



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:56 am GMT

PDB ID : 2J9P
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

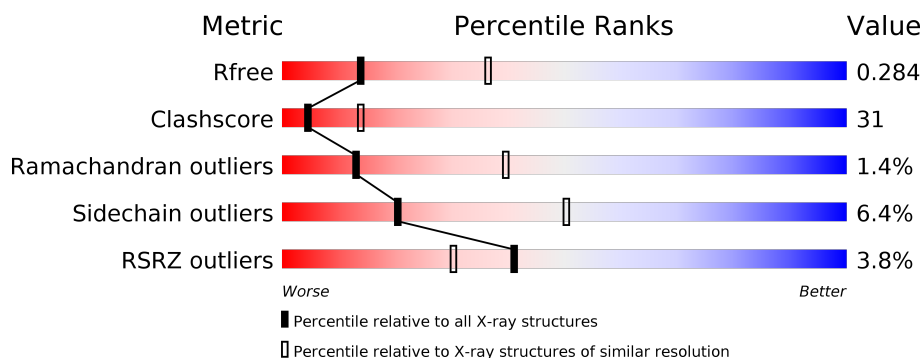
1 Overall quality at a glance

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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

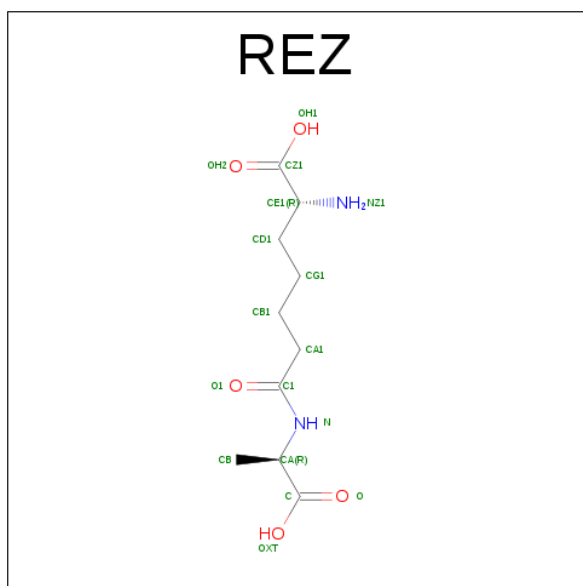
Mol	Chain	Length	Quality of chain
1	A	462	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>41%</div> <div>5% •</div> </div> </div>
1	B	462	<div> <div>5%</div> <div> <div></div> <div>46%</div> <div>49%</div> <div>• •</div> </div> </div>

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 PENICILLIN-BINDING PROTEIN.

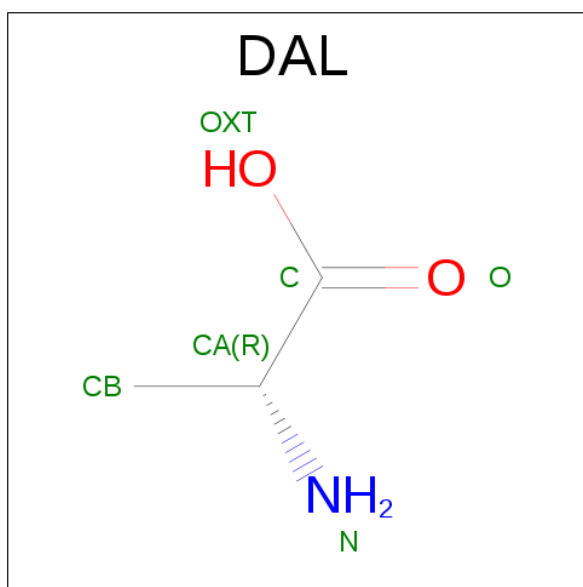
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total 3461	C 2169	N 582	O 700	S 10	0	0	0
1	B	458	Total 3461	C 2169	N 582	O 700	S 10	0	0	0

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



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

- Molecule 3 is D-ALANINE (three-letter code: DAL) (formula: $\text{C}_3\text{H}_7\text{NO}_2$).

