



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 07:02 AM GMT

PDB ID : 2RKB
Title : Serine dehydratase like-1 from human cancer cells
Authors : Yamada, T.; Komoto, J.; Kasuya, T.; Mori, H.; Ogawa, H.; Takusagawa, F.
Deposited on : 2007-10-16
Resolution : 2.80 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>

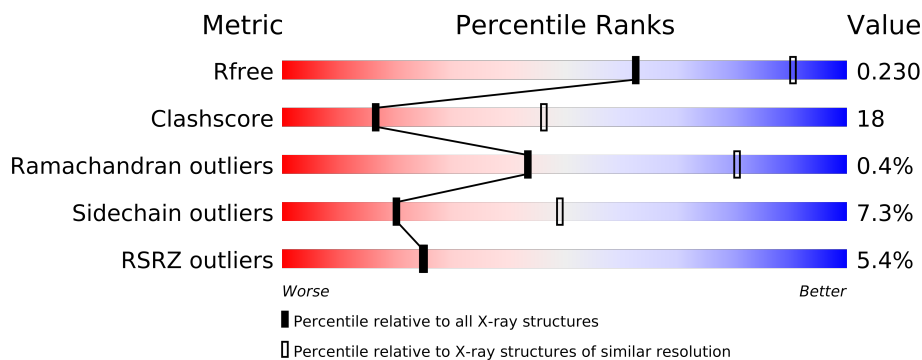
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	318	
1	B	318	
1	C	318	
1	D	318	
1	E	318	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12122 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.

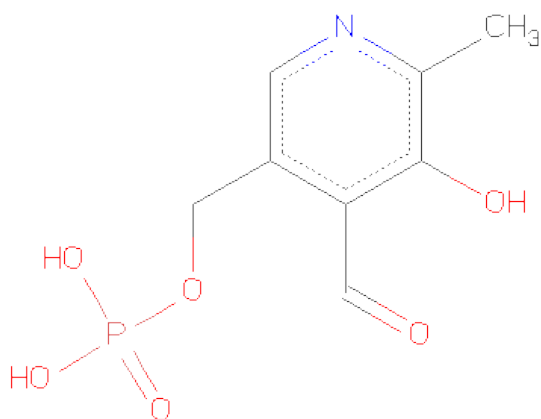
- Molecule 1 is a protein called Serine dehydratase-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2352	1487	418	432	15			
1	B	318	Total	C	N	O	S	0	0	0
			2352	1487	418	432	15			
1	C	318	Total	C	N	O	S	0	0	0
			2352	1487	418	432	15			
1	D	318	Total	C	N	O	S	0	0	0
			2352	1487	418	432	15			
1	E	318	Total	C	N	O	S	0	0	0
			2352	1487	418	432	15			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.

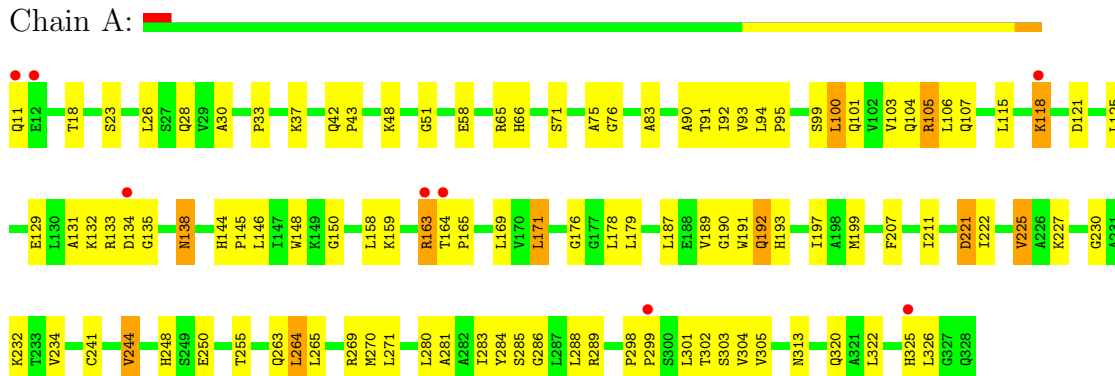
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total	O	0	0
			70	70		
4	B	74	Total	O	0	0
			74	74		
4	C	31	Total	O	0	0
			31	31		
4	D	42	Total	O	0	0
			42	42		
4	E	65	Total	O	0	0
			65	65		

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.

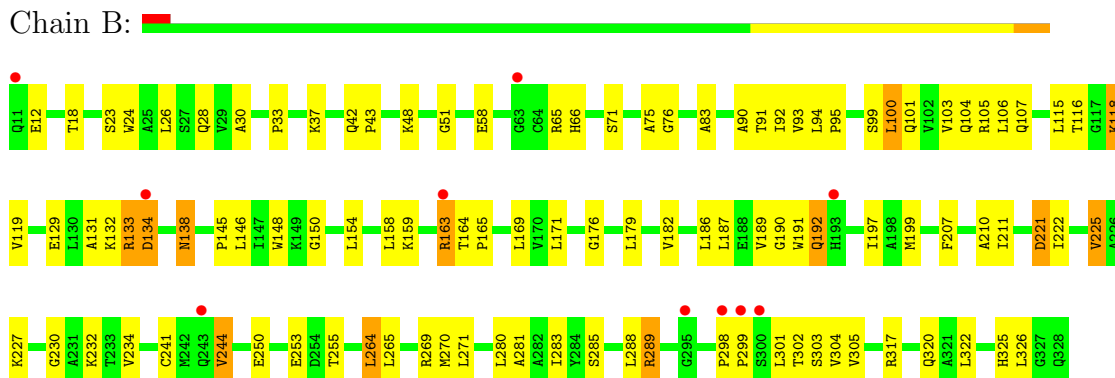
- Molecule 1: Serine dehydratase-like

Chain A:



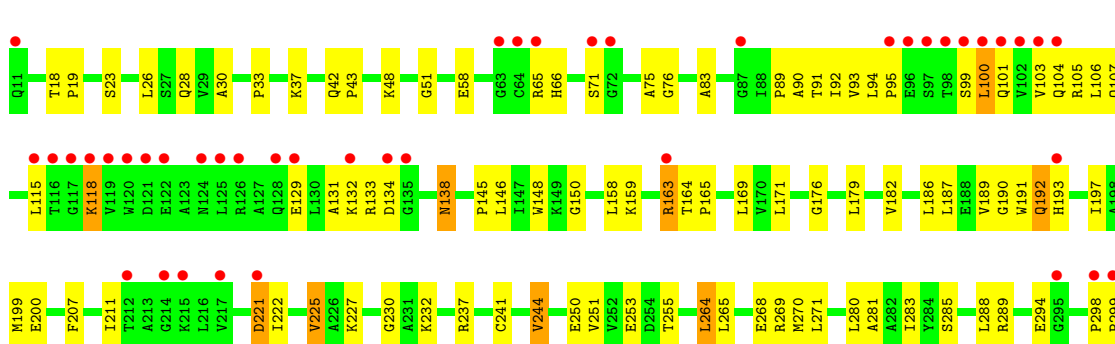
- Molecule 1: Serine dehydratase-like

Chain B:



- Molecule 1: Serine dehydratase-like

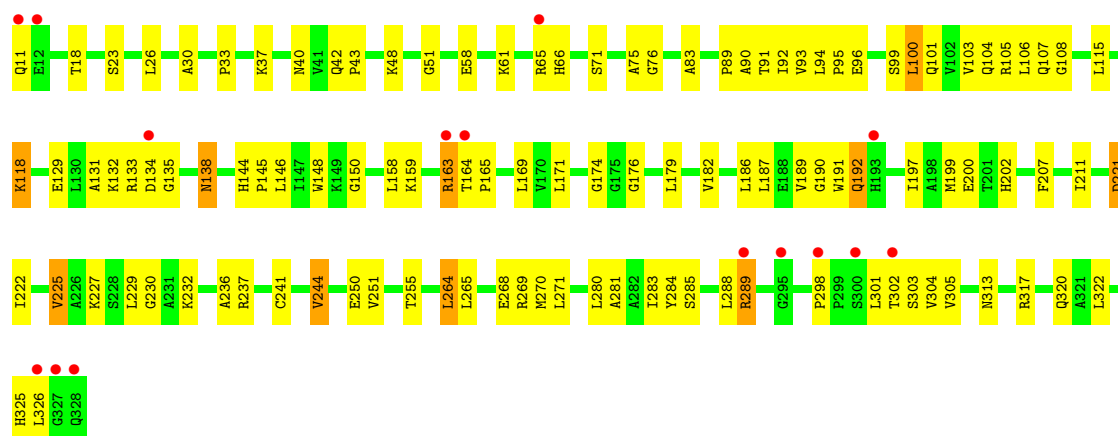
Chain C:





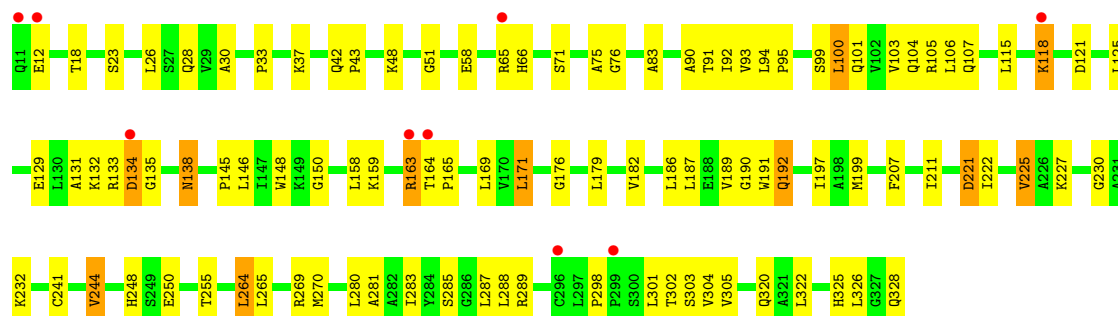
- Molecule 1: Serine dehydratase-like

Chain D:



- Molecule 1: Serine dehydratase-like

Chain E:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	97.21Å 154.74Å 306.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.80 19.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.96-2.80) 100.0 (19.95-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.65 (at 2.79Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.213 , 0.230 0.213 , 0.230	Depositor DCC
R_{free} test set	5798 reflections (10.16%)	DCC
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 29.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 57081 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12122	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: K, PLP

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	0.36	0/2395	0.59	1/3255 (0.0%)
1	B	0.34	0/2395	0.59	0/3255
1	C	0.35	0/2395	0.59	0/3255
1	D	0.36	0/2395	0.60	0/3255
1	E	0.35	0/2395	0.59	0/3255
All	All	0.35	0/11975	0.59	1/16275 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	171	LEU	CA-CB-CG	5.04	126.89	115.30

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	2352	0	2403	88	0
1	B	2352	0	2403	95	0
1	C	2352	0	2403	86	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2352	0	2403	97	2
1	E	2352	0	2403	84	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	15	0	6	1	0
3	B	15	0	7	1	0
3	C	15	0	6	1	0
3	D	15	0	6	1	0
3	E	15	0	6	1	0
4	A	70	0	0	11	0
4	B	74	0	0	10	0
4	C	31	0	0	6	0
4	D	42	0	0	9	0
4	E	65	0	0	7	0
All	All	12122	0	12046	430	2

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 18.

