



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:27 PM GMT

PDB ID : 4F2B
Title : Modulation of S.Aureus Phosphatidylinositol-Specific Phospholipase C
Membrane Binding
Authors : Cheng, J.; Goldstein, R.; Stec, B.; Gershenson, A.; Roberts, M.F.
Deposited on : 2012-05-07
Resolution : 2.16 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

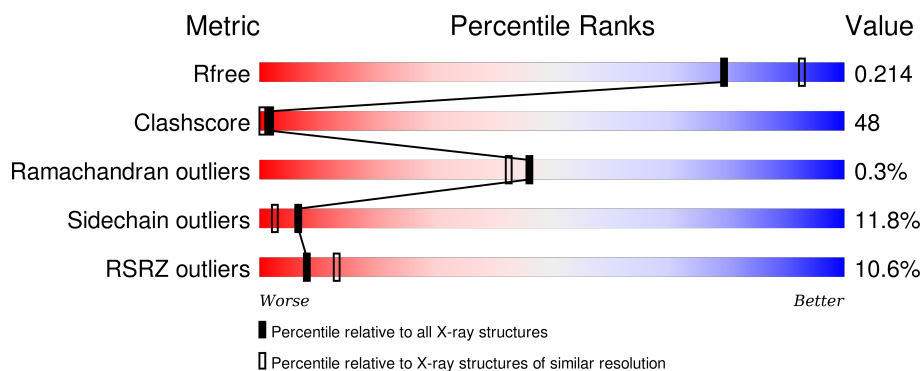
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	310	<div> <div>11%</div> <div>36%</div> <div>52%</div> <div>10%</div> <div>.</div> </div>
1	B	310	<div> <div>9%</div> <div>35%</div> <div>55%</div> <div>6%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	INS	B	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4988 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.

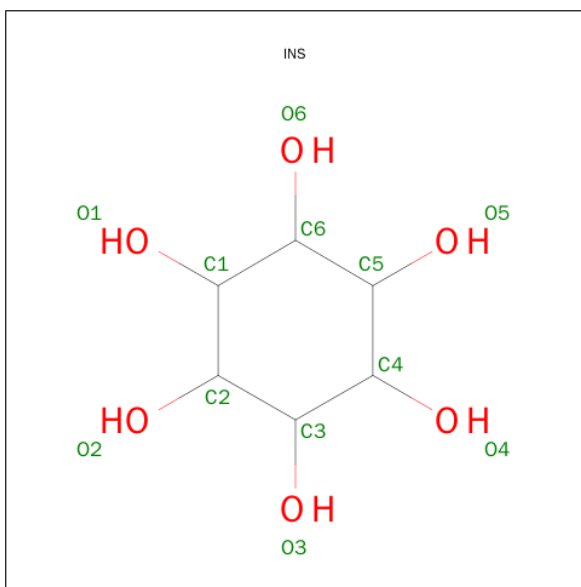
- Molecule 1 is a protein called 1-phosphatidylinositol phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2430	1541	403	479	7			
1	B	302	Total	C	N	O	S	0	0	0
			2411	1530	399	475	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	LEU	-	EXPRESSION TAG	UNP P45723
A	304	GLU	-	EXPRESSION TAG	UNP P45723
A	305	HIS	-	EXPRESSION TAG	UNP P45723
A	306	HIS	-	EXPRESSION TAG	UNP P45723
A	307	HIS	-	EXPRESSION TAG	UNP P45723
A	308	HIS	-	EXPRESSION TAG	UNP P45723
A	309	HIS	-	EXPRESSION TAG	UNP P45723
A	310	HIS	-	EXPRESSION TAG	UNP P45723
B	303	LEU	-	EXPRESSION TAG	UNP P45723
B	304	GLU	-	EXPRESSION TAG	UNP P45723
B	305	HIS	-	EXPRESSION TAG	UNP P45723
B	306	HIS	-	EXPRESSION TAG	UNP P45723
B	307	HIS	-	EXPRESSION TAG	UNP P45723
B	308	HIS	-	EXPRESSION TAG	UNP P45723
B	309	HIS	-	EXPRESSION TAG	UNP P45723
B	310	HIS	-	EXPRESSION TAG	UNP P45723

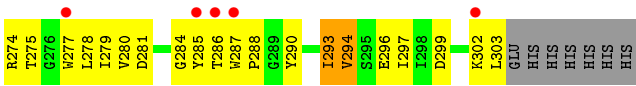
- Molecule 2 is 1,2,3,4,5,6-HEXAHYDROXY-CYCLOHEXANE (three-letter code: INS) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	61	Total	O	0	0
			61	61		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.36Å 133.38Å 50.19Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	50.00 – 2.16 36.35 – 2.16	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.16) 95.4 (36.35-2.16)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.215 , 0.250 0.221 , 0.214	Depositor DCC
R_{free} test set	1481 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.8	EDS
Estimated twinning fraction	0.545 for H, K, L 0.455 for -H, -K, L 0.449 for h,-k,-l	Xtriage
Reported twinning fraction	0.545 for H, K, L 0.455 for -H, -K, L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 29020 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4988	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: INS

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	1.10	3/2488 (0.1%)	0.98	6/3363 (0.2%)
1	B	1.15	1/2468 (0.0%)	0.99	1/3336 (0.0%)
All	All	1.13	4/4956 (0.1%)	0.99	7/6699 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	SER	C-N	5.92	1.47	1.34
1	B	294	VAL	CB-CG1	5.25	1.63	1.52
1	A	68	GLY	C-O	-5.20	1.15	1.23
1	A	246	GLY	C-O	-5.14	1.15	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ASP	CB-CG-OD2	5.96	123.67	118.30
1	A	112	MET	CG-SD-CE	-5.57	91.29	100.20
1	A	223	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	200	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	52	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	109	VAL	N-CA-C	-5.30	96.70	111.00
1	B	166	ARG	NE-CZ-NH1	-5.11	117.74	120.30

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	2430	0	2338	235	0
1	B	2411	0	2325	232	0
2	A	12	0	12	1	0
2	B	12	0	12	4	0
3	A	62	0	0	20	0
3	B	61	0	0	17	0
All	All	4988	0	4687	457	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 48.

