



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:09 PM UTC

PDB ID : 2NX3 / pdb_00002nx3
Title : Structural and mechanistic changes along an engineered path from metallo to non-metallo KDO8P synthase
Authors : Kona, F.; Xu, X.; Martin, P.; Kuzmic, P.; Gatti, D.L.
Deposited on : 2006-11-16
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

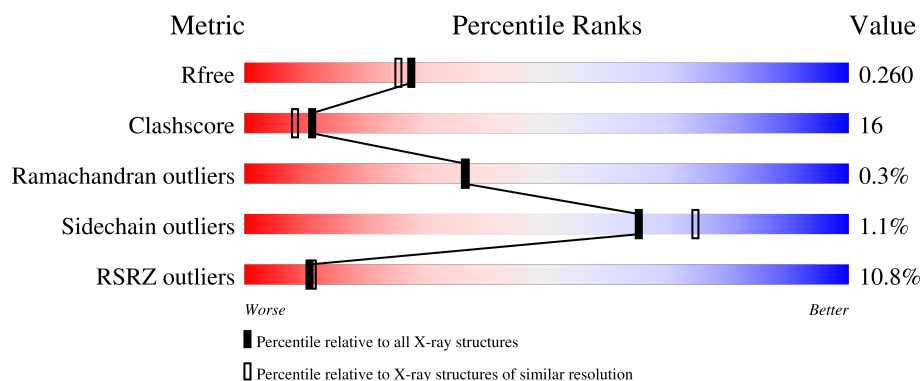
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	267	2% 82% 16% .
1	B	267	4% 75% 22% ..
1	C	267	9% 70% 27% ..
1	D	267	17% 64% 33% ..
1	E	267	21% 63% 34% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	267	
1	G	267	
1	H	267	
1	I	267	
1	J	267	
1	K	267	
1	L	267	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEP	B	268	-	-	X	-
2	PEP	H	268	-	-	X	-
2	PEP	I	268	-	-	X	-
3	A5P	B	269	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26573 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 2-dehydro-3-deoxyphosphooctonate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	B	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	C	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	D	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	E	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	F	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	G	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	H	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	I	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	J	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	K	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	L	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			

There are 36 discrepancies between the modelled and reference sequences:

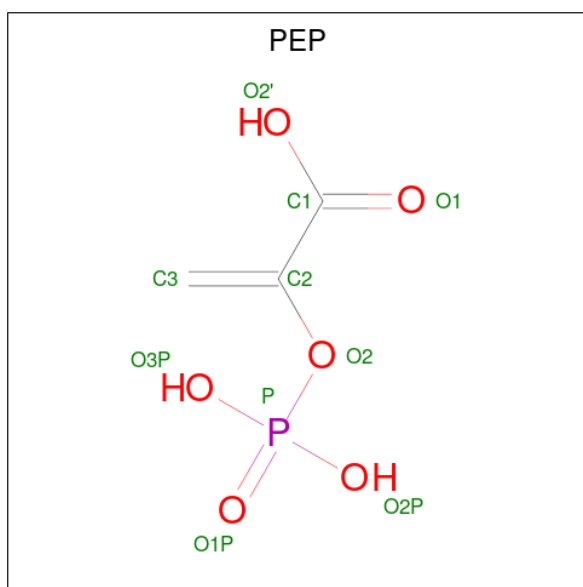
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ASN	CYS	engineered mutation	UNP O66496
A	235	PRO	SER	engineered mutation	UNP O66496
A	237	ALA	GLN	engineered mutation	UNP O66496
B	11	ASN	CYS	engineered mutation	UNP O66496
B	235	PRO	SER	engineered mutation	UNP O66496

Continued on next page...

Continued from previous page...

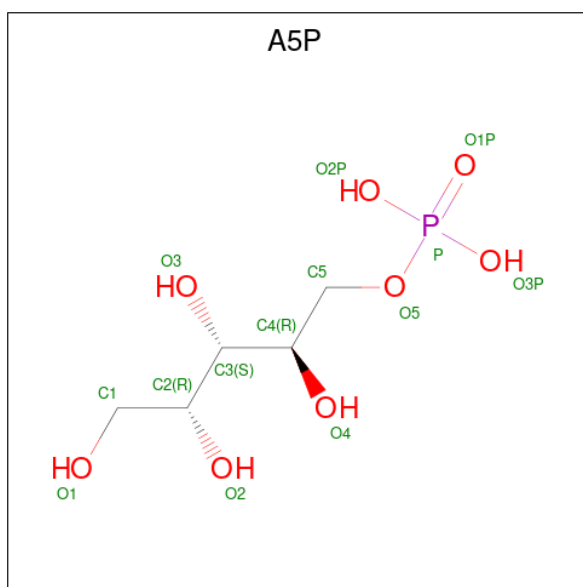
Chain	Residue	Modelled	Actual	Comment	Reference
B	237	ALA	GLN	engineered mutation	UNP O66496
C	11	ASN	CYS	engineered mutation	UNP O66496
C	235	PRO	SER	engineered mutation	UNP O66496
C	237	ALA	GLN	engineered mutation	UNP O66496
D	11	ASN	CYS	engineered mutation	UNP O66496
D	235	PRO	SER	engineered mutation	UNP O66496
D	237	ALA	GLN	engineered mutation	UNP O66496
E	11	ASN	CYS	engineered mutation	UNP O66496
E	235	PRO	SER	engineered mutation	UNP O66496
E	237	ALA	GLN	engineered mutation	UNP O66496
F	11	ASN	CYS	engineered mutation	UNP O66496
F	235	PRO	SER	engineered mutation	UNP O66496
F	237	ALA	GLN	engineered mutation	UNP O66496
G	11	ASN	CYS	engineered mutation	UNP O66496
G	235	PRO	SER	engineered mutation	UNP O66496
G	237	ALA	GLN	engineered mutation	UNP O66496
H	11	ASN	CYS	engineered mutation	UNP O66496
H	235	PRO	SER	engineered mutation	UNP O66496
H	237	ALA	GLN	engineered mutation	UNP O66496
I	11	ASN	CYS	engineered mutation	UNP O66496
I	235	PRO	SER	engineered mutation	UNP O66496
I	237	ALA	GLN	engineered mutation	UNP O66496
J	11	ASN	CYS	engineered mutation	UNP O66496
J	235	PRO	SER	engineered mutation	UNP O66496
J	237	ALA	GLN	engineered mutation	UNP O66496
K	11	ASN	CYS	engineered mutation	UNP O66496
K	235	PRO	SER	engineered mutation	UNP O66496
K	237	ALA	GLN	engineered mutation	UNP O66496
L	11	ASN	CYS	engineered mutation	UNP O66496
L	235	PRO	SER	engineered mutation	UNP O66496
L	237	ALA	GLN	engineered mutation	UNP O66496

- Molecule 2 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: $C_3H_5O_6P$).



