Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:59 AM GMT

PDB ID	:	3QML
Title	:	The structural analysis of Sil1-Bip complex reveals the mechanism for Sil1 to function as a novel nucleotide exchange factor
Authors	:	Yan, M.; Li, J.Z.; Sha, B.D.
Deposited on	:	2011-02-04
Resolution	:	2.31 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:

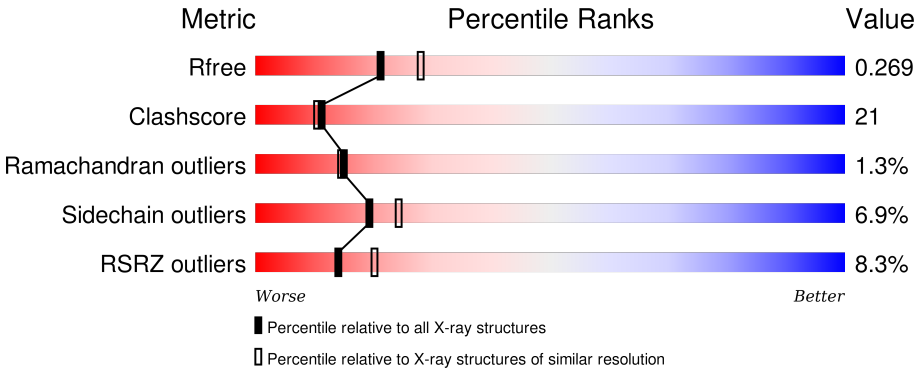
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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 <=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	390	77% 18%
1	B	390	21% 53% 37% 5% 5%
2	C	315	2% 58% 19% 6% 17%
2	D	315	5% 49% 34% 13%

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
3	PO4	A	2	-	-	-	X
3	PO4	A	4	-	-	X	X
3	PO4	B	1	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10378 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 78 kDa glucose-regulated protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2893	1825	495	568	5			
1	B	370	Total	C	N	O	S	0	0	0
			2830	1788	483	554	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLY	-	EXPRESSION TAG	UNP P16474
A	38	MET	-	EXPRESSION TAG	UNP P16474
A	39	SER	-	EXPRESSION TAG	UNP P16474
A	40	HIS	-	EXPRESSION TAG	UNP P16474
A	41	ALA	-	EXPRESSION TAG	UNP P16474
A	42	SER	-	EXPRESSION TAG	UNP P16474
B	37	GLY	-	EXPRESSION TAG	UNP P16474
B	38	MET	-	EXPRESSION TAG	UNP P16474
B	39	SER	-	EXPRESSION TAG	UNP P16474
B	40	HIS	-	EXPRESSION TAG	UNP P16474
B	41	ALA	-	EXPRESSION TAG	UNP P16474
B	42	SER	-	EXPRESSION TAG	UNP P16474

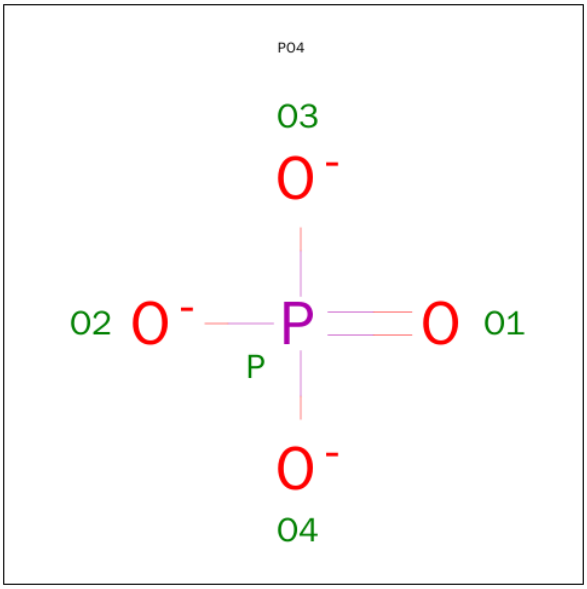
- Molecule 2 is a protein called Nucleotide exchange factor SIL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	262	Total	C	N	O	S	0	0	0
			2160	1367	367	419	7			
2	D	273	Total	C	N	O	S	0	0	0
			2246	1423	384	432	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	107	GLY	-	EXPRESSION TAG	UNP Q08199
C	108	MET	-	EXPRESSION TAG	UNP Q08199
C	109	SER	-	EXPRESSION TAG	UNP Q08199
C	110	HIS	-	EXPRESSION TAG	UNP Q08199
C	111	ALA	-	EXPRESSION TAG	UNP Q08199
C	112	SER	-	EXPRESSION TAG	UNP Q08199
D	107	GLY	-	EXPRESSION TAG	UNP Q08199
D	108	MET	-	EXPRESSION TAG	UNP Q08199
D	109	SER	-	EXPRESSION TAG	UNP Q08199
D	110	HIS	-	EXPRESSION TAG	UNP Q08199
D	111	ALA	-	EXPRESSION TAG	UNP Q08199
D	112	SER	-	EXPRESSION TAG	UNP Q08199

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	C	1	Total Mg 1 1	0	0

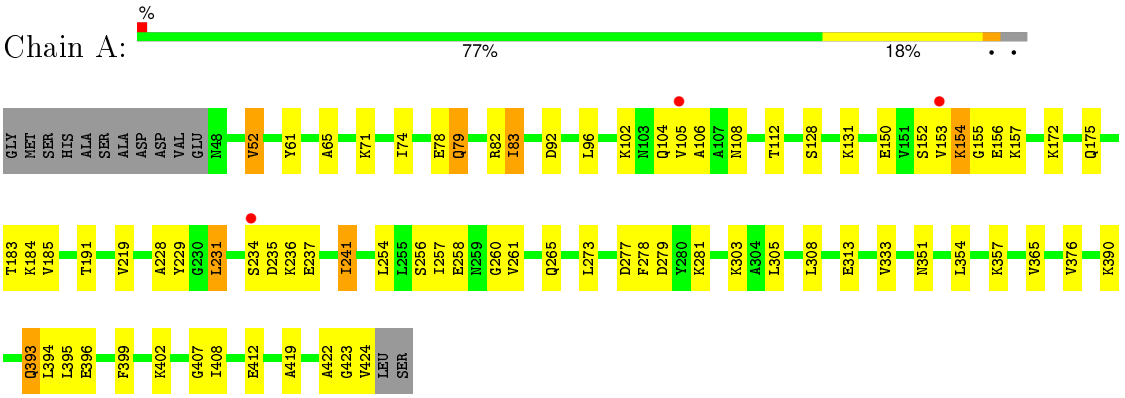
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	96	Total O 96 96	0	0
5	B	48	Total O 48 48	0	0
5	C	34	Total O 34 34	0	0
5	D	28	Total O 28 28	0	0

