



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:29 AM UTC

PDB ID : 2J9P / pdb_00002j9p
Title : Crystal structure of the Bacillus subtilis PBP4a, and its complex with a peptidoglycan mimetic peptide.
Authors : Sauvage, E.; Herman, R.; Kerff, F.; Duez, C.; Charlier, P.
Deposited on : 2006-11-15
Resolution : 2.80 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)
Validation Pipeline (wwPDB-VP) : 2.49

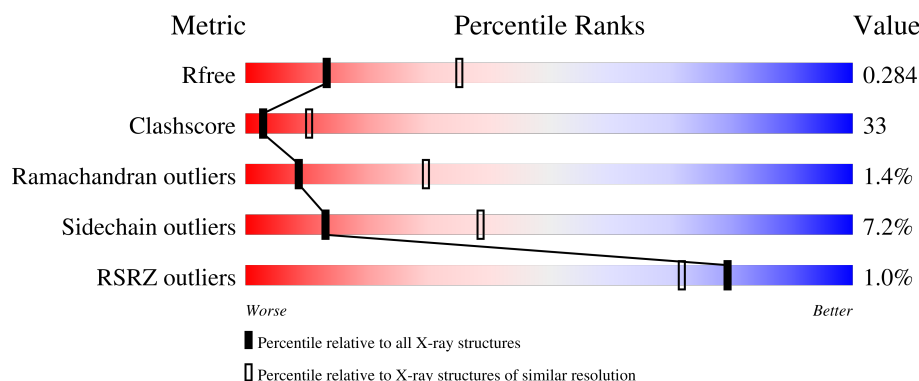
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	462	% 48% 43% 7% ..
1	B	462	% 44% 49% 6% .

2 Entry composition [i](#)

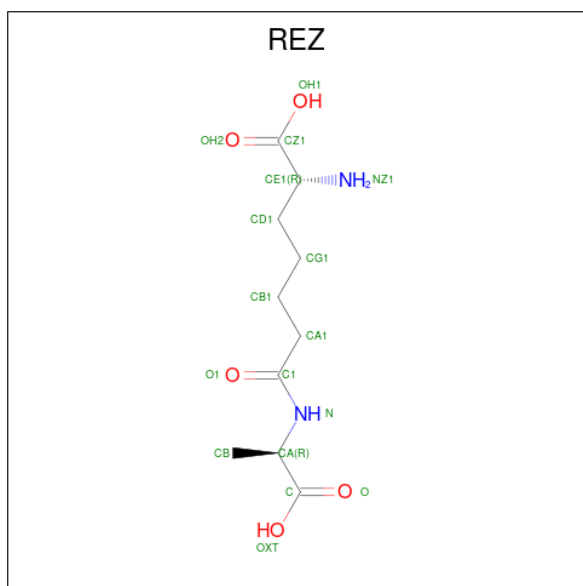
There are 3 unique types of molecules in this entry. The entry contains 6966 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-alanyl-D-alanine carboxypeptidase DacC.

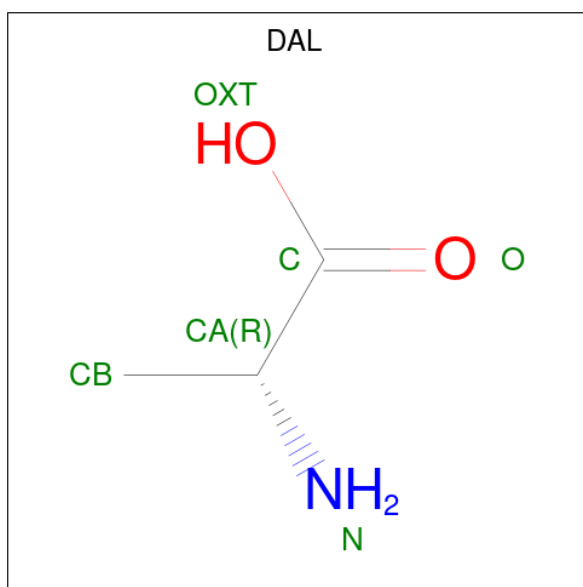
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3461	2169	582	700	10			
1	B	458	Total	C	N	O	S	0	0	0
			3461	2169	582	700	10			

- Molecule 2 is (2R)-2-AMINO-7-[(1R)-1-CARBOXYETHYL]AMINO}-7-OXOHEPTANOIC ACID (CCD ID: REZ) (formula: $C_{10}H_{18}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	10	2	4		
2	B	1	Total	C	N	O	0	0
			16	10	2	4		

- Molecule 3 is D-ALANINE (CCD ID: DAL) (formula: $C_3H_7NO_2$).

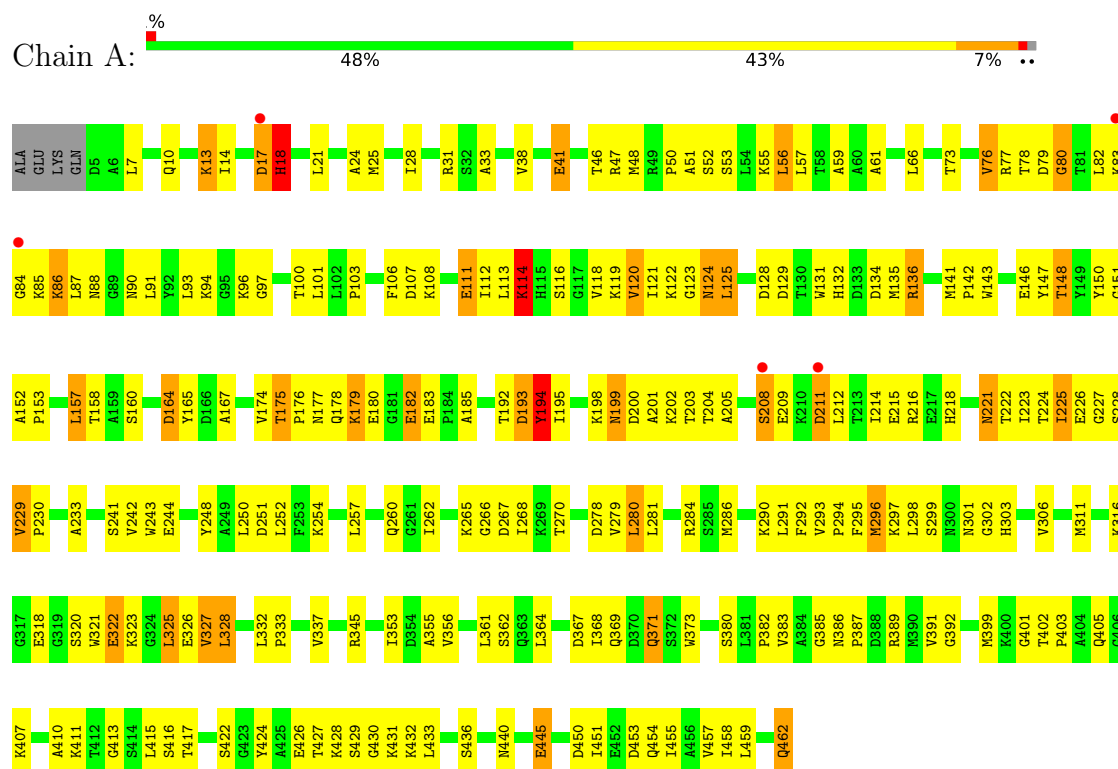


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	3	1	2		
3	B	1	Total	C	N	O	0	0
			6	3	1	2		