All (457) 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:33:GLY:HA3	3:B:508:HOH:O	1.35	1.23
1:A:151:ASN:OD1	1:A:200:LEU:HD21	1.46	1.15
1:A:242:VAL:HG12	1:A:255:TYR:CE2	1.83	1.13
1:B:173:LYS:CE	1:B:179:ASP:HA	1.78	1.13
1:B:173:LYS:HE3	1:B:179:ASP:CA	1.79	1.10
1:B:78:VAL:HG11	3:B:508:HOH:O	1.53	1.06
1:B:217:GLU:HB3	3:B:509:HOH:O	1.56	1.02
1:B:43:SER:HB3	1:B:47:LYS:HB2	1.03	1.00
1:B:264:ALA:HB2	1:B:293:ILE:HA	1.40	1.00
1:A:42:LYS:HA	3:A:518:HOH:O	1.61	0.99
1:B:238:ASN:HB3	1:B:278:LEU:CD2	1.95	0.97
1:A:53:TYR:O	1:A:57:MET:HG3	1.64	0.97
1:A:160:LYS:HE3	3:A:507:HOH:O	1.65	0.97
1:A:97:LYS:HA	1:A:143:LEU:HD11	1.47	0.96
1:A:125:THR:O	1:A:129:ILE:HG13	1.65	0.96
1:A:249:PHE:CE2	1:A:258:HIS:CD2	2.54	0.95
1:A:58:LYS:HG2	3:A:537:HOH:O	1.67	0.95
1:A:17:ASP:HB3	1:A:158:LYS:HZ3	1.31	0.94
1:B:43:SER:CB	1:B:47:LYS:HB2	1.96	0.94
1:B:143:LEU:HD21	1:B:161:ILE:HD12	1.50	0.94
1:B:51:LYS:HZ1	1:B:284:GLY:C	1.71	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:PHE:O	1:B:160:LYS:HD3	1.66	0.93
1:A:38:LYS:HE3	1:B:285:TYR:HE1	1.33	0.92
1:B:58:LYS:HD3	3:B:532:HOH:O	1.68	0.91
1:B:153:THR:OG1	1:B:156:GLU:HG3	1.69	0.91
1:B:43:SER:HB3	1:B:47:LYS:CB	1.99	0.90
1:A:285:TYR:CE2	1:B:38:LYS:HG3	2.07	0.90
1:A:249:PHE:CZ	1:A:258:HIS:CD2	2.60	0.89
1:B:143:LEU:CD2	1:B:161:ILE:HD12	2.03	0.89
1:B:92:PHE:CE2	1:B:93:LEU:HD23	2.08	0.89
1:B:143:LEU:HD21	1:B:161:ILE:CD1	2.03	0.88
1:A:45:TRP:CD1	3:A:506:HOH:O	2.27	0.88
1:B:9:GLU:CD	1:B:9:GLU:H	1.78	0.87
1:A:138:PRO:O	1:A:141:GLN:HG2	1.72	0.87
1:A:74:ASN:HB2	1:A:133:TYR:CD1	2.09	0.87
1:A:74:ASN:HB2	1:A:133:TYR:HD1	1.40	0.86
1:A:137:ASN:CG	1:A:138:PRO:HD2	1.96	0.86
1:B:127:GLU:OE2	1:B:170:THR:HA	1.74	0.85
1:A:302:LYS:C	1:A:303:LEU:HG	1.95	0.85
1:A:105:ASN:HA	1:A:158:LYS:HG2	1.59	0.84
1:B:51:LYS:NZ	1:B:284:GLY:C	2.30	0.84
1:A:249:PHE:CE2	1:A:258:HIS:NE2	2.46	0.83
1:B:72:ALA:HB3	1:B:75:MET:HB2	1.59	0.83
1:B:72:ALA:HB3	1:B:75:MET:CB	2.07	0.83
1:B:222:LEU:HA	1:B:225:LYS:HE2	1.59	0.82
1:A:74:ASN:HA	1:A:133:TYR:CD1	2.14	0.82
1:A:205:GLN:NE2	1:A:207:GLU:H	1.77	0.81
1:B:58:LYS:CD	3:B:532:HOH:O	2.26	0.80
1:A:91:LYS:HE2	3:A:556:HOH:O	1.80	0.79
1:B:173:LYS:HE3	1:B:179:ASP:HA	0.89	0.79
1:A:17:ASP:CB	1:A:158:LYS:NZ	2.46	0.79
1:B:238:ASN:HB3	1:B:278:LEU:HD23	1.64	0.79
1:A:260:ASN:N	1:A:261:PRO:CD	2.45	0.79
1:A:74:ASN:CB	1:A:133:TYR:CD1	2.66	0.78
1:B:257:SER:HA	1:B:287:TRP:CZ3	2.18	0.78
1:A:222:LEU:HD23	1:A:238:ASN:HB2	1.64	0.78
1:A:267:ILE:HD11	1:A:278:LEU:HD11	1.65	0.78
1:A:163:LEU:HD21	1:A:165:ASN:HB2	1.64	0.78
1:B:302:LYS:HG3	1:B:303:LEU:N	1.98	0.78
1:A:151:ASN:OD1	1:A:200:LEU:CD2	2.30	0.77
1:B:92:PHE:HE2	1:B:93:LEU:HD23	1.49	0.76
1:B:264:ALA:CB	1:B:293:ILE:HA	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LYS:CE	3:A:556:HOH:O	2.34	0.76
1:B:131:ARG:HG3	1:B:136:ASN:ND2	2.01	0.76
1:B:287:TRP:O	1:B:290:TYR:HB2	1.86	0.75
1:A:135:TYR:CE1	1:A:144:PHE:HB3	2.22	0.75
1:A:80:HIS:HB2	1:A:85:LEU:HD11	1.69	0.74
1:A:160:LYS:CE	3:A:507:HOH:O	2.29	0.73
1:B:222:LEU:HD12	1:B:225:LYS:HE3	1.67	0.73
1:B:141:GLN:HG3	1:B:142:ASN:H	1.53	0.73
1:A:17:ASP:HB3	1:A:158:LYS:NZ	2.04	0.73
1:A:150:ALA:O	1:A:152:PRO:CD	2.37	0.72
1:A:74:ASN:CB	1:A:133:TYR:CE1	2.72	0.72
1:B:195:ILE:HG13	1:B:196:ASN:HD22	1.53	0.72
1:A:17:ASP:CB	1:A:158:LYS:HZ3	2.00	0.72
