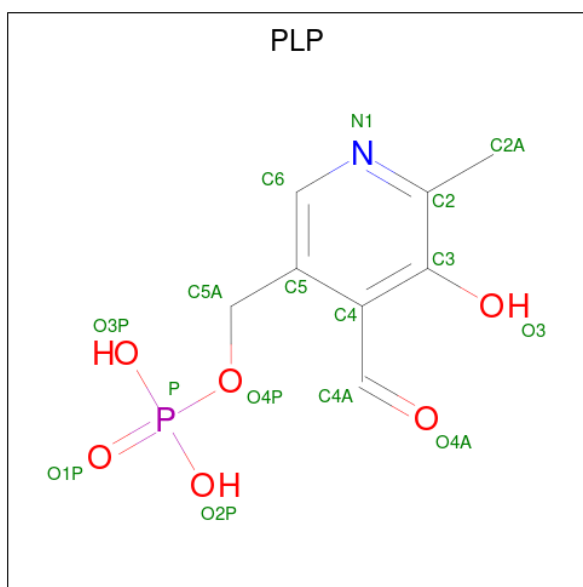
- Molecule 1 is a protein called Arginine decarboxylase.

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:

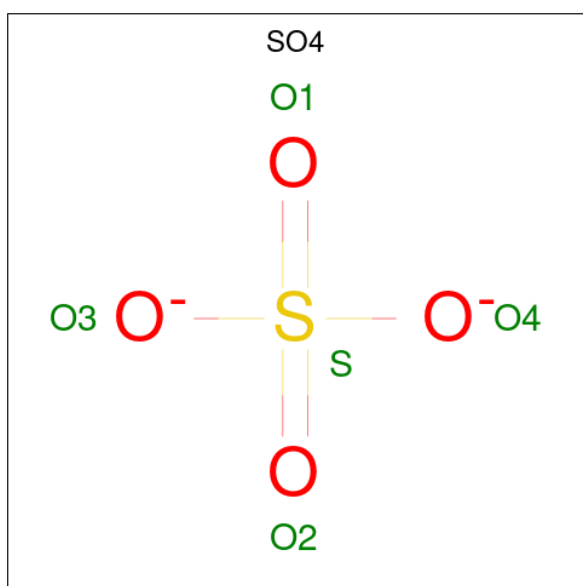
Chain	Residue	Modelled	Actual	Comment	Reference
A	612	LEU	-	expression tag	UNP Q0PAC6
A	613	GLU	-	expression tag	UNP Q0PAC6
A	614	HIS	-	expression tag	UNP Q0PAC6
A	615	HIS	-	expression tag	UNP Q0PAC6
A	616	HIS	-	expression tag	UNP Q0PAC6
A	617	HIS	-	expression tag	UNP Q0PAC6
A	618	HIS	-	expression tag	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 (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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 (CCD ID: SO₄) (formula: O₄S).



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		

Continued on next page...

Continued from previous page...