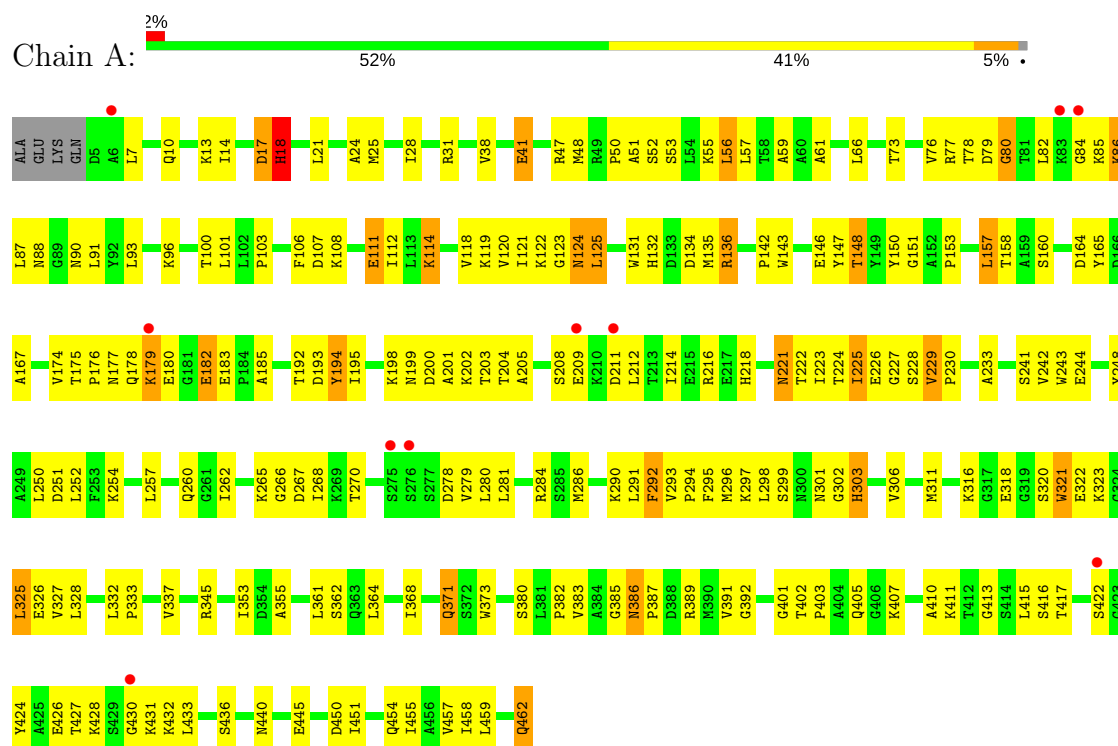


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	3	1	2		
3	B	1	Total	C	N	O	0	0
			6	3	1	2		