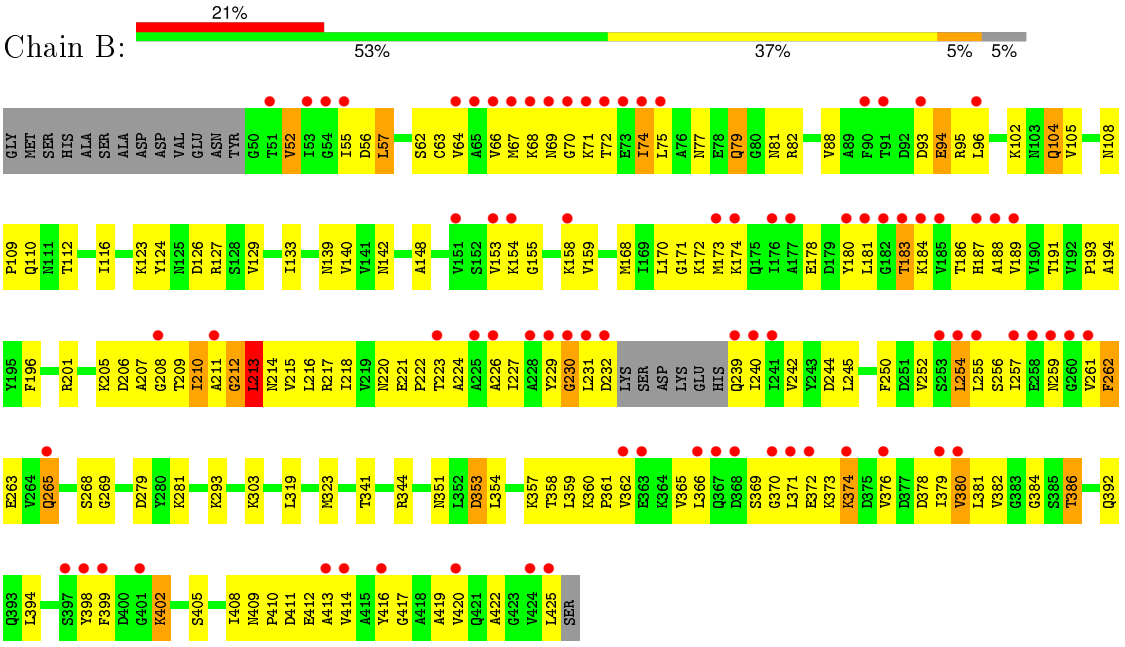
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

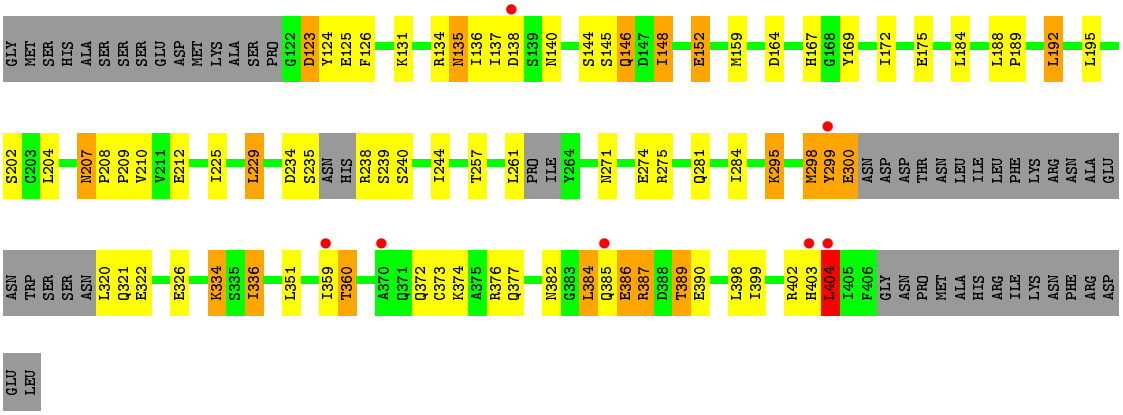
- Molecule 1: 78 kDa glucose-regulated protein homolog



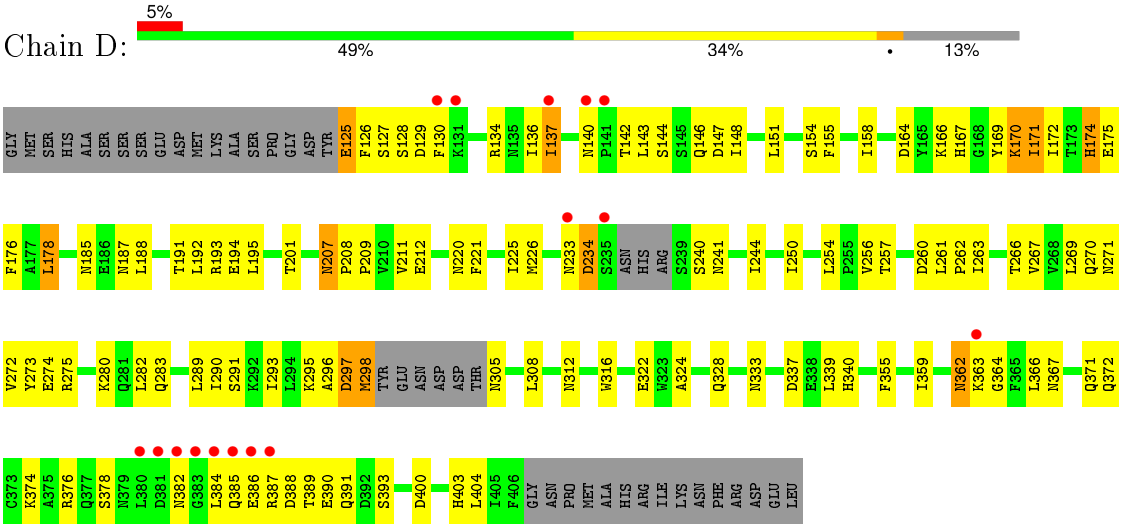
- Molecule 1: 78 kDa glucose-regulated protein homolog



- Molecule 2: Nucleotide exchange factor SIL1



- Molecule 2: Nucleotide exchange factor SIL1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	226.35Å 116.59Å 55.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.13 – 2.31 46.13 – 2.31	Depositor EDS
% Data completeness (in resolution range)	91.5 (46.13-2.31) 91.5 (46.13-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_351)	Depositor
R, R_{free}	0.210 , 0.271 0.206 , 0.269	Depositor DCC
R_{free} test set	3053 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 60114 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10378	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, MG

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	0.46	0/2931	0.60	0/3952
1	B	0.36	0/2865	0.53	0/3863
2	C	0.41	0/2194	0.57	1/2954 (0.0%)
2	D	0.37	0/2283	0.54	1/3078 (0.0%)
All	All	0.40	0/10273	0.56	2/13847 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	234	ASP	CB-CG-OD2	5.21	122.99	118.30
2	D	234	ASP	CB-CG-OD2	5.16	122.94	118.30

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	2893	0	2950	69	0
1	B	2830	0	2897	184	0
2	C	2160	0	2142	72	0
2	D	2246	0	2240	102	0
3	A	10	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	1	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	A	96	0	0	3	0
5	B	48	0	0	9	0
5	C	34	0	0	4	0
5	D	28	0	0	2	0
All	All	10378	0	10229	422	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 21.