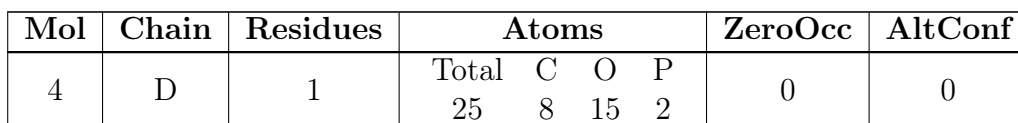
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		
2	B	1	Total	C	O	P	0	0
			10	3	6	1		
2	C	1	Total	C	O	P	0	0
			10	3	6	1		
2	E	1	Total	C	O	P	0	0
			10	3	6	1		
2	F	1	Total	C	O	P	0	0
			10	3	6	1		
2	G	1	Total	C	O	P	0	0
			10	3	6	1		
2	H	1	Total	C	O	P	0	0
			10	3	6	1		
2	I	1	Total	C	O	P	0	0
			10	3	6	1		
2	J	1	Total	C	O	P	0	0
			10	3	6	1		
2	K	1	Total	C	O	P	0	0
			10	3	6	1		
2	L	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 3 is ARABINOSE-5-PHOSPHATE (CCD ID: A5P) (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		
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	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 (2R,4R,5R,6R,7R)-2,4,5,6,7-PENTAHYDROXY-2,8-BIS(PHOSPHONOOXY)OCTANOIC ACID (CCD ID: 1NT) (formula: C₈H₁₈O₁₅P₂).



- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5 | A | 194 | Total O
194 194 | 0 | 0 |
| 5 | B | 197 | Total O
197 197 | 0 | 0 |
| 5 | C | 108 | Total O
108 108 | 0 | 0 |
| 5 | D | 88 | Total O
88 88 | 0 | 0 |
| 5 | E | 71 | Total O
71 71 | 0 | 0 |
| 5 | F | 55 | Total O
55 55 | 0 | 0 |
| 5 | G | 177 | Total O
177 177 | 0 | 0 |
| 5 | H | 191 | Total O
191 191 | 0 | 0 |
| 5 | I | 191 | Total O
191 191 | 0 | 0 |
| 5 | J | 184 | Total O
184 184 | 0 | 0 |
| 5 | K | 56 | Total O
56 56 | 0 | 0 |

Continued on next page...

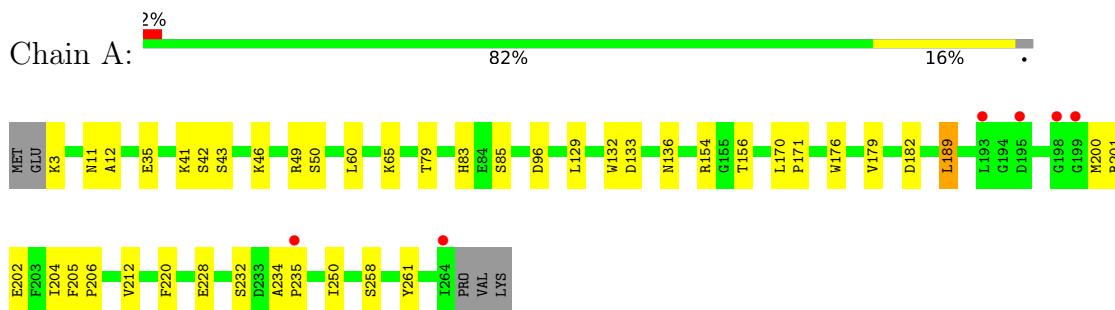
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	112	Total 112	O 112	0	0

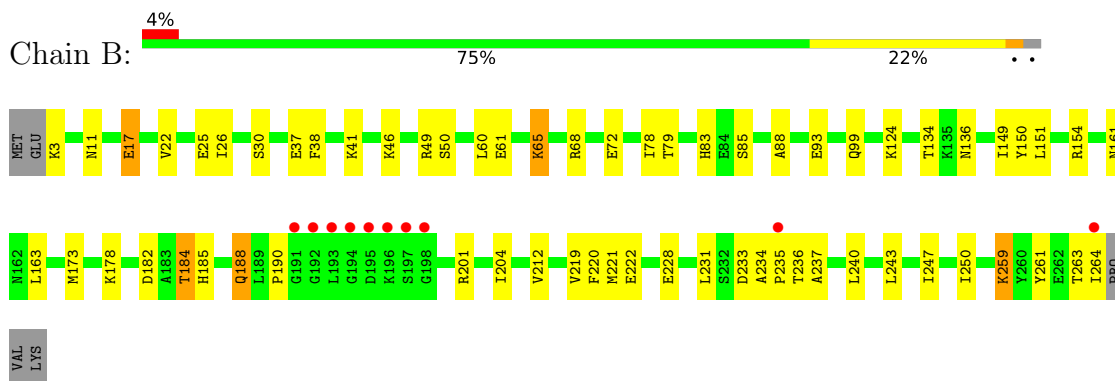
3 Residue-property plots

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

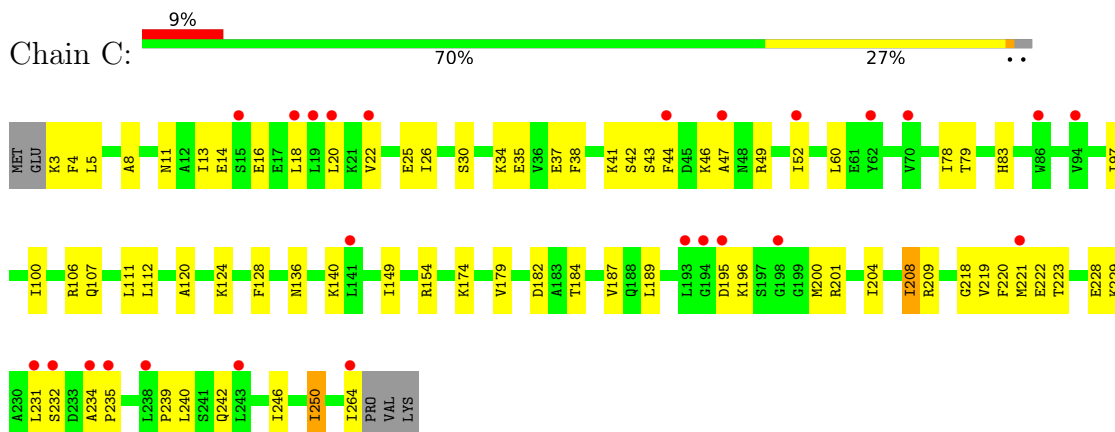
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



