



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2026 – 04:08 pm BST

PDB ID : 9TCF / pdb_00009tcf
Title : Crystal Structure of Cystathionine beta-Synthase from *Pseudomonas aeruginosa*
Authors : Conter, C.; Martinez-Cruz, L.A.
Deposited on : 2025-11-21
Resolution : 3.43 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 Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

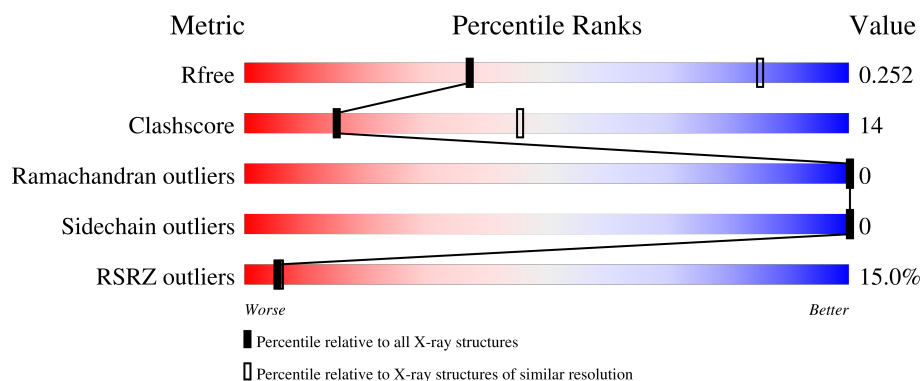
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)

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	E	457	16% 76% 24%
2	G	457	15% 73% 27%
2	I	457	15% 76% 24%
2	K	457	14% 75% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13807 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 Cysteine synthase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	457	Total	C	N	O	S	0	0	0
			3421	2139	612	657	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	457	ALA	-	expression tag	UNP A0A7M2ZYJ1

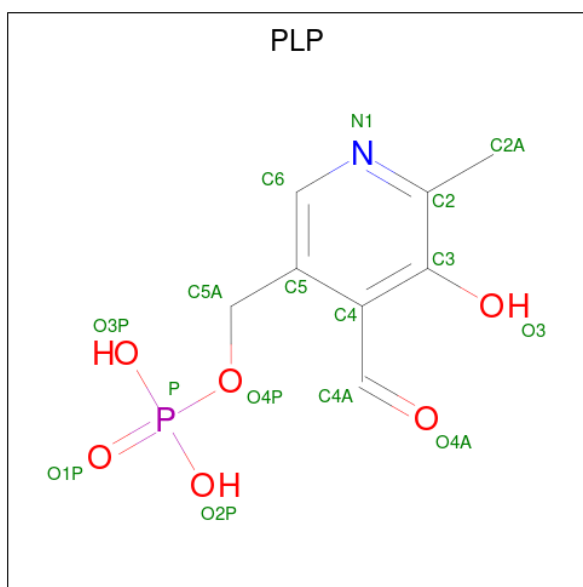
- Molecule 2 is a protein called Cysteine synthase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	457	Total	C	N	O	P	S	0	0	0
			3454	2160	614	666	1	13			
2	I	457	Total	C	N	O	P	S	0	0	0
			3451	2160	611	666	1	13			
2	K	457	Total	C	N	O	P	S	0	0	0
			3466	2166	620	666	1	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	457	ALA	-	expression tag	UNP A0A7M2ZYJ1
I	457	ALA	-	expression tag	UNP A0A7M2ZYJ1
K	457	ALA	-	expression tag	UNP A0A7M2ZYJ1

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).