1:A:97:LYS:HA	1:A:143:LEU:CD1	2.19	0.72
1:B:264:ALA:HB2	1:B:293:ILE:CA	2.18	0.71
1:A:102:ALA:O	1:A:104:PRO:HD3	1.91	0.71
1:B:128:GLU:HG3	1:B:132:GLU:OE2	1.91	0.70
1:A:150:ALA:O	1:A:152:PRO:HD3	1.90	0.70
1:B:179:ASP:OD1	1:B:179:ASP:C	2.28	0.70
1:A:211:TYR:CE1	1:A:213:ASP:OD1	2.45	0.70
1:B:135:TYR:CE2	1:B:172:ILE:HG23	2.26	0.70
1:A:89:LEU:HD12	1:A:89:LEU:O	1.92	0.69
1:A:47:LYS:NZ	1:A:49:GLN:O	2.24	0.69
1:B:150:ALA:O	1:B:200:LEU:HD11	1.92	0.69
1:B:153:THR:OG1	1:B:156:GLU:CG	2.41	0.69
1:A:135:TYR:HE1	1:A:144:PHE:HB3	1.57	0.69
1:A:305:HIS:C	1:A:305:HIS:CD2	2.66	0.69
1:B:73:ASP:O	1:B:124:LYS:HD2	1.93	0.68
1:A:20:HIS:ND1	1:A:151:ASN:HB3	2.08	0.68
1:A:84:TYR:CE2	1:A:86:HIS:HA	2.28	0.68
1:B:163:LEU:HD12	1:B:164:PHE:N	2.07	0.68
1:A:27:PRO:CB	1:A:294:VAL:HG13	2.24	0.68
1:A:4:LEU:HD21	1:A:14:LYS:HD3	1.75	0.68
1:B:114:LYS:HB2	1:B:126:PHE:CD2	2.29	0.67
1:B:121:LYS:C	3:B:510:HOH:O	2.33	0.67
1:A:38:LYS:O	1:A:40:PRO:HD3	1.94	0.67
1:B:72:ALA:CB	1:B:75:MET:HB2	2.26	0.66
1:A:7:SER:OG	1:A:10:ASN:ND2	2.24	0.66
1:A:62:ARG:HH21	1:A:106:GLU:CD	1.98	0.66
1:A:177:GLY:N	1:A:196:ASN:OD1	2.29	0.66
1:A:150:ALA:C	1:A:152:PRO:HD3	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:HE3	1:B:285:TYR:CE1	2.24	0.66
1:A:293:ILE:O	1:A:297:ILE:HG13	1.95	0.66
1:B:92:PHE:CD2	1:B:93:LEU:HD23	2.30	0.65
1:A:74:ASN:CA	1:A:133:TYR:CD1	2.78	0.65
1:B:222:LEU:HA	1:B:225:LYS:CE	2.25	0.65
1:A:272:LYS:NZ	1:A:299:ASP:O	2.28	0.65
1:A:260:ASN:N	1:A:261:PRO:HD2	2.12	0.65
1:A:155:LYS:HA	1:A:158:LYS:HE3	1.79	0.65
1:A:193:THR:O	1:A:202:LEU:N	2.25	0.65
1:B:257:SER:HA	1:B:287:TRP:CH2	2.31	0.65
1:B:47:LYS:HE3	1:B:49:GLN:O	1.96	0.64
1:B:163:LEU:HD12	1:B:164:PHE:H	1.62	0.64
1:A:12:MET:HB2	1:A:106:GLU:OE1	1.97	0.64
1:A:41:VAL:O	1:A:44:VAL:HG23	1.96	0.64
1:B:252:THR:O	1:B:252:THR:HG22	1.96	0.64
1:B:88:GLU:CD	1:B:88:GLU:N	2.51	0.64
1:A:180:THR:HG23	3:A:553:HOH:O	1.97	0.64
1:A:227:LYS:HA	1:A:274:ARG:O	1.97	0.64
1:B:128:GLU:CG	1:B:132:GLU:OE2	2.44	0.64
1:B:197:ASN:HB2	3:B:530:HOH:O	1.97	0.64
1:A:137:ASN:C	1:A:137:ASN:OD1	2.36	0.64
1:A:137:ASN:OD1	1:A:139:GLN:N	2.31	0.64
1:B:73:ASP:HB3	1:B:124:LYS:HE3	1.79	0.64
1:B:100:LEU:HD12	1:B:143:LEU:HD11	1.80	0.63
1:A:97:LYS:O	1:A:101:SER:HB3	1.98	0.63
1:B:13:SER:OG	1:B:105:ASN:HB2	1.98	0.63
1:A:179:ASP:HB2	3:A:553:HOH:O	1.98	0.63
1:A:119:ASP:OD2	1:A:120:SER:N	2.30	0.63
1:A:102:ALA:C	1:A:104:PRO:HD3	2.19	0.63
1:B:68:GLY:HA2	1:B:77:SER:O	1.99	0.63
1:B:107:THR:CG2	1:B:107:THR:O	2.47	0.62
1:A:240:LEU:HD22	1:A:280:VAL:HG12	1.80	0.62
1:B:9:GLU:OE1	1:B:9:GLU:N	2.30	0.62
1:A:278:LEU:HB2	1:A:297:ILE:HD13	1.81	0.62
1:B:30:HIS:NE2	2:B:401:INS:O2	2.24	0.62
1:A:153:THR:OG1	1:A:156:GLU:HG3	1.98	0.62
1:B:240:LEU:HB2	1:B:280:VAL:HG12	1.82	0.62
1:B:173:LYS:HA	1:B:178:ALA:O	1.99	0.62
1:B:125:THR:O	1:B:129:ILE:HG13	2.00	0.62
1:A:205:GLN:HE21	1:A:207:GLU:H	1.45	0.61
1:A:146:THR:C	1:A:174:SER:OG	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ASP:HA	3:B:512:HOH:O	1.98	0.61
1:A:45:TRP:CZ3	1:A:251:SER:HA	2.35	0.61
1:B:113:LYS:NZ	2:B:401:INS:O6	2.33	0.61
1:A:294:VAL:O	1:A:294:VAL:HG12	1.99	0.61
1:B:88:GLU:OE1	1:B:88:GLU:N	2.33	0.61
1:A:302:LYS:O	1:A:303:LEU:HG	1.99	0.61
1:B:219:VAL:O	1:B:223:LEU:HB2	2.01	0.61
1:A:285:TYR:HE2	1:B:38:LYS:HG3	1.62	0.60