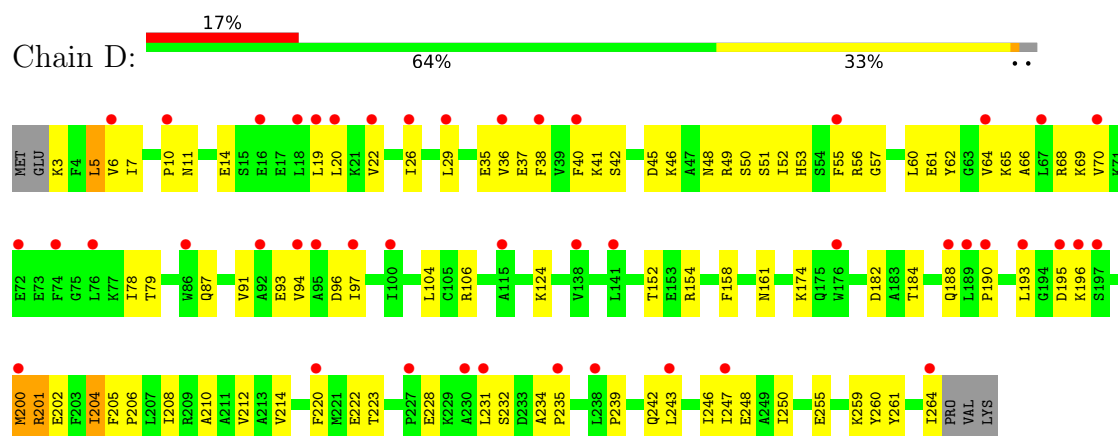
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



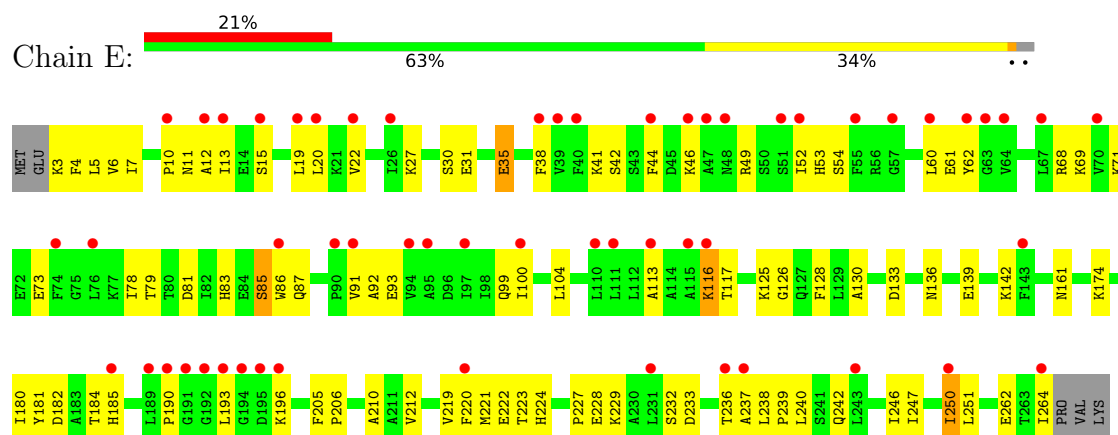
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



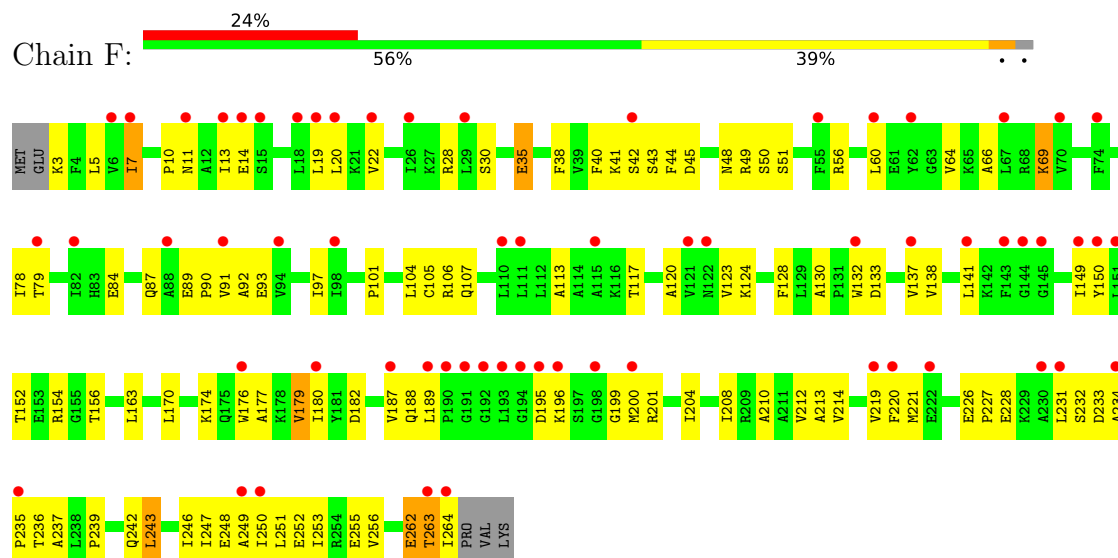
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



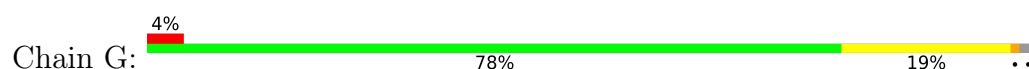
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