All (422) 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:213:LEU:HD12	1:B:214:ASN:H	1.14	1.10
1:A:234:SER:HA	1:A:235:ASP:HB2	1.32	1.05
1:A:52:VAL:HG22	1:A:422:ALA:HB1	1.38	1.00
2:D:233:ASN:ND2	2:D:271:ASN:ND2	2.12	0.97
2:D:382:ASN:HB2	2:D:387:ARG:HH22	1.29	0.95
2:D:164:ASP:OD2	2:D:166:LYS:HG2	1.67	0.95
2:C:334:LYS:H	2:C:334:LYS:HD2	1.31	0.94
1:B:252:VAL:HG21	1:B:362:VAL:HG12	1.50	0.93
1:B:52:VAL:HG22	1:B:422:ALA:HB1	1.52	0.89
2:D:386:GLU:HB3	2:D:387:ARG:HA	1.54	0.88
1:B:74:ILE:HD11	1:B:82:ARG:HB3	1.54	0.88
2:D:271:ASN:HD21	2:D:275:ARG:HH21	1.22	0.87
1:B:94:GLU:HG3	1:B:95:ARG:H	1.39	0.87
1:B:213:LEU:HA	5:B:461:HOH:O	1.77	0.84
1:B:216:LEU:HD23	1:B:425:LEU:HD13	1.60	0.83
2:C:351:LEU:HB3	2:C:359:ILE:HD13	1.62	0.82
2:C:123:ASP:HA	2:C:124:TYR:HB3	1.61	0.82
2:D:266:THR:HG22	2:D:316:TRP:CH2	2.15	0.81
1:B:105:VAL:HG22	1:B:112:THR:HG21	1.62	0.80
2:C:239:SER:CA	2:C:240:SER:HB3	2.11	0.80
2:D:372:GLN:HE21	2:D:376:ARG:HH11	1.30	0.79
2:D:403:HIS:CD2	2:D:404:LEU:HG	2.18	0.79
2:D:372:GLN:HG3	2:D:376:ARG:HD2	1.64	0.79
1:B:244:ASP:HA	1:B:382:VAL:HG23	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:GLU:HG2	1:B:414:VAL:HG11	1.64	0.78
1:B:360:LYS:HB2	1:B:361:PRO:HD3	1.64	0.78
1:B:370:GLY:HA3	1:B:371:LEU:HB2	1.62	0.78
1:B:213:LEU:HD12	1:B:214:ASN:N	1.96	0.78
1:B:57:LEU:HA	1:B:62:SER:HB3	1.64	0.78
2:C:372:GLN:HG3	2:C:376:ARG:HD2	1.65	0.78
1:B:66:VAL:HG21	1:B:181:LEU:HD11	1.64	0.78
2:D:233:ASN:ND2	2:D:271:ASN:HD22	1.79	0.77
1:A:153:VAL:HA	1:A:154:LYS:HB2	1.67	0.77
2:C:135:ASN:HA	2:C:138:ASP:HB2	1.66	0.77
1:B:52:VAL:HG11	1:B:425:LEU:HB2	1.65	0.76
2:C:239:SER:HA	2:C:240:SER:HB3	1.67	0.76
2:D:155:PHE:HB3	2:D:195:LEU:HD12	1.68	0.75
1:B:210:ILE:HD12	1:B:211:ALA:HB2	1.68	0.75
1:B:254:LEU:HD23	1:B:365:VAL:HG12	1.68	0.75
1:A:234:SER:HA	1:A:235:ASP:CB	2.12	0.75
2:C:159:MET:HE2	5:C:427:HOH:O	1.87	0.74
2:D:388:ASP:O	2:D:390:GLU:N	2.20	0.74
2:C:298:MET:O	2:C:298:MET:SD	2.46	0.74
2:D:233:ASN:HD21	2:D:271:ASN:ND2	1.86	0.74
1:B:227:ILE:HD11	1:B:262:PHE:HE2	1.53	0.73
1:B:265:GLN:HE21	1:B:265:GLN:HA	1.54	0.73
1:B:187:HIS:CD2	1:B:216:LEU:HD13	2.24	0.73
1:B:79:GLN:HE22	1:B:81:ASN:HB2	1.54	0.72
1:A:106:ALA:HA	5:A:486:HOH:O	1.90	0.72
1:B:220:ASN:O	1:B:223:THR:HG22	1.89	0.72
1:B:77:ASN:HD21	1:B:79:GLN:HE21	1.38	0.71
1:B:174:LYS:NZ	5:B:460:HOH:O	2.20	0.71
2:D:385:GLN:HA	2:D:387:ARG:HH11	1.54	0.71
2:C:298:MET:HA	2:C:299:TYR:HB3	1.73	0.71
1:A:104:GLN:HE22	1:A:112:THR:HG22	1.56	0.71
1:B:172:LYS:N	5:B:450:HOH:O	2.22	0.71
2:C:229:LEU:HD21	2:C:244:ILE:HG23	1.73	0.70
2:C:124:TYR:HE2	2:C:175:GLU:OE1	1.73	0.70
1:B:370:GLY:CA	1:B:371:LEU:HB2	2.20	0.70
1:B:102:LYS:O	1:B:105:VAL:HG23	1.91	0.70
2:C:131:LYS:HE2	2:C:131:LYS:HA	1.74	0.70
1:B:208:GLY:O	1:B:213:LEU:HB3	1.91	0.69
2:D:256:VAL:HG23	2:D:296:ALA:HB2	1.73	0.69
2:D:296:ALA:O	2:D:312:ASN:ND2	2.26	0.69
1:B:194:ALA:HB2	1:B:222:PRO:HG2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:152:GLU:HG3	2:C:195:LEU:HD11	1.75	0.69
1:B:213:LEU:CD1	1:B:214:ASN:H	1.99	0.68
1:B:231:LEU:HG	1:B:240:ILE:HG12	1.72	0.68
1:B:268:SER:HB2	1:B:365:VAL:HG23	1.73	0.68
1:A:393:GLN:HG3	1:A:394:LEU:N	2.08	0.68
1:B:402:LYS:HD3	1:B:402:LYS:O	1.93	0.68
1:B:52:VAL:HG22	1:B:422:ALA:CB	2.22	0.68
2:D:240:SER:O	2:D:244:ILE:HG12	1.94	0.68
2:D:363:LYS:HG3	2:D:366:LEU:HB2	1.76	0.68
1:A:104:GLN:HE22	1:A:112:THR:CG2	2.07	0.67
1:B:261:VAL:HG12	1:B:262:PHE:H	1.59	0.67
1:A:234:SER:CA	1:A:235:ASP:HB2	2.16	0.67
1:B:372:GLU:HG2	1:B:374:LYS:H	1.60	0.67
2:D:233:ASN:HD22	2:D:271:ASN:HD22	1.43	0.67
2:C:235:SER:HB3	2:C:238:ARG:HB3	1.76	0.67
1:B:212:GLY:O	1:B:213:LEU:HB2	1.94	0.66
2:C:152:GLU:HG3	2:C:195:LEU:CD1	2.25	0.66
2:C:239:SER:HA	2:C:240:SER:CB	2.23	0.66
1:B:239:GLN:N	1:B:257:ILE:HG22	2.10	0.66
2:C:334:LYS:N	2:C:334:LYS:HD2	2.08	0.66
1:B:254:LEU:HD23	1:B:365:VAL:CG1	2.24	0.66
1:A:102:LYS:O	1:A:105:VAL:HG23	1.96	0.66
1:A:52:VAL:CG2	1:A:422:ALA:HB1	2.21	0.66
1:B:79:GLN:NE2	1:B:81:ASN:HB2	2.11	0.66
2:D:372:GLN:HE21	2:D:376:ARG:NH1	1.94	0.65
2:D:271:ASN:HD21	2:D:275:ARG:NH2	1.93	0.65
1:B:399:PHE:HB2	1:B:402:LYS:HG3	1.79	0.65
2:C:372:GLN:HE21	2:C:376:ARG:HH11	1.42	0.65
1:B:191:THR:HA	5:B:446:HOH:O	1.97	0.64
2:D:337:ASP:HB3	2:D:340:HIS:HB2	1.78	0.64
1:B:174:LYS:HE3	1:B:178:GLU:OE2	1.97	0.64
2:D:266:THR:HG22	2:D:316:TRP:CZ3	2.33	0.64
1:B:70:GLY:C	1:B:71:LYS:HD2	2.17	0.64
2:C:351:LEU:HB3	2:C:359:ILE:CD1	2.28	0.64
2:D:362:ASN:HD22	2:D:364:GLY:HA3	1.62	0.63
2:D:209:PRO:HA	2:D:212:GLU:OE1	1.99	0.63
2:D:261:LEU:HD22	2:D:293:ILE:HG23	1.81	0.63
1:B:359:LEU:O	1:B:362:VAL:HG22	1.99	0.63
2:C:164:ASP:HB3	2:C:167:HIS:HB2	1.80	0.63
1:B:205:LYS:HG3	1:B:218:ILE:HD13	1.81	0.63
2:C:281:GLN:NE2	5:C:40:HOH:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:THR:HB	1:B:221:GLU:HG3	1.79	0.63
2:D:386:GLU:OE2	2:D:386:GLU:HA	1.99	0.62
1:B:239:GLN:OE1	1:B:371:LEU:HD21	1.99	0.62
1:B:341:THR:HG23	2:D:337:ASP:OD1	1.99	0.62
1:B:227:ILE:HD11	1:B:262:PHE:CE2	2.35	0.62
2:D:385:GLN:HA	2:D:387:ARG:NH1	2.14	0.62
1:B:66:VAL:HG12	1:B:75:LEU:HD21	1.81	0.62
1:B:411:ASP:OD1	1:B:412:GLU:HG3	1.99	0.62
2:D:372:GLN:O	2:D:376:ARG:HG3	2.00	0.62
2:D:363:LYS:CG	2:D:366:LEU:HB2	2.29	0.62
2:D:295:LYS:O	2:D:298:MET:HG3	1.99	0.62
2:D:271:ASN:ND2	2:D:275:ARG:HH21	1.96	0.62
2:D:388:ASP:HB3	2:D:391:GLN:HB3	1.81	0.61
1:B:173:MET:SD	5:B:436:HOH:O	2.56	0.61
1:A:150:GLU:OE1	1:A:157:LYS:HD3	1.99	0.61
1:B:224:ALA:O	1:B:417:GLY:HA3	2.00	0.61
1:B:63:CYS:HA	5:B:439:HOH:O	1.99	0.61
1:B:223:THR:HA	1:B:255:LEU:HD11	1.82	0.61
2:D:127:SER:HA	2:D:130:PHE:HB3	1.82	0.60
1:B:77:ASN:ND2	1:B:79:GLN:HE21	1.99	0.60
2:D:191:THR:O	2:D:195:LEU:HD23	2.00	0.60
2:C:403:HIS:O	2:C:404:LEU:HB2	2.01	0.60
2:D:372:GLN:NE2	2:D:376:ARG:HH11	1.97	0.60
2:D:295:LYS:HD3	2:D:295:LYS:N	2.17	0.60
1:B:154:LYS:HD3	1:B:155:GLY:CA	2.32	0.60
1:B:265:GLN:HB3	1:B:369:SER:HB2	1.84	0.60
2:C:239:SER:N	2:C:240:SER:HB3	2.15	0.59
1:B:341:THR:HG21	2:D:337:ASP:OD2	2.02	0.59
1:A:128:SER:HA	1:A:131:LYS:HG2	1.84	0.59
2:C:148:ILE:HD12	2:C:189:PRO:HG2	1.84	0.59
1:B:74:ILE:HD12	1:B:412:GLU:HG2	1.84	0.59
1:B:209:THR:O	1:B:211:ALA:HA	2.01	0.59
1:A:78:GLU:OE2	1:A:172:LYS:NZ	2.34	0.59
1:A:228:ALA:O	1:A:408:ILE:HD11	2.03	0.59
2:C:184:LEU:HD21	2:C:225:ILE:HD13	1.83	0.58