All (430) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:134:ASP:HA	4:B:453:HOH:O	1.65	0.94
1:C:264:LEU:HG	1:C:280:LEU:HD13	1.54	0.90
1:A:264:LEU:HG	1:A:280:LEU:HD13	1.53	0.89
1:E:264:LEU:HG	1:E:280:LEU:HD13	1.53	0.89
1:D:264:LEU:HG	1:D:280:LEU:HD13	1.54	0.89
1:C:118:LYS:HE3	1:C:118:LYS:HA	1.55	0.88
1:B:264:LEU:HG	1:B:280:LEU:HD13	1.55	0.88
1:B:118:LYS:HE3	1:B:118:LYS:HA	1.56	0.87
1:D:118:LYS:HE3	1:D:118:LYS:HA	1.59	0.85
1:E:118:LYS:HA	1:E:118:LYS:HE3	1.58	0.85
1:A:313:ASN:HB2	4:A:440:HOH:O	1.76	0.84
1:C:163:ARG:HB3	4:C:413:HOH:O	1.76	0.84
1:C:192:GLN:HB3	4:C:402:HOH:O	1.75	0.84
1:C:269:ARG:HB2	1:D:271:LEU:HB3	1.59	0.83
1:A:118:LYS:HA	1:A:118:LYS:HE3	1.60	0.81
1:A:248:HIS:HB3	4:A:418:HOH:O	1.84	0.78
1:E:265:LEU:O	1:E:269:ARG:HA	1.85	0.77
1:B:298:PRO:HG2	1:B:301:LEU:HG	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:298:PRO:HG2	1:D:301:LEU:HG	1.67	0.77
1:B:104:GLN:HE21	1:D:104:GLN:NE2	1.82	0.76
1:A:298:PRO:HG2	1:A:301:LEU:HG	1.67	0.76
1:C:265:LEU:O	1:C:269:ARG:HA	1.86	0.76
1:B:104:GLN:NE2	1:D:104:GLN:HE21	1.83	0.76
1:E:298:PRO:HG2	1:E:301:LEU:HG	1.67	0.76
1:B:104:GLN:HE21	1:D:104:GLN:HE21	1.34	0.75
1:B:265:LEU:O	1:B:269:ARG:HA	1.87	0.75
1:A:265:LEU:O	1:A:269:ARG:HA	1.86	0.75
1:D:265:LEU:O	1:D:269:ARG:HA	1.86	0.74
1:C:298:PRO:HG2	1:C:301:LEU:HG	1.67	0.73
1:E:264:LEU:HG	1:E:280:LEU:CD1	2.19	0.72
1:A:269:ARG:HB2	1:B:271:LEU:HB3	1.70	0.72
1:D:264:LEU:HG	1:D:280:LEU:CD1	2.19	0.72
1:C:264:LEU:HG	1:C:280:LEU:CD1	2.19	0.72
1:A:264:LEU:HG	1:A:280:LEU:CD1	2.20	0.71
1:B:264:LEU:HG	1:B:280:LEU:CD1	2.21	0.71
1:D:163:ARG:HE	1:D:164:THR:H	1.40	0.70
1:C:163:ARG:HE	1:C:164:THR:H	1.41	0.69
1:E:92:ILE:HG21	1:E:106:LEU:HD13	1.75	0.69
1:B:163:ARG:HE	1:B:164:THR:H	1.41	0.68
1:B:92:ILE:HG21	1:B:106:LEU:HD13	1.75	0.68
1:B:163:ARG:HG2	1:B:164:THR:HG23	1.75	0.68
1:A:163:ARG:HE	1:A:164:THR:H	1.42	0.68
1:E:163:ARG:HE	1:E:164:THR:H	1.42	0.68
1:B:28:GLN:HE22	1:E:28:GLN:HE22	1.42	0.68
1:B:289:ARG:HG2	4:B:430:HOH:O	1.93	0.68
1:A:99:SER:OG	1:A:101:GLN:HG2	1.94	0.68
1:C:163:ARG:HG2	1:C:164:THR:HG23	1.75	0.67
1:D:92:ILE:HG21	1:D:106:LEU:HD13	1.75	0.67
1:B:187:LEU:HD23	1:B:192:GLN:HG3	1.77	0.67
1:C:187:LEU:HD23	1:C:192:GLN:HG3	1.75	0.67
1:D:163:ARG:HG2	1:D:164:THR:HG23	1.78	0.66
1:E:187:LEU:HD23	1:E:192:GLN:HG3	1.78	0.66
1:C:92:ILE:HG21	1:C:106:LEU:HD13	1.78	0.66
1:E:99:SER:OG	1:E:101:GLN:HG2	1.96	0.66
1:C:99:SER:OG	1:C:101:GLN:HG2	1.95	0.66
1:A:92:ILE:HG21	1:A:106:LEU:HD13	1.76	0.65
1:A:187:LEU:HD23	1:A:192:GLN:HG3	1.78	0.65
1:D:165:PRO:HG3	1:D:191:TRP:NE1	2.11	0.65
1:E:192:GLN:NE2	1:E:192:GLN:H	1.95	0.65
1:D:159:LYS:HG3	1:D:189:VAL:HB	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:159:LYS:HG3	1:B:189:VAL:HB	1.79	0.65
1:D:11:GLN:HG2	4:D:428:HOH:O	1.96	0.65
1:D:192:GLN:HB3	4:D:442:HOH:O	1.96	0.65
1:D:187:LEU:HD23	1:D:192:GLN:HG3	1.78	0.65
1:D:61:LYS:HE3	4:D:428:HOH:O	1.98	0.65
1:C:159:LYS:HG3	1:C:189:VAL:HB	1.79	0.64
1:C:165:PRO:HG3	1:C:191:TRP:NE1	2.13	0.64
1:E:163:ARG:HG2	1:E:164:THR:HG23	1.80	0.64
1:C:241:CYS:HA	1:C:244:VAL:CG1	2.28	0.63
1:B:99:SER:OG	1:B:101:GLN:HG2	1.99	0.63
1:D:99:SER:OG	1:D:101:GLN:HG2	1.99	0.63
1:E:159:LYS:HG3	1:E:189:VAL:HB	1.79	0.63
1:A:163:ARG:HG2	1:A:164:THR:HG23	1.78	0.63
1:D:51:GLY:HA2	1:D:150:GLY:HA3	1.81	0.63
1:B:255:THR:HG23	4:B:429:HOH:O	1.98	0.62
1:A:192:GLN:NE2	1:A:192:GLN:H	1.97	0.62
1:E:248:HIS:HB3	4:E:468:HOH:O	1.98	0.62
1:C:192:GLN:H	1:C:192:GLN:NE2	1.97	0.62
1:E:328:GLN:O	4:E:499:HOH:O	2.16	0.62
1:B:51:GLY:HA2	1:B:150:GLY:HA3	1.82	0.62
1:C:94:LEU:HB3	1:C:95:PRO:HD2	1.82	0.61
1:E:134:ASP:HB3	4:E:506:HOH:O	2.00	0.61
1:B:192:GLN:HB3	4:B:447:HOH:O	2.00	0.61
1:C:51:GLY:HA2	1:C:150:GLY:HA3	1.81	0.61
1:A:159:LYS:HG3	1:A:189:VAL:HB	1.81	0.61
1:A:283:ILE:HD13	1:A:288:LEU:HD22	1.83	0.61
1:E:165:PRO:HG3	1:E:191:TRP:NE1	2.16	0.60
1:A:66:HIS:HE1	1:A:91:THR:OG1	1.85	0.60
1:E:283:ILE:HD13	1:E:288:LEU:HD22	1.83	0.60
1:E:287:LEU:HD11	4:E:471:HOH:O	2.01	0.60
1:A:165:PRO:HG3	1:A:191:TRP:NE1	2.16	0.60
1:D:241:CYS:HA	1:D:244:VAL:CG1	2.32	0.60
1:C:271:LEU:HB3	1:D:269:ARG:HB2	1.81	0.60
1:A:271:LEU:HB3	1:B:269:ARG:HB2	1.83	0.59
1:B:241:CYS:HA	1:B:244:VAL:CG1	2.32	0.59
1:B:163:ARG:HB3	4:B:406:HOH:O	2.02	0.59
1:D:221:ASP:HB3	4:D:417:HOH:O	2.02	0.59
1:B:283:ILE:HD13	1:B:288:LEU:HD22	1.84	0.59
1:C:30:ALA:HB2	1:C:283:ILE:HG23	1.83	0.59
1:B:165:PRO:HG3	1:B:191:TRP:NE1	2.18	0.59
1:C:66:HIS:HE1	1:C:91:THR:OG1	1.86	0.59
1:C:33:PRO:HG2	1:C:303:SER:HA	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:42:GLN:OE1	1:E:43:PRO:HD2	2.03	0.59
1:B:192:GLN:NE2	1:B:192:GLN:H	1.99	0.59
1:A:192:GLN:HB3	4:A:410:HOH:O	2.03	0.59
1:B:30:ALA:HB2	1:B:283:ILE:HG23	1.85	0.59
1:D:313:ASN:HB2	4:D:434:HOH:O	2.02	0.59
1:D:192:GLN:NE2	1:D:192:GLN:H	2.00	0.59
1:A:51:GLY:HA2	1:A:150:GLY:HA3	1.85	0.59
1:A:241:CYS:HA	1:A:244:VAL:CG1	2.33	0.58
1:C:283:ILE:HD13	1:C:288:LEU:HD22	1.85	0.58
1:B:42:GLN:OE1	1:B:43:PRO:HD2	2.02	0.58
1:D:283:ILE:HD13	1:D:288:LEU:HD22	1.85	0.58
1:C:42:GLN:OE1	1:C:43:PRO:HD2	2.04	0.58
1:A:42:GLN:OE1	1:A:43:PRO:HD2	2.04	0.58
1:D:42:GLN:OE1	1:D:43:PRO:HD2	2.04	0.57
1:D:30:ALA:HB2	1:D:283:ILE:HG23	1.86	0.57
1:D:66:HIS:HE1	1:D:91:THR:OG1	1.87	0.57
1:A:33:PRO:HG2	1:A:303:SER:HA	1.87	0.57
1:A:30:ALA:HB2	1:A:283:ILE:HG23	1.87	0.57
1:E:51:GLY:HA2	1:E:150:GLY:HA3	1.86	0.57
1:C:301:LEU:HD12	1:C:301:LEU:N	2.20	0.56
1:E:241:CYS:HA	1:E:244:VAL:CG1	2.35	0.56
1:B:94:LEU:HB3	1:B:95:PRO:HD2	1.86	0.56
1:D:301:LEU:HD12	1:D:301:LEU:N	2.21	0.56
1:E:94:LEU:HB3	1:E:95:PRO:HD2	1.87	0.56
1:E:66:HIS:HE1	1:E:91:THR:OG1	1.88	0.56
1:D:94:LEU:HB3	1:D:95:PRO:HD2	1.87	0.56
1:E:33:PRO:HG2	1:E:303:SER:HA	1.87	0.56
1:A:178:LEU:HB3	4:A:407:HOH:O	2.06	0.55
1:B:66:HIS:HE1	1:B:91:THR:OG1	1.90	0.55
1:A:197:ILE:N	1:A:197:ILE:HD12	2.21	0.55
1:B:33:PRO:HG2	1:B:303:SER:HA	1.87	0.55
1:C:283:ILE:CD1	1:C:288:LEU:HD22	2.36	0.55
1:D:33:PRO:HG2	1:D:303:SER:HA	1.87	0.55
1:D:169:LEU:HD12	1:D:305:VAL:HB	1.89	0.55
1:A:94:LEU:HB3	1:A:95:PRO:HD2	1.89	0.55
1:B:301:LEU:HD12	1:B:301:LEU:N	2.21	0.55
1:E:30:ALA:HB2	1:E:283:ILE:HG23	1.89	0.54
1:E:169:LEU:HD12	1:E:305:VAL:HB	1.89	0.54
1:A:283:ILE:CD1	1:A:288:LEU:HD22	2.37	0.54
1:A:301:LEU:HD12	1:A:301:LEU:N	2.23	0.54