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

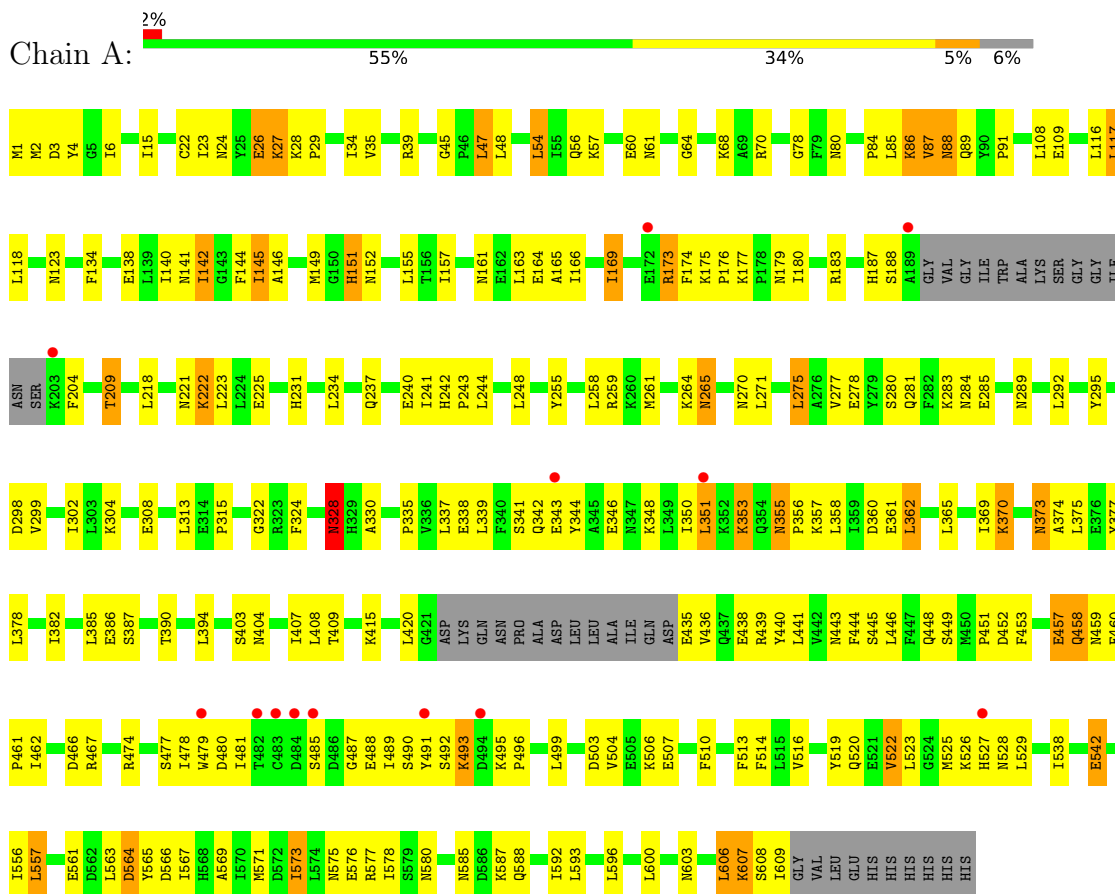
- Molecule 4 is water.

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

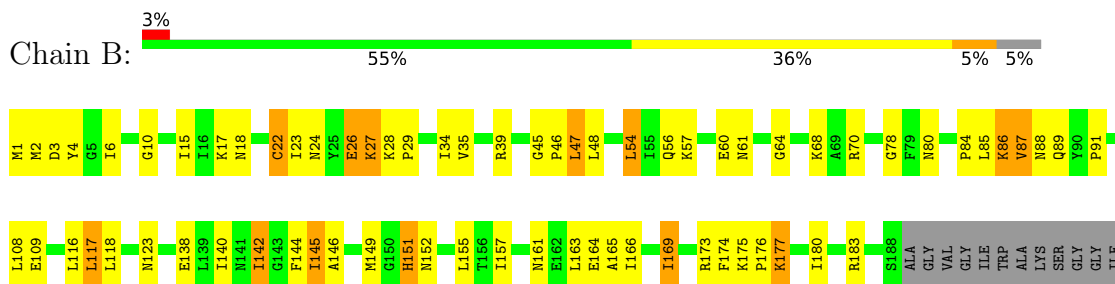
3 Residue-property plots

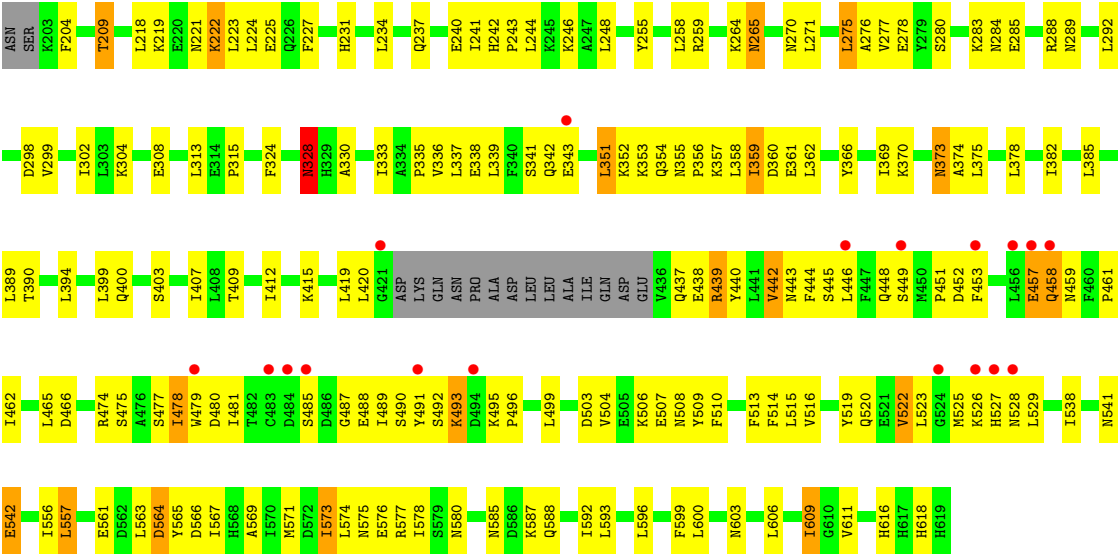
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Arginine decarboxylase