1:B:211:ALA:N	5:B:440:HOH:O	2.36	0.58
2:C:384:LEU:HD13	2:C:386:GLU:H	1.68	0.58
1:A:258:GLU:O	1:A:261:VAL:HG22	2.03	0.58
1:A:153:VAL:HA	1:A:154:LYS:CB	2.32	0.58
1:B:281:LYS:HG3	1:B:351:ASN:ND2	2.19	0.58
1:B:256:SER:HB3	1:B:263:GLU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:SER:HB3	1:A:265:GLN:HE21	1.69	0.58
1:B:231:LEU:HD11	1:B:378:ASP:OD2	2.03	0.58
1:B:74:ILE:CD1	1:B:412:GLU:HG2	2.33	0.57
2:D:388:ASP:O	2:D:388:ASP:OD1	2.22	0.57
1:A:396:GLU:HG2	1:A:402:LYS:O	2.04	0.57
1:B:268:SER:CB	1:B:365:VAL:HG23	2.34	0.57
1:A:357:LYS:NZ	5:A:462:HOH:O	2.36	0.57
1:B:399:PHE:HB2	1:B:402:LYS:CG	2.34	0.57
1:B:153:VAL:HA	1:B:154:LYS:CB	2.33	0.57
2:D:290:ILE:HD12	2:D:316:TRP:CH2	2.40	0.57
2:D:155:PHE:CB	2:D:195:LEU:HD12	2.33	0.57
2:D:126:PHE:HB2	2:D:170:LYS:HE2	1.86	0.57
1:A:313:GLU:OE1	3:A:4:PO4:O1	2.23	0.57
1:B:210:ILE:HD12	1:B:211:ALA:CB	2.35	0.57
1:A:279:ASP:OD2	3:A:4:PO4:P	2.62	0.57
1:B:399:PHE:HB2	1:B:402:LYS:HD2	1.86	0.57
2:C:124:TYR:CE2	2:C:175:GLU:OE1	2.56	0.56
2:D:144:SER:O	2:D:148:ILE:HG12	2.05	0.56
1:B:242:VAL:HG22	1:B:380:VAL:CG1	2.35	0.56
1:A:241:ILE:HD13	1:A:399:PHE:HZ	1.71	0.56
2:D:125:GLU:N	2:D:127:SER:HG	2.03	0.56
2:D:400:ASP:HB3	2:D:404:LEU:HD12	1.87	0.56
2:D:257:THR:HG22	2:D:260:ASP:OD2	2.06	0.56
1:B:188:ALA:HB3	1:B:213:LEU:HD21	1.88	0.56
1:B:351:ASN:HD22	1:B:354:LEU:HD12	1.69	0.56
1:B:154:LYS:HD3	1:B:155:GLY:HA2	1.87	0.55
1:B:207:ALA:HA	1:B:210:ILE:HG23	1.86	0.55
1:B:379:ILE:HD12	1:B:402:LYS:HE2	1.89	0.55
2:D:170:LYS:O	2:D:174:HIS:HB2	2.07	0.55
1:B:94:GLU:CG	1:B:95:ARG:H	2.14	0.55
2:D:291:SER:O	2:D:295:LYS:HD3	2.07	0.55
2:D:280:LYS:HD2	2:D:283:GLN:OE1	2.07	0.55
1:B:75:LEU:HD22	1:B:180:TYR:CG	2.42	0.54
1:B:210:ILE:CD1	1:B:211:ALA:HB2	2.36	0.54
1:A:108:ASN:O	1:A:112:THR:HG23	2.08	0.54
1:B:221:GLU:N	1:B:222:PRO:CD	2.71	0.54
2:D:241:ASN:HA	2:D:244:ILE:HG13	1.88	0.54
2:C:145:SER:HB3	2:C:146:GLN:HE21	1.72	0.54
1:B:93:ASP:O	1:B:94:GLU:HB2	2.08	0.54
2:C:145:SER:HB3	2:C:146:GLN:NE2	2.23	0.54
1:B:229:TYR:HE1	1:B:408:ILE:HG22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ILE:CD1	1:B:82:ARG:HB3	2.32	0.53
1:A:423:GLY:O	1:A:424:VAL:O	2.25	0.53
1:B:183:THR:HG22	1:B:184:LYS:H	1.73	0.53
1:B:419:ALA:O	1:B:422:ALA:HB3	2.08	0.53
2:C:204:LEU:HD23	2:C:210:VAL:HG12	1.90	0.53
2:C:123:ASP:CA	2:C:124:TYR:HB3	2.35	0.53
2:C:240:SER:O	2:C:244:ILE:HG12	2.09	0.53
2:C:372:GLN:NE2	2:C:376:ARG:HH11	2.07	0.53
1:A:256:SER:CB	1:A:265:GLN:HE21	2.21	0.53
1:B:66:VAL:HG21	1:B:181:LEU:HD21	1.90	0.53
2:C:398:LEU:HD23	2:C:398:LEU:C	2.29	0.53
1:B:319:LEU:HD13	1:B:344:ARG:HA	1.91	0.53
2:D:126:PHE:HB2	2:D:170:LYS:CD	2.39	0.52
1:B:158:LYS:HD3	1:B:159:VAL:H	1.74	0.52
2:D:305:ASN:N	5:D:88:HOH:O	2.42	0.52
1:B:226:ALA:HB1	1:B:231:LEU:HD23	1.92	0.52
1:B:217:ARG:HG3	1:B:217:ARG:HH11	1.76	0.51
1:A:105:VAL:HG12	5:A:486:HOH:O	2.10	0.51
2:C:144:SER:O	2:C:148:ILE:HG23	2.10	0.51
1:B:171:GLY:C	5:B:450:HOH:O	2.49	0.51
2:C:385:GLN:O	2:C:387:ARG:HG2	2.11	0.51
1:B:231:LEU:HG	1:B:240:ILE:CG1	2.38	0.51
1:B:232:ASP:HA	1:B:257:ILE:HD11	1.93	0.51
1:B:75:LEU:HD22	1:B:180:TYR:CD2	2.46	0.51
1:A:153:VAL:HG12	1:A:153:VAL:O	2.11	0.51
1:B:79:GLN:HE22	1:B:81:ASN:CB	2.21	0.50
2:D:137:ILE:HG22	2:D:143:LEU:HD21	1.92	0.50
1:B:223:THR:HA	1:B:255:LEU:CD1	2.41	0.50
2:C:124:TYR:CE1	2:C:126:PHE:HB2	2.46	0.50
1:A:261:VAL:O	1:A:261:VAL:HG23	2.11	0.50
1:B:158:LYS:HD3	1:B:159:VAL:N	2.26	0.50
1:B:408:ILE:HG12	1:B:416:TYR:CD1	2.47	0.50
1:B:56:ASP:HA	1:B:191:THR:OG1	2.12	0.50
2:C:134:ARG:O	2:C:137:ILE:HG13	2.10	0.50
2:D:130:PHE:CD1	2:D:175:GLU:HG2	2.45	0.50
2:C:208:PRO:HB2	2:C:209:PRO:HD3	1.92	0.50
2:D:172:ILE:O	2:D:176:PHE:HB2	2.11	0.50
2:C:389:THR:HG22	2:C:390:GLU:N	2.26	0.50
2:D:221:PHE:CZ	2:D:225:ILE:HD11	2.47	0.50
1:B:255:LEU:HD21	1:B:262:PHE:CD1	2.47	0.49
2:C:377:GLN:NE2	2:C:399:ILE:HD13	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:333:ASN:C	2:D:333:ASN:OD1	2.50	0.49
1:B:366:LEU:O	1:B:371:LEU:HB3	2.12	0.49
1:B:416:TYR:O	1:B:420:VAL:HG23	2.11	0.49
1:B:323:MET:HB2	2:D:390:GLU:OE2	2.11	0.49
1:B:215:VAL:HG11	1:B:218:ILE:HD12	1.93	0.49
2:D:127:SER:O	2:D:130:PHE:HB3	2.13	0.49
1:B:265:GLN:NE2	1:B:265:GLN:HA	2.24	0.49
1:A:96:LEU:HD12	1:A:104:GLN:HG2	1.94	0.49
1:B:242:VAL:HG22	1:B:380:VAL:HG13	1.94	0.49
2:C:238:ARG:HG2	2:C:239:SER:N	2.28	0.49
1:B:71:LYS:N	1:B:71:LYS:HD2	2.27	0.49
1:B:153:VAL:HG13	1:B:153:VAL:O	2.13	0.49
1:A:278:PHE:HA	1:A:351:ASN:HD21	1.77	0.49
1:B:357:LYS:HA	1:B:360:LYS:NZ	2.28	0.49
2:C:135:ASN:HD22	2:C:136:ILE:N	2.10	0.49
1:A:241:ILE:HD12	1:A:376:VAL:HG21	1.94	0.49
1:B:206:ASP:O	1:B:210:ILE:HG22	2.13	0.48
1:A:423:GLY:O	1:A:424:VAL:C	2.51	0.48
2:D:167:HIS:O	2:D:171:ILE:HG12	2.13	0.48
2:C:298:MET:CG	2:C:298:MET:O	2.61	0.48
1:A:74:ILE:HG12	1:A:412:GLU:HB3	1.96	0.48
1:B:109:PRO:HG2	1:B:110:GLN:OE1	2.14	0.48
1:B:384:GLY:C	1:B:386:THR:H	2.17	0.48
1:B:402:LYS:HD3	1:B:402:LYS:C	2.33	0.48
1:B:174:LYS:O	1:B:178:GLU:HG3	2.14	0.48
1:B:399:PHE:CD1	1:B:402:LYS:HD2	2.48	0.48
1:A:102:LYS:C	1:A:105:VAL:HG23	2.34	0.48
1:B:370:GLY:HA3	1:B:371:LEU:CB	2.33	0.48
1:A:254:LEU:C	1:A:254:LEU:HD13	2.34	0.48
1:A:313:GLU:HB2	3:A:4:PO4:O1	2.13	0.48
2:C:321:GLN:OE1	2:C:360:THR:HG23	2.14	0.47
2:D:126:PHE:HB2	2:D:170:LYS:CE	2.44	0.47
1:A:254:LEU:HD12	1:A:265:GLN:HB2	1.96	0.47
1:B:205:LYS:HG3	1:B:218:ILE:CD1	2.44	0.47
2:C:403:HIS:O	2:C:404:LEU:CB	2.62	0.47
2:C:373:CYS:SG	2:C:402:ARG:HD3	2.55	0.47
1:A:105:VAL:HA	1:A:112:THR:HG21	1.96	0.47
1:B:193:PRO:HG2	1:B:196:PHE:CE1	2.50	0.47
1:B:262:PHE:N	1:B:262:PHE:CD2	2.83	0.46
2:D:261:LEU:N	2:D:262:PRO:CD	2.78	0.46
2:C:123:ASP:HA	2:C:124:TYR:CB	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:PRO:O	1:B:365:VAL:HB	2.15	0.46
2:C:159:MET:HE3	2:C:202:SER:OG	2.16	0.46
2:D:125:GLU:HG2	2:D:170:LYS:HZ3	1.80	0.46
2:D:273:TYR:CE1	2:D:283:GLN:HB3	2.51	0.46
2:C:295:LYS:HD3	2:C:300:GLU:C	2.36	0.46
2:D:382:ASN:HB2	2:D:387:ARG:NH2	2.13	0.46
1:A:104:GLN:NE2	1:A:112:THR:HG22	2.29	0.46
1:A:258:GLU:C	1:A:260:GLY:H	2.19	0.46
2:C:188:LEU:HD13	2:C:192:LEU:CD1	2.46	0.46
1:B:229:TYR:CE1	1:B:408:ILE:HG22	2.51	0.46
2:C:207:ASN:HD22	2:C:209:PRO:HD2	1.81	0.46
2:C:271:ASN:O	2:C:275:ARG:HG2	2.16	0.45
1:B:381:LEU:HB3	1:B:386:THR:HG21	1.98	0.45
2:D:372:GLN:NE2	2:D:376:ARG:NH1	2.60	0.45