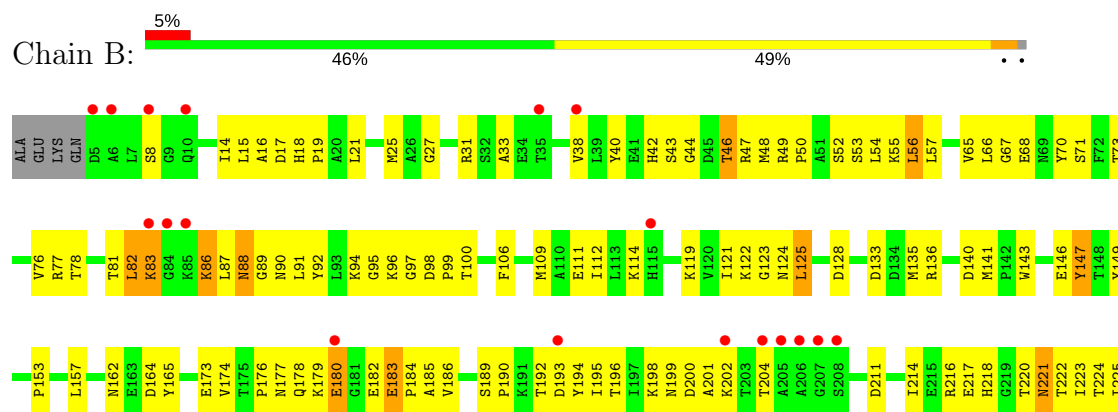
3 Residue-property plots

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

• Molecule 1: PENICILLIN-BINDING PROTEIN



• Molecule 1: PENICILLIN-BINDING PROTEIN





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 24.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.7 (19.90-2.80) 89.8 (24.59-2.80)	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	1049 reflections (4.88%)	DCC
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.5	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	0.92	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: REZ, DAL

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	0.41	0/3520	0.69	0/4765
1	B	0.34	0/3520	0.61	0/4765
All	All	0.38	0/7040	0.65	0/9530

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3461	0	3463	199	1
1	B	3461	0	3463	234	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	435	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 31.

