



Full wwPDB X-ray Structure Validation Report

Jun 10, 2014 – 01:27 PM EDT

PDB ID : 3WCE
Title : The complex structure of TcSQS with ligand, ER119884
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Zhu, Z.; Chen, C.C.; Guo, R.T.
Deposited on : 2013-05-27
Resolution : 2.75 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

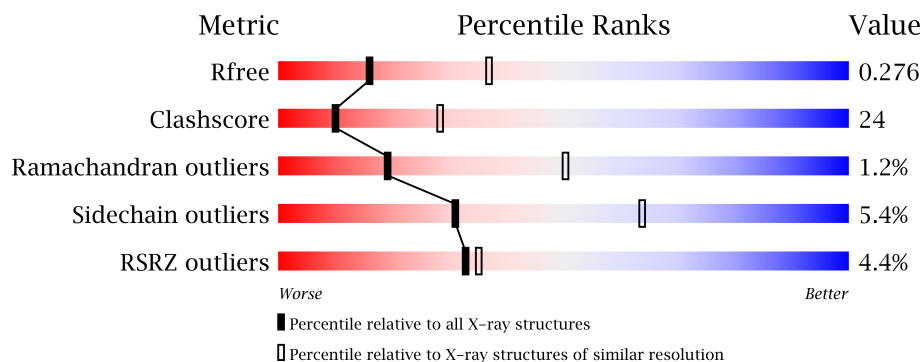
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : **FAILED**
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.75 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}	66092	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	365	
1	B	365	
1	C	365	
1	D	365	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ER4	A	401	-	X
2	ER4	B	401	-	X
2	ER4	C	401	-	X
2	ER4	D	401	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11468 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

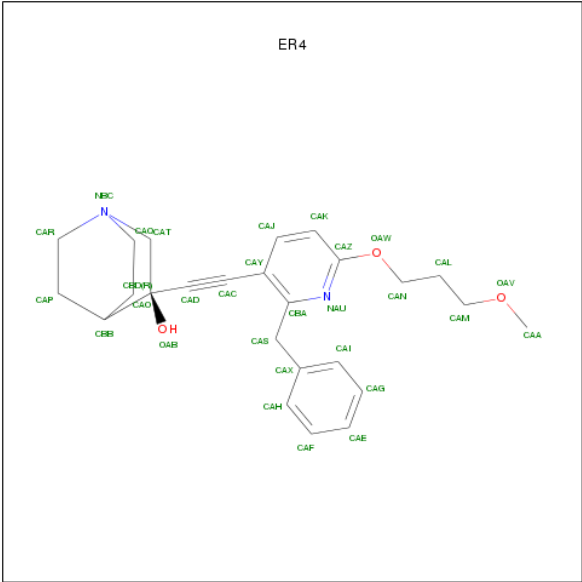
- Molecule 1 is a protein called Farnesyltransferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	B	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	C	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	D	341	Total	C	N	O	S	0	0	0
			2748	1743	473	510	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4
B	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4
C	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4
D	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4

- Molecule 2 is (3R)-3-{[2-BENZYL-6-(3-METHOXYPROPOXY)PYRIDIN-3-YL]ETHYNYL}-1-AZABICYCLO[2.2.2]OCTAN-3-OL (three-letter code: ER4) (formula: C₂₅H₃₀N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	25	2	3		
2	B	1	Total	C	N	O	0	0
			30	25	2	3		
2	C	1	Total	C	N	O	0	0
			30	25	2	3		
2	D	1	Total	C	N	O	0	0
			30	25	2	3		

- Molecule 3 is water.

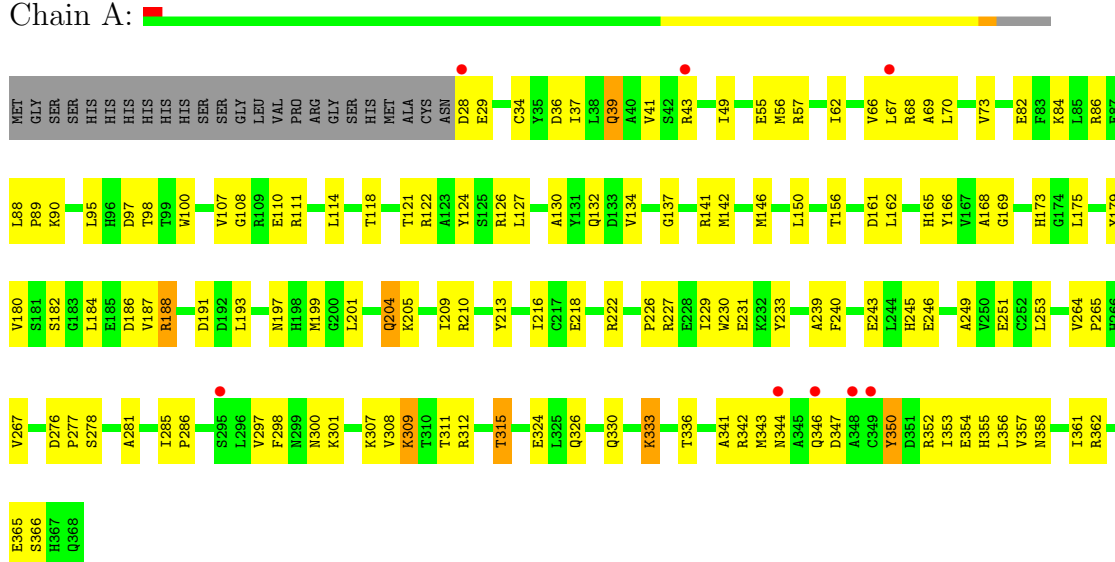
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	99	Total	O	0	0
			99	99		
3	B	100	Total	O	0	0
			100	100		
3	C	78	Total	O	0	0
			78	78		
3	D	70	Total	O	0	0
			70	70		

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 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.

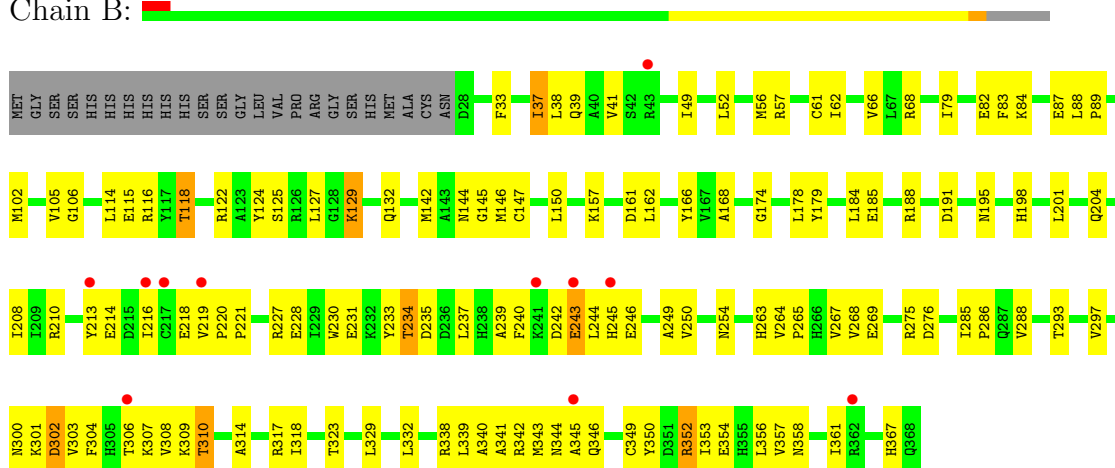
- Molecule 1: Farnesyltransferase, putative

Chain A:



- Molecule 1: Farnesyltransferase, putative

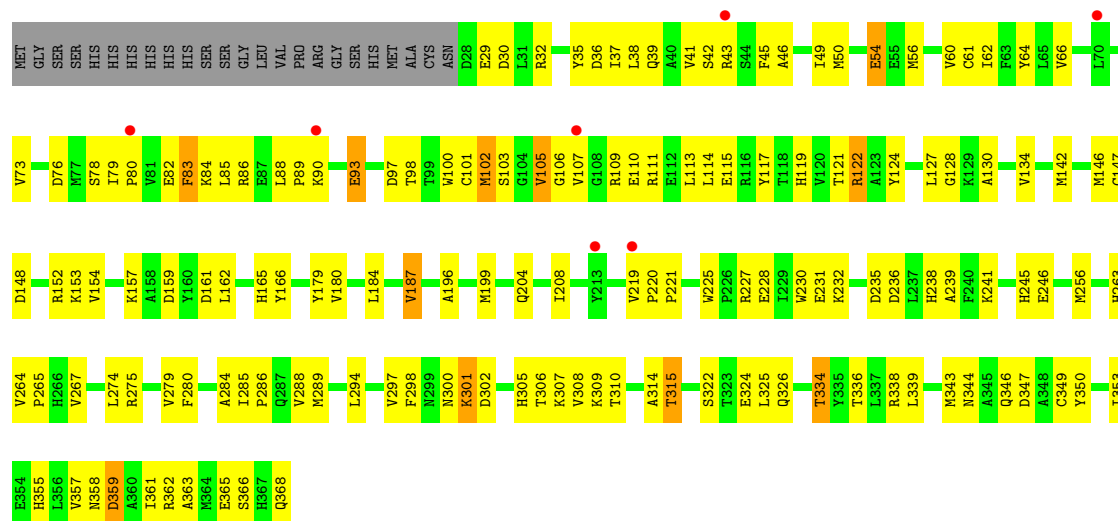
Chain B:



- Molecule 1: Farnesyltransferase, putative

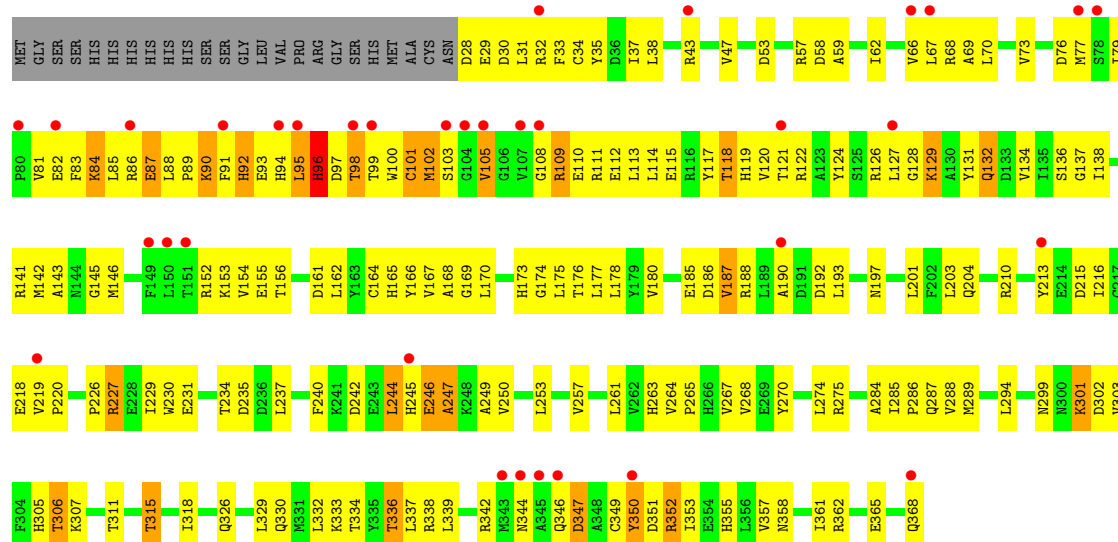
Chain C:





● Molecule 1: Farnesyltransferase, putative

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.81Å 131.42Å 142.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.75 24.93 – 2.74	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.75) 95.5 (24.93-2.74)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 2.76Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.213 , 0.262 0.228 , 0.276	Depositor DCC
R_{free} test set	1874 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	58.8	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 37796 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11468	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ER4

