



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:07 AM GMT

PDB ID : 2FLI
Title : The crystal structure of D-ribulose 5-phosphate 3-epimerase from Streptococcus pyogenes complexed with D-xylitol 5-phosphate
Authors : Fedorov, A.A.; Fedorov, E.V.; Akana, J.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2006-01-06
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

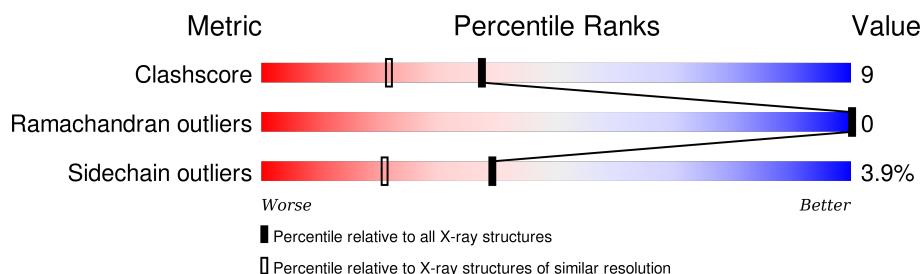
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	220	
1	B	220	
1	C	220	
1	D	220	
1	E	220	
1	F	220	
1	G	220	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	220	<div><div></div><div>78%</div><div>18%</div><div></div><div>• •</div></div>
1	I	220	<div><div></div><div>77%</div><div>19%</div><div></div><div>• •</div></div>
1	J	220	<div><div></div><div>83%</div><div>15%</div><div></div><div>• •</div></div>
1	K	220	<div><div></div><div>77%</div><div>20%</div><div></div><div>• •</div></div>
1	L	220	<div><div></div><div>83%</div><div>15%</div><div></div><div>• •</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20886 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 ribulose-phosphate 3-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1645	1046	276	314	9			
1	B	217	Total	C	N	O	S	0	0	0
			1643	1045	275	314	9			
1	C	219	Total	C	N	O	S	0	0	0
			1659	1054	278	318	9			
1	D	217	Total	C	N	O	S	0	0	0
			1643	1045	275	314	9			
1	E	216	Total	C	N	O	S	0	0	0
			1637	1042	274	312	9			
1	F	216	Total	C	N	O	S	0	0	0
			1637	1042	274	312	9			
1	G	218	Total	C	N	O	S	0	0	0
			1651	1049	277	316	9			
1	H	216	Total	C	N	O	S	0	0	0
			1637	1042	274	312	9			
1	I	217	Total	C	N	O	S	0	0	0
			1645	1046	276	314	9			
1	J	218	Total	C	N	O	S	0	0	0
			1651	1049	277	316	9			
1	K	216	Total	C	N	O	S	0	0	0
			1637	1042	274	312	9			
1	L	218	Total	C	N	O	S	0	0	0
			1653	1051	277	316	9			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

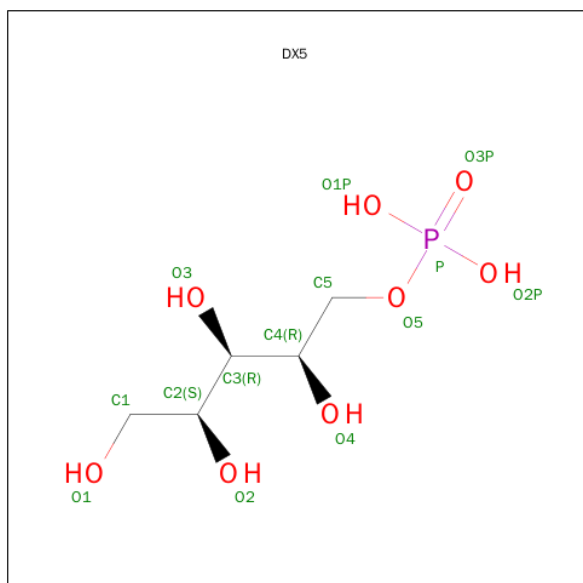
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	J	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	K	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	I	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	L	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is D-XYLITOL-5-PHOSPHATE (three-letter code: DX5) (formula: $C_5H_{13}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			14	5	8	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			14	5	8	1		
3	C	1	Total	C	O	P	0	0
			14	5	8	1		
3	D	1	Total	C	O	P	0	0
			14	5	8	1		
3	E	1	Total	C	O	P	0	0
			14	5	8	1		
3	F	1	Total	C	O	P	0	0
			14	5	8	1		
3	G	1	Total	C	O	P	0	0
			14	5	8	1		
3	H	1	Total	C	O	P	0	0
			14	5	8	1		
3	I	1	Total	C	O	P	0	0
			14	5	8	1		
3	J	1	Total	C	O	P	0	0
			14	5	8	1		
3	K	1	Total	C	O	P	0	0
			14	5	8	1		
3	L	1	Total	C	O	P	0	0
			14	5	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total	O	0	0
			97	97		
4	B	86	Total	O	0	0
			86	86		
4	C	102	Total	O	0	0
			102	102		
4	D	85	Total	O	0	0
			85	85		
4	E	89	Total	O	0	0
			89	89		
4	F	69	Total	O	0	0
			69	69		
4	G	55	Total	O	0	0
			55	55		
4	H	104	Total	O	0	0
			104	104		

Continued on next page...

Continued from previous page...

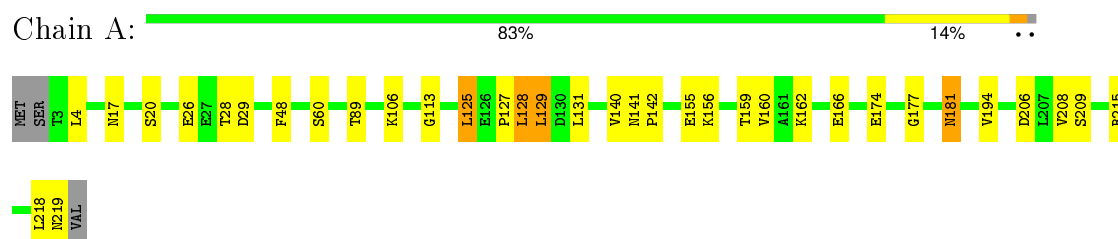
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	53	Total 53	O 53	0	0
4	J	94	Total 94	O 94	0	0
4	K	62	Total 62	O 62	0	0
4	L	72	Total 72	O 72	0	0

3 Residue-property plots

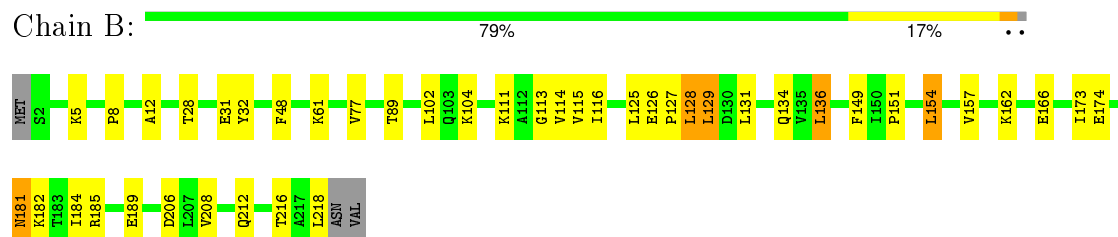
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