All (435) 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	1.26	0.99
1:A:415:LEU:O	1:A:445:GLU:HG2	1.66	0.96
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:321:TRP:O	1:A:325:LEU:HB2	1.75	0.86
1:A:47:ARG:HG2	1:A:355:ALA:HB1	1.54	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: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:121:ILE:HG22	1:B:123:GLY:H	1.54	0.73
1:B:97:GLY:O	1:B:99:PRO:HD3	1.87	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	0.72
1:B:401:GLY:H	1:B:405:GLN:HE22	1.37	0.71
1:A:431:LYS:HE3	1:A:433:LEU:HD21	1.70	0.71
1:A:426:GLU:HG2	1:A:432:LYS:NZ	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ILE:O	1:B:225:ILE:HG13	1.91	0.71
1:A:322:GLU:O	1:A:326:GLU:HG3	1.91	0.70
1:B:310:GLU:HA	1:B:310:GLU:OE2	1.90	0.70
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: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:445:GLU:H	1:A:445:GLU:CD	1.96	0.66
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:HG13	1:A:268:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:HB3	1:A:13:LYS:NZ	2.15	0.62
1:B:196:THR:OG1	1:B:222:THR:HG22	1.99	0.62
1:B:54:LEU:HD12	1:B:57:LEU:HD12	1.80	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: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:O	1:A:291:LEU:HD13	2.01	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: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:230:PRO:HG2	1:A:233:ALA:HB2	1.84	0.59
1:A:31:ARG:HD2	1:A:362:SER:OG	2.02	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:B:180:GLU:H	1:B:180:GLU:CD	2.05	0.58
1:A:61:ALA:HB1	1:A:311:MET:HE1	1.84	0.58
1:B:178:GLN:O	1:B:179:LYS:HB2	2.02	0.58
1:B:54:LEU:HD23	1:B:349:GLY:HA2	1.85	0.58
1:A:214:ILE:HG12	1:A:225:ILE:HG12	1.84	0.58
1:A:426:GLU:HG2	1:A:432:LYS:HZ1	1.69	0.58
1:B:82:LEU:CD1	1:B:86:LYS:HE2	2.31	0.58
1:A:100:THR:HG22	1:A:165:TYR:CG	2.38	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NZ	1:B:258:LYS:HB3	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: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:B:54:LEU:CD1	1:B:57:LEU:HD12	2.34	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: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:211:ASP:O	1:A:227:GLY:HA3	2.05	0.56
1:B:230:PRO:HG2	1:B:233:ALA:HB2	1.86	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:386:ASN:HD22	1:A:387:PRO:N	2.03	0.56
1:A:21:LEU:HD11	1:A:451:ILE:CD1	2.34	0.56
1:A:124:ASN:N	1:A:124:ASN:ND2	2.52	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: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:454:GLN:O	1:B:458:ILE:HG12	2.05	0.56
1:B:342:LEU:HD13	1:B:344:LEU:HD21	1.88	0.55
1:B:140:ASP:OD1	1:B:353:ILE:HD12	2.05	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:369:GLN:HA	1:B:374:PHE:CD1	2.42	0.55
1:B:65:VAL:CG2	1:B:331:THR:HG21	2.37	0.55
1:B:81:THR:HA	1:B:87:LEU:HD12	1.87	0.55
1:B:141:MET:HE1	1:B:146:GLU:HA	1.88	0.55
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:322:GLU:CD	1:A:322:GLU:H	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:345:ARG:CZ	1:A:353:ILE:HG21	2.38	0.53
1:A:142:PRO:HG2	2:A:500:REZ:NZ1	2.22	0.53
1:B:189:SER:HA	1:B:190:PRO:C	2.28	0.53
1:B:415:LEU:O	1:B:445:GLU:HG2	2.08	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:178:GLN:HE21	1:B:178:GLN:HA	1.74	0.53
1:B:251:ASP:O	1:B:255:GLN:HG3	2.09	0.52