1:B:51:LYS:HZ1	1:B:285:TYR:N	1.98	0.60
1:B:275:THR:HA	3:B:561:HOH:O	2.00	0.60
1:A:5:SER:O	1:A:8:PRO:HD3	2.00	0.60
1:A:50:ASP:HB2	3:A:544:HOH:O	2.00	0.60
1:B:21:LEU:HD23	1:B:24:ILE:HD12	1.83	0.60
1:A:242:VAL:HG12	1:A:255:TYR:CZ	2.33	0.60
1:B:43:SER:O	1:B:44:VAL:C	2.39	0.60
1:A:4:LEU:CD2	1:A:14:LYS:HD3	2.32	0.60
1:B:192:GLU:HG3	1:B:202:LEU:O	2.01	0.60
1:A:74:ASN:HB3	1:A:133:TYR:CE1	2.37	0.60
1:B:45:TRP:CE3	1:B:244:SER:HA	2.37	0.59
1:B:135:TYR:OH	1:B:174:SER:HB2	2.01	0.59
1:A:10:ASN:H	1:A:10:ASN:HD22	1.50	0.59
1:B:302:LYS:CG	1:B:303:LEU:N	2.65	0.59
1:B:93:LEU:HD21	1:B:110:MET:SD	2.42	0.59
1:A:10:ASN:H	1:A:10:ASN:ND2	1.99	0.59
1:B:28:GLY:N	1:B:278:LEU:O	2.31	0.59
1:A:177:GLY:CA	1:A:196:ASN:OD1	2.50	0.59
1:B:268:LYS:HB2	1:B:296:GLU:OE1	2.03	0.58
1:B:96:ALA:HB1	1:B:161:ILE:HD11	1.86	0.58
1:B:139:GLN:NE2	1:B:140:TYR:CE1	2.65	0.58
1:A:150:ALA:O	1:A:152:PRO:HD2	2.03	0.58
1:A:229:ASP:C	3:A:531:HOH:O	2.41	0.57
1:B:256:ALA:O	1:B:260:ASN:HB2	2.05	0.57
1:B:153:THR:HG1	1:B:156:GLU:HG3	1.70	0.57
1:A:69:ARG:HH12	1:A:119:ASP:HB2	1.68	0.57
1:A:145:TYR:CE1	1:A:147:GLY:HA3	2.39	0.57
1:A:137:ASN:CG	1:A:138:PRO:CD	2.72	0.57
1:B:136:ASN:ND2	3:B:526:HOH:O	2.37	0.57
1:A:29:SER:OG	1:A:32:SER:OG	2.22	0.57
1:B:8:PRO:HD2	1:B:9:GLU:OE2	2.05	0.57
1:B:131:ARG:CG	1:B:136:ASN:ND2	2.68	0.56
1:A:133:TYR:N	1:A:133:TYR:CD2	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASP:HB2	1:A:158:LYS:NZ	2.21	0.56
1:A:304:GLU:O	1:A:305:HIS:C	2.40	0.56
1:B:210:ASP:CB	1:B:215:LYS:HB2	2.35	0.56
1:B:252:THR:CG2	1:B:252:THR:O	2.53	0.56
1:A:133:TYR:N	1:A:133:TYR:HD2	2.02	0.56
1:A:48:THR:O	1:A:282:TYR:N	2.28	0.56
1:A:87:HIS:CB	1:A:91:LYS:HD2	2.35	0.56
1:B:43:SER:O	1:B:45:TRP:N	2.38	0.56
1:A:74:ASN:HB3	1:A:133:TYR:HE1	1.70	0.56
1:A:146:THR:O	1:A:174:SER:OG	2.24	0.56
1:A:27:PRO:CG	1:A:294:VAL:HG13	2.36	0.55
1:B:272:LYS:NZ	1:B:299:ASP:O	2.38	0.55
1:A:229:ASP:O	1:A:274:ARG:HD3	2.07	0.55
1:A:20:HIS:HB2	1:A:23:GLU:HG3	1.89	0.55
1:A:17:ASP:CB	1:A:158:LYS:HZ1	2.20	0.55
1:B:67:ARG:HB3	1:B:115:ASP:HB2	1.89	0.55
1:B:177:GLY:H	1:B:196:ASN:ND2	2.04	0.55
1:A:84:TYR:CZ	1:A:86:HIS:HA	2.40	0.55
1:B:24:ILE:CD1	1:B:154:LEU:HD13	2.37	0.55
1:A:125:THR:OG1	1:A:128:GLU:HG3	2.06	0.55
1:B:20:HIS:CD2	1:B:232:LYS:HD2	2.42	0.55
1:A:232:LYS:NZ	3:A:533:HOH:O	2.40	0.54
1:A:285:TYR:CZ	1:B:38:LYS:HG3	2.42	0.54
1:B:130:PHE:O	1:B:134:TYR:HB2	2.08	0.54
1:A:97:LYS:HG3	1:A:143:LEU:HD13	1.90	0.54
1:B:52:ASP:O	1:B:56:GLN:HG3	2.08	0.54
1:B:190:THR:HA	1:B:204:VAL:O	2.07	0.54
1:A:293:ILE:HG23	1:A:294:VAL:N	2.23	0.54
1:B:107:THR:HG23	1:B:107:THR:O	2.08	0.54
1:B:76:ILE:HD12	1:B:134:TYR:CD2	2.43	0.53
1:A:257:SER:O	1:A:261:PRO:HG2	2.08	0.53
1:A:229:ASP:OD1	1:A:229:ASP:C	2.42	0.53
1:A:222:LEU:HD23	1:A:238:ASN:CB	2.34	0.53
1:A:67:ARG:HB2	1:A:79:HIS:O	2.08	0.53
1:B:92:PHE:HD2	1:B:93:LEU:HG	1.74	0.53
1:A:20:HIS:HD1	1:A:151:ASN:HB3	1.72	0.53
1:B:238:ASN:HB3	1:B:278:LEU:HD22	1.85	0.53
1:B:93:LEU:HA	1:B:96:ALA:HB3	1.90	0.53
1:A:246:GLY:C	1:A:248:ALA:H	2.13	0.53
1:B:103:TYR:N	1:B:104:PRO:HD3	2.23	0.53
1:B:12:MET:O	1:B:15:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLU:OE2	1:B:203:LYS:HE2	2.09	0.53
1:B:260:ASN:HB2	1:B:261:PRO:HD3	1.91	0.52
1:B:138:PRO:O	1:B:141:GLN:HG2	2.09	0.52
1:A:232:LYS:HG2	1:A:233:ASP:N	2.25	0.52