2:D:233:ASN:HD21	2:D:271:ASN:CG	2.20	0.45
1:B:384:GLY:C	1:B:386:THR:N	2.70	0.45
1:B:399:PHE:HB2	1:B:402:LYS:CD	2.46	0.45
1:B:72:THR:HG21	1:B:416:TYR:CZ	2.52	0.45
1:B:373:LYS:HG3	1:B:374:LYS:HD3	1.99	0.45
2:D:169:TYR:CE1	2:D:209:PRO:HG2	2.51	0.45
1:A:61:TYR:CD1	1:A:83:ILE:HG23	2.52	0.45
2:D:324:ALA:O	2:D:328:GLN:HG3	2.17	0.45
1:B:68:LYS:NZ	5:B:462:HOH:O	2.50	0.45
2:D:185:ASN:OD1	2:D:187:ASN:HB2	2.17	0.45
2:D:220:ASN:HB2	3:D:7:PO4:O1	2.17	0.45
1:B:409:ASN:HB3	1:B:412:GLU:CD	2.37	0.45
1:A:92:ASP:OD1	1:A:154:LYS:HG3	2.18	0.45
1:B:96:LEU:H	1:B:96:LEU:HD12	1.82	0.45
1:B:129:VAL:O	1:B:133:ILE:HG13	2.17	0.45
2:D:296:ALA:O	2:D:312:ASN:CG	2.55	0.44
2:D:134:ARG:O	2:D:137:ILE:HG12	2.17	0.44
2:C:322:GLU:O	2:C:326:GLU:HG2	2.18	0.44
1:B:67:MET:CE	1:B:72:THR:HB	2.48	0.44
1:A:154:LYS:N	1:A:156:GLU:HG2	2.32	0.44
2:D:154:SER:O	2:D:158:ILE:HG13	2.15	0.44
2:C:274:GLU:HG2	5:C:436:HOH:O	2.17	0.44
2:C:284:ILE:HG12	2:C:336:ILE:HD11	1.98	0.44
1:B:379:ILE:CG2	1:B:380:VAL:N	2.80	0.44
2:D:192:LEU:O	2:D:192:LEU:HD13	2.17	0.44
2:C:123:ASP:CA	2:C:124:TYR:CB	2.96	0.44
2:D:270:GLN:HG3	2:D:274:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:TYR:HB2	1:A:231:LEU:HD22	1.99	0.44
1:A:235:ASP:O	1:A:236:LYS:HB2	2.17	0.44
2:D:295:LYS:CD	2:D:295:LYS:N	2.81	0.44
2:D:269:LEU:HA	2:D:269:LEU:HD23	1.83	0.44
1:B:379:ILE:HD11	1:B:399:PHE:CE1	2.53	0.44
1:A:172:LYS:O	1:A:175:GLN:HG2	2.18	0.44
1:A:79:GLN:HG3	2:C:125:GLU:CD	2.38	0.44
2:D:178:LEU:HA	2:D:178:LEU:HD22	1.80	0.44
2:D:136:ILE:HG21	2:D:151:LEU:HD11	1.98	0.44
1:B:244:ASP:CA	1:B:382:VAL:HG23	2.39	0.44
1:B:96:LEU:N	1:B:96:LEU:HD12	2.33	0.44
1:B:257:ILE:HD13	1:B:262:PHE:CE1	2.53	0.43
2:D:296:ALA:HA	2:D:297:ASP:HA	1.66	0.43
1:A:254:LEU:HB2	1:A:365:VAL:CG1	2.48	0.43
2:C:169:TYR:HB2	5:C:432:HOH:O	2.18	0.43
1:A:183:THR:HB	1:A:184:LYS:H	1.51	0.43
1:B:359:LEU:HA	1:B:359:LEU:HD23	1.83	0.43
2:C:372:GLN:HE21	2:C:376:ARG:HD2	1.84	0.43
1:A:154:LYS:HA	1:A:155:GLY:HA2	1.70	0.43
2:C:299:TYR:O	2:C:300:GLU:CG	2.66	0.43
1:B:409:ASN:HA	1:B:410:PRO:HD2	1.90	0.43
1:A:102:LYS:HA	1:A:105:VAL:CG2	2.47	0.43
2:C:384:LEU:CD1	2:C:386:GLU:HG2	2.48	0.43
1:B:359:LEU:O	1:B:360:LYS:C	2.57	0.43
1:A:128:SER:HA	1:A:131:LYS:HE2	2.00	0.43
1:B:88:VAL:HG11	1:B:168:MET:SD	2.57	0.43
1:B:104:GLN:HE22	1:B:108:ASN:HD22	1.67	0.43
1:B:212:GLY:O	1:B:213:LEU:CB	2.66	0.43
1:B:66:VAL:HG21	1:B:181:LEU:CD1	2.44	0.43
1:B:126:ASP:O	1:B:127:ARG:C	2.55	0.43
1:B:239:GLN:C	1:B:240:ILE:HD12	2.39	0.43
1:B:413:ALA:O	1:B:416:TYR:HB3	2.18	0.43
1:B:398:TYR:HD2	1:B:399:PHE:CD1	2.37	0.43
2:C:207:ASN:ND2	2:C:209:PRO:HD2	2.33	0.43
2:D:188:LEU:HD13	2:D:192:LEU:HD12	2.01	0.43
2:C:372:GLN:HG3	2:C:376:ARG:CD	2.43	0.43
1:B:193:PRO:HG2	1:B:196:PHE:CD1	2.54	0.43
2:C:257:THR:O	2:C:261:LEU:HD13	2.19	0.43
2:D:207:ASN:HD22	2:D:207:ASN:C	2.22	0.43
1:B:379:ILE:HG13	1:B:402:LYS:HZ1	1.83	0.42
2:C:135:ASN:C	2:C:135:ASN:HD22	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLN:CD	1:A:104:GLN:O	2.57	0.42
2:C:207:ASN:HD22	2:C:207:ASN:C	2.22	0.42
2:D:211:VAL:HG13	2:D:254:LEU:HD23	2.01	0.42
1:B:170:LEU:HD13	1:B:208:GLY:HA2	2.01	0.42
1:B:357:LYS:HA	1:B:360:LYS:HZ3	1.84	0.42
1:B:245:LEU:HA	1:B:245:LEU:HD12	1.83	0.42
1:B:379:ILE:O	1:B:405:SER:HB2	2.19	0.42
1:A:191:THR:HA	1:A:219:VAL:O	2.19	0.42
2:D:201:THR:HG22	2:D:250:ILE:HG13	2.01	0.42
1:B:362:VAL:O	1:B:366:LEU:HB2	2.19	0.42
1:B:408:ILE:HD12	1:B:409:ASN:H	1.84	0.42
1:B:229:TYR:O	1:B:230:GLY:C	2.57	0.42
2:D:174:HIS:HB3	2:D:175:GLU:HG3	2.02	0.42
1:B:116:ILE:HD12	1:B:116:ILE:HA	1.87	0.42
1:A:237:GLU:HA	1:A:257:ILE:O	2.20	0.42
2:D:130:PHE:CE1	2:D:175:GLU:HG2	2.55	0.42
1:B:153:VAL:HA	1:B:154:LYS:HB2	2.01	0.42
2:D:282:LEU:HD23	2:D:282:LEU:C	2.39	0.42
1:B:154:LYS:HA	1:B:155:GLY:HA2	1.72	0.42
1:A:281:LYS:HG3	1:A:351:ASN:ND2	2.34	0.42
1:A:150:GLU:CD	1:A:157:LYS:HD3	2.40	0.42
1:B:55:ILE:CD1	1:B:64:VAL:HG23	2.50	0.42
1:B:242:VAL:O	1:B:252:VAL:HA	2.20	0.41
1:B:201:ARG:HG2	1:B:218:ILE:HG21	2.02	0.41
1:B:279:ASP:OD2	3:B:3:PO4:O3	2.38	0.41
1:B:357:LYS:HA	1:B:360:LYS:HD3	2.02	0.41
1:B:341:THR:HG22	2:D:339:LEU:HD12	2.02	0.41
2:D:143:LEU:HD22	2:D:147:ASP:HB3	2.01	0.41
1:A:277:ASP:O	1:A:281:LYS:HG2	2.21	0.41
2:D:208:PRO:HA	2:D:212:GLU:OE1	2.20	0.41
1:A:308:LEU:HA	1:A:308:LEU:HD12	1.90	0.41
2:C:137:ILE:HD12	2:C:137:ILE:C	2.41	0.41
2:D:233:ASN:HB2	2:D:272:VAL:HG22	2.02	0.41
1:B:359:LEU:HA	1:B:362:VAL:HG22	2.02	0.41
1:B:221:GLU:HG2	1:B:414:VAL:CG1	2.42	0.41
1:B:210:ILE:HA	1:B:211:ALA:HA	1.68	0.41
2:D:355:PHE:HB2	2:D:359:ILE:HD13	2.01	0.41
1:A:104:GLN:NE2	1:A:112:THR:CG2	2.81	0.41
1:B:140:VAL:HA	1:B:148:ALA:O	2.20	0.41
1:A:234:SER:HB3	1:A:236:LYS:O	2.21	0.41
2:C:238:ARG:HG2	2:C:240:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:374:LYS:HE2	2:D:374:LYS:HB3	1.89	0.41
1:A:79:GLN:HE21	1:A:79:GLN:HA	1.86	0.41
2:C:384:LEU:HD12	2:C:384:LEU:H	1.85	0.41
1:A:241:ILE:HD13	1:A:399:PHE:CZ	2.53	0.41
1:B:68:LYS:HD3	1:B:69:ASN:N	2.36	0.41
2:D:363:LYS:HG3	2:D:366:LEU:CB	2.49	0.41
1:B:360:LYS:HB2	1:B:361:PRO:CD	2.45	0.40
2:C:351:LEU:O	2:C:359:ILE:HD12	2.22	0.40
1:A:154:LYS:O	1:A:154:LYS:HD3	2.21	0.40
1:A:281:LYS:HE2	1:A:354:LEU:HD11	2.01	0.40
2:D:171:ILE:H	2:D:171:ILE:HG12	1.42	0.40
2:D:185:ASN:O	2:D:193:ARG:HD3	2.21	0.40
1:B:257:ILE:HD13	1:B:262:PHE:HE1	1.87	0.40
1:A:78:GLU:HG3	1:A:79:GLN:HE22	1.86	0.40
2:D:322:GLU:HB3	5:D:46:HOH:O	2.20	0.40
1:A:65:ALA:HB3	1:A:419:ALA:HB2	2.03	0.40
1:B:250:PHE:CZ	1:B:358:THR:HB	2.56	0.40
1:B:210:ILE:HG13	1:B:210:ILE:O	2.22	0.40
1:B:354:LEU:HD23	1:B:354:LEU:HA	1.93	0.40
1:B:250:PHE:O	1:B:269:GLY:HA3	2.20	0.40
2:D:384:LEU:HD12	2:D:384:LEU:HA	1.90	0.40
1:B:353:ASP:N	1:B:353:ASP:OD1	2.53	0.40
2:D:367:ASN:O	2:D:371:GLN:HG3	2.21	0.40
1:B:124:TYR:CD1	1:B:142:ASN:HB2	2.56	0.40
2:D:226:MET:HG2	2:D:263:ILE:O	2.20	0.40
1:B:265:GLN:HB3	1:B:369:SER:CB	2.51	0.40
1:A:390:LYS:HD2	1:A:393:GLN:HG2	2.02	0.40
1:B:394:LEU:HA	1:B:394:LEU:HD23	1.92	0.40
1:B:386:THR:O	1:B:392:GLN:HG3	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	375/390 (96%)	361 (96%)	13 (4%)	1 (0%)	46 56
1	B	366/390 (94%)	327 (89%)	32 (9%)	7 (2%)	10 8
2	C	254/315 (81%)	242 (95%)	8 (3%)	4 (2%)	12 10
2	D	267/315 (85%)	241 (90%)	21 (8%)	5 (2%)	10 8
All	All	1262/1410 (90%)	1171 (93%)	74 (6%)	17 (1%)	15 14