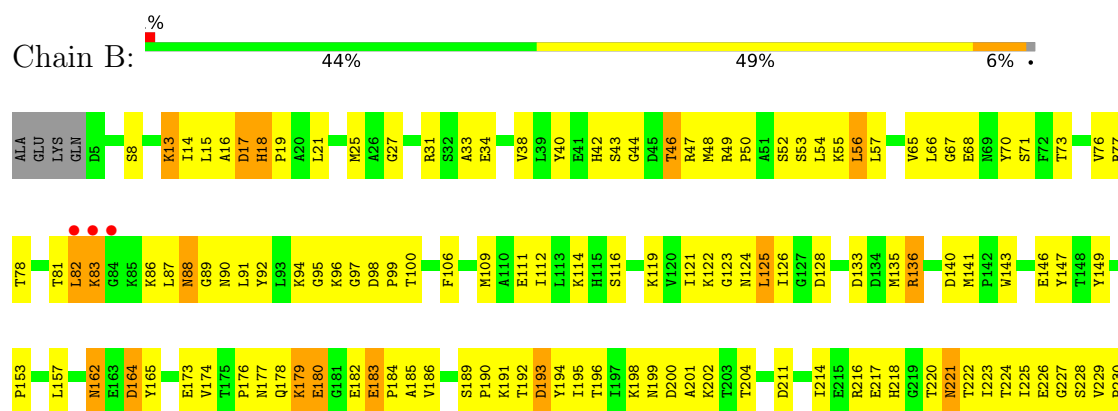
3 Residue-property plots

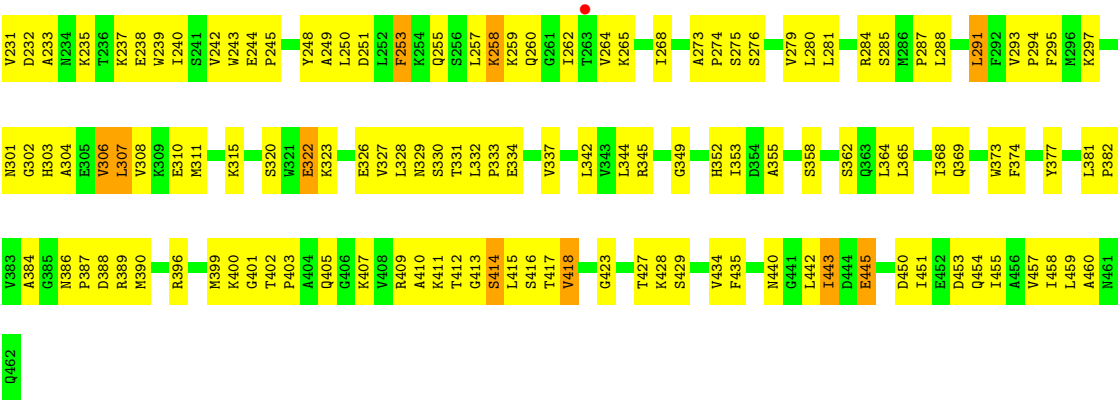
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: D-alanyl-D-alanine carboxypeptidase DacC





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.86Å 77.59Å 164.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.80 19.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.7 (19.90-2.80) 89.5 (19.90-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.290 0.208 , 0.284	Depositor DCC
R_{free} test set	1051 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6966	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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

5.1 Standard geometry

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

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	0.53	0/3520	1.06	20/4765 (0.4%)
1	B	0.42	0/3520	0.95	12/4765 (0.3%)
All	All	0.48	0/7040	1.01	32/9530 (0.3%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ASP	N-CA-C	-9.83	101.04	113.23
1	A	211	ASP	N-CA-C	-8.87	102.55	112.57
1	B	164	ASP	N-CA-C	-7.84	103.50	113.23
1	B	18	HIS	CA-C-N	7.30	126.97	119.82
1	B	18	HIS	C-N-CA	7.30	126.97	119.82
1	A	369	GLN	N-CA-C	6.96	118.86	111.28
1	B	443	ILE	N-CA-C	-6.39	104.11	110.62
1	B	253	PHE	N-CA-C	-6.38	104.76	112.54
1	A	33	ALA	N-CA-C	-6.34	104.81	112.54
1	A	193	ASP	N-CA-C	-6.29	105.64	113.38
1	A	367	ASP	N-CA-C	6.18	117.82	111.14
1	A	113	LEU	N-CA-C	-6.08	106.18	113.97
1	A	83	LYS	N-CA-C	-5.85	106.38	112.93
1	B	126	ILE	N-CA-C	5.83	116.47	107.78
1	A	194	TYR	N-CA-C	-5.75	106.87	112.97
1	B	17	ASP	N-CA-C	5.64	119.16	112.72
1	B	193	ASP	N-CA-C	-5.58	106.14	113.17
1	A	114	LYS	N-CA-C	-5.50	105.19	111.14
1	B	136	ARG	N-CA-C	5.46	118.28	111.24
1	A	296	MET	N-CA-C	5.35	118.97	112.23
1	B	418	VAL	N-CA-C	5.33	115.80	108.12
1	A	76	VAL	N-CA-C	-5.33	100.71	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	SER	N-CA-C	5.26	117.07	108.55
1	A	328	LEU	N-CA-C	-5.24	105.21	111.03
1	A	215	GLU	N-CA-C	5.18	116.16	108.60
1	A	152	ALA	CA-C-N	5.17	125.11	119.78
1	A	152	ALA	C-N-CA	5.17	125.11	119.78
1	B	307	LEU	N-CA-C	-5.17	105.73	111.36
1	A	97	GLY	N-CA-C	5.17	120.96	114.25
1	A	199	ASN	N-CA-C	5.16	116.98	109.71
1	A	141	MET	N-CA-C	5.11	116.34	109.24
1	A	116	SER	N-CA-C	-5.01	106.42	112.54