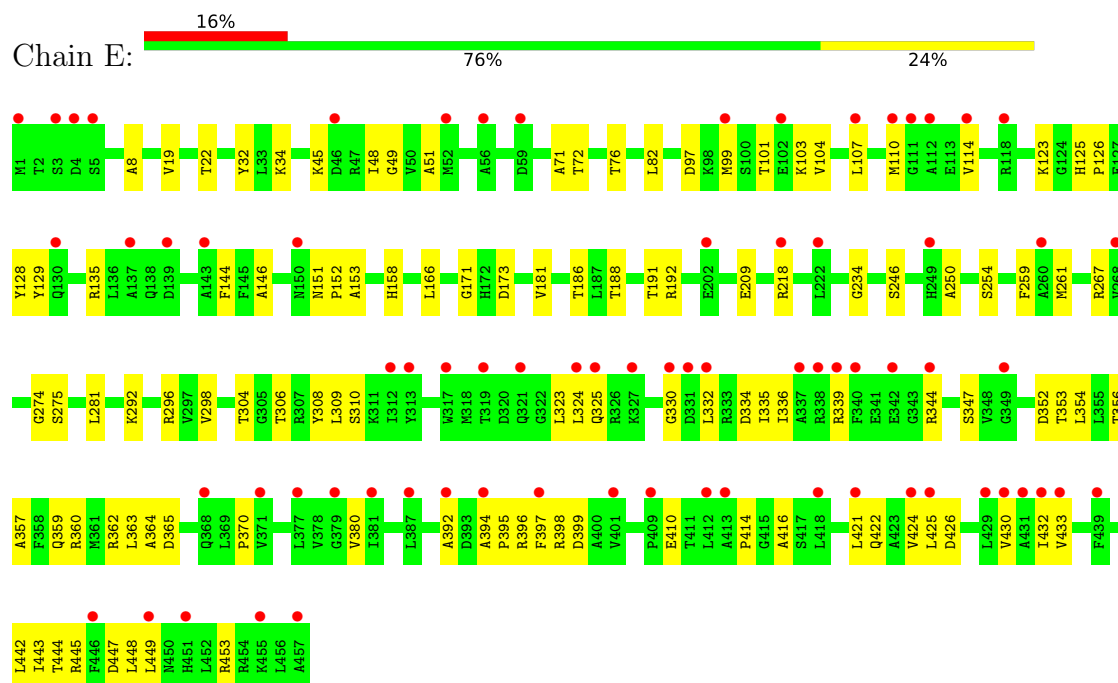


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	E	1	15	8	1	5	1	0	0

3 Residue-property plots [i](#)

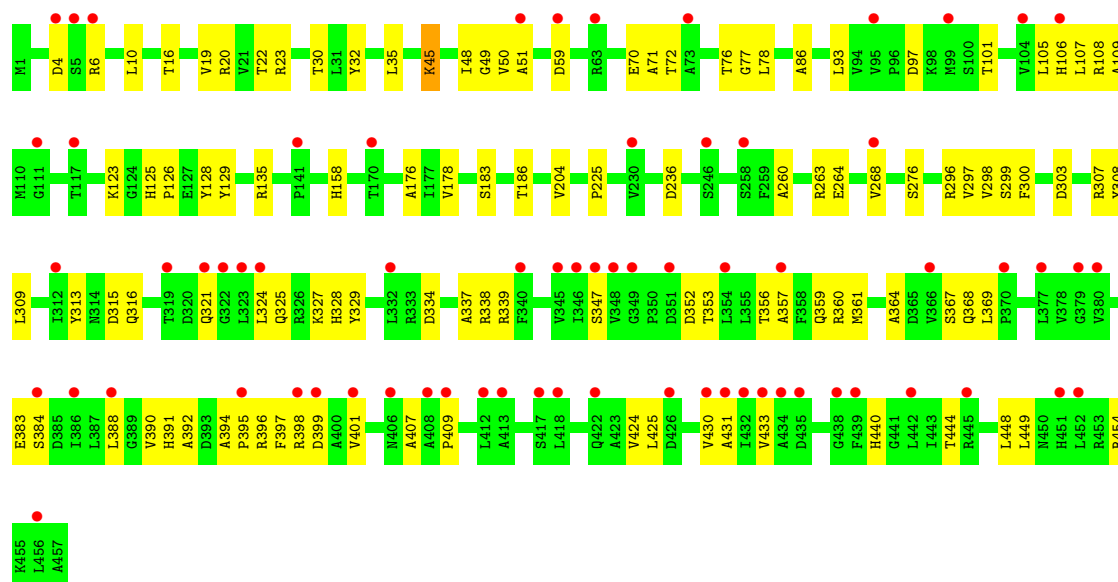
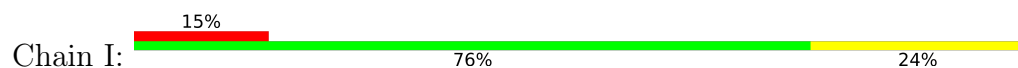
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cysteine synthase B

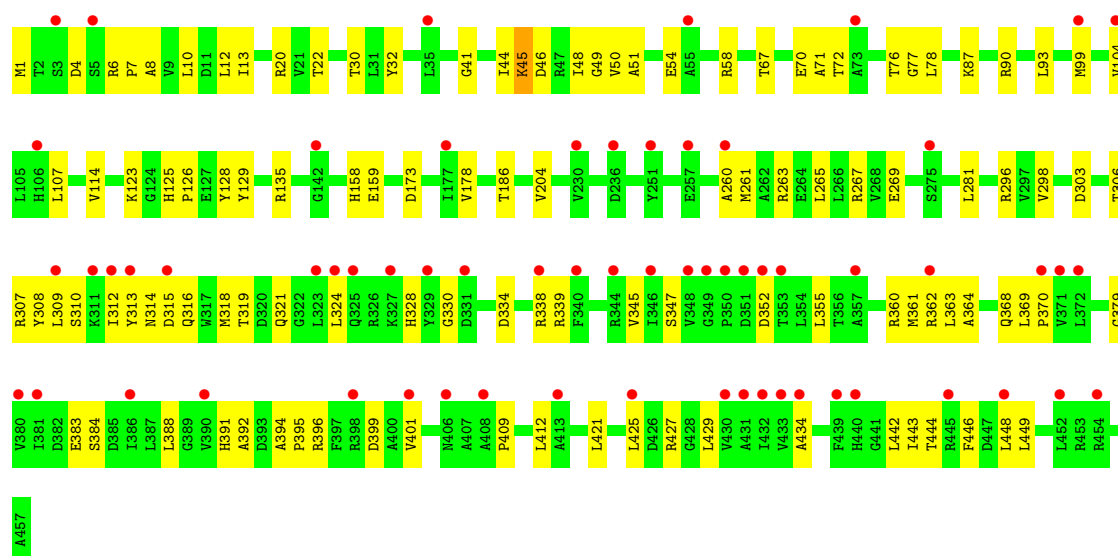
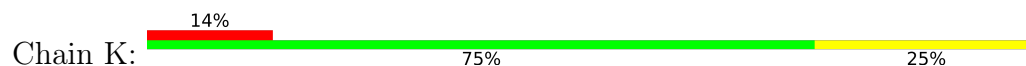




● Molecule 2: Cysteine synthase B



● Molecule 2: Cysteine synthase B



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	341.83Å 109.55Å 69.98Å 90.00° 100.47° 90.00°	Depositor
Resolution (Å)	68.81 – 3.43 68.81 – 3.44	Depositor EDS
% Data completeness (in resolution range)	90.1 (68.81-3.43) 83.1 (68.81-3.44)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.41Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.247 , 0.286 0.246 , 0.252	Depositor DCC
R_{free} test set	1678 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	109.6	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 147.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.155 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	13807	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: LLP, 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	E	0.26	0/3480	0.61	0/4722
2	G	0.23	0/3490	0.56	0/4734
2	I	0.24	0/3487	0.56	1/4731 (0.0%)
2	K	0.23	0/3502	0.54	0/4748
All	All	0.24	0/13959	0.57	1/18935 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	59	ASP	CA-CB-CG	5.09	117.69	112.60

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	E	3421	0	3405	117	0
2	G	3454	0	3424	117	0
2	I	3451	0	3422	101	0
2	K	3466	0	3446	103	0
3	E	15	0	6	3	0
All	All	13807	0	13703	373	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 14.