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	GLN
2	C	404	LEU
2	D	389	THR
1	B	213	LEU
1	B	230	GLY
1	B	376	VAL
2	C	386	GLU
2	C	123	ASP
2	D	362	ASN
1	B	94	GLU
2	C	387	ARG
2	D	140	ASN
1	A	407	GLY
1	B	259	ASN
2	D	128	SER
2	D	234	ASP
1	B	212	GLY

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	313/323 (97%)	297 (95%)	16 (5%)	29 39
1	B	306/323 (95%)	285 (93%)	21 (7%)	19 24
2	C	248/295 (84%)	225 (91%)	23 (9%)	11 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	259/295 (88%)	241 (93%)	18 (7%)	19 24
All	All	1126/1236 (91%)	1048 (93%)	78 (7%)	19 24

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	71	LYS
1	A	79	GLN
1	A	82	ARG
1	A	83	ILE
1	A	152	SER
1	A	154	LYS
1	A	185	VAL
1	A	231	LEU
1	A	241	ILE
1	A	273	LEU
1	A	303	LYS
1	A	305	LEU
1	A	333	VAL
1	A	393	GLN
1	A	395	LEU
1	B	52	VAL
1	B	57	LEU
1	B	74	ILE
1	B	104	GLN
1	B	123	LYS
1	B	139	ASN
1	B	183	THR
1	B	186	THR
1	B	189	VAL
1	B	210	ILE
1	B	213	LEU
1	B	254	LEU
1	B	262	PHE
1	B	265	GLN
1	B	293	LYS
1	B	303	LYS
1	B	353	ASP
1	B	374	LYS
1	B	380	VAL
1	B	386	THR