1:B:48:THR:HG22	1:B:252:THR:HG21	1.92	0.52
1:A:55:THR:O	1:A:56:GLN:C	2.47	0.52
1:B:130:PHE:HE2	1:B:172:ILE:CD1	2.23	0.52
1:B:4:LEU:CD2	1:B:14:LYS:HD2	2.39	0.52
1:B:215:LYS:NZ	3:B:511:HOH:O	2.30	0.52
1:B:76:ILE:HD12	1:B:134:TYR:CE2	2.45	0.51
1:A:272:LYS:HB3	1:A:302:LYS:HG2	1.91	0.51
1:B:205:GLN:OE1	1:B:205:GLN:C	2.49	0.51
1:A:72:ALA:HB3	1:A:75:MET:HB2	1.92	0.51
1:B:51:LYS:NZ	1:B:285:TYR:N	2.55	0.51
1:B:9:GLU:CD	1:B:9:GLU:N	2.54	0.51
1:A:189:ALA:HA	1:A:207:GLU:HG2	1.92	0.51
1:B:186:ALA:HB3	1:B:191:PHE:CD2	2.45	0.51
1:B:194:LYS:HE3	1:B:201:ASN:OD1	2.09	0.51
1:B:80:HIS:N	1:B:83:VAL:O	2.28	0.51
1:A:137:ASN:ND2	1:A:138:PRO:HD2	2.26	0.51
1:B:217:GLU:C	3:B:509:HOH:O	2.48	0.51
1:A:53:TYR:O	1:A:57:MET:CG	2.49	0.51
1:B:177:GLY:H	1:B:196:ASN:HD21	1.59	0.51
1:A:305:HIS:HD2	1:A:305:HIS:O	1.93	0.51
1:A:97:LYS:CA	1:A:143:LEU:HD11	2.30	0.50
1:B:202:LEU:HD12	1:B:203:LYS:H	1.76	0.50
1:B:210:ASP:HB3	1:B:215:LYS:HB2	1.94	0.50
1:B:51:LYS:HE2	1:B:284:GLY:O	2.10	0.50
1:A:211:TYR:HE1	1:A:213:ASP:OD1	1.93	0.50
1:A:286:THR:HG22	1:A:292:ASP:OD2	2.11	0.50
1:A:73:ASP:O	1:A:129:ILE:HG23	2.11	0.50
1:B:30:HIS:CD2	2:B:401:INS:HO2	2.25	0.50
1:A:285:TYR:CD1	1:A:285:TYR:C	2.84	0.50
1:A:69:ARG:HG3	1:A:116:TYR:HB3	1.94	0.50
1:A:201:ASN:HB2	1:A:234:ASN:OD1	2.11	0.50
1:A:97:LYS:NZ	1:A:139:GLN:O	2.35	0.50
1:A:12:MET:SD	1:A:62:ARG:HG3	2.52	0.50
1:B:205:GLN:OE1	1:B:205:GLN:O	2.30	0.49
1:B:96:ALA:O	1:B:100:LEU:HG	2.12	0.49
1:A:294:VAL:O	1:A:298:ILE:HG13	2.12	0.49
1:A:149:ASN:OD1	1:A:150:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:CG	1:A:188:ASN:O	2.48	0.49
1:A:160:LYS:NZ	3:A:507:HOH:O	2.43	0.49
1:B:217:GLU:CB	3:B:509:HOH:O	2.36	0.49
1:A:35:PHE:C	1:A:35:PHE:CD1	2.86	0.49
1:A:87:HIS:HB2	1:A:91:LYS:HD2	1.94	0.49
1:A:151:ASN:ND2	1:A:233:ASP:OD1	2.46	0.49
1:A:62:ARG:HD2	1:A:107:THR:O	2.13	0.49
1:B:210:ASP:HB2	1:B:215:LYS:HB2	1.95	0.49
1:B:48:THR:O	1:B:49:GLN:CD	2.52	0.48
1:A:260:ASN:HB2	1:A:261:PRO:HD3	1.95	0.48
1:A:151:ASN:CG	1:A:200:LEU:HD21	2.26	0.48
1:A:194:LYS:HG2	1:A:201:ASN:OD1	2.14	0.48
1:B:26:ILE:HG23	1:B:62:ARG:HB2	1.94	0.48
1:A:291:ASP:HA	3:A:523:HOH:O	2.13	0.48
1:A:150:ALA:C	1:A:152:PRO:CD	2.81	0.48
1:A:7:SER:O	1:A:10:ASN:ND2	2.46	0.48
1:A:98:TYR:O	1:A:98:TYR:CD1	2.67	0.48
1:B:143:LEU:HD21	1:B:161:ILE:HD11	1.94	0.48
1:B:58:LYS:CE	3:B:532:HOH:O	2.58	0.48
1:A:205:GLN:NE2	1:A:207:GLU:N	2.55	0.48
1:B:51:LYS:NZ	1:B:284:GLY:O	2.36	0.48
1:B:277:TRP:CD1	1:B:277:TRP:N	2.82	0.48
1:B:8:PRO:O	1:B:11:TRP:HD1	1.96	0.48
1:A:17:ASP:O	1:A:155:LYS:HB2	2.14	0.47
1:A:278:LEU:HB2	1:A:297:ILE:CD1	2.43	0.47
1:B:21:LEU:HD21	1:B:154:LEU:HD12	1.96	0.47
1:B:214:LYS:O	1:B:217:GLU:HB2	2.14	0.47
1:B:76:ILE:HG12	1:B:126:PHE:CE1	2.48	0.47
1:B:92:PHE:CD2	1:B:92:PHE:C	2.85	0.47
1:B:302:LYS:HG3	1:B:303:LEU:H	1.76	0.47
1:B:165:ASN:O	1:B:183:ILE:HD12	2.14	0.47
1:B:205:GLN:HE21	1:B:218:ALA:HB1	1.78	0.47
1:A:185:TRP:HA	1:A:191:PHE:CZ	2.49	0.47
1:A:51:LYS:HB3	1:A:55:THR:HB	1.96	0.47
1:A:52:ASP:OD1	1:A:55:THR:OG1	2.20	0.47
1:A:165:ASN:OD1	1:A:167:MET:N	2.35	0.47
1:A:202:LEU:HG	1:A:204:VAL:HG23	1.97	0.47
1:A:72:ALA:HB3	1:A:75:MET:CB	2.45	0.47
1:A:294:VAL:O	1:A:294:VAL:CG1	2.62	0.47
1:B:51:LYS:HZ1	1:B:285:TYR:CA	2.27	0.47