• Molecule 1: Arginine decarboxylase





4 Data and refinement statistics

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 19.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.6 (19.96-3.00) 94.1 (19.96-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 3.00Å)	Xtriage
Refinement program	REFMAC, CNS 1.2	Depositor
R, R_{free}	0.180 , 0.219 0.194 , 0.233	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)	0.35 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.52	0/4784	0.85	1/6440 (0.0%)
1	B	0.51	0/4864	0.84	3/6549 (0.0%)
All	All	0.52	0/9648	0.85	4/12989 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	ASN	N-CA-C	5.20	119.25	113.01
1	B	478	ILE	N-CA-C	5.19	115.79	109.30
1	B	328	ASN	N-CA-C	5.19	119.24	113.01
1	B	504	VAL	N-CA-C	5.05	115.66	110.36

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	4701	0	4734	212	0
1	B	4775	0	4794	221	0
2	A	15	0	7	2	0
2	B	15	0	7	1	0
3	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	0	0
4	A	93	0	0	4	0
4	B	71	0	0	2	0
All	All	9685	0	9542	410	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 22.

All (410) 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:ND2	1:A:355:ASN:H	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:A:650:HOH:O	1:B:599:PHE:HB3	1.95	0.66
1:B:493:LYS:N	1:B:493:LYS:HE3	2.11	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:HD3	1:A:353:LYS:N	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:373:ASN:C	1:B:373:ASN:HD22	2.04	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:A:117:LEU:HD23	1:B:556:ILE:HD13	1.80	0.62
1:B:15:ILE:HB	1:B:24:ASN:HD22	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:222:LYS:HE2	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:341:SER:HB3	1:A:438:GLU:HG2	1.81	0.61
1:A:369:ILE:HD11	1:A:374:ALA:HA	1.82	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:373:ASN:HD22	1:A:373:ASN:C	2.09	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
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: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:A:608:SER:C	1:A:609:ILE:HD13	2.29	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:A:697:HOH:O	1:B:523:LEU:HD21	2.04	0.57
1:B:225:GLU:HA	1:B:265:ASN:HD22	1.68	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: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
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:O	1:A:375:LEU:HD13	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:149:MSE:HE2	1:B:578:ILE:HG12	1.89	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:359:ILE:HD13	1:B:359:ILE:C	2.33	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:H	1:A:351:LEU:HD22	1.74	0.53
1:A:578:ILE:HG12	1:B:149:MSE:HE2	1.90	0.53
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:35:VAL:O	1:A:39:ARG:HG3	2.08	0.52
1:A:242:HIS:N	1:A:243:PRO:HD2	2.25	0.52
1:B:23:ILE:O	1:B:28:LYS:HA	2.09	0.52