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	3461	0	3463	206	1
1	B	3461	0	3463	245	1
2	A	16	0	16	5	0
2	B	16	0	16	2	0
3	A	6	0	6	2	0
3	B	6	0	6	0	0
All	All	6966	0	6970	453	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (453) 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:111:GLU:HA	1:B:260:GLN:HE21	1.03	1.05
1:B:57:LEU:HD23	1:B:364:LEU:HD22	1.39	1.00
1:B:407:LYS:HZ3	1:B:428:LYS:HD3	1.30	0.97
1:A:415:LEU:O	1:A:445:GLU:HG2	1.66	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:HB3	1:A:120:VAL:HG13	1.47	0.94
1:A:112:ILE:HD11	1:A:281:LEU:HD22	1.53	0.90
1:B:111:GLU:HA	1:B:260:GLN:NE2	1.88	0.88
1:B:76:VAL:HB	1:B:281:LEU:HG	1.55	0.88
1:A:91:LEU:HD22	1:A:121:ILE:HD13	1.56	0.88
1:B:82:LEU:HD11	1:B:86:LYS:HE2	1.56	0.86
1:A:192:THR:HG22	1:A:194:TYR:H	1.40	0.86
1:A:47:ARG:HG2	1:A:355:ALA:HB1	1.54	0.86
1:A:321:TRP:O	1:A:325:LEU:HB2	1.75	0.86
1:B:401:GLY:H	1:B:405:GLN:NE2	1.75	0.85
1:A:82:LEU:HG	1:A:84:GLY:H	1.40	0.85
1:A:177:ASN:HD21	1:A:182:GLU:HB3	1.43	0.82
1:B:87:LEU:HG	1:B:88:ASN:H	1.43	0.82
1:B:192:THR:HG22	1:B:194:TYR:H	1.43	0.82
1:B:331:THR:O	1:B:334:GLU:HG2	1.82	0.80
1:A:25:MET:HG3	1:A:48:MET:HE3	1.63	0.79
1:A:82:LEU:HD23	1:A:86:LYS:O	1.82	0.79
1:B:47:ARG:HB3	1:B:355:ALA:HB1	1.64	0.78
1:B:77:ARG:HA	1:B:280:LEU:HD13	1.65	0.78
1:A:86:LYS:HB3	1:A:120:VAL:CG1	2.15	0.77
1:B:71:SER:HB3	1:B:284:ARG:HH11	1.48	0.76
1:B:125:LEU:HD22	1:B:250:LEU:HD11	1.68	0.75
1:B:82:LEU:HD13	1:B:86:LYS:HG2	1.67	0.75
1:A:21:LEU:HD11	1:A:451:ILE:HD13	1.68	0.75
1:B:192:THR:HG23	1:B:251:ASP:OD2	1.87	0.74
1:A:401:GLY:H	1:A:405:GLN:NE2	1.84	0.74
1:A:212:LEU:HD11	1:A:225:ILE:HD11	1.69	0.74
1:B:217:GLU:HB2	1:B:220:THR:OG1	1.88	0.74
1:A:143:TRP:O	1:A:146:GLU:HG3	1.87	0.73
1:B:14:ILE:HG13	1:B:454:GLN:NE2	2.03	0.73
1:B:311:MET:HB3	1:B:327:VAL:HG21	1.68	0.73
1:B:97:GLY:O	1:B:99:PRO:HD3	1.87	0.73
1:B:121:ILE:HG22	1:B:123:GLY:H	1.54	0.73
1:A:90:ASN:HD22	1:A:123:GLY:HA3	1.54	0.72
1:B:407:LYS:HZ3	1:B:428:LYS:CD	2.02	0.71
1:B:401:GLY:H	1:B:405:GLN:HE22	1.37	0.71
1:A:426:GLU:HG2	1:A:432:LYS:NZ	2.06	0.71
1:A:431:LYS:HE3	1:A:433:LEU:HD21	1.70	0.71
1:B:225:ILE:HG13	1:B:225:ILE:O	1.91	0.71
1:A:322:GLU:O	1:A:326:GLU:HG3	1.91	0.70
1:B:310:GLU:OE2	1:B:310:GLU:HA	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLU:CD	1:A:445:GLU:H	1.96	0.69
1:B:403:PRO:HD2	1:B:457:VAL:HG13	1.75	0.69
1:B:211:ASP:O	1:B:227:GLY:HA3	1.93	0.69
1:A:426:GLU:HG2	1:A:432:LYS:HZ3	1.56	0.69
1:B:176:PRO:HB3	1:B:229:VAL:HG22	1.75	0.68
1:A:86:LYS:CB	1:A:120:VAL:HG13	2.21	0.68
1:A:57:LEU:HD23	1:A:364:LEU:HD22	1.76	0.68
1:A:296:MET:HB2	1:A:380:SER:HB2	1.74	0.68
1:A:422:SER:HB3	1:A:436:SER:HA	1.75	0.68
1:A:91:LEU:HD22	1:A:121:ILE:CD1	2.22	0.68
1:B:90:ASN:HD22	1:B:124:ASN:HB2	1.59	0.68
1:A:177:ASN:ND2	1:A:182:GLU:HB3	2.09	0.67
1:B:106:PHE:HA	1:B:109:MET:HE3	1.75	0.67
1:B:330:SER:O	1:B:333:PRO:HD2	1.95	0.67
1:A:293:VAL:O	1:A:297:LYS:HB2	1.95	0.66
1:A:195:ILE:HD12	1:A:223:ILE:CD1	2.25	0.66
1:B:44:GLY:HA2	1:B:358:SER:OG	1.96	0.66
1:B:82:LEU:HB3	1:B:86:LYS:O	1.96	0.65
1:A:195:ILE:HD12	1:A:223:ILE:HD11	1.78	0.65
1:A:177:ASN:H	1:A:203:THR:HG21	1.60	0.65
1:B:66:LEU:HD21	1:B:311:MET:HG2	1.77	0.65
1:B:78:THR:HG22	1:B:280:LEU:HD11	1.78	0.65
1:B:33:ALA:HB1	1:B:369:GLN:HE22	1.62	0.65
1:A:124:ASN:N	1:A:124:ASN:HD22	1.94	0.64
1:A:134:ASP:HA	1:A:136:ARG:HH21	1.62	0.64
1:A:431:LYS:CE	1:A:433:LEU:HD21	2.26	0.64
1:B:143:TRP:HA	1:B:146:GLU:HG3	1.80	0.64
1:B:73:THR:HG22	1:B:284:ARG:HG2	1.78	0.64
1:B:88:ASN:HA	1:B:122:LYS:HD2	1.80	0.64
1:A:221:ASN:HD21	1:A:243:TRP:H	1.46	0.63
1:B:221:ASN:HD21	1:B:243:TRP:H	1.44	0.63
1:A:268:ILE:O	1:A:268:ILE:HG13	1.97	0.63
1:B:221:ASN:ND2	1:B:243:TRP:H	1.97	0.63
1:A:254:LYS:HD3	1:A:268:ILE:HG21	1.80	0.63
1:B:204:THR:HG23	1:B:228:SER:HB2	1.81	0.63
1:A:146:GLU:OE1	1:A:218:HIS:NE2	2.31	0.62
1:B:179:LYS:HE2	1:B:179:LYS:HA	1.81	0.62
1:B:329:ASN:OD1	1:B:344:LEU:HD12	1.99	0.62
1:B:389:ARG:HG3	1:B:396:ARG:CZ	2.30	0.62
1:A:13:LYS:NZ	1:A:13:LYS:HB3	2.15	0.62
1:B:54:LEU:HD12	1:B:57:LEU:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:THR:OG1	1:B:222:THR:HG22	1.99	0.62
1:B:180:GLU:CD	1:B:180:GLU:H	2.05	0.62
1:A:203:THR:HA	1:A:229:VAL:O	2.00	0.62
1:B:53:SER:O	1:B:56:LEU:HB2	1.99	0.62
1:A:293:VAL:HB	1:A:294:PRO:HD3	1.81	0.61
1:B:230:PRO:HB2	1:B:232:ASP:OD2	1.99	0.61
1:B:407:LYS:NZ	1:B:428:LYS:HD3	2.12	0.61
1:B:384:ALA:HB1	1:B:399:MET:HE3	1.82	0.61
1:A:198:LYS:HE2	1:A:200:ASP:OD2	2.00	0.61
1:B:111:GLU:CA	1:B:260:GLN:HE21	1.95	0.61
1:B:214:ILE:HB	1:B:238:GLU:OE2	2.00	0.60
1:A:291:LEU:HD13	1:A:291:LEU:O	2.01	0.60
1:B:293:VAL:HG12	1:B:390:MET:HE3	1.82	0.60
1:A:76:VAL:HB	1:A:281:LEU:HG	1.84	0.60
1:B:95:GLY:HA3	1:B:157:LEU:HD23	1.84	0.60
1:A:454:GLN:O	1:A:458:ILE:HG12	2.01	0.60
1:B:77:ARG:O	1:B:91:LEU:HD12	2.01	0.60
1:B:18:HIS:HD2	1:B:19:PRO:HD2	1.67	0.60
1:A:47:ARG:HG2	1:A:355:ALA:CB	2.31	0.59
1:B:177:ASN:OD1	1:B:178:GLN:N	2.35	0.59
1:A:194:TYR:O	1:A:195:ILE:HG12	2.01	0.59