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	0.27	0/2809	0.47	0/3806
1	B	0.25	0/2809	0.46	0/3806
1	C	0.25	0/2809	0.48	0/3806
1	D	0.26	0/2806	0.52	1/3801 (0.0%)
All	All	0.26	0/11233	0.49	1/15219 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	HIS	N-CA-C	-6.10	94.52	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2751	0	2698	99	0
1	B	2751	0	2698	89	0
1	C	2751	0	2698	117	0
1	D	2748	0	2694	218	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	30	0	0	1	0
2	B	30	0	0	0	0
2	C	30	0	0	0	0
2	D	30	0	0	1	0
3	A	99	0	0	4	0
3	B	100	0	0	0	0
3	C	78	0	0	2	0
3	D	70	0	0	1	0
All	All	11468	0	10788	521	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (521) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:85:LEU:O	1:D:89:PRO:HD2	1.59	1.03
1:D:29:GLU:HA	1:D:32:ARG:HE	1.24	0.99
1:D:98:THR:HA	1:D:121:THR:HG21	1.46	0.96
1:D:59:ALA:HA	1:D:127:LEU:HD11	1.49	0.94
1:D:92:HIS:O	1:D:95:LEU:HG	1.67	0.92
1:B:297:VAL:HG23	1:B:303:VAL:HG21	1.52	0.91
1:D:62:ILE:HD12	1:D:127:LEU:HD12	1.55	0.87
1:A:168:ALA:HB2	1:A:204:GLN:HG3	1.57	0.86
1:C:62:ILE:HD12	1:C:127:LEU:HD11	1.56	0.86
1:C:56:MET:HE1	1:C:179:TYR:HA	1.54	0.86
1:A:366:SER:HA	1:D:108:GLY:HA2	1.57	0.85
1:D:88:LEU:O	1:D:91:PHE:HB2	1.78	0.82
1:D:227:ARG:HG3	1:D:230:TRP:CZ2	2.15	0.81
1:D:186:ASP:N	1:D:275:ARG:HH12	1.77	0.81
1:D:180:VAL:HG13	1:D:187:VAL:HA	1.64	0.80
1:D:153:LYS:HD2	1:D:227:ARG:CZ	2.12	0.80
1:D:98:THR:O	1:D:118:THR:HG22	1.83	0.78
1:D:127:LEU:HD23	1:D:128:GLY:N	1.99	0.78
1:D:301:LYS:HD3	1:D:301:LYS:H	1.49	0.78
1:D:344:ASN:HD21	1:D:346:GLN:HB3	1.50	0.77
1:D:103:SER:HA	1:D:115:GLU:HG2	1.67	0.77
1:D:90:LYS:HD3	1:D:93:GLU:HB2	1.67	0.77
1:A:227:ARG:HA	1:A:230:TRP:NE1	2.00	0.76
1:D:124:TYR:CZ	1:D:132:GLN:HG3	2.21	0.76
1:D:28:ASP:O	1:D:32:ARG:HG3	1.86	0.75
1:A:186:ASP:OD2	1:A:188:ARG:HB2	1.87	0.75
1:C:114:LEU:HA	1:C:117:TYR:HB2	1.68	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:37:ILE:HG21	1:C:113:LEU:HD13	1.69	0.74
1:D:121:THR:O	1:D:124:TYR:HB3	1.88	0.74
1:D:127:LEU:HD23	1:D:128:GLY:H	1.52	0.74
1:B:41:VAL:HG22	1:B:68:ARG:NH1	2.03	0.73
1:D:76:ASP:OD2	1:D:79:ILE:HB	1.89	0.73
1:A:344:ASN:HB3	1:A:346:GLN:HG2	1.71	0.73
1:C:80:PRO:HB2	1:C:82:GLU:HG2	1.70	0.72
1:D:117:TYR:O	1:D:120:VAL:HG12	1.90	0.71
1:D:155:GLU:HA	1:D:227:ARG:HB2	1.71	0.71
1:D:264:VAL:HB	1:D:265:PRO:HD3	1.71	0.71
1:A:285:ILE:HB	1:A:286:PRO:HD3	1.72	0.71
1:B:62:ILE:HD12	1:B:127:LEU:HD11	1.72	0.70
1:C:43:ARG:HB2	1:C:43:ARG:NH1	2.06	0.70
1:C:358:ASN:HB3	1:C:362:ARG:NH2	2.06	0.70
1:B:297:VAL:HG23	1:B:303:VAL:CG2	2.22	0.70
1:D:152:ARG:HG2	1:D:153:LYS:H	1.56	0.69
1:D:85:LEU:HD12	1:D:89:PRO:HG2	1.74	0.69
1:D:362:ARG:HH11	1:D:362:ARG:HG3	1.58	0.69
1:A:298:PHE:O	1:A:342:ARG:NH1	2.25	0.68
1:C:83:PHE:O	1:C:86:ARG:HG2	1.93	0.67
1:C:29:GLU:O	1:C:32:ARG:HB2	1.94	0.67
1:C:46:ALA:O	1:C:50:MET:HG2	1.93	0.67
1:D:210:ARG:HD3	1:D:307:LYS:HG3	1.77	0.67
1:D:95:LEU:HD13	1:D:124:TYR:CE2	2.30	0.67
1:D:59:ALA:CA	1:D:127:LEU:HD11	2.24	0.67
1:D:311:THR:O	1:D:315:THR:HG22	1.94	0.67
1:D:180:VAL:HG21	1:D:190:ALA:HB2	1.78	0.66
1:C:106:GLY:O	1:C:111:ARG:HB2	1.96	0.65
1:C:41:VAL:HG23	1:C:42:SER:H	1.60	0.65
1:C:79:ILE:HG23	1:C:80:PRO:HD2	1.78	0.65
1:D:174:GLY:O	1:D:178:LEU:HD12	1.96	0.65
1:A:168:ALA:HB2	1:A:204:GLN:CG	2.27	0.65
1:B:293:THR:O	1:B:297:VAL:HG12	1.97	0.65
1:D:82:GLU:O	1:D:86:ARG:HD3	1.96	0.64
1:D:98:THR:HA	1:D:121:THR:CG2	2.24	0.64
1:A:88:LEU:HB2	1:A:89:PRO:HD3	1.77	0.64
1:A:330:GLN:HA	1:A:333:LYS:HZ2	1.63	0.64
1:B:213:TYR:O	1:B:216:ILE:HG22	1.97	0.64
1:C:309:LYS:NZ	1:C:309:LYS:HB2	2.12	0.64
1:D:30:ASP:OD2	1:D:122:ARG:HD2	1.98	0.64
1:B:142:MET:HG3	1:B:166:TYR:O	1.97	0.64
1:D:246:GLU:O	1:D:249:ALA:N	2.31	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:109:ARG:NH1	1:D:109:ARG:HB3	2.13	0.63
1:D:250:VAL:O	1:D:253:LEU:HB3	1.99	0.62
1:B:214:GLU:O	1:B:218:GLU:HG3	2.00	0.62
1:B:88:LEU:HB2	1:B:89:PRO:HD3	1.81	0.62
1:A:264:VAL:HB	1:A:265:PRO:HD3	1.82	0.62
1:C:35:TYR:O	1:C:39:GLN:HG3	1.99	0.62
1:C:42:SER:O	1:C:46:ALA:HB2	1.99	0.62
1:D:352:ARG:O	1:D:355:HIS:HB3	2.00	0.62
1:C:285:ILE:HB	1:C:286:PRO:HD3	1.82	0.62
1:C:355:HIS:O	1:C:359:ASP:HB2	2.00	0.62
1:D:154:VAL:O	1:D:227:ARG:HD3	2.00	0.62
1:D:138:ILE:CG2	1:D:170:LEU:HB3	2.30	0.61
1:D:30:ASP:HB2	1:D:126:ARG:NH1	2.14	0.61
1:C:30:ASP:CG	1:C:122:ARG:HD2	2.20	0.61
1:C:79:ILE:HD11	1:C:105:VAL:HG12	1.81	0.61
1:D:43:ARG:O	1:D:47:VAL:HG23	2.00	0.61
1:A:97:ASP:OD2	1:A:100:TRP:HB2	2.01	0.61
1:C:83:PHE:C	1:C:83:PHE:CD2	2.72	0.61
1:D:333:LYS:O	1:D:337:LEU:HD13	2.01	0.61
1:C:41:VAL:HG23	1:C:42:SER:N	2.15	0.61
1:A:67:LEU:HD22	1:A:142:MET:SD	2.41	0.61
1:C:42:SER:HB2	1:C:64:TYR:OH	2.00	0.61
1:B:243:GLU:O	1:B:246:GLU:HB2	2.01	0.60
1:D:240:PHE:HE1	1:D:249:ALA:HA	1.66	0.60
1:D:242:ASP:OD1	1:D:245:HIS:HB3	2.02	0.60
1:C:102:MET:CE	1:C:105:VAL:HG21	2.32	0.60
1:D:244:LEU:HD23	1:D:244:LEU:N	2.17	0.60
1:A:118:THR:O	1:A:122:ARG:HG2	2.02	0.59
1:A:199:MET:SD	1:A:267:VAL:HG13	2.42	0.59
1:B:33:PHE:CZ	1:B:37:ILE:HD12	2.37	0.59
1:D:186:ASP:N	1:D:275:ARG:NH1	2.49	0.59
1:B:285:ILE:HB	1:B:286:PRO:HD3	1.84	0.59
3:A:540:HOH:O	1:B:323:THR:HG21	2.01	0.59
1:A:184:LEU:HD23	1:A:276:ASP:OD2	2.02	0.59
1:B:340:ALA:HB2	1:B:357:VAL:HG21	1.84	0.59
1:A:343:MET:SD	1:A:350:TYR:HA	2.42	0.59
1:D:185:GLU:C	1:D:275:ARG:HH12	2.06	0.59
1:D:240:PHE:CE1	1:D:249:ALA:HA	2.38	0.59
1:D:117:TYR:CE1	1:D:120:VAL:HG11	2.37	0.58
1:D:68:ARG:O	1:D:68:ARG:HD3	2.03	0.58
1:B:246:GLU:OE2	1:B:301:LYS:HD2	2.03	0.58
1:D:100:TRP:O	1:D:101:CYS:HB3	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:227:ARG:O	1:C:231:GLU:HG2	2.02	0.58
1:A:182:SER:OG	1:A:184:LEU:HD12	2.04	0.58
1:B:264:VAL:HB	1:B:265:PRO:HD3	1.83	0.58
1:D:77:MET:HG3	1:D:220:PRO:HG2	1.86	0.58
1:D:102:MET:HE2	1:D:105:VAL:HG22	1.84	0.58