1:B:66:LEU:CD2	1:B:311:MET:HG2	2.39	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:B:178:GLN:NE2	1:B:178:GLN:HA	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:162:ASN:OD1	1:B:162:ASN:C	2.47	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:B:221:ASN:HD21	1:B:242:VAL:HG13	1.75	0.52
1:B:55:LYS:NZ	1:B:301:ASN:ND2	2.58	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
1:A:298:LEU:O	1:A:299:SER:HB3	2.10	0.51
1:B:302:GLY:O	1:B:306:VAL:HG13	2.10	0.51
1:B:31:ARG:HD2	1:B:362:SER:OG	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:147:TYR:CD1	1:B:147:TYR:C	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:90:ASN:HD22	1:B:124:ASN:H	1.56	0.51
1:B:73:THR:O	1:B:96:LYS:HB2	2.11	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: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: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:B:82:LEU:HD23	1:B:82:LEU:C	2.32	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:242:VAL:HG11	1:A:248:TYR:HB2	1.94	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:H	1:A:124:ASN:HD22	1.60	0.49
1:B:164:ASP:OD2	1:B:389:ARG:NH2	2.45	0.49
1:B:297:LYS:HA	1:B:382:PRO:HG3	1.94	0.49
1:A:401:GLY:H	1:A:405:GLN:HE22	1.57	0.49
1:B:83:LYS:O	1:B:83:LYS:HG2	2.13	0.49
1:B:281:LEU:C	1:B:281:LEU:HD12	2.33	0.49
1:B:301:ASN:OD1	2:B:500:REZ:HBC2	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:50:PRO:O	1:A:51:ALA:HB3	2.13	0.49
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PRO:HB2	1:B:245:PRO:HG2	1.96	0.48
1:B:407:LYS:NZ	1:B:428:LYS:HD3	2.12	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:410:ALA:HA	1:B:423:GLY:HA3	1.95	0.47
1:A:281:LEU:C	1:A:281:LEU:HD12	2.35	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: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:386:ASN:HD22	1:A:386:ASN:C	2.17	0.47
1:A:38:VAL:HG21	1:A:41:GLU:HB3	1.97	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: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
1:B:217:GLU:HB2	1:B:220:THR:HG1	1.81	0.46
1:B:216:ARG:HH21	1:B:243:TRP:HE3	1.63	0.46
1:B:52:SER:HB2	1:B:413:GLY:HA2	1.96	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:85:LYS:HZ2	1:A:119:LYS:HD2	1.81	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:H	1:B:235:LYS:HD2	1.81	0.46
1:B:405:GLN:C	1:B:407:LYS:H	2.18	0.46
1:B:43:SER:HB3	1:B:46:THR:HG21	1.98	0.46
1:B:274:PRO:C	1:B:276:SER:H	2.18	0.46
1:B:86:LYS:H	1:B:86:LYS:HD3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:426:GLU:HG2	1:A:432:LYS:HZ3	1.78	0.45
1:A:295:PHE:HB2	1:A:303:HIS:HD2	1.81	0.45
1:A:257:LEU:HB3	1:A:262:ILE:HB	1.98	0.45
1:A:142:PRO:HG2	2:A:500:REZ:HZ11	1.81	0.45
1:B:195:ILE:HD11	1:B:242:VAL:HG13	1.98	0.45
1:B:153:PRO:HB2	1:B:245:PRO:CG	2.46	0.45
1:A:284:ARG:CG	1:A:284:ARG:HH21	2.29	0.45
1:A:176:PRO:HB3	1:A:229:VAL:HG22	1.98	0.45
1:B:128:ASP:C	1:B:128:ASP:OD2	2.54	0.45
1:B:268:ILE:O	1:B:268:ILE:HG23	2.16	0.45
1:A:325:LEU:HA	1:A:325:LEU:HD12	1.87	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:B:95:GLY:CA	1:B:157:LEU:HD23	2.46	0.45
1:A:311:MET:HB3	1:A:327:VAL:CG2	2.47	0.44
1:A:85:LYS:NZ	1:A:119:LYS:HD2	2.32	0.44
1:B:255:GLN:O	1:B:259:LYS:HG3	2.17	0.44
1:B:260:GLN:C	1:B:262:ILE:H	2.20	0.44
1:B:291:LEU:O	1:B:294:PRO:HD2	2.18	0.44
1:A:17:ASP:CG	1:A:18:HIS:H	2.20	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
1:A:122:LYS:HA	1:A:265:LYS:HB2	1.98	0.44
1:A:13:LYS:HB3	1:A:13:LYS:HZ2	1.82	0.44
1:A:143:TRP:C	1:A:146:GLU:HG3	2.38	0.44
1:B:55:LYS:HZ1	1:B:301:ASN:ND2	2.15	0.44
1:A:417:THR:H	1:A:445:GLU:HG3	1.82	0.44
1:B:428:LYS:HA	1:B:428:LYS:HE3	2.00	0.44