1:A:249:PHE:CD2	1:A:258:HIS:CD2	3.01	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:TYR:N	1:B:171:TYR:CD2	2.84	0.47
1:B:173:LYS:HA	1:B:173:LYS:HD3	1.63	0.46
1:B:211:TYR:CE1	1:B:213:ASP:HB2	2.50	0.46
1:A:137:ASN:OD1	1:A:138:PRO:HD2	2.13	0.46
1:B:222:LEU:HD12	1:B:225:LYS:CE	2.41	0.46
1:A:100:LEU:HD13	1:A:159:GLY:O	2.15	0.46
1:A:21:LEU:HD21	1:A:107:THR:HG21	1.96	0.46
1:B:287:TRP:HA	1:B:288:PRO:HD2	1.80	0.46
1:B:17:ASP:HA	1:B:154:LEU:HB3	1.96	0.46
1:B:135:TYR:CZ	1:B:172:ILE:HG23	2.51	0.46
1:A:12:MET:C	1:A:14:LYS:N	2.69	0.46
1:A:35:PHE:CB	1:A:51:LYS:O	2.63	0.46
1:A:253:TYR:CD2	1:B:39:ASP:HA	2.50	0.46
1:B:80:HIS:ND1	1:B:80:HIS:O	2.45	0.46
1:B:197:ASN:C	1:B:199:SER:H	2.16	0.46
1:B:206:ASP:OD1	2:B:401:INS:O1	2.34	0.46
1:A:212:TYR:CD2	1:A:212:TYR:C	2.89	0.46
1:A:67:ARG:HB3	1:A:115:ASP:HB2	1.98	0.46
1:A:103:TYR:N	1:A:104:PRO:HD3	2.30	0.46
1:B:90:GLY:O	1:B:94:ASP:CG	2.54	0.46
1:A:285:TYR:HE2	1:B:38:LYS:CD	2.29	0.45
1:B:141:GLN:HG3	1:B:142:ASN:N	2.25	0.45
1:B:78:VAL:CG1	3:B:508:HOH:O	2.31	0.45
1:B:43:SER:C	1:B:45:TRP:N	2.69	0.45
1:A:39:ASP:O	1:A:43:SER:HB2	2.16	0.45
1:B:153:THR:H	1:B:156:GLU:HB2	1.81	0.45
1:B:234:ASN:O	1:B:274:ARG:NH2	2.49	0.45
1:B:144:PHE:O	1:B:160:LYS:CD	2.53	0.45
1:A:305:HIS:CD2	1:A:305:HIS:O	2.70	0.45
1:A:21:LEU:HB2	1:A:176:TYR:OH	2.17	0.45
1:A:4:LEU:HD21	1:A:14:LYS:CD	2.44	0.45
1:B:20:HIS:O	1:B:23:GLU:HB2	2.17	0.45
1:B:59:SER:O	1:B:294:VAL:HG11	2.16	0.45
1:B:86:HIS:ND1	1:B:86:HIS:N	2.63	0.45
1:B:92:PHE:CD2	1:B:93:LEU:CD2	2.98	0.45
1:A:265:LYS:HG2	3:A:538:HOH:O	2.16	0.45
1:A:183:ILE:HG23	1:A:195:ILE:HG21	1.99	0.45
1:A:78:VAL:O	1:A:85:LEU:HB2	2.17	0.44
1:B:185:TRP:HD1	1:B:186:ALA:O	2.00	0.44
1:A:181:SER:O	1:A:182:GLY:C	2.56	0.44
1:A:119:ASP:O	1:A:122:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LYS:CE	1:B:284:GLY:O	2.64	0.44
1:B:223:LEU:HD12	3:B:561:HOH:O	2.17	0.44
1:B:140:TYR:O	1:B:141:GLN:C	2.54	0.44
1:A:241:SER:HB3	1:A:281:ASP:OD1	2.17	0.44
1:B:302:LYS:CG	1:B:303:LEU:H	2.29	0.44
1:B:48:THR:HB	1:B:281:ASP:OD1	2.18	0.44
1:A:285:TYR:HE2	1:B:38:LYS:CG	2.27	0.44
1:B:262:GLU:O	1:B:262:GLU:HG3	2.18	0.44
1:A:255:TYR:O	1:A:256:ALA:C	2.56	0.44
1:A:27:PRO:HG3	1:A:297:ILE:HB	1.99	0.44
1:B:89:LEU:HD11	1:B:93:LEU:HD11	2.00	0.44
1:A:192:GLU:HA	1:A:202:LEU:O	2.18	0.44
1:B:130:PHE:HE2	1:B:172:ILE:HD12	1.82	0.44
1:A:65:ASP:OD2	1:A:67:ARG:NH2	2.49	0.44
1:B:4:LEU:HA	1:B:4:LEU:HD23	1.56	0.44
1:B:85:LEU:O	1:B:86:HIS:HB2	2.17	0.44
1:B:177:GLY:HA2	1:B:195:ILE:HB	1.99	0.43
1:A:249:PHE:CZ	1:A:258:HIS:CG	3.06	0.43
1:A:285:TYR:CE2	1:B:38:LYS:CG	2.91	0.43
1:B:39:ASP:OD2	1:B:40:PRO:HD2	2.18	0.43
1:B:137:ASN:OD1	1:B:139:GLN:HB3	2.18	0.43
1:B:155:LYS:HE3	1:B:155:LYS:HB2	1.66	0.43
1:A:184:GLN:HB2	1:A:184:GLN:HE21	1.55	0.43
1:B:128:GLU:OE2	1:B:132:GLU:OE2	2.37	0.43
1:A:12:MET:CB	1:A:106:GLU:OE1	2.63	0.43
1:B:73:ASP:CB	1:B:124:LYS:HE3	2.46	0.43
1:A:100:LEU:HD22	1:A:106:GLU:O	2.18	0.43
1:B:89:LEU:HD23	1:B:134:TYR:CG	2.53	0.43
1:A:253:TYR:CZ	1:B:38:LYS:HB2	2.54	0.43
1:A:285:TYR:C	1:A:285:TYR:HD1	2.22	0.43
1:B:13:SER:OG	1:B:105:ASN:CB	2.65	0.43
1:A:183:ILE:HG23	1:A:195:ILE:CG2	2.48	0.43
1:B:100:LEU:HD21	1:B:108:ILE:HD12	2.01	0.43
1:A:45:TRP:NE1	3:A:506:HOH:O	2.44	0.43
1:A:149:ASN:HB2	3:A:521:HOH:O	2.19	0.43
1:B:227:LYS:HA	1:B:274:ARG:O	2.18	0.43