1:D:118:THR:O	1:D:121:THR:HG22	2.03	0.58
1:D:102:MET:CE	1:D:105:VAL:HG22	2.34	0.58
1:D:155:GLU:HB2	1:D:227:ARG:NH1	2.19	0.58
1:C:246:GLU:OE2	1:C:301:LYS:HE3	2.04	0.58
1:A:210:ARG:HD2	1:A:308:VAL:O	2.03	0.57
1:C:280:PHE:CZ	1:C:325:LEU:HA	2.39	0.57
1:A:142:MET:HG3	1:A:166:TYR:O	2.04	0.57
1:D:142:MET:HG2	1:D:146:MET:CE	2.34	0.57
1:D:301:LYS:HD3	1:D:301:LYS:N	2.17	0.57
1:C:310:THR:HG22	1:C:314:ALA:HB3	1.86	0.57
1:D:88:LEU:HB2	1:D:89:PRO:HD3	1.87	0.57
1:D:118:THR:HB	1:D:122:ARG:HH12	1.70	0.57
1:D:353:ILE:HG22	1:D:357:VAL:HG23	1.87	0.57
1:D:73:VAL:O	1:D:84:LYS:HE2	2.04	0.57
1:A:43:ARG:HB2	1:A:43:ARG:NH2	2.20	0.56
1:D:285:ILE:HB	1:D:286:PRO:HD3	1.86	0.56
1:D:90:LYS:NZ	1:D:93:GLU:HG2	2.20	0.56
1:D:227:ARG:O	1:D:231:GLU:HB3	2.05	0.56
1:C:142:MET:O	1:C:146:MET:HG3	2.04	0.56
1:D:43:ARG:HG3	3:D:539:HOH:O	2.05	0.56
1:C:264:VAL:HB	1:C:265:PRO:HD3	1.87	0.56
1:C:79:ILE:HD12	1:C:79:ILE:N	2.21	0.56
1:D:244:LEU:HD23	1:D:244:LEU:H	1.70	0.56
1:D:83:PHE:O	1:D:87:GLU:HB2	2.06	0.56
1:B:56:MET:HE1	1:B:179:TYR:HA	1.88	0.55
1:D:84:LYS:O	1:D:88:LEU:N	2.30	0.55
1:B:142:MET:O	1:B:146:MET:HG3	2.06	0.55
1:D:76:ASP:O	1:D:79:ILE:HG22	2.06	0.55
1:C:90:LYS:O	1:C:93:GLU:HB2	2.07	0.55
1:D:302:ASP:HA	1:D:305:HIS:CE1	2.41	0.55
1:B:338:ARG:O	1:B:342:ARG:HG3	2.07	0.55
1:C:227:ARG:HA	1:C:230:TRP:NE1	2.22	0.55
1:D:173:HIS:O	1:D:177:LEU:HG	2.07	0.55
1:D:93:GLU:N	1:D:93:GLU:OE2	2.38	0.55
1:D:94:HIS:HD2	1:D:100:TRP:CE2	2.24	0.55
1:A:62:ILE:HD12	1:A:127:LEU:HD11	1.88	0.55
1:C:130:ALA:O	1:C:134:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:324:GLU:OE1	1:C:326:GLN:HB2	2.07	0.55
1:D:109:ARG:HH11	1:D:109:ARG:HB3	1.72	0.55
1:D:213:TYR:HA	1:D:216:ILE:HG22	1.88	0.55
1:C:56:MET:O	1:C:60:VAL:HG23	2.07	0.54
1:D:142:MET:HG3	1:D:166:TYR:O	2.06	0.54
1:C:38:LEU:HD23	1:C:50:MET:HE2	1.90	0.54
1:D:339:LEU:HD23	1:D:339:LEU:O	2.07	0.54
1:C:111:ARG:O	1:C:115:GLU:HG3	2.07	0.54
1:B:102:MET:HB2	1:B:114:LEU:HB3	1.89	0.54
1:B:227:ARG:HG2	1:B:231:GLU:HB3	1.90	0.54
1:B:268:VAL:HG13	1:B:329:LEU:HD21	1.89	0.54
1:C:76:ASP:HB3	1:C:79:ILE:HD13	1.90	0.54
1:D:102:MET:HB3	1:D:105:VAL:CG2	2.38	0.54
1:D:70:LEU:HA	1:D:91:PHE:CZ	2.43	0.54
1:C:110:GLU:O	1:C:113:LEU:HB3	2.07	0.54
1:A:311:THR:O	1:A:315:THR:HG22	2.07	0.53
1:B:129:LYS:HD2	1:B:129:LYS:O	2.08	0.53
1:D:358:ASN:O	1:D:362:ARG:HG2	2.09	0.53
1:B:249:ALA:HB1	1:B:304:PHE:CE2	2.43	0.53
1:C:289:MET:CE	1:C:315:THR:HB	2.38	0.53
1:D:110:GLU:O	1:D:113:LEU:HB3	2.08	0.53
1:D:96:HIS:O	1:D:97:ASP:C	2.45	0.53
1:C:157:LYS:HG3	1:C:228:GLU:OE1	2.07	0.53
1:D:347:ASP:HB2	1:D:350:TYR:HB2	1.89	0.53
1:D:85:LEU:CD1	1:D:89:PRO:HG2	2.38	0.53
1:B:303:VAL:HG22	1:B:308:VAL:HG21	1.91	0.53
1:A:358:ASN:O	1:A:362:ARG:HB2	2.09	0.53
1:A:361:ILE:O	1:A:365:GLU:HG3	2.09	0.53
1:B:227:ARG:HA	1:B:230:TRP:NE1	2.24	0.53
1:B:125:SER:HA	1:B:132:GLN:NE2	2.24	0.53
1:D:59:ALA:HA	1:D:127:LEU:CD1	2.31	0.53
1:A:41:VAL:HG11	1:A:68:ARG:HE	1.74	0.52
1:A:142:MET:O	1:A:146:MET:HG3	2.09	0.52
1:D:162:LEU:O	1:D:165:HIS:HB3	2.09	0.52
1:A:175:LEU:HD12	2:A:401:ER4:CAM	2.39	0.52
1:B:314:ALA:O	1:B:318:ILE:HG13	2.10	0.52
1:B:244:LEU:O	1:B:245:HIS:HB2	2.10	0.52
1:C:88:LEU:HB2	1:C:89:PRO:HD3	1.90	0.52
1:B:244:LEU:C	1:B:246:GLU:H	2.12	0.52
1:D:237:LEU:HD12	1:D:240:PHE:CE2	2.45	0.52
1:D:250:VAL:CG2	1:D:301:LYS:HG3	2.40	0.52
1:B:242:ASP:OD2	1:B:244:LEU:HB3	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:180:VAL:CG1	1:D:187:VAL:HA	2.38	0.52
1:D:337:LEU:HD11	1:D:361:ILE:HD11	1.92	0.52
1:A:69:ALA:HB1	1:A:114:LEU:HD21	1.93	0.51
1:C:62:ILE:O	1:C:66:VAL:HG23	2.11	0.51
1:A:34:CYS:O	1:A:37:ILE:HG22	2.10	0.51
1:A:108:GLY:O	1:A:111:ARG:HB3	2.10	0.51
1:A:86:ARG:O	1:A:90:LYS:HE3	2.10	0.51
1:D:67:LEU:HD22	1:D:142:MET:SD	2.50	0.51
1:B:353:ILE:O	1:B:357:VAL:HG23	2.10	0.51
1:A:62:ILE:O	1:A:66:VAL:HG23	2.10	0.51
1:D:90:LYS:HZ2	1:D:93:GLU:HG2	1.75	0.51
1:D:362:ARG:NH1	1:D:362:ARG:HG3	2.25	0.51
1:D:88:LEU:CB	1:D:89:PRO:HD3	2.40	0.51
1:B:49:ILE:HG12	1:B:57:ARG:HG3	1.93	0.51
1:C:302:ASP:O	1:C:306:THR:HG22	2.11	0.51
1:D:164:CYS:HB2	1:D:201:LEU:HD22	1.93	0.51
1:C:220:PRO:HB2	1:C:221:PRO:HD2	1.93	0.51
1:C:336:THR:HG22	1:C:357:VAL:HG13	1.92	0.50
1:A:180:VAL:HG13	1:A:187:VAL:HA	1.92	0.50
1:C:274:LEU:HD13	1:C:279:VAL:HG12	1.93	0.50
1:D:137:GLY:O	1:D:141:ARG:HG3	2.11	0.50
1:D:153:LYS:HG3	1:D:227:ARG:NH1	2.27	0.50
1:D:174:GLY:C	1:D:178:LEU:HD12	2.31	0.50
1:D:284:ALA:O	1:D:288:VAL:HG23	2.11	0.50
1:D:81:VAL:C	1:D:83:PHE:H	2.13	0.50
1:D:203:LEU:HG	1:D:287:GLN:HE22	1.77	0.50
1:D:97:ASP:O	1:D:99:THR:N	2.44	0.50
1:C:236:ASP:OD2	1:C:238:HIS:HB2	2.11	0.50
1:D:210:ARG:C	1:D:210:ARG:HD2	2.32	0.50
1:C:56:MET:CE	1:C:179:TYR:HA	2.37	0.50
1:C:358:ASN:HB3	1:C:362:ARG:HH21	1.74	0.50
1:C:42:SER:HB2	1:C:64:TYR:CZ	2.47	0.50
1:D:97:ASP:C	1:D:99:THR:H	2.13	0.50
1:A:205:LYS:O	1:A:209:ILE:HG13	2.11	0.49
1:D:164:CYS:CB	1:D:201:LEU:HD22	2.41	0.49
1:D:250:VAL:HG21	1:D:301:LYS:HG3	1.93	0.49
1:C:196:ALA:O	1:C:199:MET:HB2	2.12	0.49
1:C:45:PHE:O	1:C:49:ILE:HG13	2.12	0.49
1:C:152:ARG:HG2	1:C:153:LYS:N	2.27	0.49
1:D:117:TYR:CZ	1:D:120:VAL:HG11	2.47	0.49
1:B:102:MET:O	1:B:115:GLU:HA	2.11	0.49
1:D:226:PRO:HB2	1:D:229:ILE:HG13	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:185:GLU:HA	1:D:275:ARG:NH1	2.27	0.49
1:A:69:ALA:HB1	1:A:114:LEU:CD2	2.43	0.49
1:B:306:THR:OG1	1:B:307:LYS:N	2.45	0.49
1:B:188:ARG:HG3	1:B:191:ASP:OD2	2.12	0.49
1:C:97:ASP:OD2	1:C:100:TRP:HB2	2.12	0.49
1:C:79:ILE:HD11	1:C:105:VAL:CG1	2.42	0.49
1:C:142:MET:HG3	1:C:166:TYR:O	2.13	0.49
1:C:38:LEU:HD22	1:C:61:CYS:SG	2.53	0.49
1:C:37:ILE:O	1:C:41:VAL:HG22	2.12	0.49
1:D:142:MET:HG2	1:D:146:MET:HE3	1.95	0.49
1:D:111:ARG:O	1:D:115:GLU:HG3	2.13	0.49
1:D:90:LYS:HD3	1:D:93:GLU:CB	2.41	0.49
1:A:197:ASN:O	1:A:201:LEU:HG	2.12	0.49
1:D:230:TRP:CG	1:D:237:LEU:HD13	2.48	0.49