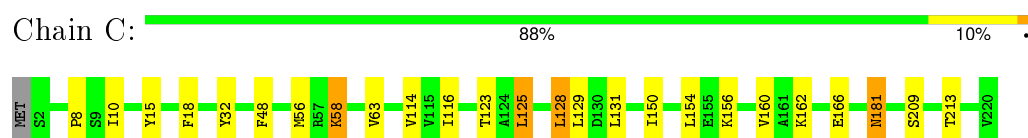
- Molecule 1: ribulose-phosphate 3-epimerase



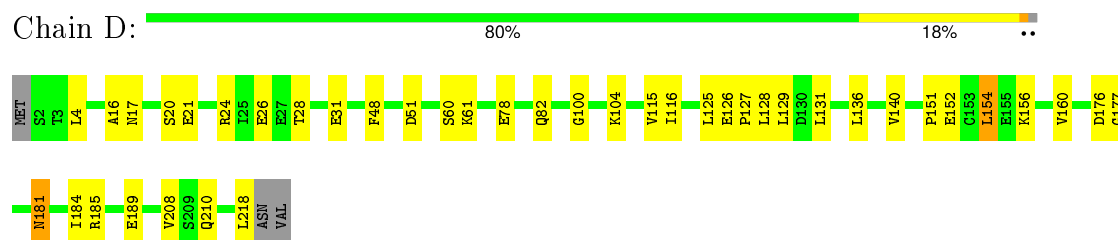
- Molecule 1: ribulose-phosphate 3-epimerase



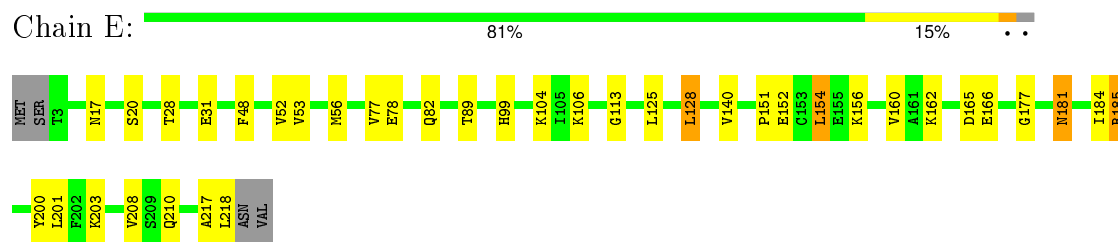
- Molecule 1: ribulose-phosphate 3-epimerase



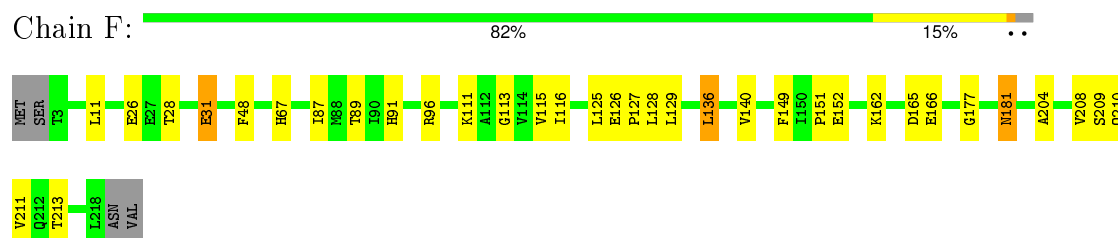
- Molecule 1: ribulose-phosphate 3-epimerase



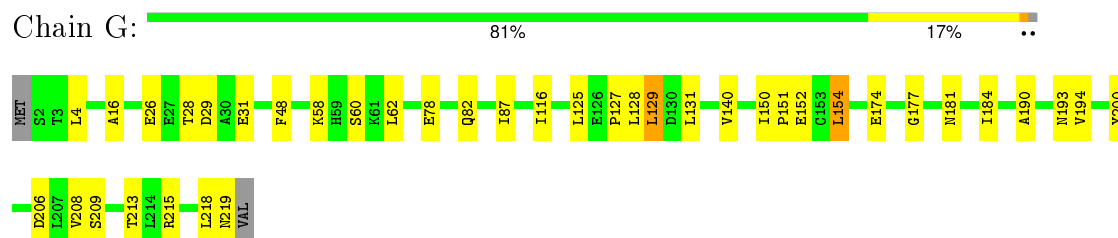
- Molecule 1: ribulose-phosphate 3-epimerase



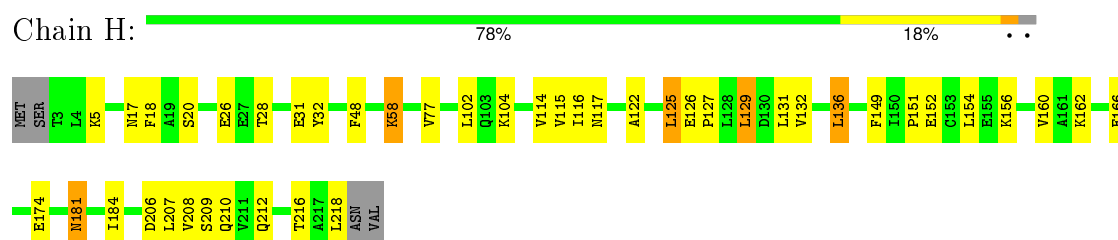
- Molecule 1: ribulose-phosphate 3-epimerase



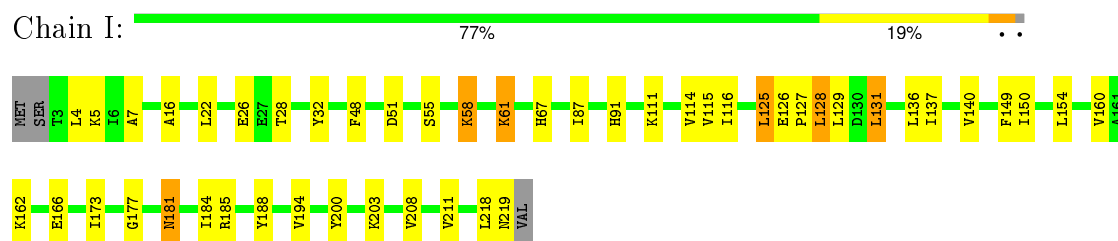
- Molecule 1: ribulose-phosphate 3-epimerase



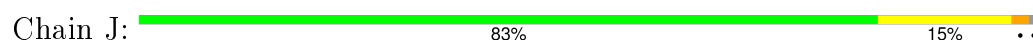
- Molecule 1: ribulose-phosphate 3-epimerase