1:B:352:LYS:HB3	1:B:355:ASN:CG	2.35	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:56:GLN:O	1:A:60:GLU:HG2	2.10	0.52
1:A:259:ARG:HH12	1:A:313:LEU:CD2	2.23	0.52
1:B:35:VAL:O	1:B:39:ARG:HG3	2.10	0.52
1:A:134:PHE:O	1:B:606:LEU:HD21	2.10	0.51
1:A:261:MSE:HE1	1:B:399:LEU:HD23	1.92	0.51
1:B:259:ARG:HH12	1:B:313:LEU:CD2	2.23	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:A:152:ASN:C	1:A:152:ASN:HD22	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:HD23	1:B:328:ASN:O	2.10	0.50
1:B:439:ARG:HG2	1:B:479:TRP:CZ3	2.46	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:23:ILE:O	1:A:28:LYS:HA	2.12	0.50
1:A:283:LYS:HG2	1:A:284:ASN:OD1	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:H	1:B:609:ILE:CD1	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
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:54:LEU:HD23	1:A:328:ASN:O	2.11	0.49
1:A:138:GLU:O	1:A:142:ILE:HG22	2.12	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:H	1:A:353:LYS:CD	2.14	0.48
1:A:526:LYS:HB3	1:A:526:LYS:HE2	1.62	0.48
1:B:222:LYS:NZ	1:B:225:GLU:HG2	2.28	0.48
1:B:152:ASN:HD22	1:B:152:ASN:C	2.20	0.48
1:B:481:ILE:O	1:B:481:ILE:HG13	2.14	0.48
1:A:343:GLU:HB2	1:A:348:LYS:HE3	1.94	0.48
1:A:481:ILE:HG13	1:A:481:ILE:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:HG12	1:A:519:TYR:CZ	2.49	0.48
1:A:592:ILE:HD11	1:B:174:PHE:HE2	1.78	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: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:B:275:LEU:HD13	1:B:324:PHE:CG	2.49	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:373:ASN:ND2	1:B:373:ASN:C	2.72	0.47
1:B:378:LEU:O	1:B:382:ILE:HG12	2.13	0.47
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:A:375:LEU:HD13	1:A:375:LEU:C	2.40	0.47
1:B:221:ASN:O	1:B:222:LYS:C	2.57	0.47
1:A:344:TYR:CD1	1:A:407:ILE:HD13	2.50	0.47
1:B:70:ARG:NH2	1:B:78:GLY:HA2	2.30	0.47
1:B:283:LYS:HG2	1:B:284:ASN:OD1	2.13	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:84:PRO:HG3	2:B:701:PLP:H5A2	1.95	0.47
1:B:448:GLN:NE2	1:B:526:LYS:HA	2.29	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:A:221:ASN:O	1:A:222:LYS:C	2.58	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:ARG:NH2	1:A:78:GLY:HA2	2.30	0.46
1:A:441:LEU:HD11	1:A:481:ILE:HG22	1.98	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:15:ILE:CB	1:B:24:ASN:HD22	2.30	0.45
1:B:165:ALA:O	1:B:169:ILE:HG23	2.17	0.45
1:B:385:LEU:HD22	1:B:409:THR:HG21	1.99	0.45
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:A:152:ASN:C	1:A:152:ASN:ND2	2.75	0.44
1:A:480:ASP:OD2	1:A:480:ASP:C	2.60	0.44
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:338:GLU:HG3	1:B:609:ILE:HD11	1.99	0.44
1:B:351:LEU:HD12	1:B:351:LEU:H	1.82	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:480:ASP:OD2	1:B:480:ASP:C	2.59	0.44
1:A:27:LYS:HE2	1:A:542:GLU:C	2.42	0.44
1:A:350:ILE:H	1:A:404:ASN:HD21	1.65	0.44
1:A:557:LEU:HD12	1:A:557:LEU:HA	1.80	0.44
1:B:526:LYS:HB3	1:B:526:LYS:HE2	1.62	0.44