1:A:322:GLU:CD	1:A:322:GLU:H	2.10	0.59
1:B:245:PRO:O	1:B:248:TYR:HB3	2.03	0.59
1:A:286:MET:HB2	1:A:290:LYS:HD2	1.84	0.59
1:A:31:ARG:HD2	1:A:362:SER:OG	2.02	0.59
1:A:230:PRO:HG2	1:A:233:ALA:HB2	1.84	0.59
1:B:27:GLY:HA2	1:B:42:HIS:O	2.03	0.59
1:B:345:ARG:HG3	1:B:353:ILE:HB	1.85	0.59
1:A:221:ASN:ND2	1:A:243:TRP:H	2.00	0.59
1:B:83:LYS:H	1:B:83:LYS:HD3	1.68	0.59
1:A:108:LYS:O	1:A:112:ILE:HG23	2.03	0.58
1:A:243:TRP:O	1:A:244:GLU:HB2	2.02	0.58
1:B:323:LYS:HA	1:B:326:GLU:OE2	2.02	0.58
1:A:14:ILE:HD12	1:A:454:GLN:HB3	1.85	0.58
1:A:61:ALA:HB1	1:A:311:MET:HE1	1.84	0.58
1:B:54:LEU:HD23	1:B:349:GLY:HA2	1.85	0.58
1:B:178:GLN:O	1:B:179:LYS:HB2	2.02	0.58
1:A:214:ILE:HG12	1:A:225:ILE:HG12	1.84	0.58
1:B:82:LEU:CD1	1:B:86:LYS:HE2	2.31	0.58
1:B:189:SER:HA	1:B:190:PRO:C	2.28	0.58
1:A:100:THR:HG22	1:A:165:TYR:CG	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:SER:O	1:A:230:PRO:HG3	2.04	0.57
1:A:371:GLN:HG2	1:A:373:TRP:CZ2	2.39	0.57
1:A:385:GLY:HA3	1:A:405:GLN:HG3	1.85	0.57
1:A:422:SER:CB	1:A:436:SER:HA	2.34	0.57
1:B:258:LYS:HB3	1:B:258:LYS:NZ	2.19	0.57
1:A:225:ILE:HD13	1:A:226:GLU:N	2.20	0.57
1:B:112:ILE:HD11	1:B:281:LEU:HD22	1.86	0.57
1:A:82:LEU:CG	1:A:84:GLY:H	2.16	0.57
1:B:54:LEU:CD1	1:B:57:LEU:HD12	2.34	0.57
1:B:90:ASN:ND2	1:B:124:ASN:H	2.03	0.57
1:B:320:SER:OG	1:B:322:GLU:HG2	2.04	0.57
1:A:174:VAL:HG11	1:A:212:LEU:HD21	1.87	0.57
1:A:403:PRO:HG2	1:A:457:VAL:HG13	1.85	0.57
1:B:332:LEU:HB3	1:B:337:VAL:CG2	2.35	0.57
1:A:297:LYS:HD2	1:A:380:SER:O	2.04	0.57
1:B:162:ASN:C	1:B:162:ASN:OD1	2.47	0.57
1:B:18:HIS:HD2	1:B:19:PRO:CD	2.18	0.56
1:B:25:MET:HG3	1:B:440:ASN:HB2	1.87	0.56
1:A:134:ASP:HA	1:A:136:ARG:NH2	2.20	0.56
1:A:175:THR:HG23	1:A:176:PRO:HD2	1.87	0.56
1:A:211:ASP:O	1:A:227:GLY:HA3	2.05	0.56
1:A:386:ASN:HD22	1:A:387:PRO:N	2.03	0.56
1:B:230:PRO:HG2	1:B:233:ALA:HB2	1.86	0.56
1:A:21:LEU:HD11	1:A:451:ILE:CD1	2.34	0.56
1:A:53:SER:O	1:A:56:LEU:HB2	2.05	0.56
1:A:59:ALA:HB1	1:A:292:PHE:CE1	2.41	0.56
1:A:124:ASN:N	1:A:124:ASN:ND2	2.52	0.56
1:B:253:PHE:O	1:B:257:LEU:HG	2.06	0.56
1:A:107:ASP:O	1:A:111:GLU:HB2	2.06	0.56
1:A:302:GLY:O	1:A:306:VAL:HG23	2.06	0.56
1:B:67:GLY:O	1:B:288:LEU:HD12	2.06	0.56
1:B:14:ILE:HG13	1:B:454:GLN:HE21	1.70	0.56
1:B:147:TYR:CD1	1:B:147:TYR:C	2.83	0.56
1:B:454:GLN:O	1:B:458:ILE:HG12	2.05	0.56
1:B:140:ASP:OD1	1:B:353:ILE:HD12	2.05	0.55
1:B:342:LEU:HD13	1:B:344:LEU:HD21	1.88	0.55
1:A:112:ILE:CD1	1:A:281:LEU:HD22	2.32	0.55
1:B:8:SER:HA	1:B:40:TYR:CD2	2.42	0.55
1:B:65:VAL:CG2	1:B:331:THR:HG21	2.37	0.55
1:B:369:GLN:HA	1:B:374:PHE:CD1	2.42	0.55
1:B:81:THR:HA	1:B:87:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:500:REZ:C	3:A:501:DAL:H2	2.20	0.55
1:B:70:TYR:O	1:B:287:PRO:HA	2.07	0.55
1:A:296:MET:CE	1:A:411:LYS:HD3	2.37	0.54
1:A:201:ALA:HB2	1:A:226:GLU:HA	1.89	0.54
1:B:427:THR:HA	1:B:460:ALA:O	2.08	0.54
1:A:148:THR:HG21	1:A:150:TYR:CE2	2.43	0.54
1:B:18:HIS:CD2	1:B:19:PRO:HD2	2.43	0.54
1:B:82:LEU:C	1:B:82:LEU:HD23	2.32	0.54
1:B:146:GLU:OE1	1:B:218:HIS:NE2	2.40	0.54
1:B:411:LYS:NZ	1:B:412:THR:O	2.40	0.54
1:B:281:LEU:HD12	1:B:281:LEU:C	2.33	0.54
1:A:142:PRO:HG2	2:A:500:REZ:NZ1	2.22	0.53
1:A:345:ARG:CZ	1:A:353:ILE:HG21	2.38	0.53
1:B:415:LEU:O	1:B:445:GLU:HG2	2.08	0.53
1:B:55:LYS:HZ3	1:B:301:ASN:ND2	2.07	0.53
1:B:114:LYS:HD3	1:B:260:GLN:HB3	1.90	0.53
1:B:173:GLU:CG	1:B:237:LYS:HG2	2.39	0.53
1:A:143:TRP:HA	1:A:146:GLU:HG3	1.91	0.53
2:A:500:REZ:C	3:A:501:DAL:N	2.71	0.53
1:B:442:LEU:HD13	1:B:445:GLU:HA	1.90	0.53
1:A:85:LYS:HG3	1:A:119:LYS:HB3	1.91	0.53
1:B:141:MET:HE1	1:B:146:GLU:HA	1.91	0.53
1:B:178:GLN:HE21	1:B:178:GLN:HA	1.74	0.53
1:B:384:ALA:CB	1:B:399:MET:HE3	2.38	0.53
1:B:66:LEU:CD2	1:B:311:MET:HG2	2.39	0.52
1:B:251:ASP:O	1:B:255:GLN:HG3	2.09	0.52
1:B:100:THR:HG22	1:B:165:TYR:CD1	2.44	0.52
1:A:164:ASP:OD1	1:A:389:ARG:NH2	2.41	0.52
1:A:198:LYS:HD3	1:A:224:THR:HG22	1.92	0.52
1:A:281:LEU:C	1:A:281:LEU:HD12	2.35	0.52
1:B:178:GLN:HA	1:B:178:GLN:NE2	2.25	0.52
1:B:235:LYS:N	1:B:235:LYS:HD2	2.24	0.52
1:B:304:ALA:O	1:B:308:VAL:HG23	2.09	0.52
1:B:364:LEU:O	1:B:368:ILE:HG12	2.10	0.52
1:B:100:THR:HG22	1:B:165:TYR:CG	2.45	0.52
1:A:178:GLN:O	1:A:179:LYS:HB2	2.09	0.52
1:A:386:ASN:HD22	1:A:386:ASN:C	2.17	0.52
1:B:55:LYS:NZ	1:B:301:ASN:ND2	2.58	0.52
1:B:221:ASN:HD21	1:B:242:VAL:HG13	1.75	0.52
1:A:455:ILE:O	1:A:459:LEU:HG	2.10	0.52
1:B:90:ASN:HD22	1:B:124:ASN:CB	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LEU:O	1:A:299:SER:HB3	2.10	0.51
1:B:31:ARG:HD2	1:B:362:SER:OG	2.10	0.51
1:B:302:GLY:O	1:B:306:VAL:HG13	2.10	0.51
1:A:77:ARG:NH1	1:A:279:VAL:HG22	2.26	0.51
1:A:52:SER:HB2	1:A:413:GLY:HA2	1.92	0.51
1:B:65:VAL:HG21	1:B:331:THR:HG21	1.92	0.51
1:B:94:LYS:HA	1:B:128:ASP:HB3	1.92	0.51
1:A:212:LEU:CD1	1:A:225:ILE:HD11	2.41	0.51
1:A:407:LYS:HE3	1:A:428:LYS:HZ2	1.76	0.51
1:B:73:THR:O	1:B:96:LYS:HB2	2.11	0.51
1:B:90:ASN:HD22	1:B:124:ASN:H	1.56	0.51
1:B:386:ASN:ND2	1:B:388:ASP:HB2	2.26	0.51
1:B:443:ILE:N	1:B:443:ILE:HD12	2.25	0.51