1:D:344:ASN:ND2	1:D:346:GLN:HB3	2.25	0.49
1:A:336:THR:HG22	1:A:357:VAL:HG13	1.95	0.49
1:A:298:PHE:O	1:A:342:ARG:NH2	2.46	0.49
1:C:101:CYS:HB2	1:C:114:LEU:O	2.12	0.48
1:D:155:GLU:OE2	1:D:227:ARG:CZ	2.61	0.48
1:D:83:PHE:CE2	1:D:102:MET:HE3	2.47	0.48
1:D:129:LYS:HA	1:D:132:GLN:CB	2.43	0.48
1:D:85:LEU:HD12	1:D:89:PRO:CG	2.40	0.48
1:A:169:GLY:HA3	1:A:197:ASN:OD1	2.14	0.48
1:A:239:ALA:HB1	1:A:245:HIS:CD2	2.49	0.48
1:C:162:LEU:O	1:C:165:HIS:HB3	2.13	0.48
1:C:43:ARG:CB	1:C:43:ARG:HH11	2.26	0.48
1:D:185:GLU:HA	1:D:275:ARG:HH12	1.79	0.48
1:D:62:ILE:O	1:D:66:VAL:HG23	2.13	0.48
1:A:127:LEU:O	1:A:132:GLN:NE2	2.47	0.48
1:A:182:SER:CB	1:A:184:LEU:HD12	2.44	0.48
1:D:326:GLN:O	1:D:330:GLN:HG3	2.14	0.48
1:C:148:ASP:OD2	1:C:152:ARG:NH2	2.46	0.48
1:A:56:MET:HE3	1:A:179:TYR:HD1	1.79	0.48
1:C:219:VAL:O	1:C:219:VAL:HG23	2.12	0.48
1:D:131:TYR:O	1:D:134:VAL:N	2.46	0.48
1:C:80:PRO:HG2	1:C:83:PHE:HB3	1.94	0.48
1:D:168:ALA:HB2	1:D:204:GLN:HB2	1.96	0.48
1:D:95:LEU:HD21	1:D:136:SER:OG	2.14	0.48
1:B:300:ASN:HD21	1:B:302:ASP:HB2	1.78	0.48
1:D:169:GLY:HA3	1:D:197:ASN:OD1	2.14	0.48
1:A:41:VAL:HG11	1:A:68:ARG:NE	2.29	0.47
1:B:219:VAL:O	1:B:219:VAL:HG13	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:56:MET:HE2	1:C:184:LEU:HD12	1.95	0.47
1:C:204:GLN:HE21	1:C:208:ILE:HG13	1.79	0.47
1:C:225:TRP:CG	1:C:256:MET:HE2	2.49	0.47
1:D:120:VAL:O	1:D:124:TYR:HB2	2.14	0.47
1:D:246:GLU:O	1:D:247:ALA:C	2.52	0.47
1:C:85:LEU:HD23	1:C:147:CYS:HB3	1.97	0.47
1:D:344:ASN:ND2	1:D:346:GLN:H	2.12	0.47
1:A:233:TYR:CE1	1:A:251:GLU:HG2	2.50	0.47
1:B:124:TYR:CE1	1:B:132:GLN:HA	2.50	0.47
1:B:41:VAL:HG22	1:B:68:ARG:CZ	2.44	0.47
1:C:353:ILE:O	1:C:357:VAL:HG23	2.15	0.47
1:A:146:MET:O	1:A:150:LEU:HB2	2.14	0.47
1:B:268:VAL:HG13	1:B:329:LEU:CD2	2.44	0.47
1:B:52:LEU:HD13	1:B:56:MET:HG3	1.96	0.47
1:D:263:HIS:O	1:D:267:VAL:HG23	2.14	0.47
1:D:28:ASP:OD2	1:D:32:ARG:HD3	2.15	0.47
1:D:215:ASP:HA	1:D:218:GLU:HG2	1.96	0.47
1:A:353:ILE:O	1:A:356:LEU:N	2.47	0.47
1:D:145:GLY:HA3	1:D:166:TYR:CG	2.50	0.47
1:A:49:ILE:HG12	1:A:57:ARG:HG3	1.97	0.47
1:B:168:ALA:HB2	1:B:204:GLN:HB2	1.95	0.47
1:B:345:ALA:HA	1:B:350:TYR:CG	2.49	0.47
1:C:307:LYS:HD3	1:C:309:LYS:HD3	1.97	0.47
1:C:54:GLU:H	1:C:54:GLU:CD	2.17	0.47
1:A:227:ARG:HA	1:A:230:TRP:CE2	2.49	0.47
1:B:339:LEU:C	1:B:339:LEU:HD23	2.36	0.47
1:C:263:HIS:O	1:C:267:VAL:HG23	2.14	0.47
1:A:227:ARG:O	1:A:231:GLU:HB3	2.14	0.46
1:C:102:MET:HE2	1:C:105:VAL:HG21	1.97	0.46
1:D:305:HIS:O	1:D:306:THR:HB	2.15	0.46
1:B:79:ILE:HB	1:B:84:LYS:HE3	1.97	0.46
1:D:227:ARG:HA	1:D:230:TRP:NE1	2.30	0.46
1:B:185:GLU:OE1	1:B:275:ARG:HG2	2.15	0.46
1:D:69:ALA:O	1:D:73:VAL:HG23	2.14	0.46
1:D:219:VAL:HG13	1:D:219:VAL:O	2.16	0.46
1:D:270:TYR:CE1	1:D:274:LEU:HD21	2.51	0.46
1:B:83:PHE:CZ	1:B:87:GLU:HG3	2.51	0.46
1:A:226:PRO:HG2	1:A:229:ILE:HD12	1.98	0.46
1:B:244:LEU:C	1:B:246:GLU:N	2.68	0.46
1:A:95:LEU:HB3	1:A:124:TYR:CE2	2.50	0.46
1:C:30:ASP:OD2	1:C:122:ARG:HD2	2.16	0.46
1:C:365:GLU:HA	1:C:368:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:227:ARG:HA	1:A:230:TRP:CD1	2.51	0.46
1:B:210:ARG:HH11	1:B:210:ARG:HG3	1.80	0.46
1:C:285:ILE:HG12	1:C:322:SER:HB2	1.98	0.46
1:C:43:ARG:HB2	1:C:43:ARG:HH11	1.79	0.46
1:A:98:THR:HB	1:A:122:ARG:HD3	1.98	0.46
1:A:55:GLU:HG3	1:A:56:MET:N	2.31	0.46
1:C:239:ALA:O	1:C:245:HIS:HB2	2.16	0.46
1:D:268:VAL:HG13	1:D:329:LEU:HD21	1.98	0.45
1:D:29:GLU:HA	1:D:32:ARG:NE	2.09	0.45
1:B:263:HIS:O	1:B:267:VAL:HG23	2.16	0.45
1:B:341:ALA:O	1:B:342:ARG:HG2	2.16	0.45
1:B:204:GLN:HE21	1:B:208:ILE:HG13	1.82	0.45
1:C:43:ARG:NH1	1:C:43:ARG:CB	2.78	0.45
1:D:152:ARG:HG2	1:D:153:LYS:N	2.26	0.45
1:D:173:HIS:CD2	1:D:193:LEU:HB3	2.51	0.45
1:D:138:ILE:HD11	1:D:174:GLY:CA	2.47	0.45
1:B:344:ASN:C	1:B:346:GLN:H	2.19	0.45
1:A:341:ALA:C	1:A:343:MET:H	2.20	0.45
1:A:298:PHE:CZ	1:A:353:ILE:HD13	2.52	0.45
1:B:162:LEU:HG	1:B:166:TYR:CE2	2.50	0.45
1:C:78:SER:C	1:C:79:ILE:HD12	2.37	0.45
1:D:88:LEU:O	1:D:91:PHE:CB	2.59	0.45
1:C:339:LEU:HD23	1:C:339:LEU:C	2.36	0.45
1:C:154:VAL:HG13	1:C:159:ASP:HB2	1.99	0.45
1:A:68:ARG:NH2	1:A:110:GLU:OE1	2.49	0.45
1:B:357:VAL:O	1:B:361:ILE:HG13	2.16	0.45
1:C:114:LEU:HD12	1:C:114:LEU:N	2.32	0.45
1:D:185:GLU:CA	1:D:275:ARG:HH12	2.29	0.45
1:A:130:ALA:O	1:A:134:VAL:HG23	2.17	0.44
1:A:28:ASP:N	3:A:568:HOH:O	2.50	0.44
1:A:333:LYS:HZ2	1:A:333:LYS:HB3	1.82	0.44
1:D:94:HIS:HD2	1:D:100:TRP:NE1	2.14	0.44
1:D:142:MET:HG2	1:D:146:MET:HE2	1.99	0.44
1:D:138:ILE:HG23	1:D:170:LEU:HB3	1.98	0.44
1:B:174:GLY:O	1:B:178:LEU:HG	2.17	0.44
1:C:204:GLN:O	1:C:208:ILE:HG13	2.18	0.44
1:A:73:VAL:O	1:A:84:LYS:HE2	2.17	0.44
1:B:231:GLU:C	1:B:233:TYR:H	2.20	0.44
1:B:234:THR:HG21	1:B:240:PHE:CZ	2.52	0.44
1:D:98:THR:HG22	1:D:121:THR:HG23	2.00	0.44
1:D:213:TYR:O	1:D:216:ILE:HG22	2.18	0.44
1:B:184:LEU:HD22	1:B:276:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:302:ASP:HB3	1:C:306:THR:CG2	2.48	0.44
1:B:288:VAL:HA	1:B:332:LEU:CD2	2.48	0.44
1:C:121:THR:O	1:C:124:TYR:HB3	2.17	0.44
1:C:284:ALA:O	1:C:288:VAL:HG23	2.17	0.44
1:C:339:LEU:HD23	1:C:339:LEU:O	2.18	0.44
1:D:70:LEU:HD22	1:D:146:MET:CE	2.47	0.44
1:D:275:ARG:HH11	1:D:275:ARG:HG2	1.83	0.44
1:D:109:ARG:O	1:D:112:GLU:HB3	2.18	0.44
1:D:289:MET:SD	1:D:318:ILE:HD12	2.57	0.44
1:B:246:GLU:O	1:B:250:VAL:HG23	2.17	0.44
1:B:314:ALA:O	1:B:317:ARG:HG2	2.18	0.44
1:C:106:GLY:O	1:C:111:ARG:HD3	2.18	0.44
1:C:109:ARG:HD2	3:C:574:HOH:O	2.18	0.44
1:D:349:CYS:O	1:D:353:ILE:HG13	2.18	0.44
1:D:37:ILE:HG23	1:D:38:LEU:N	2.32	0.44
1:A:298:PHE:O	1:A:342:ARG:CZ	2.66	0.43
1:B:254:ASN:HD22	1:B:254:ASN:N	2.15	0.43
1:B:352:ARG:O	1:B:356:LEU:HG	2.18	0.43
1:C:308:VAL:HA	3:C:535:HOH:O	2.18	0.43
1:D:134:VAL:O	1:D:138:ILE:HG13	2.17	0.43
1:D:352:ARG:C	1:D:352:ARG:HD2	2.39	0.43
1:D:365:GLU:HA	1:D:368:GLN:OE1	2.17	0.43
1:A:330:GLN:HA	1:A:333:LYS:NZ	2.31	0.43