All (373) 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)
2:I:353:THR:O	2:I:356:THR:HG22	1.41	1.15
1:E:353:THR:O	1:E:356:THR:HG22	1.51	1.09
1:E:449:LEU:HD22	2:G:392:ALA:HB2	1.35	1.09
2:I:352:ASP:HB3	2:I:356:THR:HG21	1.36	1.08
2:G:353:THR:O	2:G:356:THR:HG22	1.58	1.01
1:E:425:LEU:O	1:E:445:ARG:NH2	2.00	0.93
1:E:352:ASP:HB3	1:E:356:THR:HG21	1.53	0.89
2:K:308:TYR:O	2:K:312:ILE:N	2.07	0.88
1:E:444:THR:OG1	1:E:447:ASP:OD1	1.95	0.84
2:I:108:ARG:HD2	2:K:363:LEU:HD11	1.62	0.81
2:G:352:ASP:HB3	2:G:356:THR:HG21	1.64	0.80
1:E:453:ARG:HD3	2:G:392:ALA:HA	1.62	0.80
2:K:334:ASP:OD1	2:K:339:ARG:NH2	2.16	0.79
1:E:99:MET:O	2:G:359:GLN:NE2	2.15	0.79
2:G:71:ALA:HB1	2:G:129:TYR:CD2	2.17	0.78
1:E:359:GLN:NE2	2:G:99:MET:O	2.16	0.78
1:E:453:ARG:CD	2:G:392:ALA:HA	2.14	0.77
2:I:263:ARG:NH1	2:I:315:ASP:OD1	2.18	0.77
1:E:396:ARG:NH1	1:E:399:ASP:OD2	2.18	0.76
2:G:263:ARG:NH1	2:G:315:ASP:OD1	2.20	0.75
2:K:32:TYR:HB2	2:K:298:VAL:HG22	1.69	0.74
2:G:338:ARG:HH22	2:G:364:ALA:HB1	1.52	0.74
2:K:78:LEU:HD13	2:K:307:ARG:NH1	2.03	0.74
1:E:449:LEU:HD22	2:G:392:ALA:CB	2.15	0.74
2:G:71:ALA:HB1	2:G:129:TYR:HD2	1.54	0.73
2:I:32:TYR:HB2	2:I:298:VAL:HG22	1.69	0.73
1:E:363:LEU:HD13	2:G:104:VAL:HG12	1.70	0.73
1:E:218:ARG:NH1	1:E:250:ALA:O	2.22	0.72
2:G:396:ARG:NH1	2:G:399:ASP:OD2	2.22	0.72
2:K:425:LEU:HD12	2:K:448:LEU:HD22	1.71	0.72
2:K:396:ARG:NH1	2:K:399:ASP:OD2	2.23	0.71
2:G:424:VAL:HG13	2:G:427:ARG:NH2	2.07	0.70
2:I:359:GLN:NE2	2:K:99:MET:O	2.23	0.70
2:I:309:LEU:O	2:I:313:TYR:HB3	1.91	0.69
2:K:338:ARG:HB2	2:K:345:VAL:HG22	1.73	0.69
1:E:309:LEU:HD12	1:E:310:SER:N	2.07	0.69
2:I:324:LEU:HD13	2:I:337:ALA:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:196:LYS:NZ	2:K:159:GLU:OE2	2.26	0.68
2:K:126:PRO:HA	2:K:135:ARG:HH22	1.59	0.68
2:K:104:VAL:HG13	2:K:114:VAL:HG11	1.75	0.68
2:I:338:ARG:HH22	2:I:364:ALA:HB1	1.59	0.68
2:I:328:HIS:HB3	2:I:334:ASP:OD1	1.94	0.68
2:I:353:THR:O	2:I:356:THR:CG2	2.32	0.68
2:I:425:LEU:HD12	2:I:448:LEU:HD22	1.74	0.68
2:I:101:THR:OG1	2:K:362:ARG:CZ	2.42	0.68
2:I:396:ARG:NH1	2:I:399:ASP:OD2	2.27	0.68
2:K:71:ALA:HB1	2:K:129:TYR:CD2	2.29	0.67
2:I:324:LEU:O	2:I:339:ARG:NH1	2.27	0.67
1:E:324:LEU:HD12	1:E:325:GLN:HG2	1.76	0.67
2:I:391:HIS:NE2	2:K:446:PHE:HA	2.10	0.66
1:E:324:LEU:HD23	1:E:344:ARG:NE	2.11	0.66
2:G:324:LEU:O	2:G:339:ARG:NH1	2.28	0.66
2:G:315:ASP:OD1	2:G:316:GLN:N	2.29	0.65
1:E:449:LEU:CD2	2:G:392:ALA:HB2	2.20	0.65
1:E:324:LEU:HD23	1:E:344:ARG:CZ	2.26	0.65
2:K:71:ALA:HB1	2:K:129:TYR:HD2	1.60	0.65
2:G:181:VAL:O	2:G:234:GLY:N	2.29	0.65
2:G:309:LEU:HD12	2:G:310:SER:N	2.12	0.64
2:G:412:LEU:HD11	2:G:424:VAL:HG21	1.77	0.64
2:I:264:GLU:O	2:I:268:VAL:HG22	1.96	0.64
1:E:425:LEU:HD12	1:E:448:LEU:HD22	1.78	0.64
2:I:407:ALA:C	2:I:409:PRO:HD3	2.22	0.64
2:I:433:VAL:HG12	2:I:440:HIS:HB2	1.81	0.63
1:E:324:LEU:HD12	1:E:325:GLN:N	2.14	0.63
2:I:78:LEU:HD13	2:I:307:ARG:NH1	2.14	0.63
2:K:312:ILE:HA	2:K:315:ASP:OD2	1.99	0.63
2:I:71:ALA:HB1	2:I:129:TYR:CD2	2.33	0.63
2:G:304:THR:OG1	2:G:306:THR:HG23	1.98	0.62
1:E:71:ALA:HB1	1:E:129:TYR:CD2	2.34	0.62
1:E:104:VAL:HG13	1:E:114:VAL:HG11	1.82	0.62
1:E:304:THR:OG1	1:E:306:THR:HG23	1.99	0.62
1:E:362:ARG:HE	2:G:101:THR:HB	1.64	0.62
2:I:106:HIS:NE2	2:K:306:THR:HG22	2.13	0.62
2:K:421:LEU:HD21	2:K:443:ILE:HG21	1.83	0.61
2:K:158:HIS:CD2	2:K:186:THR:HA	2.36	0.60
2:K:54:GLU:HB3	2:K:58:ARG:NH1	2.17	0.59
1:E:158:HIS:ND1	1:E:186:THR:HA	2.18	0.59
2:G:356:THR:HG23	2:G:357:ALA:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:347:SER:O	2:I:360:ARG:NH1	2.35	0.59
1:E:356:THR:HG23	1:E:357:ALA:N	2.15	0.59
1:E:104:VAL:HB	2:G:363:LEU:CD1	2.33	0.59
2:G:82:LEU:HB2	2:G:110:MET:HE3	1.85	0.59
2:I:356:THR:HG23	2:I:357:ALA:N	2.18	0.59
2:I:158:HIS:CD2	2:I:186:THR:HA	2.37	0.58
2:K:338:ARG:HH22	2:K:364:ALA:HB1	1.68	0.58
2:G:292:LYS:HD3	2:G:292:LYS:N	2.19	0.58
2:K:263:ARG:HH11	2:K:315:ASP:CG	2.11	0.58
2:I:4:ASP:O	2:K:22:THR:HB	2.03	0.58
1:E:71:ALA:HB1	1:E:129:TYR:HD2	1.68	0.58
2:I:32:TYR:OH	2:I:296:ARG:NH2	2.37	0.58
2:K:13:ILE:HD12	2:K:50:VAL:HG21	1.86	0.57
1:E:292:LYS:HD3	1:E:292:LYS:N	2.18	0.57
2:G:424:VAL:HG13	2:G:427:ARG:HH21	1.68	0.57
2:K:32:TYR:OH	2:K:296:ARG:NH2	2.37	0.57
1:E:425:LEU:HD13	1:E:445:ARG:HG2	1.86	0.57
1:E:392:ALA:HA	2:G:453:ARG:HD3	1.85	0.57
1:E:19:VAL:CG1	2:G:8:ALA:HB1	2.33	0.57
1:E:19:VAL:HG11	2:G:8:ALA:HB1	1.84	0.57
1:E:380:VAL:HG11	1:E:430:VAL:CG1	2.34	0.57
2:G:332:LEU:HD13	2:G:335:ILE:HD12	1.87	0.57
2:G:410:GLU:OE2	2:G:424:VAL:HG21	2.05	0.57
1:E:364:ALA:O	1:E:365:ASP:OD1	2.22	0.57
1:E:8:ALA:HB1	2:G:19:VAL:CG1	2.35	0.56
2:G:218:ARG:NH1	2:G:250:ALA:O	2.38	0.56
2:I:22:THR:HB	2:K:4:ASP:O	2.05	0.56
1:E:332:LEU:HD13	1:E:335:ILE:HD12	1.88	0.56
2:G:364:ALA:O	2:G:365:ASP:OD1	2.23	0.56
1:E:309:LEU:HD12	1:E:309:LEU:C	2.31	0.56
2:K:347:SER:O	2:K:360:ARG:NH1	2.38	0.56
1:E:363:LEU:HD21	2:G:108:ARG:NH1	2.21	0.56
2:K:328:HIS:HB2	2:K:339:ARG:HH12	1.70	0.56
1:E:363:LEU:HD22	2:G:104:VAL:HG11	1.88	0.55
2:K:352:ASP:O	2:K:401:VAL:HG23	2.07	0.55
2:K:315:ASP:OD1	2:K:316:GLN:N	2.40	0.55
2:K:330:GLY:HA2	2:K:334:ASP:OD2	2.07	0.55
1:E:363:LEU:HD22	2:G:104:VAL:CG1	2.36	0.55
2:G:103:LYS:HZ1	2:G:308:TYR:HE1	1.52	0.55
1:E:45:LYS:NZ	3:E:601:PLP:C4A	2.70	0.55
2:G:421:LEU:HD21	2:G:443:ILE:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:425:LEU:HD12	2:G:448:LEU:HD22	1.88	0.54
2:I:325:GLN:OE1	2:I:454:ARG:NH1	2.40	0.54
2:K:312:ILE:HA	2:K:315:ASP:CG	2.32	0.54
2:K:370:PRO:HD3	2:K:442:LEU:HD11	1.89	0.54
1:E:51:ALA:HB1	1:E:153:ALA:HB1	1.89	0.54
1:E:363:LEU:HD11	2:G:108:ARG:HD2	1.89	0.54
2:G:410:GLU:OE2	2:G:412:LEU:HD11	2.08	0.54
2:K:368:GLN:NE2	2:K:444:THR:HG22	2.23	0.54
2:G:368:GLN:HG3	2:G:430:VAL:HG21	1.90	0.54