1:B:98:ASP:OD2	1:B:285:SER:HB3	2.10	0.51
1:A:90:ASN:ND2	1:A:123:GLY:HA3	2.23	0.50
1:B:173:GLU:HG2	1:B:237:LYS:HG2	1.93	0.50
1:B:405:GLN:C	1:B:407:LYS:H	2.18	0.50
1:A:28:ILE:O	1:A:41:GLU:HA	2.11	0.50
1:B:146:GLU:OE2	1:B:218:HIS:CD2	2.64	0.50
1:B:274:PRO:C	1:B:276:SER:H	2.18	0.50
1:B:399:MET:O	1:B:405:GLN:HB2	2.10	0.50
1:A:204:THR:HG23	1:A:228:SER:HB2	1.93	0.50
1:A:417:THR:N	1:A:445:GLU:HG3	2.26	0.50
1:A:386:ASN:HD22	1:A:387:PRO:CD	2.25	0.50
1:B:442:LEU:CD1	1:B:445:GLU:HA	2.42	0.50
1:A:136:ARG:HG2	1:A:153:PRO:HB3	1.94	0.49
1:A:180:GLU:OE1	1:A:205:ALA:HA	2.12	0.49
1:B:176:PRO:HG3	1:B:233:ALA:HB3	1.94	0.49
1:A:13:LYS:HB3	1:A:13:LYS:HZ2	1.77	0.49
1:A:242:VAL:HG11	1:A:248:TYR:HB2	1.94	0.49
1:B:128:ASP:C	1:B:128:ASP:OD2	2.54	0.49
1:B:202:LYS:O	1:B:228:SER:HA	2.13	0.49
1:A:318:GLU:HB3	1:A:323:LYS:HG3	1.93	0.49
1:B:195:ILE:HD11	1:B:242:VAL:HG22	1.93	0.49
1:A:87:LEU:HD23	1:A:121:ILE:HG23	1.93	0.49
1:A:124:ASN:HD22	1:A:124:ASN:H	1.60	0.49
1:B:164:ASP:OD2	1:B:389:ARG:NH2	2.45	0.49
1:B:260:GLN:C	1:B:262:ILE:H	2.20	0.49
1:B:297:LYS:HA	1:B:382:PRO:HG3	1.94	0.49
1:A:17:ASP:CG	1:A:18:HIS:H	2.20	0.49
1:A:401:GLY:H	1:A:405:GLN:HE22	1.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ASN:OD1	2:B:500:REZ:HBC2	2.13	0.49
1:A:50:PRO:O	1:A:51:ALA:HB3	2.13	0.49
1:A:316:LYS:HE3	1:A:326:GLU:HB2	1.95	0.49
1:A:407:LYS:HE3	1:A:428:LYS:NZ	2.28	0.49
1:A:143:TRP:C	1:A:146:GLU:HG3	2.38	0.48
1:A:192:THR:HG23	1:A:251:ASP:OD2	2.13	0.48
1:B:48:MET:O	1:B:50:PRO:HD3	2.13	0.48
1:B:21:LEU:HD21	1:B:451:ILE:HD13	1.95	0.48
1:B:401:GLY:N	1:B:405:GLN:NE2	2.52	0.48
1:A:55:LYS:HZ2	1:A:301:ASN:HA	1.78	0.48
1:A:293:VAL:HG13	1:A:297:LYS:HD3	1.95	0.48
1:A:61:ALA:CB	1:A:328:LEU:HD12	2.43	0.48
1:B:153:PRO:HB2	1:B:245:PRO:HG2	1.96	0.48
1:B:83:LYS:O	1:B:83:LYS:HG2	2.13	0.48
1:B:13:LYS:HZ3	1:B:13:LYS:HB3	1.78	0.48
1:A:148:THR:HG22	1:A:151:GLY:N	2.29	0.48
1:A:345:ARG:NH2	1:A:353:ILE:HD13	2.29	0.48
1:A:21:LEU:HA	1:A:24:ALA:HB3	1.96	0.47
1:B:204:THR:CG2	1:B:228:SER:HB2	2.44	0.47
1:B:279:VAL:C	1:B:280:LEU:HD12	2.38	0.47
1:B:410:ALA:HA	1:B:423:GLY:HA3	1.95	0.47
1:B:157:LEU:HD13	1:B:249:ALA:HB3	1.96	0.47
1:B:328:LEU:HD22	1:B:344:LEU:HD13	1.97	0.47
1:A:25:MET:HG3	1:A:440:ASN:HB2	1.96	0.47
1:A:368:ILE:HD11	1:A:424:TYR:OH	2.14	0.47
1:B:87:LEU:CG	1:B:88:ASN:H	2.17	0.47
1:A:85:LYS:HZ2	1:A:119:LYS:HD2	1.80	0.47
1:A:459:LEU:O	1:A:462:GLN:HB2	2.15	0.47
1:B:365:LEU:HB2	1:B:434:VAL:CG1	2.44	0.47
1:B:157:LEU:CD1	1:B:249:ALA:HB3	2.43	0.47
1:B:186:VAL:HG23	1:B:199:ASN:ND2	2.29	0.47
1:A:38:VAL:HG21	1:A:41:GLU:HB3	1.97	0.47
1:A:428:LYS:C	1:A:430:GLY:H	2.23	0.47
1:A:82:LEU:HG	1:A:84:GLY:N	2.19	0.47
1:B:149:TYR:HB3	1:B:239:TRP:HB3	1.96	0.47
1:A:311:MET:HB3	1:A:327:VAL:HG21	1.96	0.47
1:B:184:PRO:HD2	1:B:201:ALA:O	2.15	0.47
1:A:386:ASN:ND2	1:A:387:PRO:HD2	2.30	0.47
1:B:239:TRP:C	1:B:240:ILE:HD12	2.39	0.47
1:B:223:ILE:HG12	1:B:240:ILE:HG21	1.97	0.46
1:A:73:THR:O	1:A:96:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:SER:HB2	1:B:413:GLY:HA2	1.96	0.46
1:B:216:ARG:HH21	1:B:243:TRP:HE3	1.63	0.46
1:A:90:ASN:ND2	1:A:124:ASN:H	2.14	0.46
1:B:403:PRO:HD2	1:B:457:VAL:CG1	2.43	0.46
1:B:417:THR:H	1:B:445:GLU:HG3	1.81	0.46
1:B:43:SER:HB3	1:B:46:THR:CG2	2.46	0.46
1:A:382:PRO:HD2	1:A:410:ALA:O	2.15	0.46
1:B:119:LYS:O	1:B:262:ILE:HA	2.16	0.46
1:B:235:LYS:HD2	1:B:235:LYS:H	1.81	0.46
1:B:43:SER:HB3	1:B:46:THR:HG21	1.98	0.46
1:B:86:LYS:H	1:B:86:LYS:HD3	1.80	0.46
1:B:257:LEU:O	1:B:260:GLN:N	2.47	0.45
1:B:301:ASN:N	1:B:301:ASN:HD22	2.14	0.45
1:A:86:LYS:HE3	1:A:120:VAL:HG11	1.98	0.45
1:A:93:LEU:HD23	1:A:157:LEU:HD11	1.97	0.45
1:B:232:ASP:OD2	1:B:232:ASP:N	2.49	0.45
1:B:260:GLN:OE1	1:B:260:GLN:HA	2.15	0.45
1:A:332:LEU:N	1:A:333:PRO:CD	2.78	0.45
1:A:295:PHE:HB2	1:A:303:HIS:HD2	1.81	0.45
1:A:142:PRO:HG2	2:A:500:REZ:HZ11	1.81	0.45
1:A:257:LEU:HB3	1:A:262:ILE:HB	1.98	0.45
1:B:153:PRO:HB2	1:B:245:PRO:CG	2.46	0.45
1:B:195:ILE:HD11	1:B:242:VAL:HG13	1.98	0.45
1:A:284:ARG:HH21	1:A:284:ARG:CG	2.29	0.45
1:A:176:PRO:HB3	1:A:229:VAL:HG22	1.98	0.45
1:B:48:MET:HE3	1:B:440:ASN:HB2	1.99	0.45
1:B:268:ILE:O	1:B:268:ILE:HG23	2.16	0.45
1:A:325:LEU:HD12	1:A:325:LEU:HA	1.87	0.45
1:B:95:GLY:CA	1:B:157:LEU:HD23	2.46	0.45
1:B:332:LEU:HB3	1:B:337:VAL:HG21	1.98	0.45
1:B:427:THR:O	1:B:428:LYS:HB2	2.17	0.45
1:A:85:LYS:NZ	1:A:119:LYS:HD2	2.32	0.44
1:A:311:MET:HB3	1:A:327:VAL:CG2	2.47	0.44
1:B:255:GLN:O	1:B:259:LYS:HG3	2.17	0.44
1:B:291:LEU:O	1:B:294:PRO:HD2	2.18	0.44
1:B:92:TYR:CD2	1:B:273:ALA:HA	2.53	0.44
1:B:407:LYS:HA	1:B:407:LYS:HD3	1.84	0.44
1:A:143:TRP:CA	1:A:146:GLU:HG3	2.48	0.44
1:A:148:THR:CG2	1:A:151:GLY:N	2.80	0.44
1:A:183:GLU:HA	1:A:202:LYS:HA	1.99	0.44
1:B:121:ILE:HB	1:B:264:VAL:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LYS:HA	1:A:265:LYS:HB2	1.98	0.44
1:B:330:SER:C	1:B:333:PRO:HD2	2.42	0.44
1:A:417:THR:H	1:A:445:GLU:HG3	1.82	0.44
1:B:428:LYS:HE3	1:B:428:LYS:HA	2.00	0.44
1:A:216:ARG:NH2	1:A:243:TRP:HE3	2.16	0.43
1:A:225:ILE:HD13	1:A:225:ILE:C	2.43	0.43