1:A:161:ILE:HD13	1:A:161:ILE:HG21	1.76	0.43
1:B:188:ASN:CG	1:B:188:ASN:O	2.56	0.43
1:A:20:HIS:CE1	1:A:151:ASN:HB3	2.53	0.43
1:B:21:LEU:HD21	1:B:154:LEU:CD1	2.48	0.43
1:B:204:VAL:HG12	1:B:205:GLN:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLY:C	1:A:248:ALA:N	2.72	0.43
1:B:92:PHE:CE2	1:B:93:LEU:CD2	2.91	0.42
1:A:267:ILE:HD11	1:A:278:LEU:CD1	2.41	0.42
1:B:109:VAL:O	1:B:109:VAL:HG12	2.17	0.42
1:B:173:LYS:HD3	1:B:178:ALA:O	2.19	0.42
1:B:52:ASP:HB2	3:B:516:HOH:O	2.19	0.42
1:A:45:TRP:HA	1:A:252:THR:OG1	2.19	0.42
1:A:265:LYS:HB2	1:A:265:LYS:HE3	1.51	0.42
1:A:302:LYS:O	1:A:303:LEU:C	2.57	0.42
1:B:26:ILE:CG2	1:B:62:ARG:HB2	2.50	0.42
1:B:7:SER:C	1:B:9:GLU:OE1	2.57	0.42
1:A:163:LEU:HD21	1:A:165:ASN:CB	2.42	0.42
1:B:141:GLN:CG	1:B:142:ASN:N	2.82	0.42
1:A:190:THR:HA	1:A:204:VAL:O	2.20	0.42
1:B:222:LEU:HG	1:B:222:LEU:O	2.20	0.42
1:A:260:ASN:H	1:A:261:PRO:CD	2.30	0.42
1:B:302:LYS:CD	1:B:303:LEU:H	2.33	0.42
1:A:10:ASN:N	1:A:10:ASN:HD22	2.10	0.42
1:A:87:HIS:HD2	1:A:91:LYS:HB3	1.84	0.42
1:A:145:TYR:CZ	1:A:147:GLY:HA3	2.54	0.42
1:B:208:TYR:HA	1:B:242:VAL:HG23	2.00	0.42
1:A:63:PHE:CE2	1:A:279:ILE:HD12	2.55	0.42
1:B:121:LYS:HB3	1:B:121:LYS:HZ2	1.84	0.42
1:A:196:ASN:O	1:A:199:SER:OG	2.31	0.42
1:B:240:LEU:HD21	1:B:263:ILE:HG21	2.01	0.42
1:B:211:TYR:CD1	1:B:214:LYS:HE3	2.55	0.42
1:A:213:ASP:N	1:A:213:ASP:OD1	2.50	0.42
1:A:287:TRP:HB2	1:A:290:TYR:HD2	1.84	0.42
1:B:76:ILE:HG23	1:B:126:PHE:HE1	1.84	0.42
1:A:266:THR:O	1:A:267:ILE:C	2.55	0.42
1:A:7:SER:O	1:A:7:SER:OG	2.30	0.41
1:A:52:ASP:O	1:A:56:GLN:HG3	2.20	0.41
1:A:127:GLU:O	1:A:128:GLU:C	2.56	0.41
1:B:112:MET:O	1:B:166:ARG:HB2	2.20	0.41
1:A:55:THR:C	1:A:57:MET:N	2.72	0.41
1:A:222:LEU:HB3	1:A:238:ASN:ND2	2.35	0.41
1:B:2:ASP:HB3	1:B:3:SER:H	1.62	0.41
1:A:176:TYR:CE2	1:A:277:TRP:HH2	2.38	0.41
1:B:21:LEU:HA	1:B:21:LEU:HD23	1.73	0.41
1:A:24:ILE:O	1:A:277:TRP:CD1	2.74	0.41
1:B:67:ARG:O	1:B:78:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLN:NE2	1:B:64:PHE:HE1	2.18	0.41
1:B:26:ILE:HA	1:B:27:PRO:HD3	1.77	0.41
1:B:179:ASP:OD1	1:B:179:ASP:O	2.38	0.41
1:B:167:MET:HB2	1:B:167:MET:HE3	1.93	0.41
1:B:11:TRP:CZ3	1:B:12:MET:HG2	2.55	0.41
1:A:80:HIS:CE1	3:A:505:HOH:O	2.73	0.41
1:A:213:ASP:HB3	3:A:519:HOH:O	2.21	0.41
1:B:42:LYS:HE2	1:B:42:LYS:HB3	1.59	0.41
1:B:64:PHE:HD2	1:B:108:ILE:HG23	1.86	0.41
1:B:72:ALA:HB3	1:B:75:MET:HB3	1.95	0.41
1:B:137:ASN:OD1	1:B:139:GLN:N	2.50	0.41
1:A:35:PHE:CD2	1:A:52:ASP:HA	2.56	0.40
1:A:47:LYS:HZ1	1:A:50:ASP:HA	1.86	0.40
1:B:93:LEU:O	1:B:97:LYS:N	2.44	0.40
1:B:111:SER:HA	1:B:164:PHE:O	2.21	0.40
1:A:12:MET:C	1:A:14:LYS:H	2.25	0.40
1:A:30:HIS:CD2	2:A:401:INS:HO2	2.39	0.40
1:A:232:LYS:HD2	3:A:534:HOH:O	2.20	0.40
1:A:238:ASN:HB3	1:A:278:LEU:HD23	2.03	0.40
1:A:179:ASP:OD1	1:A:179:ASP:C	2.60	0.40
1:A:263:ILE:HA	1:A:263:ILE:HD13	1.87	0.40
1:B:149:ASN:ND2	1:B:156:GLU:OE1	2.54	0.40
1:A:205:GLN:C	1:A:205:GLN:CD	2.79	0.40
1:B:105:ASN:HD22	1:B:105:ASN:N	2.18	0.40
1:A:25:ASN:ND2	1:A:275:THR:HG23	2.37	0.40
1:B:25:ASN:O	1:B:297:ILE:HG22	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	A	302/310 (97%)	288 (95%)	12 (4%)	2 (1%)	26	18
1	B	300/310 (97%)	292 (97%)	8 (3%)	0	100	100
All	All	602/620 (97%)	580 (96%)	20 (3%)	2 (0%)	46	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	182	GLY