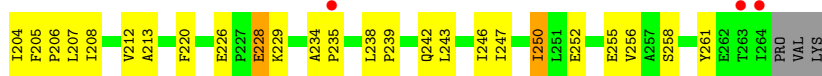


• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

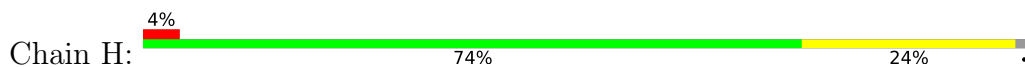


• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

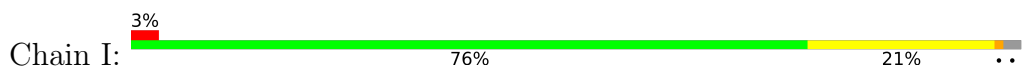




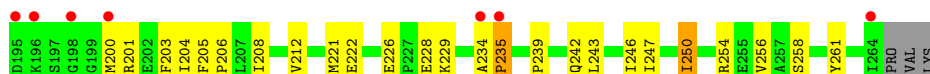
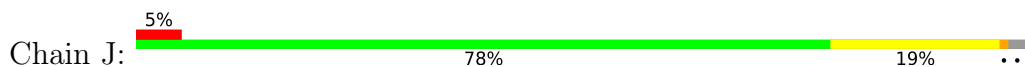
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



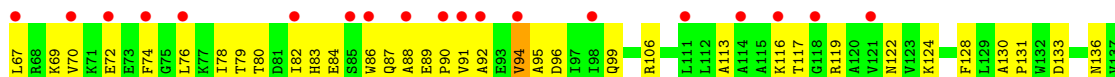
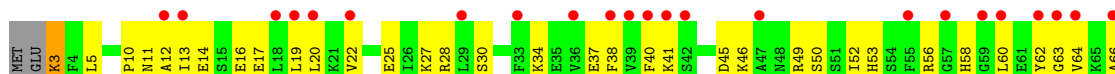
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

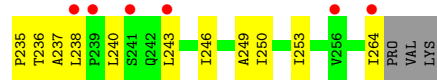
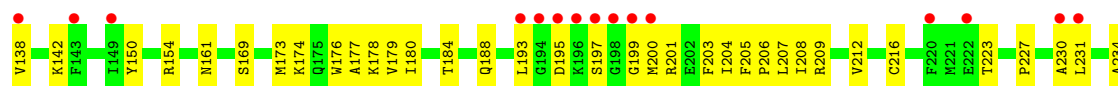


• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

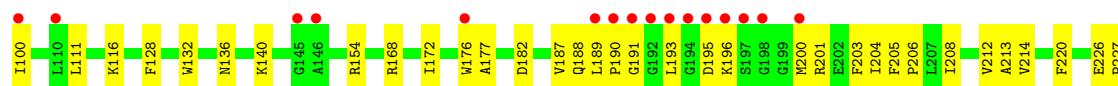
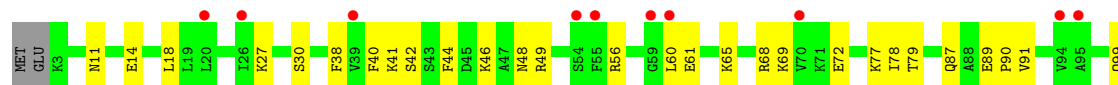


• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase





● Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.38Å 198.53Å 125.83Å 90.00° 94.19° 90.00°	Depositor
Resolution (Å)	29.79 – 2.10 29.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.9 (29.79-2.10) 95.0 (29.79-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.261 0.214 , 0.260	Depositor DCC
R_{free} test set	20582 reflections (9.53%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26573	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6054e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEP, 1NT, A5P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/2097	0.90	5/2830 (0.2%)
1	B	0.46	0/2097	0.91	4/2830 (0.1%)
1	C	0.38	0/2097	0.84	4/2830 (0.1%)
1	D	0.35	0/2097	0.84	1/2830 (0.0%)
1	E	0.36	0/2097	0.81	0/2830
1	F	0.33	0/2097	0.82	5/2830 (0.2%)
1	G	0.43	0/2097	0.88	4/2830 (0.1%)
1	H	0.44	0/2097	0.89	1/2830 (0.0%)
1	I	0.45	0/2097	0.88	4/2830 (0.1%)
1	J	0.42	0/2097	0.89	3/2830 (0.1%)
1	K	0.34	0/2097	0.83	1/2830 (0.0%)
1	L	0.36	0/2097	0.84	2/2830 (0.1%)
All	All	0.40	0/25164	0.86	34/33960 (0.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	85	SER	N-CA-C	6.84	119.61	111.33
1	J	226	GLU	CA-C-N	6.68	126.18	119.24
1	J	226	GLU	C-N-CA	6.68	126.18	119.24
1	B	85	SER	N-CA-C	6.32	118.97	111.33
1	A	189	LEU	CA-C-N	5.95	126.30	119.93
1	A	189	LEU	C-N-CA	5.95	126.30	119.93
1	F	179	VAL	N-CA-C	5.84	116.29	108.11
1	F	48	ASN	N-CA-C	5.81	117.87	110.61
1	B	236	THR	N-CA-C	5.76	121.74	114.31
1	I	78	ILE	N-CA-C	5.73	116.73	108.48
1	C	208	ILE	N-CA-C	-5.62	105.05	110.72
1	A	179	VAL	N-CA-C	5.60	115.94	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ASP	N-CA-C	-5.52	105.66	112.90
1	F	263	THR	CB-CA-C	-5.51	109.14	117.07
1	L	226	GLU	CA-C-N	5.44	125.52	119.32
1	L	226	GLU	C-N-CA	5.44	125.52	119.32
1	J	179	VAL	N-CA-C	5.38	115.70	108.17
1	G	78	ILE	N-CA-C	5.38	116.22	108.48
1	K	34	LYS	N-CA-C	5.35	117.86	111.71
1	H	243	LEU	N-CA-C	5.33	116.78	111.07
1	C	25	GLU	N-CA-C	-5.29	105.59	111.36
1	B	17	GLU	N-CA-C	-5.29	105.60	111.36
1	I	51	SER	N-CA-C	5.25	118.03	109.59
1	A	85	SER	N-CA-C	5.22	117.65	111.33
1	D	204	ILE	N-CA-C	5.14	115.36	110.53
1	I	226	GLU	CA-C-N	5.10	126.22	119.84
1	I	226	GLU	C-N-CA	5.10	126.22	119.84
1	B	149	ILE	N-CA-C	5.09	115.24	108.11
1	C	179	VAL	N-CA-C	5.09	115.30	108.17
1	C	149	ILE	N-CA-C	5.08	115.28	108.17
1	G	226	GLU	CA-C-N	5.02	126.11	119.84
1	G	226	GLU	C-N-CA	5.02	126.11	119.84
1	F	226	GLU	CA-C-N	5.01	124.61	119.05
1	F	226	GLU	C-N-CA	5.01	124.61	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2055	0	2095	34	0
1	B	2055	0	2095	63	0
1	C	2055	0	2095	64	0
1	D	2055	0	2095	78	0
1	E	2055	0	2095	81	0
1	F	2055	0	2095	104	0
1	G	2055	0	2095	46	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2055	0	2095	68	0
1	I	2055	0	2095	54	0
1	J	2055	0	2095	58	0
1	K	2055	0	2095	111	0
1	L	2055	0	2095	71	0
2	A	10	0	2	2	0
2	B	10	0	2	4	0
2	C	10	0	2	2	0
2	E	10	0	2	1	0
2	F	10	0	2	2	0
2	G	10	0	2	1	0
2	H	10	0	2	5	0
2	I	10	0	2	5	0
2	J	10	0	2	3	0
2	K	10	0	2	2	0
2	L	10	0	2	2	0
3	A	14	0	10	2	0
3	B	14	0	10	6	0
3	C	14	0	10	3	0
3	E	14	0	10	0	0
3	F	14	0	10	4	0
3	G	14	0	10	3	0
3	H	14	0	10	3	0
3	I	14	0	10	3	0
3	J	14	0	10	2	0
3	K	14	0	10	1	0
3	L	14	0	10	1	0
4	D	25	0	13	3	0
5	A	194	0	0	4	0
5	B	197	0	0	10	0
5	C	108	0	0	7	0
5	D	88	0	0	10	0
5	E	71	0	0	6	0
5	F	55	0	0	5	0
5	G	177	0	0	8	0
5	H	191	0	0	12	0
5	I	191	0	0	12	0
5	J	184	0	0	10	0
5	K	56	0	0	12	0
5	L	112	0	0	9	0
All	All	26573	0	25285	819	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 16.