2:K:263:ARG:NH2	2:K:319:THR:OG1	2.42	0.53
2:I:368:GLN:NE2	2:I:444:THR:HG22	2.24	0.53
1:E:335:ILE:HG22	1:E:447:ASP:HB2	1.90	0.53
2:I:352:ASP:HB3	2:I:356:THR:CG2	2.25	0.53
2:G:158:HIS:ND1	2:G:186:THR:HA	2.24	0.53
2:K:313:TYR:O	2:K:316:GLN:HG3	2.08	0.53
2:I:327:LYS:HB2	2:I:339:ARG:NH1	2.23	0.53
2:K:303:ASP:OD2	2:K:308:TYR:OH	2.24	0.53
2:G:123:LYS:HA	2:G:128:TYR:CD2	2.44	0.52
2:I:19:VAL:HG11	2:K:8:ALA:HB1	1.89	0.52
2:G:309:LEU:HD12	2:G:309:LEU:C	2.35	0.52
1:E:171:GLY:O	2:I:6:ARG:NH2	2.42	0.52
2:I:19:VAL:CG1	2:K:8:ALA:HB1	2.39	0.52
2:I:315:ASP:OD1	2:I:316:GLN:N	2.41	0.52
2:K:361:MET:HG2	2:K:369:LEU:HG	1.91	0.52
2:K:310:SER:O	2:K:314:ASN:HB2	2.09	0.52
1:E:104:VAL:HG12	2:G:363:LEU:HD11	1.91	0.51
1:E:347:SER:O	1:E:360:ARG:NH1	2.43	0.51
2:G:51:ALA:HB1	2:G:153:ALA:HB1	1.91	0.51
2:G:321:GLN:O	2:G:324:LEU:HG	2.10	0.51
2:K:338:ARG:CB	2:K:345:VAL:HG22	2.41	0.51
2:I:391:HIS:HE2	2:K:446:PHE:HA	1.76	0.51
1:E:8:ALA:HB1	2:G:19:VAL:HG12	1.92	0.51
2:I:424:VAL:HG11	2:I:430:VAL:O	2.10	0.51
2:K:44:ILE:HD11	2:K:158:HIS:CE1	2.45	0.51
1:E:354:LEU:HB2	1:E:397:PHE:HA	1.93	0.51
2:I:352:ASP:O	2:I:401:VAL:HG23	2.11	0.51
1:E:356:THR:CG2	1:E:357:ALA:N	2.75	0.50
2:G:394:ALA:O	2:G:395:PRO:C	2.55	0.50
2:G:338:ARG:NH2	2:G:364:ALA:HB1	2.23	0.50
2:G:126:PRO:HA	2:G:135:ARG:HH22	1.75	0.50
2:G:312:ILE:HA	2:G:315:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:ASP:O	1:E:296:ARG:HD3	2.11	0.50
1:E:104:VAL:CG1	2:G:363:LEU:CD1	2.90	0.50
2:I:72:THR:HG21	2:I:77:GLY:HA3	1.94	0.50
2:I:123:LYS:HA	2:I:128:TYR:CD2	2.46	0.50
2:K:45:LLP:HB2	2:K:76:THR:HA	1.93	0.50
2:K:126:PRO:O	2:K:135:ARG:NH2	2.44	0.50
2:K:379:GLY:HA2	2:K:409:PRO:HG3	1.93	0.50
1:E:125:HIS:ND1	1:E:126:PRO:HD2	2.27	0.49
1:E:394:ALA:O	1:E:395:PRO:C	2.55	0.49
2:I:398:ARG:N	2:I:398:ARG:HD2	2.27	0.49
2:K:6:ARG:HG3	2:K:10:LEU:HD12	1.93	0.49
2:K:263:ARG:HD2	2:K:315:ASP:HB2	1.94	0.49
1:E:123:LYS:HA	1:E:128:TYR:CD2	2.47	0.49
2:K:321:GLN:O	2:K:324:LEU:HG	2.12	0.49
1:E:422:GLN:HG3	1:E:448:LEU:HD21	1.93	0.49
2:K:412:LEU:O	2:K:434:ALA:O	2.31	0.49
1:E:82:LEU:HB2	1:E:110:MET:HE3	1.95	0.49
2:G:332:LEU:HB2	2:G:414:PRO:O	2.13	0.49
1:E:181:VAL:O	1:E:234:GLY:N	2.43	0.49
2:G:48:ILE:HG13	2:G:49:GLY:N	2.27	0.49
2:I:23:ARG:NH1	2:K:7:PRO:HG3	2.27	0.49
1:E:330:GLY:HA2	1:E:334:ASP:CG	2.38	0.49
1:E:274:GLY:HA2	1:E:308:TYR:CD2	2.48	0.49
2:G:332:LEU:HD23	2:G:416:ALA:O	2.12	0.49
1:E:332:LEU:HB2	1:E:414:PRO:O	2.13	0.49
2:G:356:THR:CG2	2:G:357:ALA:N	2.76	0.48
2:I:225:PRO:HB3	2:I:236:ASP:HB2	1.95	0.48
1:E:267:ARG:HG2	1:E:267:ARG:HH11	1.77	0.48
2:I:45:LLP:HB2	2:I:76:THR:HA	1.95	0.48
2:I:101:THR:OG1	2:K:362:ARG:NE	2.46	0.48
1:E:191:THR:HG23	1:E:246:SER:OG	2.14	0.48
1:E:398:ARG:HD2	1:E:398:ARG:N	2.29	0.48
2:I:126:PRO:HA	2:I:135:ARG:HH22	1.79	0.48
2:G:45:LLP:HB2	2:G:76:THR:HA	1.96	0.48
2:G:54:GLU:HB3	2:G:58:ARG:NH1	2.29	0.48
2:I:313:TYR:O	2:I:316:GLN:HG3	2.12	0.48
1:E:188:THR:O	1:E:192:ARG:HG3	2.14	0.48
2:G:259:PHE:HE1	2:G:275:SER:HB3	1.78	0.48
1:E:209:GLU:HG3	1:E:254:SER:HA	1.96	0.48
2:G:125:HIS:ND1	2:G:126:PRO:HD2	2.28	0.48
2:I:394:ALA:O	2:I:395:PRO:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:104:VAL:HA	2:K:107:LEU:HD12	1.96	0.48
2:K:309:LEU:O	2:K:313:TYR:HB3	2.13	0.47
2:I:391:HIS:NE2	2:K:449:LEU:HB2	2.29	0.47
2:I:48:ILE:O	2:I:49:GLY:C	2.58	0.47
2:I:176:ALA:HB3	2:I:297:VAL:HG22	1.97	0.47
1:E:101:THR:HG23	2:G:363:LEU:HD12	1.96	0.47
2:G:45:LLP:CD	2:G:48:ILE:HD11	2.44	0.47
2:G:393:ASP:O	2:G:394:ALA:C	2.57	0.47
2:G:191:THR:HG23	2:G:246:SER:OG	2.14	0.47
2:I:356:THR:CG2	2:I:357:ALA:N	2.77	0.47
2:G:171:GLY:O	2:K:6:ARG:NH2	2.48	0.47
2:I:6:ARG:HG3	2:I:10:LEU:HD12	1.96	0.47
2:I:97:ASP:O	2:K:355:LEU:CD2	2.63	0.47
2:K:72:THR:OG1	2:K:76:THR:HB	2.15	0.47
2:K:303:ASP:OD2	2:K:308:TYR:CZ	2.68	0.47
2:G:26:THR:OG1	2:G:29:CYS:O	2.32	0.47
2:K:48:ILE:O	2:K:49:GLY:C	2.58	0.47
2:K:178:VAL:HG22	2:K:204:VAL:HB	1.97	0.47
2:K:328:HIS:CB	2:K:339:ARG:HH22	2.28	0.47
2:G:72:THR:OG1	2:G:76:THR:HB	2.14	0.47
2:I:328:HIS:HB2	2:I:339:ARG:CZ	2.44	0.47
1:E:45:LYS:HZ3	3:E:601:PLP:C4A	2.26	0.47
2:I:338:ARG:NH2	2:I:364:ALA:HB1	2.27	0.47
1:E:453:ARG:HD2	2:G:392:ALA:HA	1.94	0.46
1:E:330:GLY:HA2	1:E:334:ASP:OD2	2.15	0.46
1:E:422:GLN:HG2	1:E:426:ASP:OD1	2.14	0.46
2:G:364:ALA:O	2:G:366:VAL:HG13	2.15	0.46
2:K:384:SER:O	2:K:388:LEU:HG	2.14	0.46
1:E:126:PRO:O	1:E:135:ARG:NH2	2.44	0.46
1:E:370:PRO:HD3	1:E:442:LEU:HD11	1.96	0.46
2:G:398:ARG:N	2:G:398:ARG:HD2	2.29	0.46
2:I:368:GLN:O	2:I:369:LEU:HD23	2.14	0.46
2:K:20:ARG:HE	2:K:30:THR:HG23	1.81	0.46
2:K:394:ALA:O	2:K:395:PRO:C	2.58	0.46
2:G:328:HIS:HB3	2:G:334:ASP:OD1	2.14	0.46
1:E:103:LYS:HZ2	1:E:308:TYR:HE1	1.62	0.46
1:E:356:THR:HA	2:G:97:ASP:HB2	1.96	0.46
1:E:380:VAL:HG11	1:E:430:VAL:HG11	1.98	0.46
2:I:367:SER:HA	2:I:383:GLU:OE1	2.16	0.46
2:I:392:ALA:HB2	2:K:449:LEU:CD1	2.46	0.46
1:E:267:ARG:HG2	1:E:267:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:93:LEU:CD1	2:I:107:LEU:HD22	2.46	0.45
1:E:34:LYS:HD3	1:E:166:LEU:HD21	1.99	0.45
1:E:104:VAL:CG1	2:G:363:LEU:HD11	2.46	0.45
2:G:31:LEU:HD12	2:G:297:VAL:O	2.16	0.45
2:K:123:LYS:HA	2:K:128:TYR:CD2	2.52	0.45
1:E:335:ILE:O	1:E:447:ASP:HB3	2.17	0.45
1:E:410:GLU:OE2	1:E:424:VAL:HG21	2.17	0.45
2:I:327:LYS:HB2	2:I:339:ARG:HH11	1.81	0.45
2:I:72:THR:OG1	2:I:76:THR:HB	2.17	0.45
1:E:421:LEU:HD21	1:E:443:ILE:HG21	1.98	0.45
2:G:48:ILE:O	2:G:49:GLY:C	2.60	0.45
2:G:98:LYS:O	2:G:98:LYS:HG2	2.17	0.45
2:I:384:SER:O	2:I:388:LEU:HG	2.17	0.45
2:K:93:LEU:CD1	2:K:107:LEU:HD22	2.47	0.45
2:G:261:MET:HG3	2:G:281:LEU:HD23	1.97	0.44
2:G:282:ALA:O	2:G:286:ARG:HG3	2.17	0.44
1:E:324:LEU:CD1	1:E:325:GLN:HG2	2.44	0.44
1:E:352:ASP:HB3	1:E:356:THR:CG2	2.38	0.44
1:E:425:LEU:HD13	1:E:445:ARG:CG	2.46	0.44