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Mol	Chain	Res	Type
1	B	402	LYS
2	C	135	ASN
2	C	140	ASN
2	C	146	GLN
2	C	148	ILE
2	C	152	GLU
2	C	172	ILE
2	C	192	LEU
2	C	207	ASN
2	C	212	GLU
2	C	229	LEU
2	C	295	LYS
2	C	298	MET
2	C	299	TYR
2	C	300	GLU
2	C	320	LEU
2	C	334	LYS
2	C	336	ILE
2	C	360	THR
2	C	374	LYS
2	C	382	ASN
2	C	384	LEU
2	C	389	THR
2	C	404	LEU
2	D	125	GLU
2	D	129	ASP
2	D	137	ILE
2	D	142	THR
2	D	146	GLN
2	D	170	LYS
2	D	171	ILE
2	D	174	HIS
2	D	178	LEU
2	D	194	GLU
2	D	207	ASN
2	D	267	VAL
2	D	289	LEU
2	D	297	ASP
2	D	298	MET
2	D	308	LEU
2	D	378	SER
2	D	393	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	79	GLN
1	A	104	GLN
1	A	108	ASN
1	A	175	GLN
1	A	265	GLN
1	A	285	GLN
1	A	351	ASN
1	A	367	GLN
1	B	79	GLN
1	B	103	ASN
1	B	104	GLN
1	B	125	ASN
1	B	135	HIS
1	B	187	HIS
1	B	265	GLN
1	B	285	GLN
1	B	351	ASN
2	C	135	ASN
2	C	146	GLN
2	C	167	HIS
2	C	174	HIS
2	C	207	ASN
2	C	215	ASN
2	C	233	ASN
2	C	271	ASN
2	C	372	GLN
2	C	377	GLN
2	D	187	ASN
2	D	206	ASN
2	D	207	ASN
2	D	215	ASN
2	D	233	ASN
2	D	271	ASN
2	D	362	ASN
2	D	372	GLN
2	D	403	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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	PO4	A	2	-	4,4,4	0.63	0	6,6,6	0.28	0
3	PO4	A	4	-	4,4,4	0.83	0	6,6,6	0.28	0
3	PO4	B	1	-	4,4,4	0.48	0	6,6,6	0.27	0
3	PO4	B	3	-	4,4,4	0.76	0	6,6,6	0.28	0
3	PO4	C	5	-	4,4,4	0.43	0	6,6,6	0.27	0
3	PO4	C	6	-	4,4,4	0.39	0	6,6,6	0.27	0
3	PO4	D	7	-	4,4,4	0.39	0	6,6,6	0.28	0
3	PO4	D	8	-	4,4,4	0.42	0	6,6,6	0.28	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	PO4	A	2	-	-	0/0/0/0	0/0/0/0
3	PO4	A	4	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1	-	-	0/0/0/0	0/0/0/0
3	PO4	B	3	-	-	0/0/0/0	0/0/0/0
3	PO4	C	5	-	-	0/0/0/0	0/0/0/0
3	PO4	C	6	-	-	0/0/0/0	0/0/0/0
3	PO4	D	7	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	D	8	-	-	0/0/0/0	0/0/0/0