All (819) 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:H:184:THR:HG21	1:H:222:GLU:H	1.15	1.12
1:B:134:THR:HG21	1:B:173:MET:HE3	1.30	1.11
1:B:184:THR:HG21	1:B:222:GLU:H	1.17	1.06
1:I:189:LEU:HD21	1:I:200:MET:HE3	1.38	1.01
1:I:154:ARG:HH22	1:I:188:GLN:NE2	1.62	0.98
1:D:212:VAL:HG11	1:D:250:ILE:HG23	1.47	0.96
1:C:11:ASN:HD21	1:C:46:LYS:HE2	1.31	0.94
1:I:154:ARG:NH2	1:I:188:GLN:HE21	1.64	0.94
1:J:189:LEU:HD21	1:J:200:MET:HE2	1.54	0.90
1:I:174:LYS:HG3	1:I:264:ILE:HG12	1.53	0.90
1:H:184:THR:HG22	5:H:402:HOH:O	1.71	0.89
1:E:184:THR:HG21	1:E:222:GLU:H	1.37	0.88
1:J:184:THR:HG21	1:J:222:GLU:H	1.36	0.88
1:I:154:ARG:HH22	1:I:188:GLN:HE21	0.88	0.87
1:H:189:LEU:HD11	1:H:200:MET:HE2	1.55	0.86
1:K:161:ASN:HD21	1:L:132:TRP:HE1	1.19	0.85
1:F:188:GLN:HA	1:F:199:GLY:HA2	1.60	0.84
1:C:174:LYS:HG3	1:C:264:ILE:HD13	1.57	0.84
1:C:49:ARG:HA	3:C:269:A5P:H51	1.58	0.83
1:B:154:ARG:HH22	1:B:188:GLN:NE2	1.77	0.83
2:J:268:PEP:C3	3:J:269:A5P:H12	2.09	0.82
1:E:161:ASN:HD21	1:F:132:TRP:HE1	1.23	0.82
1:D:174:LYS:HG2	1:D:264:ILE:HD13	1.62	0.81
1:K:227:PRO:HB3	1:K:237:ALA:HB3	1.59	0.81
1:C:189:LEU:HD21	1:C:200:MET:HE2	1.62	0.81
3:G:269:A5P:H52	1:H:106:ARG:NH2	1.95	0.81
1:L:154:ARG:HH22	1:L:188:GLN:NE2	1.77	0.81
1:K:212:VAL:HG11	1:K:250:ILE:HG23	1.62	0.80
1:B:37:GLU:HG3	5:B:463:HOH:O	1.80	0.80
1:B:151:LEU:HD13	1:B:173:MET:HE2	1.63	0.79
1:E:49:ARG:HE	1:E:54:SER:HB3	1.47	0.79
1:F:10:PRO:HD3	1:F:22:VAL:HG11	1.65	0.79
1:E:35:GLU:H	1:E:35:GLU:CD	1.91	0.79
1:H:154:ARG:HH22	1:H:188:GLN:HE21	1.30	0.79
1:G:154:ARG:HH22	1:G:188:GLN:NE2	1.82	0.78
1:K:64:VAL:HG13	1:K:94:VAL:HG11	1.65	0.78
1:D:40:PHE:HB3	1:D:78:ILE:HD13	1.63	0.78
1:J:68:ARG:O	1:J:72:GLU:HG3	1.84	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:LYS:HE2	5:G:442:HOH:O	1.84	0.77
1:C:43:SER:HB2	1:C:46:LYS:HZ2	1.49	0.77
1:E:227:PRO:HB3	1:E:237:ALA:HB3	1.66	0.77
1:G:189:LEU:HD11	1:G:200:MET:HE2	1.66	0.77
1:F:189:LEU:HD11	1:F:200:MET:HE2	1.66	0.76
1:D:223:THR:HG21	1:D:243:LEU:HD11	1.67	0.76
2:I:268:PEP:C2	3:I:269:A5P:H12	2.15	0.76
3:G:269:A5P:H52	1:H:106:ARG:HH22	1.49	0.76
2:I:268:PEP:C3	3:I:269:A5P:H12	2.16	0.76
2:J:268:PEP:C2	3:J:269:A5P:H12	2.16	0.75
1:B:184:THR:CG2	1:B:222:GLU:H	1.98	0.75
1:E:11:ASN:HD21	1:E:46:LYS:HE3	1.51	0.75
1:F:256:VAL:HG21	1:G:256:VAL:HG11	1.68	0.75
1:A:65:LYS:HE3	5:G:441:HOH:O	1.84	0.75
1:I:69:LYS:HE3	1:I:73:GLU:OE1	1.87	0.75
1:D:154:ARG:HH22	1:D:188:GLN:HE21	1.35	0.74
1:A:228:GLU:CD	1:A:228:GLU:H	1.95	0.74
1:B:151:LEU:HB3	1:B:173:MET:HE2	1.68	0.74
1:E:68:ARG:HB2	1:E:68:ARG:NH1	2.02	0.73
1:G:238:LEU:HD21	1:G:246:ILE:HD12	1.70	0.73
1:H:184:THR:CG2	1:H:222:GLU:H	1.98	0.73
1:K:136:ASN:HD21	1:L:195:ASP:HA	1.52	0.73
1:K:138:VAL:O	1:K:142:LYS:HG2	1.88	0.73
1:J:154:ARG:HD2	2:J:268:PEP:O3P	1.89	0.73
1:H:184:THR:HG21	1:H:222:GLU:N	1.99	0.73
1:L:189:LEU:HD11	1:L:200:MET:HE2	1.70	0.73