1:D:35:TYR:OH	1:D:57:ARG:HG2	2.18	0.43
1:B:157:LYS:HG3	1:B:228:GLU:OE1	2.17	0.43
1:D:102:MET:HB3	1:D:105:VAL:HG21	2.00	0.43
1:D:127:LEU:CD2	1:D:128:GLY:N	2.77	0.43
1:D:342:ARG:HG2	1:D:342:ARG:HH11	1.83	0.43
1:A:243:GLU:O	1:A:246:GLU:HB2	2.19	0.43
1:A:353:ILE:O	1:A:354:GLU:C	2.56	0.43
1:D:186:ASP:OD2	1:D:187:VAL:N	2.51	0.43
1:D:70:LEU:HA	1:D:91:PHE:CE1	2.53	0.43
1:B:227:ARG:HA	1:B:230:TRP:CE2	2.53	0.43
1:C:162:LEU:HG	1:C:166:TYR:CE2	2.53	0.43
1:D:83:PHE:CZ	1:D:102:MET:HE3	2.54	0.43
1:D:33:PHE:O	1:D:37:ILE:HG22	2.17	0.43
1:B:62:ILE:O	1:B:66:VAL:HG23	2.19	0.43
1:C:334:THR:O	1:C:338:ARG:HG2	2.18	0.43
1:D:143:ALA:O	1:D:146:MET:HB2	2.18	0.43
1:D:186:ASP:H	1:D:275:ARG:NH1	2.16	0.43
1:D:299:ASN:O	1:D:299:ASN:OD1	2.37	0.43
1:A:307:LYS:HE2	1:A:309:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:343:MET:HE1	1:B:349:CYS:C	2.39	0.43
1:B:83:PHE:O	1:B:87:GLU:HG2	2.18	0.43
1:D:109:ARG:HH11	1:D:109:ARG:CB	2.30	0.43
1:D:129:LYS:HA	1:D:132:GLN:HB2	2.00	0.43
1:D:201:LEU:HD12	1:D:263:HIS:CE1	2.53	0.43
1:A:39:GLN:HE21	1:A:39:GLN:HB2	1.58	0.43
1:B:301:LYS:HG3	1:B:302:ASP:N	2.33	0.43
1:C:363:ALA:O	1:C:366:SER:HB3	2.18	0.43
1:D:175:LEU:HD12	2:D:401:ER4:CAM	2.49	0.43
1:D:332:LEU:O	1:D:336:THR:OG1	2.32	0.43
1:B:237:LEU:C	1:B:239:ALA:H	2.22	0.43
1:B:301:LYS:O	1:B:303:VAL:N	2.52	0.43
1:D:197:ASN:O	1:D:201:LEU:HG	2.19	0.43
1:D:96:HIS:HB3	1:D:97:ASP:H	1.75	0.43
1:C:102:MET:HE3	1:C:105:VAL:HG21	2.01	0.43
1:C:79:ILE:HG22	1:C:80:PRO:O	2.18	0.43
1:D:92:HIS:ND1	1:D:93:GLU:CD	2.72	0.43
1:A:281:ALA:O	1:A:285:ILE:HG13	2.18	0.42
1:B:220:PRO:HA	1:B:221:PRO:HD3	1.85	0.42
1:C:344:ASN:O	1:C:347:ASP:HB2	2.19	0.42
1:D:70:LEU:HD22	1:D:146:MET:SD	2.59	0.42
1:D:237:LEU:HD12	1:D:240:PHE:HE2	1.83	0.42
1:A:137:GLY:O	1:A:141:ARG:HG3	2.18	0.42
1:A:70:LEU:HD12	1:A:88:LEU:HD22	2.01	0.42
1:B:33:PHE:CZ	1:B:116:ARG:HB2	2.55	0.42
1:C:294:LEU:HA	1:C:297:VAL:HG22	2.00	0.42
1:A:121:THR:O	1:A:124:TYR:HB3	2.19	0.42
1:A:56:MET:HE1	1:A:179:TYR:HA	2.02	0.42
1:A:253:LEU:HD21	1:A:297:VAL:O	2.20	0.42
1:C:30:ASP:OD2	1:C:119:HIS:HA	2.19	0.42
1:D:79:ILE:HG23	1:D:84:LYS:HE3	2.00	0.42
1:D:97:ASP:C	1:D:99:THR:N	2.73	0.42
1:C:180:VAL:HG13	1:C:187:VAL:HA	2.00	0.42
1:C:338:ARG:HE	1:C:338:ARG:HB3	1.71	0.42
1:A:173:HIS:CD2	1:A:193:LEU:HB3	2.54	0.42
1:B:195:ASN:O	1:B:198:HIS:HB2	2.20	0.42
1:B:38:LEU:HD22	1:B:61:CYS:SG	2.59	0.42
1:B:82:GLU:N	1:B:82:GLU:OE1	2.49	0.42
1:C:309:LYS:HB2	1:C:309:LYS:HZ1	1.82	0.42
1:A:344:ASN:O	1:A:350:TYR:HB2	2.20	0.42
1:D:210:ARG:O	1:D:210:ARG:HD2	2.19	0.42
1:A:253:LEU:CD2	1:A:300:ASN:O	2.68	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:346:GLN:NE2	3:A:516:HOH:O	2.51	0.42
1:B:300:ASN:O	1:B:303:VAL:HG23	2.20	0.42
1:C:204:GLN:HE21	1:C:208:ILE:CG1	2.33	0.42
1:D:30:ASP:OD2	1:D:119:HIS:HA	2.20	0.42
1:D:268:VAL:HG13	1:D:329:LEU:CD2	2.50	0.42
1:A:213:TYR:O	1:A:216:ILE:HG22	2.20	0.42
1:C:238:HIS:O	1:C:241:LYS:HG3	2.20	0.42
1:C:343:MET:SD	1:C:353:ILE:HB	2.60	0.42
1:D:301:LYS:CD	1:D:301:LYS:H	2.25	0.42
1:A:122:ARG:HB3	1:A:126:ARG:HH12	1.85	0.42
1:A:182:SER:HB2	1:A:184:LEU:HD12	2.01	0.42
1:A:276:ASP:HA	1:A:277:PRO:HD3	1.84	0.42
1:B:147:CYS:HA	1:B:150:LEU:HD12	2.02	0.42
1:C:43:ARG:HB2	1:C:43:ARG:CZ	2.50	0.42
1:D:167:VAL:HG23	1:D:168:ALA:N	2.35	0.42
1:D:192:ASP:C	1:D:193:LEU:HD22	2.39	0.42
1:D:347:ASP:N	1:D:347:ASP:OD2	2.52	0.42
1:D:43:ARG:H	1:D:43:ARG:HG2	1.54	0.42
1:B:145:GLY:HA3	1:B:166:TYR:CD1	2.55	0.41
1:C:349:CYS:O	1:C:350:TYR:C	2.58	0.41
1:D:138:ILE:HD11	1:D:174:GLY:HA2	2.01	0.41
1:B:309:LYS:HG3	1:B:310:THR:O	2.20	0.41
1:C:357:VAL:O	1:C:361:ILE:HG12	2.20	0.41
1:D:227:ARG:HA	1:D:230:TRP:CE2	2.55	0.41
1:D:230:TRP:CD2	1:D:237:LEU:HD13	2.55	0.41
1:A:246:GLU:CD	1:A:301:LYS:HD2	2.40	0.41
1:B:118:THR:OG1	1:B:122:ARG:NH1	2.53	0.41
1:C:73:VAL:HG11	1:C:88:LEU:HD21	2.01	0.41
1:A:188:ARG:HG3	1:A:191:ASP:OD2	2.20	0.41
1:B:269:GLU:OE1	1:B:367:HIS:NE2	2.48	0.41
1:D:210:ARG:CD	1:D:307:LYS:HG3	2.46	0.41
1:B:301:LYS:C	1:B:303:VAL:H	2.24	0.41
1:A:346:GLN:HG3	1:A:347:ASP:H	1.85	0.41
1:A:276:ASP:OD1	1:A:278:SER:N	2.50	0.41
1:B:354:GLU:O	1:B:358:ASN:ND2	2.54	0.41
1:D:79:ILE:CG2	1:D:84:LYS:HE3	2.51	0.41
1:B:105:VAL:HG12	1:B:106:GLY:N	2.35	0.41
1:C:127:LEU:O	1:C:128:GLY:C	2.58	0.41
1:D:138:ILE:CD1	1:D:174:GLY:HA3	2.51	0.41
1:D:77:MET:HB3	1:D:220:PRO:HG3	2.02	0.41
1:D:261:LEU:HA	1:D:264:VAL:HG23	2.03	0.41
1:D:334:THR:O	1:D:338:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:83:PHE:HD2	1:C:84:LYS:N	2.19	0.41
1:D:257:VAL:HG13	1:D:294:LEU:HD11	2.03	0.41
1:A:188:ARG:HA	1:A:191:ASP:OD2	2.20	0.41
1:A:240:PHE:CE1	1:A:249:ALA:HA	2.56	0.41
1:A:43:ARG:CB	1:A:43:ARG:CZ	2.98	0.41
1:D:69:ALA:HB1	1:D:114:LEU:HD21	2.03	0.41
1:D:302:ASP:HA	1:D:305:HIS:NE2	2.36	0.41
1:D:353:ILE:O	1:D:357:VAL:HG23	2.20	0.41
1:A:312:ARG:HA	1:A:315:THR:CG2	2.50	0.40
1:C:298:PHE:C	1:C:300:ASN:H	2.23	0.40
1:C:88:LEU:N	1:C:89:PRO:CD	2.84	0.40
1:A:366:SER:O	1:D:109:ARG:HD2	2.21	0.40
1:D:70:LEU:HD21	1:D:88:LEU:HD22	2.03	0.40
1:A:324:GLU:OE1	1:A:326:GLN:HB2	2.21	0.40
1:C:239:ALA:HB1	1:C:245:HIS:CD2	2.57	0.40
1:D:186:ASP:OD1	1:D:188:ARG:HB2	2.22	0.40
1:D:97:ASP:OD1	1:D:99:THR:HG22	2.21	0.40
1:A:156:THR:HB	3:A:597:HOH:O	2.22	0.40
1:A:162:LEU:O	1:A:165:HIS:HB3	2.20	0.40
1:A:168:ALA:CB	1:A:204:GLN:HG3	2.39	0.40
1:A:218:GLU:HG2	1:A:222:ARG:CD	2.52	0.40
1:A:333:LYS:NZ	1:A:333:LYS:HB3	2.35	0.40
1:D:138:ILE:H	1:D:138:ILE:HG13	1.60	0.40
1:D:34:CYS:C	1:D:37:ILE:HG22	2.41	0.40
1:B:89:PRO:HB3	1:B:144:ASN:HD21	1.85	0.40
1:B:344:ASN:C	1:B:346:GLN:N	2.73	0.40
1:D:242:ASP:OD1	1:D:242:ASP:C	2.60	0.40
1:D:303:VAL:O	1:D:303:VAL:HG12	2.22	0.40
1:A:218:GLU:HG2	1:A:222:ARG:HD2	2.03	0.40
1:C:230:TRP:C	1:C:232:LYS:N	2.74	0.40
1:D:176:THR:O	1:D:180:VAL:HG23	2.21	0.40
1:D:245:HIS:O	1:D:246:GLU:C	2.60	0.40