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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4	PO4	3	0
3	B	3	PO4	1	0
3	D	7	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	377/390 (96%)	0.13	3 (0%) 87 91	27, 43, 78, 115	0
1	B	370/390 (94%)	1.11	81 (21%) 1 2	35, 80, 165, 252	0
2	C	262/315 (83%)	0.25	7 (2%) 58 67	35, 55, 95, 131	0
2	D	273/315 (86%)	0.47	16 (5%) 26 34	36, 67, 128, 181	0
All	All	1282/1410 (90%)	0.51	107 (8%) 14 20	27, 59, 134, 252	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	THR	20.4
1	B	366	LEU	9.0
1	B	69	ASN	8.6
1	B	71	LYS	8.1
1	B	260	GLY	7.9
1	B	67	MET	7.7
2	D	140	ASN	7.6
1	B	225	ALA	7.6
1	B	257	ILE	7.2
1	B	399	PHE	6.6
2	D	141	PRO	6.3
1	B	372	GLU	6.3
1	B	68	LYS	6.1
1	B	371	LEU	6.1
1	B	231	LEU	6.0
1	B	420	VAL	6.0
2	D	130	PHE	5.9
1	B	232	ASP	5.5
1	B	181	LEU	5.2
1	B	229	TYR	5.1
1	B	151	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
2	C	385	GLN	5.0
1	B	189	VAL	4.6
1	B	414	VAL	4.5
2	D	383	GLY	4.5
1	B	66	VAL	4.1
1	B	182	GLY	4.1
1	A	153	VAL	4.1
1	B	241	ILE	4.0
1	B	374	LYS	4.0
1	B	174	LYS	3.9
2	D	384	LEU	3.9
2	C	299	TYR	3.9
1	B	184	LYS	3.9
2	D	131	LYS	3.9
1	B	73	GLU	3.8
1	B	254	LEU	3.8
1	B	398	TYR	3.8
2	C	359	ILE	3.8
1	B	413	ALA	3.7
1	B	185	VAL	3.7
1	B	376	VAL	3.7
2	D	386	GLU	3.7
2	C	403	HIS	3.7
1	B	51	THR	3.6
1	B	53	ILE	3.6
1	B	425	LEU	3.5
2	D	235	SER	3.5
2	D	137	ILE	3.4
1	B	367	GLN	3.3
2	D	385	GLN	3.3
1	B	380	VAL	3.3
1	B	153	VAL	3.2
1	B	74	ILE	3.2
2	C	370	ALA	3.2
2	D	233	ASN	3.1
1	B	397	SER	3.1
1	B	239	GLN	3.1
1	B	226	ALA	3.0
1	B	258	GLU	3.0
1	B	176	ILE	3.0
1	B	54	GLY	3.0
1	B	177	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	91	THR	2.9
1	B	55	ILE	2.9
1	B	370	GLY	2.9
1	B	368	ASP	2.9
1	B	259	ASN	2.8
1	B	379	ILE	2.8
1	B	90	PHE	2.8
1	B	223	THR	2.8
2	D	381	ASP	2.7
1	B	240	ILE	2.7
1	B	70	GLY	2.7
1	B	261	VAL	2.7
1	B	158	LYS	2.6
1	B	265	GLN	2.5
1	B	228	ALA	2.5
1	B	424	VAL	2.5
1	B	255	LEU	2.5
1	B	64	VAL	2.5
2	C	138	ASP	2.5
1	B	188	ALA	2.5
1	B	72	THR	2.5
1	B	363	GLU	2.5
1	B	93	ASP	2.4
2	C	404	LEU	2.4
1	B	211	ALA	2.4
1	B	253	SER	2.3
1	B	180	TYR	2.3
2	D	363	LYS	2.3
1	B	208	GLY	2.3
1	B	65	ALA	2.3
1	B	75	LEU	2.3
2	D	380	LEU	2.3
1	B	230	GLY	2.3
1	B	416	TYR	2.2
1	B	401	GLY	2.2
2	D	382	ASN	2.2
1	B	173	MET	2.1
1	B	154	LYS	2.1
1	B	362	VAL	2.1
1	B	96	LEU	2.1
1	A	234	SER	2.0
1	A	105	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	387	ARG	2.0
1	B	187	HIS	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, 95^{th} 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
3	PO4	A	2	5/5	0.99	0.20	5.17	46,46,49,70	0
3	PO4	A	4	5/5	0.94	0.23	4.08	29,42,56,66	0
3	PO4	B	1	5/5	0.97	0.19	4.05	53,78,85,88	0
3	PO4	D	8	5/5	0.91	0.14	-0.22	98,100,106,107	0
3	PO4	C	5	5/5	0.96	0.11	-0.63	69,70,83,84	0
3	PO4	C	6	5/5	0.81	0.14	-0.89	109,109,115,116	0
3	PO4	D	7	5/5	0.91	0.10	-1.49	96,100,107,108	0
4	MG	A	427	1/1	0.88	0.32	-	64,64,64,64	0
4	MG	A	1	1/1	0.93	0.27	-	62,62,62,62	0
4	MG	C	1	1/1	0.98	0.12	-	58,58,58,58	0
3	PO4	B	3	5/5	0.94	0.23	-	33,41,60,70	0

6.5 Other polymers (i)

There are no such residues in this entry.