1:C:11:ASN:ND2	1:C:46:LYS:HE2	2.02	0.72
1:H:235:PRO:HA	5:H:450:HOH:O	1.89	0.72
1:K:205:PHE:HB3	1:K:206:PRO:HD3	1.70	0.72
2:B:268:PEP:C3	3:B:269:A5P:H12	2.19	0.72
1:E:11:ASN:ND2	1:E:46:LYS:HE3	2.04	0.72
2:B:268:PEP:C2	3:B:269:A5P:H12	2.19	0.72
1:A:182:ASP:HA	1:A:220:PHE:HB3	1.70	0.71
1:F:66:ALA:HA	5:F:323:HOH:O	1.90	0.71
1:G:154:ARG:HD2	2:G:268:PEP:O3P	1.91	0.71
1:J:41:LYS:HZ3	1:J:222:GLU:HG2	1.56	0.71
1:F:7:ILE:HD12	1:F:7:ILE:H	1.56	0.70
1:G:139:GLU:HG3	5:G:403:HOH:O	1.90	0.70
1:F:7:ILE:HD12	1:F:7:ILE:N	2.05	0.70
1:J:246:ILE:O	1:J:250:ILE:HG23	1.92	0.70
1:K:246:ILE:O	1:K:250:ILE:HG13	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD21	1:A:200:MET:HE2	1.74	0.70
1:G:154:ARG:HH22	1:G:188:GLN:HE21	1.37	0.70
1:D:205:PHE:HB3	1:D:206:PRO:HD3	1.73	0.70
1:K:113:ALA:HA	1:K:116:LYS:HD2	1.74	0.70
1:B:65:LYS:HE3	1:B:65:LYS:HA	1.73	0.69
1:C:200:MET:HE3	5:C:347:HOH:O	1.92	0.69
1:C:189:LEU:HD21	1:C:200:MET:CE	2.23	0.69
1:F:212:VAL:HG23	1:F:253:ILE:HG21	1.73	0.69
1:J:174:LYS:HB2	5:J:403:HOH:O	1.91	0.69
1:B:134:THR:CG2	1:B:173:MET:HE3	2.17	0.68
1:F:69:LYS:HA	1:F:69:LYS:HE3	1.76	0.68
1:F:234:ALA:HB3	1:F:235:PRO:HD3	1.76	0.68
1:G:182:ASP:HA	1:G:220:PHE:HB3	1.75	0.67
1:H:154:ARG:HD2	2:H:268:PEP:O3P	1.94	0.67
1:K:10:PRO:HD3	1:K:22:VAL:HG11	1.77	0.67
1:L:204:ILE:O	1:L:208:ILE:HG13	1.94	0.67
1:A:41:LYS:HD2	1:A:42:SER:N	2.10	0.67
1:L:248:GLU:O	1:L:252:GLU:HG3	1.94	0.67
1:H:184:THR:HG23	1:H:221:MET:HA	1.75	0.67
1:L:190:PRO:HG3	5:L:292:HOH:O	1.94	0.67
1:E:3:LYS:HG3	1:E:35:GLU:O	1.95	0.67
1:I:184:THR:HG21	1:I:222:GLU:H	1.59	0.67
1:J:201:ARG:HB2	1:J:201:ARG:NH1	2.09	0.67
1:G:246:ILE:O	1:G:250:ILE:HG23	1.94	0.66
1:F:246:ILE:O	1:F:250:ILE:HG13	1.95	0.66
1:D:234:ALA:HB3	1:D:235:PRO:HD3	1.77	0.66
1:C:22:VAL:O	1:C:26:ILE:HG12	1.96	0.66
5:I:416:HOH:O	1:J:53:HIS:HD2	1.77	0.66
1:K:223:THR:HG21	1:K:243:LEU:HD22	1.77	0.66
1:C:154:ARG:HD2	2:C:268:PEP:O3P	1.94	0.65
1:K:52:ILE:HB	1:L:140:LYS:HG2	1.77	0.65
1:D:210:ALA:O	1:D:214:VAL:HG23	1.96	0.65
1:F:123:VAL:HG11	1:F:137:VAL:HG11	1.78	0.65
1:I:235:PRO:HA	5:I:335:HOH:O	1.97	0.65
1:H:22:VAL:O	1:H:26:ILE:HG12	1.97	0.65
1:I:40:PHE:HB3	1:I:78:ILE:HD13	1.79	0.65
1:K:150:TYR:CD1	1:K:178:LYS:HB2	2.32	0.65
1:D:14:GLU:HG2	1:D:231:LEU:HD12	1.78	0.64
1:A:189:LEU:HD21	1:A:200:MET:CE	2.27	0.64
1:E:61:GLU:HG2	1:E:62:TYR:H	1.60	0.64
1:E:41:LYS:HD3	1:E:41:LYS:C	2.23	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:ARG:HB2	1:E:68:ARG:HH11	1.63	0.64
1:K:19:LEU:HD22	1:K:66:ALA:HB1	1.78	0.64
1:B:184:THR:HG21	1:B:222:GLU:N	2.03	0.63
1:D:45:ASP:HA	1:D:56:ARG:O	1.98	0.63
1:A:200:MET:HG2	5:A:443:HOH:O	1.98	0.63
1:D:19:LEU:HD12	1:D:66:ALA:HB1	1.80	0.63
1:E:5:LEU:HD23	1:E:6:VAL:N	2.14	0.63
1:A:205:PHE:HB3	1:A:206:PRO:HD3	1.81	0.63
1:B:228:GLU:H	1:B:228:GLU:CD	2.07	0.63
1:L:40:PHE:HB3	1:L:78:ILE:HD13	1.81	0.63