There are no symmetry-related clashes.

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	339/365 (93%)	314 (93%)	24 (7%)	1 (0%)	50	83
1	B	339/365 (93%)	315 (93%)	23 (7%)	1 (0%)	50	83
1	C	339/365 (93%)	312 (92%)	23 (7%)	4 (1%)	19	50
1	D	339/365 (93%)	294 (87%)	35 (10%)	10 (3%)	7	20
All	All	1356/1460 (93%)	1235 (91%)	105 (8%)	16 (1%)	19	50

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	54	GLU
1	A	29	GLU
1	D	98	THR
1	D	101	CYS
1	D	246	GLU
1	B	302	ASP
1	D	84	LYS
1	D	350	TYR
1	C	103	SER
1	D	247	ALA
1	C	305	HIS
1	D	105	VAL
1	D	132	GLN
1	D	234	THR
1	D	306	THR
1	C	107	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	298/318 (94%)	285 (96%)	13 (4%)	39	73
1	B	298/318 (94%)	287 (96%)	11 (4%)	45	80
1	C	298/318 (94%)	282 (95%)	16 (5%)	31	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	297/318 (93%)	273 (92%)	24 (8%)	17	41
All	All	1191/1272 (94%)	1127 (95%)	64 (5%)	31	64

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	39	GLN
1	A	82	GLU
1	A	107	VAL
1	A	161	ASP
1	A	188	ARG
1	A	204	GLN
1	A	309	LYS
1	A	315	THR
1	A	333	LYS
1	A	350	TYR
1	A	352	ARG
1	A	355	HIS
1	B	37	ILE
1	B	39	GLN
1	B	118	THR
1	B	129	LYS
1	B	161	ASP
1	B	201	LEU
1	B	234	THR
1	B	235	ASP
1	B	243	GLU
1	B	310	THR
1	B	352	ARG
1	C	36	ASP
1	C	83	PHE
1	C	93	GLU
1	C	98	THR
1	C	102	MET
1	C	105	VAL
1	C	122	ARG
1	C	161	ASP
1	C	187	VAL
1	C	235	ASP
1	C	275	ARG
1	C	301	LYS