1:A:114:LYS:HG3	1:A:260:GLN:OE1	2.17	0.43
1:A:17:ASP:O	1:A:18:HIS:C	2.61	0.43
1:A:79:ASP:O	1:A:80:GLY:O	2.36	0.43
1:A:88:ASN:OD1	1:A:122:LYS:HD3	2.18	0.43
1:B:71:SER:HB3	1:B:284:ARG:NH1	2.24	0.43
1:B:114:LYS:C	1:B:116:SER:N	2.75	0.43
1:B:192:THR:HG22	1:B:193:ASP:N	2.32	0.43
1:B:400:LYS:C	1:B:402:THR:H	2.25	0.43
1:A:148:THR:HG21	1:A:150:TYR:CZ	2.53	0.43
1:A:180:GLU:CD	1:A:205:ALA:HA	2.43	0.43
1:B:66:LEU:N	1:B:66:LEU:HD22	2.34	0.43
1:B:198:LYS:HB3	1:B:224:THR:HG22	2.00	0.43
1:B:235:LYS:H	1:B:235:LYS:CD	2.32	0.43
1:B:243:TRP:CD1	1:B:244:GLU:HG3	2.54	0.43
1:B:386:ASN:HA	1:B:387:PRO:HD3	1.86	0.43
1:A:125:LEU:O	1:A:268:ILE:HA	2.19	0.43
1:B:416:SER:C	1:B:417:THR:HG23	2.43	0.43
1:B:455:ILE:O	1:B:459:LEU:HG	2.19	0.43
1:B:182:GLU:O	1:B:183:GLU:HB3	2.19	0.43
1:A:103:PRO:HD3	1:A:160:SER:O	2.17	0.43
1:A:204:THR:CG2	1:A:228:SER:HB2	2.49	0.43
1:B:174:VAL:HG22	1:B:186:VAL:HG22	2.00	0.43
1:A:125:LEU:N	1:A:267:ASP:O	2.44	0.43
1:A:199:ASN:HA	1:A:225:ILE:HG22	2.01	0.43
1:B:66:LEU:HB3	1:B:70:TYR:CD2	2.54	0.43
1:B:86:LYS:CG	1:B:122:LYS:HE3	2.48	0.43
1:B:174:VAL:HA	1:B:185:ALA:O	2.19	0.43
1:B:415:LEU:HD23	2:B:500:REZ:HA11	2.01	0.43
1:B:78:THR:CG2	1:B:81:THR:HG22	2.49	0.42
1:B:200:ASP:OD1	1:B:226:GLU:HG2	2.19	0.42
1:A:123:GLY:O	1:A:266:GLY:HA3	2.19	0.42
1:A:416:SER:C	1:A:417:THR:HG23	2.43	0.42
1:B:114:LYS:C	1:B:116:SER:H	2.27	0.42
1:A:192:THR:HG22	1:A:193:ASP:N	2.34	0.42
1:A:427:THR:O	1:A:428:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:VAL:O	1:B:331:THR:HG23	2.20	0.42
1:B:328:LEU:O	1:B:332:LEU:HG	2.19	0.42
1:A:332:LEU:HB3	1:A:337:VAL:HB	2.01	0.42
1:A:427:THR:C	1:A:429:SER:H	2.26	0.42
1:A:431:LYS:NZ	1:A:433:LEU:HD21	2.33	0.42
1:A:77:ARG:HA	1:A:278:ASP:O	2.19	0.42
1:B:78:THR:HG21	1:B:81:THR:HG22	2.01	0.42
1:B:98:ASP:OD1	1:B:100:THR:OG1	2.28	0.42
1:B:204:THR:O	1:B:231:VAL:HG13	2.20	0.42
1:B:453:ASP:O	1:B:457:VAL:HG23	2.20	0.42
1:A:148:THR:HG23	1:A:150:TYR:N	2.35	0.42
1:A:94:LYS:HG3	1:A:128:ASP:CG	2.45	0.42
1:A:101:LEU:HD13	1:A:106:PHE:CE2	2.54	0.42
1:A:368:ILE:HD11	1:A:424:TYR:HH	1.85	0.42
1:B:66:LEU:HB3	1:B:70:TYR:CG	2.54	0.42
1:B:293:VAL:HG13	1:B:297:LYS:HD2	2.01	0.42
1:A:148:THR:HG21	1:A:150:TYR:CD2	2.55	0.42
1:A:415:LEU:CD2	2:A:500:REZ:HB11	2.50	0.42
1:B:38:VAL:O	1:B:38:VAL:HG23	2.19	0.42
1:B:81:THR:O	1:B:82:LEU:HB2	2.20	0.42
1:A:86:LYS:CA	1:A:120:VAL:HG13	2.49	0.42
1:A:125:LEU:HD22	1:A:250:LEU:HD11	2.01	0.42
1:B:86:LYS:HG3	1:B:122:LYS:HE3	2.02	0.42
1:B:121:ILE:CG2	1:B:264:VAL:HG13	2.50	0.42
1:B:240:ILE:HD12	1:B:240:ILE:N	2.35	0.42
1:B:435:PHE:CD1	1:B:435:PHE:C	2.98	0.42
1:A:129:ASP:OD1	1:A:129:ASP:C	2.62	0.41
1:A:131:TRP:HD1	1:A:132:HIS:CE1	2.38	0.41
1:B:389:ARG:HG3	1:B:396:ARG:NE	2.34	0.41
1:A:209:GLU:OE1	1:A:209:GLU:N	2.43	0.41
1:A:399:MET:HE2	1:A:453:ASP:OD2	2.20	0.41
1:B:68:GLU:OE2	1:B:373:TRP:HA	2.20	0.41
1:A:131:TRP:CD1	1:A:132:HIS:CE1	3.09	0.41
1:A:383:VAL:O	1:A:392:GLY:HA2	2.20	0.41
1:B:279:VAL:HG12	1:B:280:LEU:N	2.34	0.41
1:B:15:LEU:O	1:B:17:ASP:N	2.53	0.41
1:B:77:ARG:HG2	1:B:92:TYR:HB2	2.02	0.41
1:B:297:LYS:NZ	1:B:381:LEU:O	2.52	0.41
1:B:306:VAL:O	1:B:310:GLU:HB2	2.20	0.41
1:B:407:LYS:HZ3	1:B:428:LYS:CE	2.33	0.41
1:A:78:THR:HG22	1:A:280:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ASN:CG	1:A:182:GLU:HB3	2.45	0.41
1:A:298:LEU:O	1:A:299:SER:CB	2.68	0.41
1:B:83:LYS:H	1:B:83:LYS:CD	2.33	0.41
1:B:191:LYS:C	1:B:192:THR:HG1	2.29	0.41
1:B:307:LEU:O	1:B:311:MET:HG3	2.21	0.41
1:A:55:LYS:NZ	1:A:301:ASN:HA	2.36	0.41
1:A:202:LYS:HE2	1:A:202:LYS:HB3	1.89	0.41
1:B:49:ARG:HD3	1:B:352:HIS:O	2.20	0.41
1:B:92:TYR:CD1	1:B:92:TYR:N	2.89	0.41
1:B:295:PHE:CD2	1:B:303:HIS:HB2	2.56	0.41
1:A:284:ARG:HH21	1:A:284:ARG:HG3	1.86	0.41
1:B:87:LEU:HG	1:B:88:ASN:N	2.24	0.41
1:B:176:PRO:HB3	1:B:229:VAL:CG2	2.47	0.41
1:B:186:VAL:CG2	1:B:225:ILE:HD13	2.50	0.41
1:A:175:THR:O	1:A:185:ALA:N	2.54	0.41
1:B:173:GLU:O	1:B:186:VAL:HA	2.21	0.41
1:A:10:GLN:O	1:A:14:ILE:HG12	2.21	0.41
1:A:21:LEU:N	1:A:21:LEU:HD12	2.35	0.41
1:A:148:THR:CG2	1:A:151:GLY:H	2.34	0.41
1:A:174:VAL:CG1	1:A:212:LEU:HD21	2.50	0.41
1:B:89:GLY:H	1:B:122:LYS:HB2	1.86	0.41
1:B:315:LYS:HB3	1:B:327:VAL:HG11	2.03	0.41
1:A:158:THR:HG21	1:A:167:ALA:HB1	2.04	0.40
1:A:177:ASN:OD1	1:A:182:GLU:HB3	2.21	0.40
1:A:212:LEU:HD11	1:A:225:ILE:CD1	2.44	0.40
1:B:414:SER:HA	1:B:418:VAL:O	2.21	0.40
1:A:268:ILE:O	1:A:268:ILE:CG1	2.68	0.40
1:B:8:SER:HA	1:B:40:TYR:HD2	1.85	0.40
1:B:332:LEU:HB2	1:B:333:PRO:HD3	2.03	0.40
1:A:320:SER:OG	1:A:322:GLU:HG2	2.22	0.40
1:A:10:GLN:HB3	1:A:458:ILE:HD12	2.04	0.40
1:A:402:THR:HB	1:A:403:PRO:HD2	2.04	0.40
1:B:179:LYS:HA	1:B:179:LYS:CE	2.48	0.40
1:B:373:TRP:HZ3	1:B:377:TYR:CD1	2.39	0.40
1:B:450:ASP:O	1:B:454:GLN:HG3	2.22	0.40
1:A:82:LEU:CD2	1:A:86:LYS:O	2.62	0.40
1:A:147:TYR:HA	1:A:241:SER:OG	2.22	0.40
1:A:450:ASP:O	1:A:454:GLN:HG3	2.22	0.40
1:B:288:LEU:HA	1:B:291:LEU:HB3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:OE1	1:B:146:GLU:OE1[4_555]	2.05	0.15