2:K:45:LLP:HD3	2:K:48:ILE:HD11	1.99	0.44
1:E:45:LYS:HD2	1:E:76:THR:OG1	2.17	0.44
2:G:117:THR:HG21	2:G:132:VAL:HG21	1.99	0.44
1:E:186:THR:OG1	3:E:601:PLP:O2P	2.24	0.44
2:G:18:LEU:HD12	2:G:33:LEU:C	2.43	0.44
1:E:332:LEU:HD23	1:E:416:ALA:O	2.17	0.44
2:G:72:THR:HG21	2:G:77:GLY:HA3	1.99	0.44
2:G:336:ILE:HD11	2:G:433:VAL:HB	2.00	0.44
2:I:449:LEU:HD12	2:K:391:HIS:NE2	2.33	0.44
2:K:173:ASP:O	2:K:296:ARG:HD3	2.18	0.44
2:K:260:ALA:HA	2:K:263:ARG:HD3	2.00	0.44
2:K:125:HIS:CG	2:K:126:PRO:HD2	2.53	0.44
1:E:144:PHE:CE2	1:E:146:ALA:HA	2.53	0.43
2:G:34:LYS:HD3	2:G:166:LEU:HD21	2.00	0.43
2:G:347:SER:O	2:G:360:ARG:NH1	2.51	0.43
2:I:48:ILE:HG13	2:I:49:GLY:N	2.33	0.43
2:I:101:THR:OG1	2:K:362:ARG:NH2	2.51	0.43
1:E:48:ILE:O	1:E:49:GLY:C	2.60	0.43
2:I:20:ARG:HE	2:I:30:THR:HG23	1.82	0.43
2:I:125:HIS:CG	2:I:126:PRO:HD2	2.53	0.43
2:I:361:MET:HG2	2:I:369:LEU:HD21	2.01	0.43
2:I:430:VAL:HG12	2:I:431:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1:MET:HE1	2:K:87:LYS:O	2.18	0.43
1:E:45:LYS:HB3	1:E:76:THR:HA	2.00	0.43
1:E:336:ILE:HD11	1:E:433:VAL:HB	2.00	0.43
2:G:18:LEU:HD12	2:G:33:LEU:O	2.19	0.43
2:I:23:ARG:HH11	2:K:7:PRO:HG3	1.84	0.43
2:I:303:ASP:OD2	2:I:308:TYR:CZ	2.72	0.43
1:E:104:VAL:HB	2:G:363:LEU:HD13	1.99	0.43
2:G:382:ASP:O	2:G:386:ILE:HG13	2.19	0.43
2:K:70:GLU:O	2:K:93:LEU:HA	2.18	0.43
2:K:328:HIS:CD2	2:K:339:ARG:HH12	2.37	0.43
1:E:334:ASP:HA	1:E:339:ARG:HH21	1.83	0.43
2:G:179:VAL:HA	2:G:280:LEU:HD21	2.01	0.43
2:G:330:GLY:HA2	2:G:334:ASP:OD2	2.19	0.43
2:I:425:LEU:CD1	2:I:448:LEU:HD22	2.45	0.43
1:E:359:GLN:CD	2:G:99:MET:O	2.62	0.43
2:G:393:ASP:OD1	2:G:393:ASP:N	2.49	0.43
2:K:54:GLU:HB3	2:K:58:ARG:HH12	1.82	0.43
1:E:104:VAL:HA	1:E:107:LEU:HD12	2.00	0.43
1:E:453:ARG:CZ	1:E:453:ARG:HB3	2.48	0.43
2:G:268:VAL:HG23	2:G:269:GLU:HG2	2.01	0.43
2:I:45:LLP:OP3	2:I:183:SER:OG	2.35	0.43
2:K:314:ASN:O	2:K:318:MET:SD	2.76	0.43
1:E:356:THR:HA	2:G:97:ASP:CB	2.49	0.42
2:K:67:THR:HG23	2:K:90:ARG:HB3	2.01	0.42
2:I:263:ARG:HH12	2:I:316:GLN:HB3	1.84	0.42
2:I:361:MET:HG2	2:I:369:LEU:CD2	2.49	0.42
2:K:72:THR:HG21	2:K:77:GLY:HA3	2.00	0.42
2:K:334:ASP:HA	2:K:339:ARG:HH21	1.84	0.42
2:K:383:GLU:HG2	2:K:384:SER:N	2.34	0.42
2:G:171:GLY:O	2:G:172:HIS:HB2	2.18	0.42
2:G:354:LEU:HB2	2:G:397:PHE:HA	2.01	0.42
2:G:425:LEU:CD1	2:G:448:LEU:HD22	2.49	0.42
2:I:70:GLU:O	2:I:93:LEU:HA	2.20	0.42
2:I:178:VAL:HG22	2:I:204:VAL:HB	2.02	0.42
1:E:422:GLN:O	1:E:426:ASP:OD1	2.37	0.42
2:G:45:LLP:HD2	2:G:48:ILE:HD11	2.01	0.42
2:I:328:HIS:H	2:I:339:ARG:HH12	1.68	0.42
2:I:338:ARG:HH12	2:I:364:ALA:HB1	1.85	0.42
1:E:363:LEU:O	2:G:105:LEU:HD21	2.20	0.42
1:E:380:VAL:HB	1:E:432:ILE:HD11	2.02	0.42
2:K:41:GLY:N	2:K:46:ASP:OD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:48:ILE:HG13	2:K:49:GLY:N	2.35	0.42
2:I:329:TYR:C	2:I:334:ASP:OD2	2.63	0.42
2:I:392:ALA:HA	2:K:449:LEU:HD13	2.02	0.42
2:I:392:ALA:HB2	2:K:449:LEU:HD11	2.02	0.42
1:E:8:ALA:HB1	2:G:19:VAL:HG11	2.00	0.42
1:E:104:VAL:CG1	2:G:363:LEU:HD13	2.50	0.42
2:G:173:ASP:O	2:G:296:ARG:HD3	2.19	0.42
2:I:105:LEU:CD2	2:K:313:TYR:CE2	3.03	0.42
1:E:72:THR:OG1	1:E:76:THR:HB	2.20	0.41
1:E:259:PHE:HE1	1:E:275:SER:HB3	1.85	0.41
2:G:410:GLU:OE2	2:G:424:VAL:CG2	2.67	0.41
2:K:50:VAL:HG12	2:K:54:GLU:OE1	2.20	0.41
2:I:19:VAL:HG21	2:K:12:LEU:HD21	2.03	0.41
2:I:391:HIS:CE1	2:K:449:LEU:HB2	2.55	0.41
2:K:315:ASP:HA	2:K:318:MET:HE2	2.01	0.41
1:E:97:ASP:OD2	2:G:356:THR:HB	2.20	0.41
1:E:261:MET:HG3	1:E:281:LEU:HD23	2.03	0.41
1:E:425:LEU:CD1	1:E:448:LEU:HD22	2.48	0.41
2:I:361:MET:HG2	2:I:369:LEU:HG	2.02	0.41
2:I:390:VAL:HG11	2:I:397:PHE:CD2	2.56	0.41
2:K:50:VAL:O	2:K:51:ALA:C	2.62	0.41
2:I:45:LLP:H2'1	2:I:276:SER:OG	2.20	0.41
1:E:449:LEU:CD2	2:G:392:ALA:CB	2.91	0.41
2:I:299:SER:OG	2:I:300:PHE:N	2.54	0.41
2:I:391:HIS:CD2	2:K:449:LEU:HD12	2.56	0.41
2:K:265:LEU:HD12	2:K:269:GLU:HB2	2.02	0.41
1:E:32:TYR:HB2	1:E:298:VAL:HG22	2.02	0.41
1:E:335:ILE:HG22	1:E:447:ASP:CB	2.50	0.41
2:G:390:VAL:HG11	2:G:397:PHE:CE2	2.56	0.41
2:I:321:GLN:O	2:I:324:LEU:HG	2.19	0.41
2:K:261:MET:HG3	2:K:281:LEU:HD23	2.02	0.41
2:G:324:LEU:HA	2:G:327:LYS:HG2	2.02	0.41
2:I:16:THR:HB	2:I:35:LEU:O	2.21	0.41
2:I:50:VAL:O	2:I:51:ALA:C	2.63	0.41
2:G:50:VAL:O	2:G:51:ALA:C	2.64	0.41
2:I:45:LLP:HG3	2:I:45:LLP:H4'1	2.03	0.41
2:I:86:ALA:HA	2:K:267:ARG:O	2.21	0.41
2:I:260:ALA:HA	2:I:263:ARG:HD3	2.02	0.41
1:E:151:ASN:OD1	1:E:152:PRO:HD2	2.21	0.40
1:E:324:LEU:HD23	1:E:344:ARG:CD	2.51	0.40
1:E:22:THR:HB	2:G:4:ASP:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:LEU:HD23	1:E:323:LEU:HA	1.91	0.40
1:E:356:THR:HB	2:G:97:ASP:OD2	2.21	0.40
2:I:109:ALA:HB2	2:K:313:TYR:HB2	2.03	0.40
2:K:427:ARG:HH21	2:K:429:LEU:HB2	1.86	0.40
2:G:48:ILE:HG21	2:G:154:ASN:OD1	2.21	0.40
2:I:430:VAL:CG1	2:I:431:ALA:N	2.84	0.40
2:I:449:LEU:HD11	2:K:392:ALA:HB2	2.03	0.40
2:G:16:THR:OG1	2:G:34:LYS:HE3	2.21	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	E	455/457 (100%)	439 (96%)	16 (4%)	0	100	100
2	G	454/457 (99%)	437 (96%)	17 (4%)	0	100	100
2	I	454/457 (99%)	434 (96%)	20 (4%)	0	100	100
2	K	454/457 (99%)	437 (96%)	17 (4%)	0	100	100
All	All	1817/1828 (99%)	1747 (96%)	70 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	E	357/364 (98%)	357 (100%)	0	100	100
2	G	359/363 (99%)	359 (100%)	0	100	100
2	I	359/363 (99%)	359 (100%)	0	100	100
2	K	361/363 (99%)	361 (100%)	0	100	100
All	All	1436/1453 (99%)	1436 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	249	HIS
2	G	249	HIS
2	G	422	GLN
2	I	249	HIS
2	K	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	LLP	K	45	2	23,24,25	1.16	1 (4%)	25,32,34	2.45	2 (8%)
2	LLP	I	45	2	23,24,25	1.15	1 (4%)	25,32,34	2.26	3 (12%)
2	LLP	G	45	2	23,24,25	1.14	1 (4%)	25,32,34	1.92	2 (8%)