1:C:182:ASP:HA	1:C:220:PHE:HB3	1.80	0.62
1:E:212:VAL:HG11	1:E:250:ILE:HB	1.79	0.62
1:B:154:ARG:HD2	2:B:268:PEP:O3P	1.98	0.62
1:G:228:GLU:H	1:G:228:GLU:CD	2.05	0.62
1:H:16:GLU:HG3	1:H:17:GLU:N	2.15	0.62
1:G:154:ARG:NH2	1:G:188:GLN:HE21	1.97	0.62
1:K:84:GLU:HG3	5:K:310:HOH:O	1.98	0.62
1:L:263:THR:HG22	1:L:264:ILE:HG13	1.80	0.62
1:F:14:GLU:HG2	1:F:231:LEU:HD12	1.81	0.62
1:F:97:ILE:HG12	1:F:120:ALA:HB3	1.82	0.62
1:I:264:ILE:HD13	5:I:441:HOH:O	1.98	0.62
1:B:154:ARG:HH22	1:B:188:GLN:HE21	1.45	0.62
2:H:268:PEP:C2	3:H:269:A5P:H12	2.30	0.62
1:D:154:ARG:HH22	1:D:188:GLN:NE2	1.98	0.62
1:K:88:ALA:HB3	5:K:309:HOH:O	2.00	0.62
1:A:201:ARG:HG3	1:A:204:ILE:HD12	1.81	0.61
1:K:174:LYS:HE2	5:K:325:HOH:O	2.01	0.61
1:H:234:ALA:HA	5:H:274:HOH:O	2.00	0.61
4:D:268:1NT:O2P	4:D:268:1NT:HI31	1.98	0.61
1:E:237:ALA:HB2	5:E:334:HOH:O	2.00	0.61
1:D:243:LEU:O	1:D:247:ILE:HG13	2.01	0.61
1:E:250:ILE:C	1:E:250:ILE:HD12	2.26	0.61
1:G:189:LEU:HD21	1:G:200:MET:CE	2.31	0.61
1:B:201:ARG:HG3	1:B:204:ILE:HD12	1.83	0.61
1:F:101:PRO:HG2	1:F:104:LEU:HD12	1.82	0.61
1:F:200:MET:HE3	5:F:288:HOH:O	2.00	0.61
1:L:77:LYS:HG3	5:L:310:HOH:O	2.00	0.61
1:D:97:ILE:HD12	1:D:97:ILE:N	2.16	0.60
1:I:83:HIS:HD2	5:J:289:HOH:O	1.82	0.60
1:F:49:ARG:HA	3:F:269:A5P:H51	1.81	0.60
1:C:83:HIS:HD2	5:D:293:HOH:O	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:VAL:HG21	1:C:204:ILE:HG12	1.83	0.60
1:A:3:LYS:HD2	1:A:35:GLU:O	2.02	0.60
1:F:212:VAL:HG23	1:F:253:ILE:CG2	2.31	0.60
1:F:180:ILE:N	1:F:180:ILE:HD12	2.17	0.60
1:F:212:VAL:HG11	1:F:250:ILE:HG23	1.83	0.60
1:H:228:GLU:HG3	1:H:229:LYS:HG3	1.82	0.60
1:J:234:ALA:N	1:J:235:PRO:HD2	2.16	0.60
1:J:28:ARG:HD3	5:J:448:HOH:O	2.00	0.60
1:E:246:ILE:O	1:E:250:ILE:HG23	2.02	0.60
1:F:124:LYS:HD3	1:F:152:THR:HB	1.84	0.59
1:L:11:ASN:HD22	1:L:232:SER:HB3	1.66	0.59
1:H:201:ARG:HG3	1:H:204:ILE:HD12	1.84	0.59
1:B:151:LEU:HB3	1:B:173:MET:CE	2.32	0.59
1:D:61:GLU:HB3	5:D:310:HOH:O	2.02	0.59
1:E:15:SER:O	1:E:19:LEU:HD13	2.02	0.59
1:E:174:LYS:HG3	1:E:264:ILE:HG21	1.84	0.59
1:K:200:MET:HE2	1:K:203:PHE:HE2	1.67	0.59
1:F:247:ILE:O	1:F:251:LEU:HG	2.02	0.59
1:K:150:TYR:HD1	1:K:178:LYS:HB2	1.68	0.59
1:F:91:VAL:C	1:F:93:GLU:H	2.11	0.59
1:K:17:GLU:HG3	5:K:319:HOH:O	2.02	0.59
1:K:60:LEU:C	1:K:60:LEU:HD23	2.27	0.59
1:I:4:PHE:CZ	1:I:219:VAL:HG23	2.38	0.59
1:I:184:THR:HB	5:I:412:HOH:O	2.03	0.59
1:J:46:LYS:HE2	1:J:46:LYS:HA	1.84	0.59
1:K:195:ASP:HA	1:L:136:ASN:HD21	1.66	0.59
1:A:11:ASN:HD21	1:A:46:LYS:HE2	1.68	0.59
1:I:106:ARG:HA	5:I:306:HOH:O	2.03	0.58
1:K:3:LYS:N	1:K:3:LYS:HE3	2.17	0.58
1:L:11:ASN:HD21	1:L:46:LYS:HE3	1.67	0.58
1:A:11:ASN:HD21	1:A:46:LYS:CE	2.16	0.58
1:E:184:THR:HG21	1:E:222:GLU:N	2.13	0.58
1:I:182:ASP:HA	1:I:220:PHE:HB3	1.85	0.58
1:I:189:LEU:CD2	1:I:200:MET:HE3	2.26	0.58
1:E:69:LYS:NZ	1:E:73:GLU:HB2	2.18	0.58
1:H:154:ARG:HH22	1:H:188:GLN:NE2	2.01	0.58