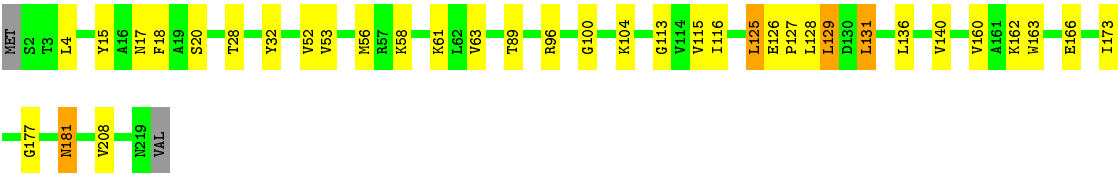


- Molecule 1: ribulose-phosphate 3-epimerase

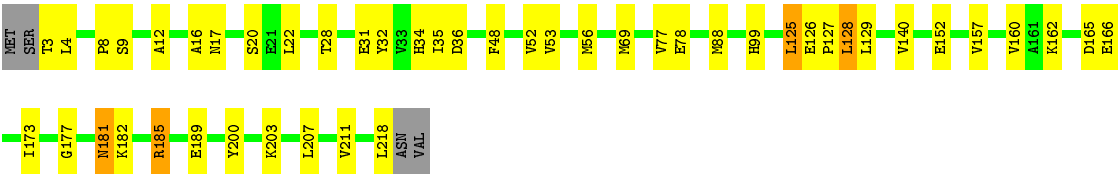


- Molecule 1: ribulose-phosphate 3-epimerase

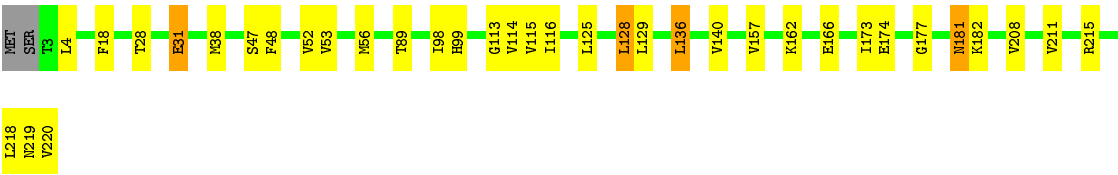
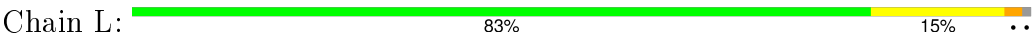




• Molecule 1: ribulose-phosphate 3-epimerase



• Molecule 1: ribulose-phosphate 3-epimerase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.02Å 199.45Å 87.62Å 90.00° 109.76° 90.00°	Depositor
Resolution (Å)	24.99 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (24.99-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20886	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DX5

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	0.32	0/1675	0.60	0/2274
1	B	0.31	0/1673	0.60	0/2271
1	C	0.34	0/1689	0.63	0/2292
1	D	0.33	0/1673	0.59	0/2271
1	E	0.31	0/1667	0.61	0/2263
1	F	0.32	0/1667	0.62	0/2263
1	G	0.31	0/1681	0.58	0/2282
1	H	0.32	0/1667	0.60	0/2263
1	I	0.32	0/1675	0.58	0/2274
1	J	0.33	0/1681	0.61	0/2282
1	K	0.31	0/1667	0.59	0/2263
1	L	0.32	0/1683	0.60	0/2284
All	All	0.32	0/20098	0.60	0/27282

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1645	0	1641	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1643	0	1640	43	0
1	C	1659	0	1655	20	0
1	D	1643	0	1640	34	0
1	E	1637	0	1635	23	0
1	F	1637	0	1635	23	0
1	G	1651	0	1646	33	0
1	H	1637	0	1635	37	0
1	I	1645	0	1641	34	0
1	J	1651	0	1646	29	0
1	K	1637	0	1635	35	0
1	L	1653	0	1650	34	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
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	14	0	11	0	0
3	B	14	0	11	0	0
3	C	14	0	11	0	0
3	D	14	0	11	0	0
3	E	14	0	11	0	0
3	F	14	0	11	0	0
3	G	14	0	11	0	0
3	H	14	0	11	0	0
3	I	14	0	11	0	0
3	J	14	0	11	0	0
3	K	14	0	11	0	0
3	L	14	0	11	0	0
4	A	97	0	0	3	0
4	B	86	0	0	2	0
4	C	102	0	0	0	0
4	D	85	0	0	1	0
4	E	89	0	0	1	0
4	F	69	0	0	0	0
4	G	55	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	104	0	0	4	0
4	I	53	0	0	0	0
4	J	94	0	0	2	0
4	K	62	0	0	3	0
4	L	72	0	0	0	0
All	All	20886	0	19831	370	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 9.