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	LLP	K	45	2	-	6/16/17/19	0/1/1/1
2	LLP	I	45	2	-	6/16/17/19	0/1/1/1
2	LLP	G	45	2	-	6/16/17/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	45	LLP	C4'-NZ	4.83	1.43	1.27
2	I	45	LLP	C4'-NZ	4.82	1.43	1.27
2	G	45	LLP	C4'-NZ	4.79	1.43	1.27

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	45	LLP	CE-NZ-C4'	8.74	145.73	118.90
2	I	45	LLP	CE-NZ-C4'	8.60	145.32	118.90
2	G	45	LLP	C4-C4'-NZ	7.76	159.94	124.31
2	K	45	LLP	C4-C4'-NZ	7.68	159.54	124.31
2	I	45	LLP	C4-C4'-NZ	6.23	152.89	124.31
2	G	45	LLP	CE-NZ-C4'	4.46	132.59	118.90
2	I	45	LLP	OP4-C5'-C5	2.33	113.79	109.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	45	LLP	C4-C4'-NZ-CE
2	G	45	LLP	C4-C5-C5'-OP4
2	G	45	LLP	C6-C5-C5'-OP4
2	I	45	LLP	C4-C5-C5'-OP4
2	I	45	LLP	C6-C5-C5'-OP4
2	K	45	LLP	C4-C5-C5'-OP4
2	K	45	LLP	C6-C5-C5'-OP4
2	K	45	LLP	C4-C4'-NZ-CE
2	I	45	LLP	CD-CE-NZ-C4'
2	I	45	LLP	C4-C4'-NZ-CE
2	K	45	LLP	CD-CE-NZ-C4'
2	G	45	LLP	C3-C4-C4'-NZ