1:D:325:HIS:ND1	1:D:326:LEU:HD12	2.23	0.54
1:B:283:ILE:CD1	1:B:288:LEU:HD22	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:283:ILE:CD1	1:E:288:LEU:HD22	2.37	0.54
1:C:18:THR:OG1	1:C:37:LYS:HE3	2.08	0.54
1:B:325:HIS:ND1	1:B:326:LEU:HD12	2.23	0.53
1:E:301:LEU:HD12	1:E:301:LEU:N	2.24	0.53
1:D:283:ILE:CD1	1:D:288:LEU:HD22	2.38	0.53
1:C:325:HIS:ND1	1:C:326:LEU:HD12	2.23	0.53
1:A:28:GLN:HE22	1:C:28:GLN:HE22	1.57	0.53
1:A:325:HIS:ND1	1:A:326:LEU:HD12	2.24	0.53
1:E:255:THR:HA	1:E:326:LEU:HD23	1.91	0.52
1:B:197:ILE:N	1:B:197:ILE:HD12	2.24	0.52
1:E:176:GLY:N	3:E:400:PLP:O2P	2.37	0.52
1:A:28:GLN:HG3	4:A:423:HOH:O	2.10	0.52
1:E:325:HIS:ND1	1:E:326:LEU:HD12	2.24	0.52
1:D:26:LEU:HD12	1:D:283:ILE:HG21	1.91	0.52
1:D:288:LEU:HD21	1:D:304:VAL:HG21	1.91	0.52
1:C:26:LEU:HD12	1:C:283:ILE:HG21	1.91	0.52
1:A:169:LEU:HD12	1:A:305:VAL:HB	1.92	0.52
1:C:169:LEU:HD12	1:C:305:VAL:HB	1.91	0.52
1:C:255:THR:HA	1:C:326:LEU:HD23	1.91	0.51
1:B:169:LEU:HD12	1:B:305:VAL:HB	1.91	0.51
1:A:193:HIS:HB2	4:A:434:HOH:O	2.09	0.51
1:E:23:SER:HB3	1:E:26:LEU:HB2	1.91	0.51
1:E:26:LEU:HD12	1:E:283:ILE:HG21	1.91	0.51
1:E:103:VAL:O	1:E:107:GLN:HG3	2.11	0.51
1:A:255:THR:HA	1:A:326:LEU:HD23	1.93	0.51
1:A:18:THR:OG1	1:A:37:LYS:HE3	2.09	0.51
1:E:197:ILE:N	1:E:197:ILE:HD12	2.25	0.51
1:C:48:LYS:HE2	1:C:75:ALA:N	2.25	0.51
1:E:138:ASN:ND2	4:E:464:HOH:O	2.36	0.51
1:B:48:LYS:HE2	1:B:75:ALA:N	2.25	0.51
1:D:23:SER:HB3	1:D:26:LEU:HB2	1.93	0.51
1:B:187:LEU:HD23	1:B:192:GLN:CG	2.41	0.51
1:D:197:ILE:N	1:D:197:ILE:HD12	2.26	0.51
1:D:255:THR:HA	1:D:326:LEU:HD23	1.92	0.51
1:D:187:LEU:HD23	1:D:192:GLN:CG	2.41	0.50
1:B:288:LEU:HD21	1:B:304:VAL:HG21	1.94	0.50
1:C:288:LEU:HD21	1:C:304:VAL:HG21	1.93	0.50
1:C:48:LYS:HE2	1:C:75:ALA:CA	2.41	0.50
1:A:284:TYR:HB3	4:A:428:HOH:O	2.09	0.50
1:E:48:LYS:HE2	1:E:75:ALA:N	2.27	0.50
1:B:119:VAL:HG22	4:B:415:HOH:O	2.12	0.50
1:D:165:PRO:HG3	1:D:191:TRP:CD1	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:302:THR:O	1:A:303:SER:HB3	2.11	0.50
1:B:210:ALA:HB2	4:B:460:HOH:O	2.11	0.50
1:A:48:LYS:HE2	1:A:75:ALA:N	2.27	0.50
1:C:23:SER:HB3	1:C:26:LEU:HB2	1.94	0.50
1:A:225:VAL:HG11	1:A:322:LEU:HD22	1.92	0.50
1:A:23:SER:HB3	1:A:26:LEU:HB2	1.94	0.50
1:E:288:LEU:HD21	1:E:304:VAL:HG21	1.94	0.50
1:C:187:LEU:HD23	1:C:192:GLN:CG	2.41	0.49
1:E:302:THR:O	1:E:303:SER:HB3	2.10	0.49
1:C:197:ILE:N	1:C:197:ILE:HD12	2.27	0.49
1:A:222:ILE:HG13	1:A:230:GLY:O	2.12	0.49
1:C:176:GLY:N	3:C:400:PLP:O2P	2.40	0.49
1:D:202:HIS:HB2	4:D:419:HOH:O	2.12	0.49
1:B:255:THR:HA	1:B:326:LEU:HD23	1.93	0.49
1:B:48:LYS:HE2	1:B:75:ALA:CA	2.43	0.49
1:E:207:PHE:O	1:E:211:ILE:HG12	2.12	0.49
1:A:26:LEU:HD12	1:A:283:ILE:HG21	1.95	0.49
1:B:23:SER:HB3	1:B:26:LEU:HB2	1.95	0.49
1:A:187:LEU:HD23	1:A:192:GLN:CG	2.43	0.49
1:A:288:LEU:HD21	1:A:304:VAL:HG21	1.95	0.49
1:A:269:ARG:HD3	4:A:412:HOH:O	2.13	0.49
1:C:193:HIS:HB2	4:C:421:HOH:O	2.13	0.49
1:C:221:ASP:HA	1:C:232:LYS:HE2	1.94	0.48
1:D:225:VAL:HG11	1:D:322:LEU:HD22	1.95	0.48
1:B:103:VAL:O	1:B:107:GLN:HG3	2.12	0.48
1:D:92:ILE:HG22	1:D:94:LEU:CD2	2.43	0.48
1:A:103:VAL:O	1:A:107:GLN:HG3	2.13	0.48
1:C:207:PHE:O	1:C:211:ILE:HG12	2.14	0.48
1:C:281:ALA:O	1:C:285:SER:HB2	2.13	0.48
1:B:118:LYS:CA	1:B:118:LYS:HE3	2.37	0.48
1:B:26:LEU:HD12	1:B:283:ILE:HG21	1.96	0.48
1:C:225:VAL:HG11	1:C:322:LEU:HD22	1.95	0.48
1:C:298:PRO:O	1:C:301:LEU:HD11	2.14	0.48
1:D:103:VAL:O	1:D:107:GLN:HG3	2.13	0.48
1:E:159:LYS:HG2	1:E:191:TRP:CZ2	2.49	0.48
1:A:159:LYS:HG2	1:A:191:TRP:CZ2	2.49	0.48
1:E:48:LYS:HE2	1:E:75:ALA:CA	2.44	0.48
1:D:221:ASP:HA	1:D:232:LYS:HE2	1.96	0.48
1:B:207:PHE:O	1:B:211:ILE:HG12	2.14	0.47
1:B:18:THR:OG1	1:B:37:LYS:HE3	2.13	0.47
1:B:176:GLY:N	3:B:400:PLP:O2P	2.43	0.47
1:D:207:PHE:O	1:D:211:ILE:HG12	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:302:THR:O	1:C:303:SER:HB3	2.14	0.47
1:C:115:LEU:N	1:C:115:LEU:HD22	2.29	0.47
1:E:281:ALA:O	1:E:285:SER:HB2	2.15	0.47
1:B:92:ILE:HG22	1:B:94:LEU:CD2	2.45	0.47
1:C:165:PRO:HG3	1:C:191:TRP:CD1	2.48	0.47
1:E:190:GLY:HA2	1:E:192:GLN:OE1	2.15	0.47
1:B:298:PRO:HA	1:B:299:PRO:HD3	1.86	0.47
1:D:48:LYS:HE2	1:D:75:ALA:CA	2.45	0.47
1:E:165:PRO:HG3	1:E:191:TRP:CD1	2.50	0.47
1:D:48:LYS:HE2	1:D:75:ALA:N	2.29	0.47
1:D:145:PRO:HA	1:D:148:TRP:CE3	2.50	0.47
1:B:225:VAL:HG11	1:B:322:LEU:HD22	1.95	0.47
1:C:103:VAL:O	1:C:107:GLN:HG3	2.15	0.47
1:A:48:LYS:HE2	1:A:75:ALA:CA	2.45	0.46
1:D:176:GLY:N	3:D:400:PLP:O2P	2.40	0.46
1:B:221:ASP:HA	1:B:232:LYS:HE2	1.95	0.46
1:E:118:LYS:HE3	1:E:118:LYS:CA	2.39	0.46
1:C:222:ILE:HG13	1:C:230:GLY:O	2.15	0.46
1:A:176:GLY:N	3:A:400:PLP:O2P	2.39	0.46
1:C:264:LEU:CD1	1:C:270:MET:HG3	2.45	0.46
1:D:92:ILE:HG22	1:D:94:LEU:HD21	1.97	0.46
1:E:221:ASP:HA	1:E:232:LYS:HE2	1.97	0.46
1:C:294:GLU:CG	4:C:422:HOH:O	2.63	0.46
1:D:289:ARG:HD3	4:D:409:HOH:O	2.15	0.46
1:E:135:GLY:N	4:E:506:HOH:O	2.25	0.46
1:A:286:GLY:HA3	1:D:89:PRO:HB3	1.97	0.46
1:D:281:ALA:O	1:D:285:SER:HB2	2.16	0.46
1:D:190:GLY:HA2	1:D:192:GLN:OE1	2.16	0.46
1:A:92:ILE:HG22	1:A:94:LEU:CD2	2.45	0.46
1:A:165:PRO:HG3	1:A:191:TRP:CD1	2.51	0.46
1:C:83:ALA:CB	1:C:90:ALA:HB2	2.46	0.46
1:C:241:CYS:HA	1:C:244:VAL:HG13	1.97	0.46
1:A:221:ASP:HA	1:A:232:LYS:HE2	1.97	0.46
1:E:18:THR:OG1	1:E:37:LYS:HE3	2.16	0.46
1:D:222:ILE:HG13	1:D:230:GLY:O	2.16	0.45
1:E:264:LEU:CD1	1:E:270:MET:HG3	2.47	0.45
1:E:187:LEU:HD23	1:E:192:GLN:CG	2.46	0.45
1:D:302:THR:O	1:D:303:SER:HB3	2.16	0.45
1:E:92:ILE:HG22	1:E:94:LEU:CD2	2.46	0.45
1:E:192:GLN:CD	1:E:192:GLN:H	2.19	0.45
1:B:302:THR:O	1:B:303:SER:HB3	2.16	0.45
1:C:48:LYS:CE	1:C:75:ALA:HB2	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:VAL:HG12	4:A:404:HOH:O	2.17	0.45
1:B:264:LEU:CD1	1:B:270:MET:HG3	2.46	0.45
1:C:145:PRO:HA	1:C:148:TRP:CE3	2.51	0.45
1:A:207:PHE:O	1:A:211:ILE:HG12	2.16	0.45
1:C:192:GLN:H	1:C:192:GLN:CD	2.20	0.45
1:B:234:VAL:HG12	4:B:460:HOH:O	2.17	0.45
1:B:225:VAL:CG1	1:B:322:LEU:HD22	2.47	0.45
1:D:18:THR:OG1	1:D:37:LYS:HE3	2.17	0.45
1:E:92:ILE:HG22	1:E:94:LEU:HD21	1.99	0.45
1:B:48:LYS:CE	1:B:75:ALA:HB2	2.47	0.45
1:C:182:VAL:O	1:C:186:LEU:HG	2.17	0.45
1:D:264:LEU:CD1	1:D:270:MET:HG3	2.47	0.45
1:B:116:THR:HG22	4:C:414:HOH:O	2.16	0.45
1:B:23:SER:HA	4:B:443:HOH:O	2.17	0.45
1:E:227:LYS:HE2	1:E:227:LYS:HA	1.99	0.45