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	264/270 (98%)	231 (88%)	33 (12%)	6	2
1	B	262/270 (97%)	233 (89%)	29 (11%)	8	3
All	All	526/540 (97%)	464 (88%)	62 (12%)	6	2

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	10	ASN
1	A	29	SER
1	A	32	SER
1	A	42	LYS
1	A	43	SER
1	A	50	ASP
1	A	69	ARG
1	A	79	HIS
1	A	88	GLU
1	A	89	LEU
1	A	115	ASP
1	A	117	ASP
1	A	121	LYS

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Mol	Chain	Res	Type
1	A	124	LYS
1	A	133	TYR
1	A	137	ASN
1	A	141	GLN
1	A	148	SER
1	A	165	ASN
1	A	184	GLN
1	A	199	SER
1	A	213	ASP
1	A	232	LYS
1	A	235	VAL
1	A	247	SER
1	A	265	LYS
1	A	286	THR
1	A	295	SER
1	A	302	LYS
1	A	303	LEU
1	A	304	GLU
1	A	305	HIS
1	B	2	ASP
1	B	15	LEU
1	B	19	LYS
1	B	20	HIS
1	B	43	SER
1	B	73	ASP
1	B	79	HIS
1	B	86	HIS
1	B	97	LYS
1	B	105	ASN
1	B	119	ASP
1	B	121	LYS
1	B	124	LYS
1	B	127	GLU
1	B	138	PRO
1	B	141	GLN
1	B	155	LYS
1	B	181	SER
1	B	213	ASP
1	B	227	LYS
1	B	230	SER
1	B	235	VAL
1	B	242	VAL

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Mol	Chain	Res	Type
1	B	259	ILE
1	B	265	LYS
1	B	266	THR
1	B	279	ILE
1	B	286	THR
1	B	293	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	56	GLN
1	A	79	HIS
1	A	136	ASN
1	A	141	GLN
1	A	184	GLN
1	A	197	ASN
1	A	205	GLN
1	A	250	ASN
1	A	258	HIS
1	A	305	HIS
1	B	56	GLN
1	B	105	ASN
1	B	136	ASN
1	B	141	GLN
1	B	196	ASN
1	B	205	GLN
1	B	258	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	INS	A	401	-	12,12,12	0.52	0	18,18,18	0.40	0
2	INS	B	401	-	12,12,12	0.51	0	18,18,18	0.40	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	INS	A	401	-	-	0/0/24/24	0/1/1/1
2	INS	B	401	-	-	0/0/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	INS	1	0
2	B	401	INS	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	304/310 (98%)	0.84	35 (11%) 6 11	23, 42, 55, 68	3 (0%)
1	B	302/310 (97%)	0.93	29 (9%) 10 16	25, 42, 55, 63	2 (0%)
All	All	606/620 (97%)	0.88	64 (10%) 8 13	23, 42, 55, 68	5 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	SER	7.5
1	A	2	ASP	4.1
1	B	122	VAL	4.0
1	B	176	TYR	4.0
1	B	2	ASP	3.6
1	A	129	ILE	3.5
1	A	195	ILE	3.5
1	B	200	LEU	3.4
1	B	162	VAL	3.4
1	B	133	TYR	3.3
1	B	302	LYS	3.3
1	A	151	ASN	3.3
1	B	172	ILE	3.2
1	A	250	ASN	3.1
1	B	286	THR	3.1
1	A	107	THR	3.1
1	A	4	LEU	3.0
1	A	45	TRP	2.9
1	B	135	TYR	2.9
1	B	63	PHE	2.9
1	A	255	TYR	2.8
1	B	126	PHE	2.7
1	A	236	TYR	2.7
1	B	216	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	212	TYR	2.6
1	B	277	TRP	2.6
1	B	108	ILE	2.5
1	A	121	LYS	2.5
1	B	41	VAL	2.5
1	B	98	TYR	2.5
1	A	61	VAL	2.5
1	B	253	TYR	2.5
1	A	82	MET	2.4
1	B	254	ASN	2.4
1	B	203	LYS	2.4
1	B	27	PRO	2.4
1	B	134	TYR	2.4
1	A	305	HIS	2.4
1	A	191	PHE	2.3
1	A	285	TYR	2.3
1	A	22	THR	2.3
1	A	24	ILE	2.3
1	A	159	GLY	2.2
1	A	144	PHE	2.2
1	A	26	ILE	2.2
1	A	76	ILE	2.2
1	A	89	LEU	2.2
1	A	161	ILE	2.2
1	B	189	ALA	2.2
1	A	21	LEU	2.2
1	A	211	TYR	2.2
1	A	136	ASN	2.2
1	A	164	PHE	2.2
1	A	132	GLU	2.1
1	B	287	TRP	2.1
1	B	143	LEU	2.1
1	B	201	ASN	2.1
1	B	199	SER	2.1
1	A	146	THR	2.1
1	B	222	LEU	2.1
1	A	104	PRO	2.1
1	A	101	SER	2.1
1	A	105	ASN	2.0
1	B	285	TYR	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	INS	B	401	12/12	0.48	0.22	2.17	58,60,60,60	0
2	INS	A	401	12/12	0.82	0.22	1.24	49,51,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.