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	456/462 (99%)	413 (91%)	37 (8%)	6 (1%)	9	31
1	B	456/462 (99%)	397 (87%)	52 (11%)	7 (2%)	8	28
All	All	912/924 (99%)	810 (89%)	89 (10%)	13 (1%)	9	30

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	429	SER
1	A	80	GLY
1	A	118	VAL
1	B	16	ALA
1	B	133	ASP
1	B	88	ASN
1	B	183	GLU
1	A	18	HIS
1	B	82	LEU
1	B	275	SER
1	A	17	ASP
1	A	179	LYS
1	A	391	VAL

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	382/385 (99%)	346 (91%)	36 (9%)	8	27
1	B	382/385 (99%)	363 (95%)	19 (5%)	22	54
All	All	764/770 (99%)	709 (93%)	55 (7%)	13	39

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	13	LYS
1	A	18	HIS
1	A	41	GLU
1	A	46	THR
1	A	56	LEU
1	A	66	LEU
1	A	86	LYS
1	A	111	GLU
1	A	114	LYS
1	A	120	VAL
1	A	124	ASN
1	A	125	LEU
1	A	135	MET
1	A	136	ARG
1	A	148	THR
1	A	157	LEU
1	A	175	THR
1	A	182	GLU
1	A	194	TYR
1	A	208	SER
1	A	221	ASN
1	A	222	THR
1	A	225	ILE
1	A	229	VAL
1	A	252	LEU
1	A	270	THR
1	A	280	LEU
1	A	322	GLU
1	A	325	LEU
1	A	327	VAL
1	A	356	VAL
1	A	361	LEU