1:D:40:ASN:HB2	4:D:439:HOH:O	2.17	0.45
1:A:264:LEU:CD1	1:A:270:MET:HG3	2.47	0.44
1:B:298:PRO:O	1:B:301:LEU:HD11	2.17	0.44
1:B:241:CYS:HA	1:B:244:VAL:HG13	1.99	0.44
1:C:225:VAL:CG1	1:C:322:LEU:HD22	2.48	0.44
1:A:281:ALA:O	1:A:285:SER:HB2	2.16	0.44
1:B:100:LEU:HD13	1:B:104:GLN:HG3	1.98	0.44
1:A:298:PRO:HA	1:A:299:PRO:HD3	1.87	0.44
1:D:159:LYS:HG2	1:D:191:TRP:CZ2	2.52	0.44
1:D:225:VAL:CG1	1:D:322:LEU:HD22	2.47	0.44
1:C:129:GLU:O	1:C:132:LYS:HB2	2.18	0.44
1:C:190:GLY:HA2	1:C:192:GLN:OE1	2.17	0.44
1:D:298:PRO:O	1:D:301:LEU:HD11	2.17	0.44
1:A:225:VAL:CG1	1:A:322:LEU:HD22	2.46	0.44
1:B:317:ARG:HD2	1:D:96:GLU:O	2.16	0.44
1:E:225:VAL:HG11	1:E:322:LEU:HD22	1.99	0.44
1:B:199:MET:SD	1:B:250:GLU:HB2	2.58	0.44
1:B:92:ILE:HG22	1:B:94:LEU:HD21	1.98	0.44
1:B:281:ALA:O	1:B:285:SER:HB2	2.18	0.44
1:A:145:PRO:HA	1:A:148:TRP:CE3	2.52	0.44
1:A:298:PRO:O	1:A:301:LEU:HD11	2.17	0.44
1:B:28:GLN:NE2	1:E:28:GLN:HE22	2.11	0.44
1:C:92:ILE:HG22	1:C:94:LEU:CD2	2.48	0.44
1:B:165:PRO:HG3	1:B:191:TRP:CD1	2.53	0.44
1:A:159:LYS:HA	1:A:191:TRP:CH2	2.52	0.44
1:E:58:GLU:HG3	1:E:146:LEU:HD22	1.99	0.44
1:E:145:PRO:HA	1:E:148:TRP:CE3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:199:MET:SD	1:D:250:GLU:HB2	2.58	0.44
1:D:227:LYS:HE2	1:D:227:LYS:HA	2.00	0.44
1:C:269:ARG:HG2	1:C:269:ARG:NH2	2.32	0.44
1:E:298:PRO:O	1:E:301:LEU:HD11	2.17	0.44
1:C:159:LYS:HG2	1:C:191:TRP:CZ2	2.53	0.44
1:E:199:MET:SD	1:E:250:GLU:HB2	2.57	0.44
1:D:192:GLN:CD	1:D:192:GLN:H	2.21	0.43
1:D:48:LYS:CE	1:D:75:ALA:HB2	2.48	0.43
1:A:105:ARG:HD2	1:B:24:TRP:CZ3	2.52	0.43
1:C:159:LYS:HA	1:C:191:TRP:CH2	2.54	0.43
1:E:115:LEU:N	1:E:115:LEU:HD22	2.33	0.43
1:E:71:SER:O	1:E:76:GLY:HA3	2.18	0.43
1:C:100:LEU:HD13	1:C:104:GLN:HG3	2.00	0.43
1:C:200:GLU:O	1:C:251:VAL:HA	2.19	0.43
1:A:144:HIS:HA	1:A:145:PRO:HD3	1.91	0.43
1:E:222:ILE:HG13	1:E:230:GLY:O	2.17	0.43
1:A:241:CYS:HA	1:A:244:VAL:HG13	2.00	0.43
1:E:241:CYS:HA	1:E:244:VAL:HG13	2.00	0.43
1:C:227:LYS:HA	1:C:227:LYS:HE2	2.00	0.43
1:C:71:SER:O	1:C:76:GLY:HA3	2.18	0.43
1:D:100:LEU:HD13	1:D:104:GLN:HG3	2.01	0.43
1:D:144:HIS:HA	1:D:145:PRO:HD3	1.92	0.43
1:C:237:ARG:HG2	1:C:237:ARG:HH11	1.84	0.43
1:B:58:GLU:HG3	1:B:146:LEU:HD22	2.01	0.43
1:C:92:ILE:HG22	1:C:94:LEU:HD21	2.01	0.43
1:A:190:GLY:HA2	1:A:192:GLN:OE1	2.18	0.43
1:E:159:LYS:HA	1:E:191:TRP:CH2	2.53	0.43
1:D:129:GLU:O	1:D:132:LYS:HB2	2.19	0.43
1:A:100:LEU:HD13	1:A:104:GLN:HG3	2.00	0.43
1:B:115:LEU:HD22	1:B:115:LEU:N	2.34	0.43
1:C:118:LYS:CA	1:C:118:LYS:HE3	2.36	0.43
1:B:192:GLN:CD	1:B:192:GLN:H	2.21	0.43
1:A:92:ILE:HG22	1:A:94:LEU:HD21	2.01	0.43
1:C:199:MET:SD	1:C:250:GLU:HB2	2.59	0.43
1:D:236:ALA:N	4:D:420:HOH:O	2.52	0.43
1:D:58:GLU:HG3	1:D:146:LEU:HD22	2.00	0.43
1:D:255:THR:HG22	1:D:326:LEU:HB3	2.01	0.43
1:A:48:LYS:CE	1:A:75:ALA:HB2	2.49	0.43
1:A:227:LYS:HE2	1:A:227:LYS:HA	2.00	0.43
1:B:222:ILE:HG13	1:B:230:GLY:O	2.19	0.43
1:B:190:GLY:HA2	1:B:192:GLN:OE1	2.19	0.42
1:A:192:GLN:CD	1:A:192:GLN:H	2.21	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:159:LYS:HA	1:D:191:TRP:CH2	2.54	0.42
1:D:241:CYS:HA	1:D:244:VAL:HG13	2.00	0.42
1:D:71:SER:O	1:D:76:GLY:HA3	2.18	0.42
1:D:131:ALA:HB2	1:D:138:ASN:HB2	2.01	0.42
1:B:133:ARG:NH1	1:C:253:GLU:HG3	2.34	0.42
1:B:159:LYS:HG2	1:B:191:TRP:CZ2	2.54	0.42
1:A:263:GLN:NE2	4:A:428:HOH:O	2.52	0.42
1:E:100:LEU:HD13	1:E:104:GLN:HG3	2.01	0.42
1:A:121:ASP:O	1:A:125:LEU:HD13	2.19	0.42
1:E:182:VAL:O	1:E:186:LEU:HG	2.20	0.42
1:A:23:SER:OG	1:A:26:LEU:HD23	2.19	0.42
1:B:131:ALA:HB2	1:B:138:ASN:HB2	2.01	0.42
1:B:104:GLN:HE22	1:D:101:GLN:HA	1.83	0.42
1:E:48:LYS:CE	1:E:75:ALA:HB2	2.49	0.42
1:A:58:GLU:HG3	1:A:146:LEU:HD22	2.00	0.42
1:B:145:PRO:HA	1:B:148:TRP:CE3	2.53	0.42
1:A:118:LYS:CA	1:A:118:LYS:HE3	2.40	0.42
1:C:268:GLU:C	1:C:269:ARG:HG2	2.40	0.42
1:E:131:ALA:HB2	1:E:138:ASN:HB2	2.02	0.42
1:D:182:VAL:O	1:D:186:LEU:HG	2.19	0.42
1:A:11:GLN:N	4:A:463:HOH:O	2.52	0.42
1:A:28:GLN:HE22	1:C:28:GLN:NE2	2.16	0.42
1:C:294:GLU:HG2	4:C:422:HOH:O	2.20	0.42
1:B:83:ALA:CB	1:B:90:ALA:HB2	2.50	0.42
1:B:227:LYS:HE2	1:B:227:LYS:HA	2.02	0.42
1:A:28:GLN:OE1	1:D:108:GLY:HA2	2.20	0.42
1:A:199:MET:SD	1:A:250:GLU:HB2	2.60	0.42
1:C:58:GLU:HG3	1:C:146:LEU:HD22	2.01	0.42
1:D:118:LYS:HE3	1:D:118:LYS:CA	2.40	0.41
1:E:23:SER:CB	1:E:26:LEU:HB2	2.49	0.41
1:A:71:SER:O	1:A:76:GLY:HA3	2.19	0.41
1:C:298:PRO:HA	1:C:299:PRO:HD3	1.85	0.41
1:E:192:GLN:HB3	4:E:477:HOH:O	2.19	0.41
1:E:171:LEU:O	1:E:171:LEU:HD22	2.21	0.41
1:B:182:VAL:O	1:B:186:LEU:HG	2.20	0.41
1:A:129:GLU:O	1:A:132:LYS:HB2	2.20	0.41
1:C:23:SER:CB	1:C:26:LEU:HB2	2.50	0.41
1:D:23:SER:CB	1:D:26:LEU:HB2	2.50	0.41
1:C:169:LEU:CD1	1:C:305:VAL:HB	2.51	0.41
1:A:23:SER:CB	1:A:26:LEU:HB2	2.50	0.41
1:E:26:LEU:HA	1:E:26:LEU:HD13	1.91	0.41
1:B:129:GLU:O	1:B:132:LYS:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:100:LEU:HD23	1:D:317:ARG:HH21	1.84	0.41
1:D:268:GLU:C	1:D:269:ARG:HG2	2.41	0.41
1:C:66:HIS:CD2	1:C:89:PRO:HB2	2.56	0.41
1:D:325:HIS:ND1	1:D:325:HIS:O	2.54	0.41
1:E:121:ASP:O	1:E:125:LEU:HD13	2.21	0.41
1:E:225:VAL:CG1	1:E:322:LEU:HD22	2.50	0.41
1:E:83:ALA:CB	1:E:90:ALA:HB2	2.51	0.41
1:E:192:GLN:N	1:E:192:GLN:NE2	2.67	0.41
1:B:159:LYS:HA	1:B:191:TRP:CH2	2.55	0.41
1:C:48:LYS:HE2	1:C:75:ALA:HB2	2.03	0.41
1:E:71:SER:OG	1:E:75:ALA:HB3	2.20	0.41
1:B:154:LEU:HD23	1:B:154:LEU:C	2.42	0.41
1:D:174:GLY:HA2	1:D:229:LEU:HA	2.03	0.41
1:C:131:ALA:HB2	1:C:138:ASN:HB2	2.02	0.41
1:D:83:ALA:CB	1:D:90:ALA:HB2	2.50	0.41
1:B:71:SER:O	1:B:76:GLY:HA3	2.21	0.41
1:B:104:GLN:NE2	1:D:104:GLN:NE2	2.51	0.41
1:B:28:GLN:HE22	1:E:28:GLN:NE2	2.12	0.40
1:E:255:THR:HG22	1:E:326:LEU:HB3	2.03	0.40
1:D:48:LYS:HE2	1:D:75:ALA:HB2	2.04	0.40
1:D:163:ARG:N	1:D:163:ARG:NE	2.70	0.40
1:E:129:GLU:O	1:E:132:LYS:HB2	2.20	0.40
1:D:200:GLU:O	1:D:251:VAL:HA	2.22	0.40
1:A:83:ALA:CB	1:A:90:ALA:HB2	2.52	0.40
1:D:115:LEU:HD22	1:D:115:LEU:N	2.36	0.40
1:A:131:ALA:HB2	1:A:138:ASN:HB2	2.03	0.40
1:B:100:LEU:HD22	1:B:100:LEU:HA	1.91	0.40
1:D:265:LEU:O	1:D:269:ARG:CA	2.65	0.40
1:B:253:GLU:HB3	4:B:429:HOH:O	2.21	0.40
1:C:18:THR:HA	1:C:19:PRO:HD3	1.92	0.40
1:B:12:GLU:HA	1:B:12:GLU:OE1	2.22	0.40
1:D:237:ARG:HG2	1:D:237:ARG:HH11	1.86	0.40
1:A:115:LEU:HD22	1:A:115:LEU:N	2.35	0.40
1:E:12:GLU:HA	1:E:12:GLU:OE1	2.21	0.40