All (370) 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:K:53:VAL:HA	1:K:56:MET:HE2	1.34	1.08
1:L:116:ILE:HD13	1:L:125:LEU:HD21	1.45	0.97
1:F:28:THR:HB	1:F:211:VAL:HG21	1.52	0.92
1:G:116:ILE:HD13	1:G:125:LEU:HD21	1.53	0.90
1:L:28:THR:HB	1:L:211:VAL:HG21	1.53	0.89
1:B:116:ILE:HD13	1:B:125:LEU:HD21	1.59	0.85
1:D:116:ILE:HG21	1:D:125:LEU:HD11	1.63	0.81
1:J:131:LEU:H	1:J:131:LEU:HD23	1.46	0.81
1:A:131:LEU:HD23	1:A:131:LEU:H	1.48	0.79
1:D:131:LEU:H	1:D:131:LEU:HD23	1.49	0.78
1:C:181:ASN:HD22	1:C:181:ASN:H	1.32	0.74
1:H:28:THR:HG22	1:H:208:VAL:HA	1.68	0.74
1:D:116:ILE:HD13	1:D:125:LEU:HD11	1.68	0.74
1:C:181:ASN:HD22	1:C:181:ASN:N	1.86	0.74
1:K:28:THR:HB	1:K:211:VAL:HG21	1.69	0.74
1:J:28:THR:HG22	1:J:208:VAL:HA	1.70	0.73
1:H:58:LYS:H	1:H:58:LYS:HD3	1.51	0.73
1:F:162:LYS:O	1:F:166:GLU:HG3	1.89	0.71
1:F:116:ILE:HD13	1:F:125:LEU:HD21	1.73	0.71
1:L:28:THR:HG22	1:L:208:VAL:HA	1.72	0.71
1:A:174:GLU:HA	1:A:194:VAL:HG13	1.72	0.71
1:L:116:ILE:HD13	1:L:125:LEU:CD2	2.20	0.71
1:I:28:THR:HB	1:I:211:VAL:HG21	1.72	0.70
1:C:128:LEU:O	1:C:131:LEU:HD23	1.92	0.70
1:J:131:LEU:HD23	1:J:131:LEU:N	2.07	0.69
1:C:58:LYS:HD3	1:C:58:LYS:H	1.58	0.69
1:E:156:LYS:O	1:E:160:VAL:HG12	1.93	0.68
1:I:67:HIS:HE2	1:I:91:HIS:HE2	1.39	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:126:GLU:HB3	1:I:127:PRO:HD3	1.73	0.68
1:L:162:LYS:O	1:L:166:GLU:HG3	1.93	0.68
1:A:181:ASN:HD22	1:A:181:ASN:N	1.91	0.68
1:B:77:VAL:HB	1:B:104:LYS:HE3	1.74	0.68
4:D:2019:HOH:O	1:F:96:ARG:HD2	1.93	0.68
1:B:111:LYS:HD3	4:B:2035:HOH:O	1.94	0.67
1:F:28:THR:HG22	1:F:208:VAL:HA	1.76	0.67
1:A:181:ASN:HD22	1:A:181:ASN:H	1.43	0.67
1:G:174:GLU:HA	1:G:194:VAL:HG13	1.76	0.67
1:A:156:LYS:O	1:A:160:VAL:HG12	1.94	0.67
1:B:28:THR:HG22	1:B:208:VAL:HA	1.77	0.66
1:B:102:LEU:HD21	1:B:114:VAL:HG12	1.77	0.66
1:A:206:ASP:OD2	1:A:208:VAL:HG22	1.96	0.65
1:A:174:GLU:CA	1:A:194:VAL:HG13	2.26	0.65
1:B:131:LEU:H	1:B:131:LEU:HD23	1.61	0.65
1:C:114:VAL:HG21	1:C:128:LEU:HD23	1.79	0.64
1:K:181:ASN:N	1:K:181:ASN:HD22	1.94	0.64
1:H:102:LEU:HD11	1:H:114:VAL:CG1	2.27	0.64
1:E:181:ASN:N	1:E:181:ASN:HD22	1.95	0.64
1:G:116:ILE:HD13	1:G:125:LEU:CD2	2.26	0.63
1:E:162:LYS:O	1:E:166:GLU:HG3	1.98	0.63
1:D:156:LYS:O	1:D:160:VAL:HG12	1.98	0.63
1:I:160:VAL:HG13	1:I:173:ILE:HD13	1.79	0.63
1:I:58:LYS:HD3	1:I:58:LYS:H	1.64	0.63
1:H:26:GLU:HG3	4:H:2060:HOH:O	1.98	0.62
1:F:67:HIS:HE2	1:F:91:HIS:HE2	1.47	0.62
1:L:181:ASN:HD22	1:L:182:LYS:H	1.48	0.62
1:F:204:ALA:HB3	1:F:210:GLN:HG3	1.81	0.62
1:A:26:GLU:OE2	1:A:60:SER:HA	2.00	0.62
1:J:53:VAL:HA	1:J:56:MET:HE2	1.82	0.62
1:J:53:VAL:HA	1:J:56:MET:CE	2.30	0.61
1:D:140:VAL:HG22	1:D:177:GLY:HA3	1.82	0.61
1:H:131:LEU:HD12	1:H:132:VAL:HG13	1.83	0.61
1:H:77:VAL:HB	1:H:104:LYS:HE3	1.83	0.61
1:I:149:PHE:CZ	1:I:154:LEU:HD11	2.34	0.61
1:I:26:GLU:OE2	1:I:61:LYS:HD3	2.00	0.61
1:E:28:THR:HG22	1:E:208:VAL:HA	1.82	0.60
1:H:162:LYS:O	1:H:166:GLU:HG3	2.00	0.60
1:L:181:ASN:HD22	1:L:181:ASN:N	1.98	0.60
1:K:160:VAL:HG13	1:K:173:ILE:HD13	1.83	0.60
1:G:29:ASP:CG	1:G:215:ARG:HE	2.05	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:114:VAL:HG21	1:L:128:LEU:HD23	1.83	0.60
1:D:116:ILE:CG2	1:D:125:LEU:HD11	2.29	0.60
1:H:206:ASP:OD2	1:H:208:VAL:HG22	2.02	0.59
1:F:116:ILE:HD13	1:F:125:LEU:CD2	2.32	0.59
1:E:201:LEU:HA	1:E:210:GLN:HG2	1.85	0.59
1:A:128:LEU:HD22	1:A:128:LEU:N	2.17	0.59
1:J:52:VAL:HG12	1:J:56:MET:CE	2.32	0.59
1:D:184:ILE:HG12	1:D:218:LEU:HD21	1.83	0.59
1:L:38:MET:CE	1:L:47:SER:HB3	2.33	0.59
1:K:128:LEU:N	1:K:128:LEU:HD22	2.18	0.59
1:H:181:ASN:N	1:H:181:ASN:HD22	1.98	0.59
1:B:102:LEU:HD11	1:B:114:VAL:HG11	1.85	0.58
1:J:125:LEU:O	1:J:129:LEU:HD13	2.03	0.58
1:L:38:MET:HE2	1:L:47:SER:HB3	1.85	0.58
1:B:181:ASN:N	1:B:181:ASN:HD22	2.00	0.58
1:B:185:ARG:NH1	1:B:189:GLU:HG3	2.19	0.58
1:A:4:LEU:HD23	1:A:218:LEU:HD13	1.85	0.58
1:K:140:VAL:HG22	1:K:177:GLY:HA3	1.86	0.58
1:E:52:VAL:HG12	1:E:56:MET:HE2	1.86	0.58
1:B:116:ILE:HD13	1:B:125:LEU:CD2	2.31	0.58
1:J:4:LEU:N	1:J:4:LEU:HD22	2.18	0.58
1:H:152:GLU:CD	1:H:152:GLU:H	2.07	0.58
1:C:156:LYS:O	1:C:160:VAL:HG12	2.04	0.58
1:A:162:LYS:O	1:A:166:GLU:HG3	2.03	0.58
1:D:116:ILE:HD13	1:D:125:LEU:CD1	2.34	0.57
1:E:53:VAL:HA	1:E:56:MET:CE	2.35	0.57
1:D:181:ASN:H	1:D:181:ASN:HD22	1.53	0.57
1:K:126:GLU:HB3	1:K:127:PRO:HD3	1.85	0.57
1:K:53:VAL:HA	1:K:56:MET:CE	2.23	0.57
1:D:128:LEU:N	1:D:128:LEU:HD22	2.19	0.57
1:B:128:LEU:HD22	1:B:128:LEU:N	2.20	0.57
1:K:3:THR:HB	4:K:2036:HOH:O	2.05	0.57
1:D:181:ASN:N	1:D:181:ASN:HD22	2.02	0.57
1:H:184:ILE:HG12	1:H:218:LEU:HD21	1.86	0.57
1:I:208:VAL:O	1:I:211:VAL:HG22	2.04	0.57
1:A:106:LYS:HD2	1:A:131:LEU:O	2.04	0.56
1:C:162:LYS:O	1:C:166:GLU:HG3	2.05	0.56
1:I:55:SER:HA	1:I:58:LYS:HE2	1.87	0.56
1:G:131:LEU:HD23	1:G:131:LEU:H	1.70	0.56
1:L:53:VAL:HA	1:L:56:MET:HE2	1.86	0.56
1:A:174:GLU:CB	1:A:194:VAL:HG13	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:126:GLU:HB3	1:H:127:PRO:HD3	1.86	0.56
1:G:174:GLU:CA	1:G:194:VAL:HG13	2.35	0.56
1:I:181:ASN:HD22	1:I:181:ASN:N	2.02	0.56
1:I:162:LYS:O	1:I:166:GLU:HG3	2.05	0.56
1:J:162:LYS:O	1:J:166:GLU:HG3	2.06	0.56
1:K:4:LEU:HD13	1:K:218:LEU:HD13	1.88	0.56
1:I:131:LEU:HD23	1:I:131:LEU:H	1.71	0.56
1:E:140:VAL:HG22	1:E:177:GLY:HA3	1.88	0.56
1:A:174:GLU:HG3	1:A:194:VAL:HG22	1.88	0.55
1:G:154:LEU:HG	1:G:190:ALA:HB2	1.88	0.55
1:J:52:VAL:HG12	1:J:56:MET:HE2	1.89	0.55
1:A:28:THR:HG22	1:A:208:VAL:HA	1.87	0.55
1:B:162:LYS:O	1:B:166:GLU:HG3	2.06	0.55
1:E:200:TYR:O	1:E:203:LYS:HG2	2.05	0.55
1:L:136:LEU:HG	1:L:174:GLU:OE1	2.06	0.55
1:H:136:LEU:HG	1:H:174:GLU:OE1	2.06	0.55
1:G:184:ILE:HG12	1:G:218:LEU:HD21	1.88	0.55
1:J:140:VAL:HG22	1:J:177:GLY:HA3	1.88	0.55
1:B:136:LEU:HG	1:B:174:GLU:OE1	2.06	0.55
1:H:114:VAL:HG13	1:H:132:VAL:HG11	1.88	0.55
1:J:181:ASN:N	1:J:181:ASN:HD22	2.03	0.55