1:A:216:ARG:NH2	1:A:243:TRP:HE3	2.16	0.43
1:A:114:LYS:HG3	1:A:260:GLN:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:192:THR:HG22	1:B:193:ASP:N	2.32	0.43
1:B:71:SER:HB3	1:B:284:ARG:NH1	2.24	0.43
1:A:148:THR:HG21	1:A:150:TYR:CZ	2.53	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:B:66:LEU:HD22	1:B:66:LEU:N	2.34	0.43
1:A:125:LEU:O	1:A:268:ILE:HA	2.19	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:B:279:VAL:C	1:B:280:LEU:HD12	2.38	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:B:48:MET:HE3	1:B:440:ASN:HB2	2.00	0.43
1:A:199:ASN:HA	1:A:225:ILE:HG22	2.01	0.43
1:A:125:LEU:N	1:A:267:ASP:O	2.44	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:66:LEU:HB3	1:B:70:TYR:CD2	2.54	0.43
1:B:200:ASP:OD1	1:B:226:GLU:HG2	2.19	0.42
1:B:78:THR:CG2	1:B:81:THR:HG22	2.49	0.42
1:A:123:GLY:O	1:A:266:GLY:HA3	2.19	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
1:B:328:LEU:O	1:B:332:LEU:HG	2.19	0.42
1:B:327:VAL:O	1:B:331:THR:HG23	2.20	0.42
1:A:332:LEU:HB3	1:A:337:VAL:HB	2.01	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:A:428:LYS:C	1:A:430:GLY:H	2.23	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: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:A:148:THR:HG23	1:A:150:TYR:N	2.35	0.42
1:A:101:LEU:HD13	1:A:106:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:LYS:HE3	1:A:428:LYS:HZ2	1.84	0.42
1:A:416:SER:O	1:A:417:THR:OG1	2.31	0.42
1:B:239:TRP:C	1:B:240:ILE:HD12	2.39	0.42
1:B:293:VAL:HG13	1:B:297:LYS:HD2	2.01	0.42
1:B:66:LEU:HB3	1:B:70:TYR:CG	2.54	0.42
1:A:10:GLN:HA	1:A:13:LYS:HZ2	1.85	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:279:VAL:HG12	1:B:280:LEU:N	2.34	0.42
1:B:38:VAL:HG23	1:B:38:VAL:O	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:A:55:LYS:HZ2	1:A:301:ASN:HA	1.85	0.42
1:B:240:ILE:HD12	1:B:240:ILE:N	2.35	0.42
1:B:121:ILE:CG2	1:B:264:VAL:HG13	2.50	0.42
1:B:86:LYS:HG3	1:B:122:LYS:HE3	2.02	0.42
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: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:A:25:MET:HG3	1:A:48:MET:CE	2.50	0.41
1:B:15:LEU:O	1:B:17:ASP:N	2.53	0.41
1:B:306:VAL:O	1:B:310:GLU:HB2	2.20	0.41
1:B:297:LYS:NZ	1:B:381:LEU:O	2.52	0.41
1:B:77:ARG:HG2	1:B:92:TYR:HB2	2.02	0.41
1:A:298:LEU:O	1:A:299:SER:CB	2.68	0.41
1:A:78:THR:HG22	1:A:280:LEU:HD13	2.03	0.41
1:B:307:LEU:O	1:B:311:MET:HG3	2.21	0.41
1:B:83:LYS:H	1:B:83:LYS:CD	2.33	0.41
1:A:202:LYS:HE2	1:A:202:LYS:HB3	1.89	0.41
1:A:55:LYS:NZ	1:A:301:ASN:HA	2.36	0.41
1:B:295:PHE:CD2	1:B:303:HIS:HB2	2.56	0.41
1:B:49:ARG:HD3	1:B:352:HIS:O	2.20	0.41
1:B:92:TYR:N	1:B:92:TYR:CD1	2.89	0.41
1:A:284:ARG:HH21	1:A:284:ARG:HG3	1.86	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:B:87:LEU:HG	1:B:88:ASN:N	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:174:VAL:CG1	1:A:212:LEU:HD21	2.50	0.41
1:A:21:LEU:HD12	1:A:21:LEU:N	2.35	0.41
1:B:89:GLY:H	1:B:122:LYS:HB2	1.86	0.41
1:A:148:THR:CG2	1:A:151:GLY:H	2.34	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:CG1	1:A:268:ILE:O	2.68	0.40
1:B:332:LEU:HB2	1:B:333:PRO:HD3	2.03	0.40
1:B:8:SER:HA	1:B:40:TYR:HD2	1.85	0.40
1:A:320:SER:OG	1:A:322:GLU:HG2	2.22	0.40
1:A:402:THR:HB	1:A:403:PRO:HD2	2.04	0.40
1:A:10:GLN:HB3	1:A:458:ILE:HD12	2.04	0.40
1:B:179:LYS:CE	1:B:179:LYS:HA	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: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:A:82:LEU:CD2	1:A:86:LYS:O	2.62	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