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:283:ILE:O	1:D:289:ARG:NH2[3_555]	2.17	0.03
1:D:284:TYR:O	1:D:289:ARG:NE[3_555]	2.19	0.01

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	316/318 (99%)	293 (93%)	21 (7%)	2 (1%)	33	72
1	B	316/318 (99%)	294 (93%)	21 (7%)	1 (0%)	50	84
1	C	316/318 (99%)	294 (93%)	21 (7%)	1 (0%)	50	84
1	D	316/318 (99%)	294 (93%)	20 (6%)	2 (1%)	33	72
1	E	316/318 (99%)	294 (93%)	21 (7%)	1 (0%)	50	84
All	All	1580/1590 (99%)	1469 (93%)	104 (7%)	7 (0%)	43	80

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ASP
1	B	134	ASP
1	C	134	ASP
1	D	134	ASP
1	E	134	ASP
1	D	135	GLY
1	A	135	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	248/248 (100%)	230 (93%)	18 (7%)	20	49
1	B	248/248 (100%)	230 (93%)	18 (7%)	20	49
1	C	248/248 (100%)	230 (93%)	18 (7%)	20	49
1	D	248/248 (100%)	230 (93%)	18 (7%)	20	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	248/248 (100%)	230 (93%)	18 (7%)	20	49
All	All	1240/1240 (100%)	1150 (93%)	90 (7%)	20	49