1:G:58:LYS:HG2	4:G:2037:HOH:O	2.06	0.54
1:D:125:LEU:N	1:D:125:LEU:HD12	2.23	0.54
1:D:78:GLU:O	1:D:82:GLN:HG3	2.07	0.54
1:D:116:ILE:HG21	1:D:125:LEU:CD1	2.37	0.54
1:H:58:LYS:HE3	4:K:2010:HOH:O	2.06	0.54
1:E:128:LEU:N	1:E:128:LEU:HD22	2.22	0.54
1:K:52:VAL:O	1:K:56:MET:HG3	2.08	0.54
1:A:131:LEU:HD23	1:A:131:LEU:N	2.21	0.54
1:B:102:LEU:HD21	1:B:114:VAL:CG1	2.37	0.54
1:B:61:LYS:NZ	1:B:61:LYS:HB2	2.23	0.54
1:L:208:VAL:O	1:L:211:VAL:HG22	2.07	0.54
1:B:102:LEU:HD11	1:B:114:VAL:CG1	2.38	0.54
1:A:26:GLU:HG3	4:A:2024:HOH:O	2.07	0.54
1:L:181:ASN:HD22	1:L:182:LYS:N	2.06	0.54
1:D:185:ARG:NH1	1:D:218:LEU:O	2.40	0.54
1:I:116:ILE:HG23	1:I:125:LEU:HD11	1.90	0.53
1:L:215:ARG:HA	1:L:218:LEU:HD12	1.90	0.53
1:F:152:GLU:H	1:F:152:GLU:CD	2.11	0.53
1:F:208:VAL:O	1:F:211:VAL:HG22	2.08	0.53
1:B:206:ASP:OD2	1:B:208:VAL:HG22	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:GLU:OE1	1:G:31:GLU:N	2.40	0.53
1:F:11:LEU:O	1:F:11:LEU:HD13	2.08	0.53
1:I:114:VAL:HG21	1:I:128:LEU:HD23	1.90	0.53
1:G:127:PRO:HG2	1:G:128:LEU:HD22	1.89	0.53
1:L:125:LEU:O	1:L:129:LEU:HD13	2.08	0.53
1:F:87:ILE:HG12	1:F:111:LYS:HB2	1.91	0.53
1:B:126:GLU:HB3	1:B:127:PRO:HD3	1.90	0.53
1:J:126:GLU:HG3	1:J:163:TRP:CH2	2.43	0.53
1:J:160:VAL:HG13	1:J:173:ILE:HD13	1.90	0.53
1:A:128:LEU:O	1:A:131:LEU:HD23	2.08	0.52
1:K:157:VAL:O	1:K:160:VAL:HG12	2.09	0.52
1:H:208:VAL:HG23	1:H:209:SER:N	2.23	0.52
1:E:53:VAL:HA	1:E:56:MET:HE2	1.90	0.52
1:D:131:LEU:N	1:D:131:LEU:HD23	2.21	0.52
1:H:58:LYS:H	1:H:58:LYS:CD	2.22	0.52
1:D:115:VAL:HB	1:D:136:LEU:HB3	1.92	0.52
1:L:52:VAL:HG12	1:L:56:MET:CE	2.40	0.51
1:A:127:PRO:HG2	1:A:128:LEU:HD22	1.92	0.51
1:F:129:LEU:H	1:F:129:LEU:HD22	1.76	0.51
1:J:115:VAL:HG23	1:J:136:LEU:O	2.10	0.51
1:L:31:GLU:N	1:L:31:GLU:OE1	2.43	0.51
1:A:4:LEU:HD12	1:A:4:LEU:N	2.27	0.50
1:D:152:GLU:CD	1:D:152:GLU:H	2.15	0.50
1:H:102:LEU:HD11	1:H:114:VAL:HG12	1.92	0.50
1:J:58:LYS:HE2	4:J:2013:HOH:O	2.10	0.50
1:G:151:PRO:HG2	1:G:152:GLU:OE2	2.11	0.50
1:I:58:LYS:N	1:I:58:LYS:HD3	2.27	0.50
1:E:52:VAL:HG12	1:E:56:MET:CE	2.42	0.50
1:G:131:LEU:HD23	1:G:131:LEU:N	2.27	0.50
1:G:26:GLU:OE2	1:G:60:SER:HA	2.11	0.50
4:H:2019:HOH:O	1:J:96:ARG:HD2	2.12	0.50
1:E:184:ILE:HG12	1:E:218:LEU:HD21	1.93	0.50
1:G:16:ALA:HA	1:L:18:PHE:HB2	1.92	0.50
1:J:100:GLY:O	1:J:104:LYS:HG3	2.12	0.50
1:A:159:THR:HG21	4:A:2022:HOH:O	2.12	0.50
1:G:128:LEU:O	1:G:131:LEU:HD23	2.12	0.49
1:J:32:TYR:CD1	1:J:63:VAL:HB	2.47	0.49
1:B:12:ALA:HB2	4:B:2024:HOH:O	2.13	0.49
1:I:184:ILE:HG12	1:I:218:LEU:HD21	1.94	0.49
1:L:4:LEU:HD13	1:L:218:LEU:HD13	1.94	0.49
1:B:89:THR:HA	1:B:113:GLY:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:181:ASN:ND2	1:L:182:LYS:N	2.61	0.49
1:I:22:LEU:O	1:I:26:GLU:HG3	2.13	0.49
1:I:131:LEU:HD23	1:I:131:LEU:N	2.27	0.49
1:H:125:LEU:O	1:H:129:LEU:HD13	2.12	0.49
1:J:128:LEU:N	1:J:128:LEU:HD22	2.28	0.49
1:L:140:VAL:HG22	1:L:177:GLY:HA3	1.94	0.49
1:K:77:VAL:HG22	1:K:88:MET:CE	2.43	0.49
1:D:4:LEU:N	1:D:4:LEU:HD22	2.28	0.49
1:J:127:PRO:HG2	1:J:128:LEU:HD22	1.95	0.48
1:L:125:LEU:N	1:L:125:LEU:HD22	2.29	0.48
1:I:185:ARG:NH1	1:I:218:LEU:O	2.45	0.48
1:B:157:VAL:HG13	1:B:173:ILE:HG21	1.96	0.48
1:B:77:VAL:HG11	1:B:104:LYS:HG2	1.95	0.48
1:D:28:THR:HG22	1:D:208:VAL:HA	1.94	0.48
1:D:125:LEU:N	1:D:125:LEU:CD1	2.76	0.48
1:K:77:VAL:HG22	1:K:88:MET:HE2	1.95	0.48
1:C:10:ILE:HG12	1:C:56:MET:HE3	1.94	0.48
1:A:140:VAL:HG22	1:A:177:GLY:HA3	1.96	0.48
1:A:29:ASP:CG	1:A:215:ARG:HE	2.17	0.48
1:I:140:VAL:HG22	1:I:177:GLY:HA3	1.96	0.48
1:B:185:ARG:NH1	1:B:189:GLU:CG	2.76	0.48
1:H:102:LEU:HD11	1:H:114:VAL:HG11	1.96	0.48
1:C:209:SER:O	1:C:213:THR:HG23	2.14	0.48
1:G:152:GLU:CD	1:G:152:GLU:H	2.17	0.48
1:D:210:GLN:OE1	1:D:210:GLN:HA	2.14	0.48
1:A:17:ASN:HB3	1:A:20:SER:OG	2.13	0.48
1:I:149:PHE:HZ	1:I:154:LEU:HD11	1.78	0.47
1:K:22:LEU:HD11	1:K:56:MET:HB3	1.96	0.47
1:H:102:LEU:HD21	1:H:114:VAL:HG12	1.96	0.47
1:G:206:ASP:OD2	1:G:208:VAL:HG22	2.15	0.47
1:A:89:THR:HA	1:A:113:GLY:O	2.14	0.47
1:K:35:ILE:HD13	1:K:56:MET:HE3	1.96	0.47
1:K:152:GLU:CD	1:K:152:GLU:H	2.18	0.47
1:H:156:LYS:O	1:H:160:VAL:HG12	2.14	0.47
1:K:17:ASN:HB3	1:K:20:SER:OG	2.14	0.47
1:A:208:VAL:HG23	1:A:209:SER:N	2.30	0.47
1:E:181:ASN:N	1:E:181:ASN:ND2	2.62	0.47
1:C:32:TYR:CD1	1:C:63:VAL:HB	2.50	0.47
1:G:209:SER:O	1:G:213:THR:HG23	2.15	0.47
1:E:106:LYS:NZ	4:E:2048:HOH:O	2.47	0.47
1:I:51:ASP:HB3	1:J:15:TYR:HE2	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLY:O	1:D:104:LYS:HG3	2.14	0.47
1:F:126:GLU:HB3	1:F:127:PRO:HD3	1.96	0.47
1:G:125:LEU:O	1:G:129:LEU:HD13	2.15	0.46
1:L:181:ASN:ND2	1:L:181:ASN:N	2.63	0.46
1:K:200:TYR:O	1:K:203:LYS:HG2	2.14	0.46
1:B:128:LEU:HA	1:B:131:LEU:HD21	1.97	0.46
1:F:209:SER:O	1:F:213:THR:HG23	2.16	0.46
1:A:125:LEU:O	1:A:129:LEU:HD13	2.14	0.46
1:B:125:LEU:O	1:B:129:LEU:HD13	2.16	0.46
1:F:125:LEU:O	1:F:129:LEU:HD22	2.15	0.46
1:F:31:GLU:OE1	1:F:31:GLU:N	2.46	0.46
1:K:185:ARG:HD2	1:K:189:GLU:OE2	2.16	0.46
1:K:181:ASN:HD22	1:K:182:LYS:H	1.64	0.46
1:C:18:PHE:HB2	1:D:16:ALA:HA	1.97	0.46
1:J:17:ASN:HB3	1:J:20:SER:OG	2.15	0.46
1:L:115:VAL:HB	1:L:136:LEU:HB3	1.98	0.46
1:L:52:VAL:HG12	1:L:56:MET:HE1	1.98	0.46
1:J:116:ILE:HG23	1:J:125:LEU:HD11	1.98	0.46
1:H:122:ALA:O	1:H:125:LEU:HB2	2.16	0.46
1:E:89:THR:HA	1:E:113:GLY:O	2.15	0.46
1:F:89:THR:HA	1:F:113:GLY:O	2.15	0.46
1:B:184:ILE:HG12	1:B:218:LEU:HD21	1.97	0.46
1:L:181:ASN:ND2	1:L:182:LYS:H	2.13	0.46
1:F:149:PHE:O	1:F:151:PRO:HD3	2.16	0.46
1:I:5:LYS:HE3	1:I:194:VAL:HG22	1.97	0.46
1:I:154:LEU:HD12	1:I:154:LEU:N	2.31	0.45
1:L:53:VAL:HA	1:L:56:MET:CE	2.47	0.45
1:D:17:ASN:HB3	1:D:20:SER:OG	2.15	0.45
1:I:16:ALA:HA	1:J:18:PHE:HB2	1.99	0.45
1:B:128:LEU:O	1:B:131:LEU:HD23	2.16	0.45
1:D:26:GLU:OE1	1:D:60:SER:HA	2.17	0.45
1:B:5:LYS:HD3	1:B:31:GLU:HG3	1.97	0.45