5.3.1 Protein backbone

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%)	14	41
1	B	456/462 (99%)	397 (87%)	52 (11%)	7 (2%)	12	37
All	All	912/924 (99%)	810 (89%)	89 (10%)	13 (1%)	13	39

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 ⓘ

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%)	352 (92%)	30 (8%)	14	38
1	B	382/385 (99%)	363 (95%)	19 (5%)	28	62
All	All	764/770 (99%)	715 (94%)	49 (6%)	20	50

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	18	HIS
1	A	41	GLU
1	A	56	LEU
1	A	66	LEU
1	A	86	LYS
1	A	111	GLU
1	A	114	LYS
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	182	GLU
1	A	194	TYR
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	292	PHE
1	A	303	HIS
1	A	321	TRP
1	A	325	LEU
1	A	361	LEU
1	A	371	GLN
1	A	386	ASN
1	A	462	GLN
1	B	46	THR
1	B	56	LEU
1	B	83	LYS
1	B	86	LYS
1	B	125	LEU
1	B	135	MET
1	B	136	ARG
1	B	147	TYR
1	B	180	GLU
1	B	221	ASN
1	B	235	LYS
1	B	265	LYS
1	B	291	LEU

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Mol	Chain	Res	Type
1	B	321	TRP
1	B	322	GLU
1	B	379	ASN
1	B	388	ASP
1	B	409	ARG
1	B	445	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	124	ASN
1	A	132	HIS
1	A	221	ASN
1	A	329	ASN
1	A	369	GLN
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
1	B	386	ASN
1	B	397	ASN
1	B	405	GLN
1	B	454	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	REZ	A	500	1	10,15,16	0.82	0	9,18,20	1.00	1 (11%)
3	DAL	A	501	-	2,5,5	0.60	0	2,6,6	0.32	0
2	REZ	B	500	1	10,15,16	0.71	0	9,18,20	0.69	0
3	DAL	B	501	-	2,5,5	0.34	0	2,6,6	0.52	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	REZ	A	500	1	-	0/11/17/19	0/0/0/0
3	DAL	A	501	-	-	0/0/4/4	0/0/0/0
2	REZ	B	500	1	-	0/11/17/19	0/0/0/0
3	DAL	B	501	-	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	REZ	CA-N-C1	-2.04	119.95	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	REZ	5	0
3	A	501	DAL	2	0
2	B	500	REZ	2	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	458/462 (99%)	-0.26	10 (2%) 62 52	14, 29, 57, 71	0
1	B	458/462 (99%)	0.19	25 (5%) 26 17	22, 52, 82, 102	0
All	All	916/924 (99%)	-0.03	35 (3%) 41 30	14, 42, 76, 102	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	GLY	7.9
1	B	83	LYS	4.7
1	B	180	GLU	3.8
1	B	263	THR	3.7
1	B	436	SER	3.6
1	B	208	SER	3.5
1	B	422	SER	3.4
1	B	85	LYS	3.4
1	A	84	GLY	3.4
1	A	275	SER	3.2
1	B	5	ASP	3.0
1	A	83	LYS	2.9
1	B	8	SER	2.8
1	A	276	SER	2.8
1	A	211	ASP	2.7
1	B	396	ARG	2.7
1	A	6	ALA	2.7
1	B	6	ALA	2.7
1	B	205	ALA	2.6
1	B	206	ALA	2.6
1	B	35	THR	2.5
1	A	209	GLU	2.5
1	B	207	GLY	2.4
1	B	115	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	204	THR	2.4
1	A	422	SER	2.2
1	B	274	PRO	2.2
1	B	318	GLU	2.1
1	B	202	LYS	2.1
1	B	10	GLN	2.1
1	B	38	VAL	2.1
1	B	231	VAL	2.1
1	B	193	ASP	2.0
1	A	179	LYS	2.0
1	A	430	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q < 0.9
2	REZ	A	500	16/17	0.93	0.21	1.66	41,49,54,54	0
2	REZ	B	500	16/17	0.95	0.20	1.16	47,51,55,56	0
3	DAL	B	501	6/6	0.96	0.25	0.94	46,46,46,47	0
3	DAL	A	501	6/6	0.91	0.21	0.91	37,39,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.