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	93	VAL
1	A	100	LEU
1	A	105	ARG
1	A	118	LYS
1	A	133	ARG
1	A	138	ASN
1	A	158	LEU
1	A	163	ARG
1	A	171	LEU
1	A	179	LEU
1	A	192	GLN
1	A	221	ASP
1	A	225	VAL
1	A	244	VAL
1	A	264	LEU
1	A	289	ARG
1	A	320	GLN
1	B	65	ARG
1	B	93	VAL
1	B	100	LEU
1	B	105	ARG
1	B	118	LYS
1	B	133	ARG
1	B	138	ASN
1	B	158	LEU
1	B	163	ARG
1	B	171	LEU
1	B	179	LEU
1	B	192	GLN
1	B	221	ASP
1	B	225	VAL
1	B	244	VAL
1	B	264	LEU
1	B	289	ARG
1	B	320	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	65	ARG
1	C	93	VAL
1	C	100	LEU
1	C	105	ARG
1	C	118	LYS
1	C	133	ARG
1	C	138	ASN
1	C	158	LEU
1	C	163	ARG
1	C	171	LEU
1	C	179	LEU
1	C	192	GLN
1	C	221	ASP
1	C	225	VAL
1	C	244	VAL
1	C	264	LEU
1	C	289	ARG
1	C	320	GLN
1	D	65	ARG
1	D	93	VAL
1	D	100	LEU
1	D	105	ARG
1	D	118	LYS
1	D	133	ARG
1	D	138	ASN
1	D	158	LEU
1	D	163	ARG
1	D	171	LEU
1	D	179	LEU
1	D	192	GLN
1	D	221	ASP
1	D	225	VAL
1	D	244	VAL
1	D	264	LEU
1	D	289	ARG
1	D	320	GLN
1	E	65	ARG
1	E	93	VAL
1	E	100	LEU
1	E	105	ARG
1	E	118	LYS
1	E	133	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	138	ASN
1	E	158	LEU
1	E	163	ARG
1	E	171	LEU
1	E	179	LEU
1	E	192	GLN
1	E	221	ASP
1	E	225	VAL
1	E	244	VAL
1	E	264	LEU
1	E	289	ARG
1	E	320	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	128	GLN
1	A	138	ASN
1	A	192	GLN
1	A	263	GLN
1	A	320	GLN
1	A	328	GLN
1	B	28	GLN
1	B	66	HIS
1	B	104	GLN
1	B	128	GLN
1	B	138	ASN
1	B	192	GLN
1	B	320	GLN
1	B	328	GLN
1	C	66	HIS
1	C	128	GLN
1	C	138	ASN
1	C	192	GLN
1	C	248	HIS
1	C	320	GLN
1	C	328	GLN
1	D	66	HIS
1	D	114	GLN
1	D	128	GLN
1	D	138	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	192	GLN
1	D	248	HIS
1	D	320	GLN
1	D	328	GLN
1	E	66	HIS
1	E	128	GLN
1	E	138	ASN
1	E	192	GLN
1	E	320	GLN
1	E	328	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	PLP	A	400	1	14,15,16	1.31	1 (7%)	20,22,23	1.82	5 (25%)
3	PLP	B	400	1	14,15,16	1.26	2 (14%)	20,22,23	1.86	6 (30%)
3	PLP	C	400	1	14,15,16	1.32	1 (7%)	20,22,23	1.86	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	D	400	1	14,15,16	1.43	1 (7%)	20,22,23	1.85	6 (30%)
3	PLP	E	400	1	14,15,16	1.21	1 (7%)	20,22,23	1.87	5 (25%)