1:H:212:GLN:O	1:H:216:THR:HG23	2.16	0.45
1:G:154:LEU:HG	1:G:190:ALA:CB	2.46	0.45
1:K:12:ALA:HB2	4:K:2052:HOH:O	2.16	0.45
1:C:116:ILE:HD13	1:C:125:LEU:HD22	1.98	0.45
1:G:174:GLU:CB	1:G:194:VAL:HG13	2.47	0.45
1:F:181:ASN:HD22	1:F:181:ASN:H	1.64	0.45
1:E:78:GLU:O	1:E:82:GLN:HG3	2.17	0.45
1:H:5:LYS:HD3	1:H:32:TYR:CE1	2.51	0.45
1:H:28:THR:HG22	1:H:208:VAL:CA	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:208:VAL:HG21	4:H:2073:HOH:O	2.16	0.45
1:A:181:ASN:ND2	1:A:181:ASN:N	2.62	0.45
1:B:131:LEU:HD23	1:B:131:LEU:N	2.30	0.45
1:B:185:ARG:HH12	1:B:189:GLU:CG	2.30	0.45
1:H:149:PHE:O	1:H:151:PRO:HD3	2.16	0.45
1:I:28:THR:HG22	1:I:208:VAL:HA	1.98	0.45
1:C:10:ILE:HG12	1:C:56:MET:CE	2.47	0.45
1:L:181:ASN:ND2	1:L:182:LYS:HG3	2.31	0.44
1:A:4:LEU:N	1:A:4:LEU:CD1	2.80	0.44
1:G:31:GLU:HA	1:G:62:LEU:HD22	2.00	0.44
1:I:150:ILE:HD13	1:K:99:HIS:CE1	2.53	0.44
1:F:115:VAL:HB	1:F:136:LEU:HB3	1.98	0.44
1:K:181:ASN:ND2	1:K:181:ASN:N	2.62	0.44
1:J:52:VAL:HG12	1:J:56:MET:HE1	1.99	0.44
1:L:218:LEU:C	1:L:220:VAL:H	2.20	0.44
1:C:58:LYS:H	1:C:58:LYS:CD	2.28	0.44
1:A:159:THR:HG23	4:A:2056:HOH:O	2.17	0.44
1:B:149:PHE:O	1:B:151:PRO:HD3	2.18	0.44
1:C:128:LEU:HA	1:C:131:LEU:CD2	2.47	0.44
1:E:151:PRO:HG2	1:E:152:GLU:OE2	2.17	0.44
1:K:207:LEU:O	1:K:211:VAL:HG13	2.18	0.44
1:H:17:ASN:HB3	1:H:20:SER:OG	2.17	0.44
1:H:117:ASN:HB3	4:H:2000:HOH:O	2.18	0.44
1:G:208:VAL:HG23	1:G:209:SER:N	2.33	0.44
1:B:125:LEU:N	1:B:125:LEU:HD22	2.33	0.43
1:K:162:LYS:O	1:K:166:GLU:HG3	2.18	0.43
1:D:128:LEU:O	1:D:131:LEU:HD23	2.18	0.43
1:B:181:ASN:N	1:B:181:ASN:ND2	2.66	0.43
1:G:28:THR:HG22	1:G:208:VAL:HA	2.00	0.43
1:B:116:ILE:HG21	1:B:125:LEU:HD21	2.00	0.43
1:A:155:GLU:O	1:A:159:THR:HG23	2.19	0.43
1:K:8:PRO:HD2	1:K:32:TYR:O	2.17	0.43
1:G:116:ILE:HG21	1:G:125:LEU:HD21	2.00	0.43
1:G:78:GLU:HG2	1:G:82:GLN:HE21	1.83	0.43
1:I:136:LEU:HD12	1:I:137:ILE:N	2.34	0.43
1:B:181:ASN:HD21	1:B:182:LYS:NZ	2.17	0.43
1:I:4:LEU:HD21	1:I:188:TYR:CE1	2.53	0.43
1:B:212:GLN:O	1:B:216:THR:HG23	2.19	0.43
1:L:116:ILE:CD1	1:L:125:LEU:HD21	2.32	0.43
1:H:152:GLU:CD	1:H:152:GLU:N	2.72	0.43
1:D:136:LEU:HD11	1:D:176:ASP:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:LEU:HA	1:E:154:LEU:HD12	1.85	0.43
1:L:98:ILE:HG23	1:L:99:HIS:N	2.34	0.43
1:H:102:LEU:CD1	1:H:114:VAL:CG1	2.95	0.42
1:H:162:LYS:HE2	1:H:166:GLU:OE2	2.18	0.42
1:F:126:GLU:HB3	1:F:127:PRO:CD	2.49	0.42
1:C:15:TYR:HE2	1:D:51:ASP:HB3	1.84	0.42
1:K:157:VAL:O	1:K:160:VAL:CG1	2.67	0.42
1:K:36:ASP:HB3	1:K:69:MET:CE	2.50	0.42
1:I:7:ALA:HB2	1:I:32:TYR:HB2	2.00	0.42
1:G:140:VAL:HG22	1:G:177:GLY:HA3	2.00	0.42
1:I:200:TYR:HA	1:I:203:LYS:HE3	2.00	0.42
1:B:113:GLY:HA2	1:B:134:GLN:O	2.19	0.42
1:J:89:THR:HA	1:J:113:GLY:O	2.20	0.42
1:K:181:ASN:ND2	1:K:182:LYS:N	2.68	0.42
1:G:87:ILE:HG22	4:G:2009:HOH:O	2.17	0.42
1:E:17:ASN:HB3	1:E:20:SER:OG	2.19	0.42
1:J:131:LEU:CD2	1:J:131:LEU:N	2.77	0.42
1:C:131:LEU:HD23	1:C:131:LEU:H	1.85	0.42
1:E:185:ARG:HG2	1:E:217:ALA:O	2.20	0.42
1:F:140:VAL:HG22	1:F:177:GLY:HA3	2.01	0.42
1:I:115:VAL:HB	1:I:136:LEU:HB3	2.02	0.42
1:H:181:ASN:N	1:H:181:ASN:ND2	2.67	0.42
1:H:116:ILE:HD13	1:H:125:LEU:HD22	2.01	0.42
1:G:4:LEU:HA	1:G:193:ASN:O	2.20	0.41
1:L:89:THR:HA	1:L:113:GLY:O	2.20	0.41
1:H:18:PHE:HB2	1:K:16:ALA:HA	2.02	0.41
1:B:181:ASN:HD22	1:B:182:LYS:N	2.19	0.41
1:C:8:PRO:HD2	1:C:32:TYR:O	2.19	0.41
1:D:185:ARG:NH2	1:D:189:GLU:OE2	2.53	0.41
1:B:151:PRO:O	1:B:154:LEU:HB2	2.20	0.41
1:E:77:VAL:HG21	1:E:104:LYS:HD3	2.02	0.41
1:I:87:ILE:HG12	1:I:111:LYS:HB2	2.01	0.41
1:K:9:SER:HA	1:K:34:HIS:HB3	2.02	0.41
1:A:174:GLU:HB2	1:A:194:VAL:CG1	2.51	0.41
1:J:58:LYS:HB3	4:J:2013:HOH:O	2.21	0.41
1:B:8:PRO:HD2	1:B:32:TYR:O	2.21	0.41
1:L:157:VAL:HG13	1:L:173:ILE:HG21	2.03	0.41
1:A:141:ASN:HA	1:A:142:PRO:HD3	1.93	0.41
1:B:181:ASN:HD22	1:B:182:LYS:H	1.68	0.41
1:G:150:ILE:HA	1:G:151:PRO:HD2	1.92	0.41
1:D:151:PRO:O	1:D:154:LEU:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ILE:HD13	1:E:99:HIS:CE1	2.56	0.41
1:D:126:GLU:HB2	1:D:127:PRO:HD3	2.03	0.40
1:G:181:ASN:HB3	1:G:200:TYR:OH	2.20	0.40
1:K:35:ILE:HD13	1:K:56:MET:CE	2.50	0.40
1:B:28:THR:HG22	1:B:208:VAL:CA	2.50	0.40
1:B:115:VAL:HB	1:B:136:LEU:HB3	2.03	0.40
1:D:20:SER:O	1:D:24:ARG:HG3	2.22	0.40
1:K:125:LEU:O	1:K:129:LEU:HD13	2.21	0.40
1:C:181:ASN:H	1:C:181:ASN:ND2	2.07	0.40
1:H:115:VAL:HB	1:H:136:LEU:HB3	2.03	0.40
1:K:31:GLU:N	1:K:31:GLU:OE1	2.53	0.40
1:I:55:SER:O	1:I:58:LYS:HE3	2.22	0.40
1:G:29:ASP:OD1	1:G:215:ARG:NE	2.54	0.40
1:D:21:GLU:OE2	1:D:24:ARG:HD3	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	215/220 (98%)	208 (97%)	7 (3%)	0	100	100
1	B	215/220 (98%)	208 (97%)	7 (3%)	0	100	100
1	C	217/220 (99%)	210 (97%)	7 (3%)	0	100	100
1	D	215/220 (98%)	208 (97%)	7 (3%)	0	100	100
1	E	214/220 (97%)	208 (97%)	6 (3%)	0	100	100
1	F	214/220 (97%)	207 (97%)	7 (3%)	0	100	100
1	G	216/220 (98%)	209 (97%)	7 (3%)	0	100	100
1	H	214/220 (97%)	209 (98%)	5 (2%)	0	100	100
1	I	215/220 (98%)	208 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	216/220 (98%)	210 (97%)	6 (3%)	0	100	100
1	K	214/220 (97%)	206 (96%)	8 (4%)	0	100	100
1	L	216/220 (98%)	208 (96%)	8 (4%)	0	100	100
All	All	2581/2640 (98%)	2499 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	174/177 (98%)	168 (97%)	6 (3%)	44	26
1	B	174/177 (98%)	168 (97%)	6 (3%)	44	26
1	C	176/177 (99%)	168 (96%)	8 (4%)	34	16
1	D	174/177 (98%)	168 (97%)	6 (3%)	44	26
1	E	173/177 (98%)	165 (95%)	8 (5%)	33	15
1	F	173/177 (98%)	166 (96%)	7 (4%)	38	20
1	G	175/177 (99%)	171 (98%)	4 (2%)	58	42
1	H	173/177 (98%)	163 (94%)	10 (6%)	25	9
1	I	174/177 (98%)	165 (95%)	9 (5%)	29	12
1	J	175/177 (99%)	170 (97%)	5 (3%)	50	34
1	K	173/177 (98%)	166 (96%)	7 (4%)	38	20
1	L	175/177 (99%)	169 (97%)	6 (3%)	44	26
All	All	2089/2124 (98%)	2007 (96%)	82 (4%)	39	21