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Mol	Chain	Res	Type
1	C	315	THR
1	C	334	THR
1	C	346	GLN
1	C	359	ASP
1	D	31	LEU
1	D	53	ASP
1	D	58	ASP
1	D	87	GLU
1	D	90	LYS
1	D	92	HIS
1	D	95	LEU
1	D	96	HIS
1	D	102	MET
1	D	109	ARG
1	D	118	THR
1	D	129	LYS
1	D	156	THR
1	D	161	ASP
1	D	187	VAL
1	D	227	ARG
1	D	235	ASP
1	D	244	LEU
1	D	301	LYS
1	D	315	THR
1	D	336	THR
1	D	347	ASP
1	D	351	ASP
1	D	352	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	119	HIS
1	A	144	ASN
1	A	204	GLN
1	A	245	HIS
1	A	320	HIS
1	B	132	GLN
1	B	144	ASN
1	B	204	GLN
1	B	254	ASN

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Mol	Chain	Res	Type
1	B	300	ASN
1	B	346	GLN
1	B	358	ASN
1	C	119	HIS
1	C	144	ASN
1	C	204	GLN
1	C	245	HIS
1	C	266	HIS
1	D	94	HIS
1	D	96	HIS
1	D	207	ASN
1	D	287	GLN
1	D	299	ASN
1	D	330	GLN
1	D	344	ASN
1	D	346	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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	341/365 (93%)	0.09	8 (2%) 57 61	26, 50, 75, 120	0
1	B	341/365 (93%)	0.17	11 (3%) 45 49	30, 57, 95, 107	0
1	C	341/365 (93%)	0.20	7 (2%) 60 64	26, 55, 87, 100	0
1	D	341/365 (93%)	0.59	34 (9%) 8 7	31, 76, 120, 143	0
All	All	1364/1460 (93%)	0.26	60 (4%) 33 35	26, 58, 103, 143	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	82	GLU	6.5
1	D	245	HIS	5.5
1	D	105	VAL	5.0
1	D	80	PRO	4.6
1	A	349	CYS	4.5
1	D	99	THR	4.2
1	D	346	GLN	4.0
1	D	98	THR	3.7
1	D	149	PHE	3.5
1	D	78	SER	3.5
1	D	91	PHE	3.5
1	D	32	ARG	3.4
1	C	107	VAL	3.3
1	A	346	GLN	3.1
1	D	190	ALA	3.1
1	A	344	ASN	3.1
1	C	80	PRO	3.0
1	D	127	LEU	3.0
1	B	219	VAL	3.0
1	D	103	SER	2.9
1	D	151	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	368	GLN	2.8
1	D	345	ALA	2.8
1	B	43	ARG	2.8
1	D	121	THR	2.8
1	C	43	ARG	2.7
1	B	362	ARG	2.7
1	C	213	TYR	2.6
1	A	348	ALA	2.6
1	D	344	ASN	2.5
1	B	217	CYS	2.5
1	A	43	ARG	2.5
1	D	66	VAL	2.4
1	B	213	TYR	2.4
1	D	94	HIS	2.4
1	B	306	THR	2.3
1	C	90	LYS	2.3
1	B	241	LYS	2.3
1	B	345	ALA	2.2
1	C	219	VAL	2.2
1	D	219	VAL	2.2
1	D	350	TYR	2.2
1	B	216	ILE	2.2
1	A	28	ASP	2.2
1	B	245	HIS	2.2
1	D	67	LEU	2.2
1	D	343	MET	2.1
1	D	213	TYR	2.1
1	D	86	ARG	2.1
1	D	150	LEU	2.1
1	D	108	GLY	2.1
1	D	77	MET	2.1
1	D	43	ARG	2.1
1	A	67	LEU	2.1
1	B	243	GLU	2.1
1	C	70	LEU	2.0
1	D	107	VAL	2.0
1	D	104	GLY	2.0
1	D	95	LEU	2.0
1	A	295	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ER4	C	401	30/30	0.50	5.72	79,92,111,112	0
2	ER4	B	401	30/30	0.35	4.47	68,74,82,83	0
2	ER4	D	401	30/30	0.46	4.38	91,102,111,111	0
2	ER4	A	401	30/30	0.39	3.67	69,86,103,103	0

6.5 Other polymers ⓘ

There are no such residues in this entry.