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	PLP	A	400	1	-	0/6/6/8	0/1/1/1
3	PLP	B	400	1	-	0/6/6/8	0/1/1/1
3	PLP	C	400	1	-	0/6/6/8	0/1/1/1
3	PLP	D	400	1	-	0/6/6/8	0/1/1/1
3	PLP	E	400	1	-	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	400	PLP	C3-C2	3.31	1.43	1.40
3	C	400	PLP	C3-C2	3.04	1.42	1.40
3	A	400	PLP	C3-C2	3.00	1.42	1.40
3	B	400	PLP	C3-C2	2.87	1.42	1.40
3	E	400	PLP	C3-C2	2.17	1.42	1.40
3	B	400	PLP	P-O3P	2.04	1.62	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	400	PLP	P-O4P-C5A	-5.30	102.09	121.22
3	A	400	PLP	P-O4P-C5A	-5.19	102.50	121.22
3	C	400	PLP	P-O4P-C5A	-5.07	102.93	121.22
3	D	400	PLP	P-O4P-C5A	-5.07	102.94	121.22
3	B	400	PLP	P-O4P-C5A	-5.03	103.08	121.22
3	C	400	PLP	O4P-C5A-C5	3.38	116.12	109.26
3	B	400	PLP	O4P-C5A-C5	3.30	115.96	109.26
3	E	400	PLP	O4P-C5A-C5	3.22	115.81	109.26
3	D	400	PLP	O4P-C5A-C5	3.12	115.61	109.26
3	A	400	PLP	O4P-C5A-C5	3.10	115.56	109.26
3	B	400	PLP	C5A-C5-C6	2.56	124.14	119.28
3	A	400	PLP	C5A-C5-C6	2.52	124.05	119.28
3	D	400	PLP	C5A-C5-C6	2.50	124.03	119.28
3	E	400	PLP	C5A-C5-C6	2.46	123.94	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	400	PLP	C5A-C5-C6	2.38	123.80	119.28
3	E	400	PLP	C5-C6-N1	-2.28	119.74	123.86
3	D	400	PLP	C5-C6-N1	-2.27	119.77	123.86
3	D	400	PLP	C5A-C5-C4	-2.26	116.15	121.41
3	C	400	PLP	C5-C6-N1	-2.25	119.81	123.86
3	B	400	PLP	C5A-C5-C4	-2.22	116.24	121.41
3	D	400	PLP	O3-C3-C2	2.17	121.46	117.61
3	C	400	PLP	C5A-C5-C4	-2.16	116.38	121.41
3	A	400	PLP	C5A-C5-C4	-2.14	116.42	121.41
3	C	400	PLP	O3-C3-C2	2.12	121.37	117.61
3	A	400	PLP	C5-C6-N1	-2.11	120.06	123.86
3	B	400	PLP	O3-C3-C2	2.10	121.34	117.61
3	B	400	PLP	C5-C6-N1	-2.10	120.07	123.86
3	E	400	PLP	C5A-C5-C4	-2.09	116.53	121.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	318/318 (100%)	-0.38	8 (2%) 54 55	13, 23, 45, 61	0
1	B	318/318 (100%)	-0.32	10 (3%) 47 47	12, 24, 46, 62	0
1	C	318/318 (100%)	0.30	45 (14%) 3 3	15, 27, 48, 63	0
1	D	318/318 (100%)	-0.21	15 (4%) 30 30	16, 25, 46, 63	0
1	E	318/318 (100%)	-0.37	9 (2%) 50 52	13, 23, 46, 62	0
All	All	1590/1590 (100%)	-0.20	87 (5%) 25 24	12, 25, 46, 63	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	LEU	6.4
1	C	117	GLY	6.4
1	C	72	GLY	5.8
1	D	302	THR	5.7
1	B	299	PRO	5.3
1	A	299	PRO	5.2
1	C	65	ARG	5.2
1	C	116	THR	5.1
1	C	134	ASP	5.1
1	C	103	VAL	4.8
1	C	299	PRO	4.6
1	C	97	SER	4.6
1	C	295	GLY	4.5
1	C	135	GLY	4.4
1	D	163	ARG	4.4
1	C	121	ASP	4.3
1	C	99	SER	4.3
1	D	300	SER	4.2
1	C	118	LYS	4.0
1	C	302	THR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	96	GLU	3.9
1	D	327	GLY	3.8
1	A	163	ARG	3.8
1	D	298	PRO	3.7
1	B	11	GLN	3.7
1	A	134	ASP	3.7
1	D	11	GLN	3.6
1	C	119	VAL	3.6
1	B	163	ARG	3.5
1	C	11	GLN	3.5
1	C	129	GLU	3.5
1	D	134	ASP	3.4
1	E	164	THR	3.3
1	E	299	PRO	3.2
1	C	212	THR	3.2
1	B	134	ASP	3.1
1	C	102	VAL	3.1
1	E	11	GLN	3.1
1	B	298	PRO	3.0
1	C	132	LYS	3.0
1	C	71	SER	3.0
1	E	118	LYS	3.0
1	A	11	GLN	3.0
1	C	163	ARG	3.0
1	E	65	ARG	2.9
1	C	120	TRP	2.9
1	C	98	THR	2.9
1	D	289	ARG	2.8
1	C	125	LEU	2.8
1	C	221	ASP	2.8
1	C	193	HIS	2.7
1	C	126	ARG	2.7
1	B	193	HIS	2.7
1	C	63	GLY	2.7
1	C	104	GLN	2.7
1	B	243	GLN	2.6
1	C	87	GLY	2.6
1	E	296	CYS	2.6
1	C	101	GLN	2.6
1	D	326	LEU	2.6
1	C	298	PRO	2.6
1	C	122	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	128	GLN	2.5
1	C	95	PRO	2.5
1	E	163	ARG	2.5
1	D	12	GLU	2.5
1	D	164	THR	2.4
1	C	214	GLY	2.4
1	B	295	GLY	2.4
1	A	164	THR	2.4
1	C	124	ASN	2.4
1	D	295	GLY	2.3
1	A	118	LYS	2.3
1	C	215	LYS	2.3
1	C	300	SER	2.3
1	E	134	ASP	2.3
1	D	328	GLN	2.3
1	D	65	ARG	2.2
1	C	64	CYS	2.2
1	C	217	VAL	2.2
1	B	300	SER	2.2
1	A	325	HIS	2.1
1	D	193	HIS	2.1
1	C	115	LEU	2.1
1	A	12	GLU	2.1
1	E	12	GLU	2.1
1	B	63	GLY	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(\AA^2)	Q<0.9
3	PLP	D	400	15/16	0.14	0.76	17,24,25,25	0
3	PLP	B	400	15/16	0.14	0.59	21,24,26,27	0
3	PLP	A	400	15/16	0.12	0.24	18,23,24,25	0
3	PLP	C	400	15/16	0.14	0.17	24,27,28,28	0
3	PLP	E	400	15/16	0.13	0.17	17,24,25,25	0
2	K	B	401	1/1	0.09	-1.93	26,26,26,26	0
2	K	A	401	1/1	0.09	-2.17	21,21,21,21	0
2	K	D	401	1/1	0.06	-2.29	24,24,24,24	0
2	K	C	401	1/1	0.06	-2.54	29,29,29,29	0
2	K	E	401	1/1	0.09	-2.88	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.