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	125	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	128	LEU
1	A	129	LEU
1	A	181	ASN
1	A	219	ASN
1	B	48	PHE
1	B	128	LEU
1	B	129	LEU
1	B	136	LEU
1	B	154	LEU
1	B	181	ASN
1	C	48	PHE
1	C	58	LYS
1	C	123	THR
1	C	125	LEU
1	C	128	LEU
1	C	129	LEU
1	C	154	LEU
1	C	181	ASN
1	D	31	GLU
1	D	48	PHE
1	D	61	LYS
1	D	129	LEU
1	D	154	LEU
1	D	181	ASN
1	E	31	GLU
1	E	48	PHE
1	E	125	LEU
1	E	128	LEU
1	E	154	LEU
1	E	165	ASP
1	E	181	ASN
1	E	185	ARG
1	F	26	GLU
1	F	31	GLU
1	F	48	PHE
1	F	128	LEU
1	F	136	LEU
1	F	165	ASP
1	F	181	ASN
1	G	48	PHE
1	G	129	LEU
1	G	154	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	219	ASN
1	H	31	GLU
1	H	48	PHE
1	H	58	LYS
1	H	125	LEU
1	H	129	LEU
1	H	136	LEU
1	H	154	LEU
1	H	181	ASN
1	H	207	LEU
1	H	210	GLN
1	I	48	PHE
1	I	58	LYS
1	I	61	LYS
1	I	125	LEU
1	I	128	LEU
1	I	129	LEU
1	I	131	LEU
1	I	181	ASN
1	I	219	ASN
1	J	61	LYS
1	J	125	LEU
1	J	129	LEU
1	J	131	LEU
1	J	181	ASN
1	K	48	PHE
1	K	78	GLU
1	K	125	LEU
1	K	128	LEU
1	K	165	ASP
1	K	181	ASN
1	K	185	ARG
1	L	31	GLU
1	L	48	PHE
1	L	128	LEU
1	L	136	LEU
1	L	181	ASN
1	L	219	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	147	GLN
1	A	181	ASN
1	A	219	ASN
1	B	134	GLN
1	B	147	GLN
1	B	181	ASN
1	B	210	GLN
1	C	134	GLN
1	C	147	GLN
1	C	181	ASN
1	C	212	GLN
1	C	219	ASN
1	D	134	GLN
1	D	147	GLN
1	D	181	ASN
1	E	82	GLN
1	E	134	GLN
1	E	147	GLN
1	E	181	ASN
1	E	212	GLN
1	F	134	GLN
1	F	147	GLN
1	F	181	ASN
1	G	82	GLN
1	G	134	GLN
1	G	147	GLN
1	G	219	ASN
1	H	134	GLN
1	H	147	GLN
1	H	181	ASN
1	H	210	GLN
1	I	45	ASN
1	I	147	GLN
1	I	181	ASN
1	I	219	ASN
1	J	134	GLN
1	J	147	GLN
1	J	181	ASN
1	K	103	GLN
1	K	147	GLN
1	K	181	ASN
1	K	210	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	134	GLN
1	L	147	GLN
1	L	181	ASN
1	L	219	ASN