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Mol	Chain	Res	Type	Atoms
2	I	45	LLP	C3-C4-C4'-NZ
2	K	45	LLP	C3-C4-C4'-NZ
2	G	45	LLP	CD-CE-NZ-C4'
2	I	45	LLP	C5-C4-C4'-NZ
2	K	45	LLP	C5-C4-C4'-NZ
2	G	45	LLP	CG-CD-CE-NZ

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	45	LLP	2	0
2	I	45	LLP	4	0
2	G	45	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	PLP	E	601	-	15,15,16	0.75	1 (6%)	20,22,23	0.62	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
3	PLP	E	601	-	-	0/6/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	601	PLP	C4A-C4	-2.37	1.46	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	PLP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	457/457 (100%)	0.88	73 (15%) 5 5	21, 95, 162, 254	144 (31%)
2	G	456/457 (99%)	0.97	68 (14%) 5 6	24, 94, 157, 235	143 (31%)
2	I	456/457 (99%)	0.92	69 (15%) 5 6	23, 105, 170, 223	137 (30%)
2	K	456/457 (99%)	1.00	63 (13%) 6 6	40, 111, 189, 241	140 (30%)
All	All	1825/1828 (99%)	0.94	273 (14%) 5 6	21, 100, 175, 254	564 (30%)