1:B:354:GLN:HA	1:B:354:GLN:HE21	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:HE3	1:B:2:MSE:HA	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:MSE:HE3	1:A:2:MSE:HA	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:HE2	1:B:222:LYS:CA	2.46	0.43
1:A:87:VAL:O	1:A:88:ASN:HB2	2.17	0.43
1:A:462:ILE:HG12	1:A:513:PHE:CD1	2.54	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:85:LEU:O	1:A:89:GLN:HG3	2.18	0.43
1:A:322:GLY:N	2:A:701:PLP:O3P	2.41	0.43
1:A:343:GLU:O	1:A:348:LYS:HE3	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:369:ILE:HG21	1:A:415:LYS:HD3	2.00	0.43
1:A:385:LEU:HD22	1:A:409:THR:HG21	2.00	0.43
1:B:466:ASP:OD2	1:B:466:ASP:C	2.61	0.43
1:B:248:LEU:HD21	1:B:299:VAL:HA	1.99	0.43
1:B:85:LEU:O	1:B:89:GLN:HG3	2.19	0.43
1:B:574:LEU:HD23	1:B:574:LEU:HA	1.91	0.43
1:A:281:GLN:HE22	1:A:462:ILE:H	1.66	0.42
1:A:56:GLN:O	1:A:57:LYS:C	2.62	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:A:259:ARG:HE	1:A:259:ARG:HB3	1.63	0.42
1:B:152:ASN:C	1:B:152:ASN:ND2	2.75	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:A:231:HIS:HD2	1:A:270:ASN:CG	2.27	0.42
1:A:485:SER:C	1:A:487:GLY:H	2.27	0.42
1:B:357:LYS:O	1:B:360:ASP:HB2	2.20	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:A:607:LYS:HB2	1:A:607:LYS:HZ3	1.83	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:575:ASN:OD1	1:A:593:LEU:HD21	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:CYS:HB3	1:B:29:PRO:C	2.45	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:B:17:LYS:HB3	1:B:18:ASN:H	1.57	0.41
1:B:358:LEU:HD23	1:B:358:LEU:HA	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:A:457:GLU:O	1:A:458:GLN:C	2.63	0.41
1:B:64:GLY:O	1:B:68:LYS:HG3	2.20	0.41
1:A:261:MSE:HE3	1:A:261:MSE:HB2	1.93	0.41
1:A:373:ASN:C	1:A:373:ASN:ND2	2.77	0.41
1:A:529:LEU:HG	1:B:89:GLN:OE1	2.21	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: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:A:466:ASP:OD2	1:A:466:ASP:C	2.63	0.41
1:B:26:GLU:HG2	1:B:542:GLU:CA	2.39	0.41
1:B:26:GLU:C	1:B:28:LYS:H	2.29	0.41
1:B:57:LYS:O	1:B:61:ASN:HB2	2.21	0.41
1:B:246:LYS:HE2	1:B:246:LYS:HB3	1.97	0.41
1:B:485:SER:C	1:B:487:GLY:H	2.28	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: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:B:219:LYS:HE2	1:B:224:LEU:HD11	2.03	0.40
1:B:231:HIS:HD2	1:B:270:ASN:CG	2.29	0.40
1:B:452:ASP:CG	1:B:520:GLN:HE22	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:457:GLU:O	1:B:458:GLN:C	2.64	0.40
1:B:557:LEU:HD12	1:B:557:LEU:HA	1.78	0.40
1:A:346:GLU:C	1:A:348:LYS:N	2.79	0.40
1:A:365:LEU:HD12	1:A:377:TYR:CE2	2.57	0.40
1:A:514:PHE:CD1	1:A:514:PHE:N	2.90	0.40
1:B:356:PRO:O	1:B:359:ILE:CD1	2.70	0.40
1:A:26:GLU:C	1:A:28:LYS:H	2.29	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%)	10	40
1	B	585/619 (94%)	527 (90%)	52 (9%)	6 (1%)	12	45
All	All	1162/1238 (94%)	1054 (91%)	95 (8%)	13 (1%)	11	43