5.3.3 RNA [i](#)

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 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	DX5	A	1901	2	13,13,13	1.56	2 (15%)	14,18,18	1.19	0
3	DX5	B	1902	2	13,13,13	1.50	2 (15%)	14,18,18	1.16	0
3	DX5	C	1903	2	13,13,13	1.51	2 (15%)	14,18,18	1.12	0
3	DX5	D	1904	2	13,13,13	1.46	2 (15%)	14,18,18	1.19	2 (14%)
3	DX5	E	1905	2	13,13,13	1.45	2 (15%)	14,18,18	1.21	0
3	DX5	F	1906	-	13,13,13	1.47	2 (15%)	14,18,18	1.13	1 (7%)
3	DX5	G	1911	2	13,13,13	1.57	2 (15%)	14,18,18	1.14	0
3	DX5	H	1912	2	13,13,13	1.53	2 (15%)	14,18,18	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DX5	I	1913	2	13,13,13	1.48	2 (15%)	14,18,18	1.16	1 (7%)
3	DX5	J	1914	2	13,13,13	1.50	2 (15%)	14,18,18	1.17	0
3	DX5	K	1915	2	13,13,13	1.45	2 (15%)	14,18,18	1.13	1 (7%)
3	DX5	L	1916	2	13,13,13	1.56	2 (15%)	14,18,18	1.19	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	DX5	A	1901	2	-	0/16/16/16	0/0/0/0
3	DX5	B	1902	2	-	0/16/16/16	0/0/0/0
3	DX5	C	1903	2	-	0/16/16/16	0/0/0/0
3	DX5	D	1904	2	-	0/16/16/16	0/0/0/0
3	DX5	E	1905	2	-	0/16/16/16	0/0/0/0
3	DX5	F	1906	-	-	0/16/16/16	0/0/0/0
3	DX5	G	1911	2	-	0/16/16/16	0/0/0/0
3	DX5	H	1912	2	-	0/16/16/16	0/0/0/0
3	DX5	I	1913	2	-	0/16/16/16	0/0/0/0
3	DX5	J	1914	2	-	0/16/16/16	0/0/0/0
3	DX5	K	1915	2	-	0/16/16/16	0/0/0/0
3	DX5	L	1916	2	-	0/16/16/16	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1903	DX5	P-O5	-3.69	1.47	1.60
3	H	1912	DX5	P-O5	-3.61	1.48	1.60
3	E	1905	DX5	P-O5	-3.44	1.48	1.60
3	L	1916	DX5	P-O5	-3.42	1.48	1.60
3	A	1901	DX5	P-O5	-3.38	1.48	1.60
3	D	1904	DX5	P-O5	-3.38	1.48	1.60
3	J	1914	DX5	P-O5	-3.35	1.49	1.60
3	B	1902	DX5	P-O5	-3.32	1.49	1.60
3	F	1906	DX5	P-O5	-3.32	1.49	1.60
3	I	1913	DX5	P-O5	-3.23	1.49	1.60
3	G	1911	DX5	P-O5	-3.23	1.49	1.60
3	K	1915	DX5	P-O5	-3.22	1.49	1.60
3	E	1905	DX5	P-O3P	2.84	1.60	1.51
3	C	1903	DX5	P-O3P	2.89	1.60	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1914	DX5	P-O3P	2.95	1.60	1.51
3	H	1912	DX5	P-O3P	2.97	1.61	1.51
3	K	1915	DX5	P-O3P	3.22	1.61	1.51
3	F	1906	DX5	P-O3P	3.24	1.61	1.51
3	B	1902	DX5	P-O3P	3.25	1.61	1.51
3	D	1904	DX5	P-O3P	3.30	1.62	1.51
3	A	1901	DX5	P-O3P	3.34	1.62	1.51
3	I	1913	DX5	P-O3P	3.63	1.63	1.51
3	L	1916	DX5	P-O3P	3.64	1.63	1.51
3	G	1911	DX5	P-O3P	3.66	1.63	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1904	DX5	O4-C4-C5	-2.07	105.69	110.19
3	F	1906	DX5	O4-C4-C5	-2.06	105.71	110.19
3	I	1913	DX5	O2P-P-O1P	2.01	115.02	107.38
3	K	1915	DX5	O2P-P-O1P	2.02	115.06	107.38
3	D	1904	DX5	O2P-P-O1P	2.05	115.20	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.