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	433	VAL	12.3
2	G	431	ALA	11.2
2	K	430	VAL	10.0
1	E	431	ALA	9.1
2	G	379	GLY	8.5
2	G	412	LEU	8.4
1	E	338	ARG	7.4
2	I	432	ILE	7.4
1	E	312	ILE	7.3
2	G	312	ILE	7.2
2	G	413	ALA	7.2
2	K	434	ALA	7.2
2	G	371	VAL	7.1
2	K	432	ILE	6.9
1	E	342	GLU	6.9
2	K	324	LEU	6.7
2	I	332	LEU	6.7
2	I	323	LEU	6.6
1	E	421	LEU	6.4
2	K	431	ALA	6.2
1	E	349	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
2	K	348	VAL	6.1
2	K	381	ILE	6.0
2	I	348	VAL	6.0
2	I	430	VAL	5.8
2	G	429	LEU	5.4
2	I	345	VAL	5.3
2	G	449	LEU	5.3
2	G	378	VAL	5.2
2	I	413	ALA	5.2
2	K	312	ILE	5.0
1	E	412	LEU	5.0
2	I	357	ALA	4.9
2	K	439	PHE	4.9
2	I	439	PHE	4.8
1	E	455	LYS	4.7
2	G	260	ALA	4.6
2	I	321	GLN	4.6
1	E	430	VAL	4.6
2	K	323	LEU	4.6
1	E	429	LEU	4.5
2	K	350	PRO	4.5
1	E	371	VAL	4.4
2	G	409	PRO	4.4
2	G	112	ALA	4.3
2	I	433	VAL	4.3
2	G	353	THR	4.3
2	K	315	ASP	4.3
1	E	392	ALA	4.2
2	I	370	PRO	4.2
2	G	421	LEU	4.2
2	I	409	PRO	4.2
2	G	381	ILE	4.1
2	K	349	GLY	4.1
2	K	346	ILE	4.1
1	E	313	TYR	4.1
2	I	380	VAL	4.0
1	E	137	ALA	4.0
1	E	5	SER	4.0
2	G	202	GLU	4.0
2	G	268	VAL	3.9
2	K	401	VAL	3.9
2	I	346	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
2	I	438	GLY	3.9
2	K	104	VAL	3.9
2	I	431	ALA	3.8
2	I	366	VAL	3.8
2	I	312	ILE	3.7
2	K	445	ARG	3.7
2	K	408	ALA	3.7
1	E	381	ILE	3.6
2	I	417	SER	3.6
2	K	440	HIS	3.6
2	I	349	GLY	3.6
1	E	339	ARG	3.6
2	I	434	ALA	3.6
2	I	384	SER	3.6
2	K	352	ASP	3.6
1	E	424	VAL	3.6
2	I	442	LEU	3.6
2	G	408	ALA	3.5
2	I	412	LEU	3.5
2	I	456	LEU	3.5
2	K	357	ALA	3.5
2	G	332	LEU	3.4
2	K	325	GLN	3.4
2	G	262	ALA	3.4
2	G	114	VAL	3.4
2	I	406	ASN	3.3
2	G	430	VAL	3.3
2	K	425	LEU	3.3
1	E	379	GLY	3.3
2	I	354	LEU	3.3
2	I	445	ARG	3.3
1	E	112	ALA	3.3
2	K	331	ASP	3.3
2	I	395	PRO	3.3
2	G	447	ASP	3.2
2	K	398	ARG	3.2
2	G	446	PHE	3.2
2	G	445	ARG	3.2
1	E	59	ASP	3.1
2	I	386	ILE	3.1
1	E	457	ALA	3.1
2	K	309	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	K	353	THR	3.1
1	E	268	VAL	3.1
2	I	401	VAL	3.1
1	E	56	ALA	3.1
2	K	73	ALA	3.1
2	K	372	LEU	3.1
2	K	413	ALA	3.1
2	I	451	HIS	3.0
1	E	130	GLN	3.0
1	E	321	GLN	3.0
2	K	370	PRO	3.0
2	G	142	GLY	3.0
1	E	114	VAL	3.0
1	E	418	LEU	3.0
1	E	118	ARG	3.0
2	G	313	TYR	3.0
2	K	230	VAL	3.0
2	I	258	SER	2.9
2	G	346	ILE	2.9
1	E	222	LEU	2.9
1	E	324	LEU	2.9
2	G	137	ALA	2.9
1	E	340	PHE	2.9
2	K	251	TYR	2.9
2	G	457	ALA	2.9
2	I	452	LEU	2.9
2	I	398	ARG	2.8
2	I	388	LEU	2.8
2	K	5	SER	2.8
2	G	432	ILE	2.8
2	I	340	PHE	2.8
2	K	386	ILE	2.8
1	E	102	GLU	2.8
2	G	173	ASP	2.8
2	K	327	LYS	2.8
2	K	448	LEU	2.8
2	G	343	GLY	2.8
1	E	325	GLN	2.8
2	I	422	GLN	2.8
2	K	371	VAL	2.8
1	E	449	LEU	2.8
2	G	342	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	3	SER	2.8
2	I	5	SER	2.8
2	G	4	ASP	2.7
1	E	337	ALA	2.7
2	K	329	TYR	2.7
2	K	260	ALA	2.7
2	I	104	VAL	2.7
2	K	390	VAL	2.7
2	G	222	LEU	2.7
2	G	143	ALA	2.7
1	E	377	LEU	2.7
1	E	446	PHE	2.7
2	G	293	GLU	2.7
2	G	59	ASP	2.7
2	G	315	ASP	2.7
2	K	35	LEU	2.7
2	G	319	THR	2.7
2	I	170	THR	2.7
2	I	347	SER	2.7
1	E	260	ALA	2.7
2	K	55	ALA	2.7
2	I	106	HIS	2.7
1	E	401	VAL	2.6
2	K	275	SER	2.6
2	G	338	ARG	2.6
1	E	451	HIS	2.6
1	E	46	ASP	2.6
1	E	143	ALA	2.6
2	G	99	MET	2.5
2	G	141	PRO	2.5
2	I	324	LEU	2.5
2	K	452	LEU	2.5
1	E	433	VAL	2.5
2	K	351	ASP	2.5
2	I	6	ARG	2.5
2	G	345	VAL	2.5
1	E	4	ASP	2.5
2	G	335	ILE	2.5
2	K	340	PHE	2.5
1	E	110	MET	2.5
2	I	99	MET	2.5
2	K	311	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	433	VAL	2.5
2	I	95	VAL	2.5
2	G	392	ALA	2.4
2	G	5	SER	2.4
2	G	393	ASP	2.4
2	I	51	ALA	2.4
1	E	1	MET	2.4
1	E	139	ASP	2.4
1	E	330	GLY	2.4
2	G	348	VAL	2.4
1	E	413	ALA	2.4
2	K	177	ILE	2.4
1	E	394	ALA	2.4
1	E	439	PHE	2.4
2	K	257	GLU	2.4
1	E	319	THR	2.3
2	I	426	ASP	2.3
2	G	401	VAL	2.3
2	I	319	THR	2.3
2	I	59	ASP	2.3
2	I	351	ASP	2.3
1	E	432	ILE	2.3
2	I	73	ALA	2.3
2	K	380	VAL	2.3
2	G	344	ARG	2.3
2	K	338	ARG	2.3
2	I	408	ALA	2.3
1	E	150	ASN	2.3
2	K	236	ASP	2.3
2	I	63	ARG	2.3
1	E	111	GLY	2.3
2	I	322	GLY	2.3
2	I	377	LEU	2.3
2	I	418	LEU	2.3
2	I	4	ASP	2.3
2	I	230	VAL	2.3
2	G	428	GLY	2.2
2	I	246	SER	2.2
2	G	261	MET	2.2
2	G	425	LEU	2.2
1	E	327	LYS	2.2
1	E	332	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	G	318	MET	2.2
2	G	441	GLY	2.2
2	I	379	GLY	2.2
2	K	344	ARG	2.2
2	G	321	GLN	2.2
1	E	107	LEU	2.2
1	E	425	LEU	2.2
1	E	331	ASP	2.2
1	E	218	ARG	2.2
2	I	117	THR	2.2
2	I	268	VAL	2.2
1	E	368	GLN	2.2
2	G	311	LYS	2.2
2	I	111	GLY	2.2
2	K	142	GLY	2.2
2	I	399	ASP	2.2
2	I	435	ASP	2.2
1	E	249	HIS	2.2
2	G	380	VAL	2.1
2	K	3	SER	2.1
1	E	202	GLU	2.1
2	K	454	ARG	2.1
1	E	397	PHE	2.1
2	G	451	HIS	2.1
2	G	56	ALA	2.1
1	E	409	PRO	2.1
2	G	139	ASP	2.1
2	K	106	HIS	2.1
2	G	376	LYS	2.1
2	K	313	TYR	2.1
2	G	368	GLN	2.1
1	E	317	TRP	2.1
1	E	99	MET	2.1
2	G	276	SER	2.1
1	E	52	MET	2.1
2	K	99	MET	2.1
2	I	141	PRO	2.1
1	E	344	ARG	2.0
1	E	387	LEU	2.0
2	G	17	PRO	2.0
2	K	406	ASN	2.0
2	K	362	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	LLP	G	45	24/25	0.91	0.13	39,94,135,161	0
2	LLP	K	45	24/25	0.92	0.13	59,98,130,190	0
2	LLP	I	45	24/25	0.94	0.12	51,77,107,117	0

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	PLP	E	601	15/16	0.84	0.16	75,98,136,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.