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	463 (91%)	48 (9%)	8	32
1	B	519/529 (98%)	470 (91%)	49 (9%)	8	32
All	All	1030/1058 (97%)	933 (91%)	97 (9%)	8	32

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	27	LYS
1	A	47	LEU
1	A	54	LEU
1	A	80	ASN
1	A	86	LYS
1	A	87	VAL
1	A	116	LEU
1	A	117	LEU
1	A	118	LEU
1	A	142	ILE
1	A	145	ILE
1	A	151	HIS
1	A	155	LEU
1	A	161	ASN
1	A	164	GLU
1	A	169	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	177	LYS
1	A	187	HIS
1	A	209	THR
1	A	222	LYS
1	A	223	LEU
1	A	258	LEU
1	A	264	LYS
1	A	265	ASN
1	A	275	LEU
1	A	292	LEU
1	A	328	ASN
1	A	339	LEU
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	457	GLU
1	A	459	ASN
1	A	493	LYS
1	A	507	GLU
1	A	522	VAL
1	A	542	GLU
1	A	557	LEU
1	A	564	ASP
1	A	573	ILE
1	A	587	LYS
1	A	606	LEU
1	A	607	LYS
1	B	22	CYS
1	B	26	GLU
1	B	27	LYS
1	B	47	LEU
1	B	54	LEU
1	B	80	ASN
1	B	86	LYS
1	B	87	VAL
1	B	116	LEU
1	B	117	LEU
1	B	118	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	142	ILE
1	B	145	ILE
1	B	151	HIS
1	B	155	LEU
1	B	161	ASN
1	B	164	GLU
1	B	169	ILE
1	B	177	LYS
1	B	209	THR
1	B	222	LYS
1	B	223	LEU
1	B	258	LEU
1	B	264	LYS
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	457	GLU
1	B	459	ASN
1	B	493	LYS
1	B	507	GLU
1	B	522	VAL
1	B	542	GLU
1	B	557	LEU
1	B	564	ASP
1	B	573	ILE
1	B	587	LYS
1	B	609	ILE
1	B	611	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	24	ASN
1	A	105	ASN
1	A	123	ASN
1	A	132	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	527	HIS
1	A	528	ASN
1	A	580	ASN
1	A	603	ASN
1	B	24	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	249	ASN
1	B	265	ASN
1	B	281	GLN
1	B	289	ASN
1	B	328	ASN
1	B	354	GLN
1	B	355	ASN
1	B	373	ASN
1	B	448	GLN
1	B	508	ASN
1	B	528	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	568	HIS
1	B	580	ASN
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 oligosaccharides 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	$\# Z > 2$
3	SO4	B	702	-	4,4,4	0.43	0	6,6,6	0.18	0
2	PLP	A	701	-	15,15,16	1.72	3 (20%)	21,22,23	1.02	1 (4%)
3	SO4	A	702	-	4,4,4	0.43	0	6,6,6	0.15	0
2	PLP	B	701	-	15,15,16	1.75	3 (20%)	21,22,23	1.02	1 (4%)
3	SO4	B	703	-	4,4,4	0.41	0	6,6,6	0.12	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	A	701	-	-	0/6/6/8	0/1/1/1
2	PLP	B	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	4.34	1.45	1.40
2	B	701	PLP	C5-C4	4.19	1.45	1.40
2	B	701	PLP	C3-C4	3.36	1.46	1.40
2	A	701	PLP	C3-C4	2.83	1.45	1.40
2	A	701	PLP	C3-C2	2.10	1.43	1.41
2	B	701	PLP	C3-C2	2.09	1.43	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	PLP	C6-N1-C2	2.44	123.63	119.20
2	A	701	PLP	C6-N1-C2	2.33	123.42	119.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	PLP	2	0
2	B	701	PLP	1	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, 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	573/619 (92%)	-0.25	13 (2%) 61 38	22, 44, 82, 119	0
1	B	581/619 (93%)	-0.11	18 (3%) 51 30	25, 46, 87, 121	0
All	All	1154/1238 (93%)	-0.18	31 (2%) 56 33	22, 45, 86, 121	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	483	CYS	4.4
1	B	421	GLY	3.9
1	A	172	GLU	3.5
1	A	189	ALA	3.3
1	A	494	ASP	3.2
1	B	485	SER	3.2
1	B	491	TYR	3.0
1	B	343	GLU	3.0
1	B	526	LYS	2.9
1	B	494	ASP	2.8
1	B	528	ASN	2.8
1	B	453	PHE	2.7
1	B	484	ASP	2.7
1	B	479	TRP	2.6
1	B	446	LEU	2.5
1	A	479	TRP	2.5
1	A	343	GLU	2.4
1	B	457	GLU	2.4
1	A	484	ASP	2.3
1	B	449	SER	2.3
1	A	483	CYS	2.3
1	A	491	TYR	2.2
1	A	527	HIS	2.1
1	A	482	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	203	LYS	2.1
1	A	351	LEU	2.1
1	B	524	GLY	2.1
1	B	458	GLN	2.1
1	B	456	LEU	2.1
1	B	527	HIS	2.1
1	A	485	SER	2.1

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	SO4	B	703	5/5	0.88	0.14	88,91,94,100	0
3	SO4	A	702	5/5	0.89	0.17	96,96,101,104	0
3	SO4	B	702	5/5	0.91	0.10	77,85,91,94	0
2	PLP	A	701	15/16	0.91	0.19	36,72,88,100	0
2	PLP	B	701	15/16	0.94	0.13	35,59,76,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.