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Mol	Chain	Res	Type
1	A	371	GLN
1	A	445	GLU
1	A	462	GLN
1	B	13	LYS
1	B	34	GLU
1	B	46	THR
1	B	56	LEU
1	B	83	LYS
1	B	125	LEU
1	B	135	MET
1	B	136	ARG
1	B	162	ASN
1	B	179	LYS
1	B	180	GLU
1	B	221	ASN
1	B	258	LYS
1	B	265	LYS
1	B	291	LEU
1	B	306	VAL
1	B	322	GLU
1	B	409	ARG
1	B	445	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	90	ASN
1	A	124	ASN
1	A	132	HIS
1	A	221	ASN
1	A	329	ASN
1	A	386	ASN
1	A	405	GLN
1	B	18	HIS
1	B	90	ASN
1	B	178	GLN
1	B	221	ASN
1	B	260	GLN
1	B	301	ASN
1	B	303	HIS
1	B	369	GLN

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Mol	Chain	Res	Type
1	B	379	ASN
1	B	386	ASN
1	B	397	ASN
1	B	405	GLN
1	B	454	GLN
1	B	462	GLN

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 ⓘ

4 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	DAL	A	501	-	5,5,5	1.41	1 (20%)	6,6,6	0.91	0
2	REZ	B	500	1	13,15,16	0.69	0	13,18,20	0.57	0
2	REZ	A	500	1	13,15,16	0.84	0	13,18,20	0.80	1 (7%)
3	DAL	B	501	-	5,5,5	1.13	0	6,6,6	0.93	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	DAL	A	501	-	-	0/4/4/4	-
2	REZ	B	500	1	-	3/16/17/19	-
2	REZ	A	500	1	-	3/16/17/19	-
3	DAL	B	501	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	DAL	CA-C	-2.36	1.51	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	REZ	CA-N-C1	-2.15	119.95	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	REZ	NZ1-CE1-CZ1-OH1
3	B	501	DAL	OXT-C-CA-N
3	B	501	DAL	O-C-CA-N
2	A	500	REZ	NZ1-CE1-CZ1-OH2
2	B	500	REZ	C-CA-N-C1
2	A	500	REZ	NZ1-CE1-CZ1-OH1
2	A	500	REZ	O1-C1-CA1-CB1
2	B	500	REZ	NZ1-CE1-CZ1-OH2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	DAL	2	0
2	B	500	REZ	2	0
2	A	500	REZ	5	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	458/462 (99%)	-0.44	5 (1%) 78 70	14, 29, 57, 71	0
1	B	458/462 (99%)	-0.02	4 (0%) 81 74	22, 52, 82, 102	0
All	All	916/924 (99%)	-0.23	9 (0%) 79 72	14, 42, 76, 102	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	LYS	3.4
1	A	211	ASP	3.1
1	B	263	THR	3.0
1	A	84	GLY	2.7
1	A	17	ASP	2.3
1	B	84	GLY	2.2
1	A	208	SER	2.2
1	B	82	LEU	2.1
1	A	83	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
3	DAL	A	501	6/6	0.86	0.12	37,39,39,41	0
2	REZ	B	500	16/17	0.89	0.10	47,51,55,56	0
2	REZ	A	500	16/17	0.90	0.12	41,49,54,54	0
3	DAL	B	501	6/6	0.92	0.08	46,46,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.