1:I:209:ARG:HH12	1:L:214:VAL:HA	1.68	0.58
1:K:27:LYS:HA	1:K:76:LEU:HD21	1.85	0.58
1:F:150:TYR:CD1	1:F:180:ILE:HD11	2.39	0.58
1:F:233:ASP:HB3	1:F:236:THR:OG1	2.03	0.58
1:E:52:ILE:HG23	1:E:53:HIS:CD2	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:ASN:HD22	1:E:232:SER:HB3	1.67	0.58
1:C:136:ASN:HD21	1:D:195:ASP:HA	1.67	0.58
1:F:189:LEU:HD11	1:F:200:MET:CE	2.34	0.58
1:C:41:LYS:HD2	1:C:42:SER:N	2.19	0.58
1:H:243:LEU:O	1:H:247:ILE:HG12	2.04	0.58
1:J:189:LEU:HD21	1:J:200:MET:CE	2.30	0.57
1:B:161:ASN:HA	1:B:190:PRO:HG2	1.85	0.57
1:D:242:GLN:O	1:D:246:ILE:HD13	2.04	0.57
1:I:68:ARG:O	1:I:72:GLU:HG3	2.05	0.57
1:J:41:LYS:HD2	5:J:447:HOH:O	2.04	0.57
1:L:100:ILE:HG12	1:L:111:LEU:HD23	1.86	0.57
1:L:154:ARG:HD2	2:L:268:PEP:O3P	2.04	0.57
1:D:228:GLU:HB3	5:D:346:HOH:O	2.03	0.57
1:E:41:LYS:HD3	1:E:42:SER:N	2.19	0.57
1:F:3:LYS:HB2	1:F:35:GLU:O	2.04	0.57
1:H:154:ARG:NH2	1:H:188:GLN:HE21	2.02	0.57
1:D:3:LYS:HB2	5:D:339:HOH:O	2.03	0.57
1:E:68:ARG:HH11	1:E:68:ARG:CB	2.18	0.57
1:L:41:LYS:HD3	1:L:41:LYS:C	2.29	0.57
1:E:49:ARG:HE	1:E:54:SER:CB	2.18	0.57
1:E:60:LEU:C	1:E:60:LEU:HD23	2.29	0.57
5:A:424:HOH:O	1:B:83:HIS:HD2	1.87	0.57
1:C:106:ARG:HA	5:C:376:HOH:O	2.04	0.57
1:F:263:THR:HG22	1:F:264:ILE:H	1.68	0.57
1:F:45:ASP:OD1	1:F:56:ARG:HB3	2.05	0.57
1:F:45:ASP:HA	1:F:56:ARG:O	2.05	0.57
1:G:229:LYS:HE2	5:G:414:HOH:O	2.04	0.56
1:D:41:LYS:HD3	1:D:42:SER:N	2.20	0.56
1:I:209:ARG:NH1	1:L:213:ALA:O	2.38	0.56
1:J:239:PRO:HG2	1:J:242:GLN:NE2	2.21	0.56
1:L:203:PHE:C	1:L:206:PRO:HD2	2.31	0.56
1:A:154:ARG:HD2	2:A:268:PEP:O3P	2.05	0.56
1:G:204:ILE:O	1:G:208:ILE:HG13	2.06	0.56
1:H:11:ASN:HD21	1:H:46:LYS:NZ	2.01	0.56
1:H:201:ARG:HA	1:H:204:ILE:HG13	1.87	0.56
1:H:249:ALA:O	1:H:253:ILE:HG12	2.04	0.56
1:J:41:LYS:NZ	1:J:222:GLU:HG2	2.19	0.56
1:K:188:GLN:HB3	1:K:236:THR:HG21	1.87	0.56
1:K:12:ALA:HB2	1:K:46:LYS:HD3	1.87	0.56
1:E:223:THR:OG1	1:E:240:LEU:HA	2.05	0.56
1:H:228:GLU:HG2	5:H:403:HOH:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:O	1:B:243:LEU:HD13	2.06	0.56
1:D:20:LEU:HD23	1:D:70:VAL:HG22	1.87	0.56
1:G:250:ILE:C	1:G:250:ILE:HD12	2.31	0.56
1:C:14:GLU:OE2	1:C:231:LEU:HG	2.06	0.56
1:F:40:PHE:HB3	1:F:78:ILE:HD13	1.86	0.56
1:F:219:VAL:CG1	1:F:221:MET:HE2	2.34	0.56
1:K:204:ILE:O	1:K:208:ILE:HG13	2.06	0.56
1:F:154:ARG:HD2	2:F:268:PEP:O3P	2.06	0.56
1:H:182:ASP:HA	1:H:220:PHE:HB3	1.88	0.56
1:I:31:GLU:O	1:I:34:LYS:HE3	2.05	0.56
1:K:136:ASN:ND2	1:L:195:ASP:HA	2.21	0.56
1:C:100:ILE:HG13	1:C:111:LEU:HD23	1.87	0.56
1:E:228:GLU:HG3	1:E:229:LYS:HG3	1.88	0.56
1:H:237:ALA:HB3	5:H:274:HOH:O	2.06	0.56
1:A:41:LYS:HB2	1:A:79:THR:CG2	2.36	0.55
1:B:212:VAL:HG11	1:B:250:ILE:HG23	1.87	0.55
1:B:237:ALA:HB3	5:B:301:HOH:O	2.04	0.55
1:E:242:GLN:O	1:E:246:ILE:HD13	2.06	0.55
1:H:201:ARG:HH12	1:H:227:PRO:HB2	1.72	0.55
1:H:201:ARG:NH2	1:H:234:ALA:O	2.38	0.55
1:F:28:ARG:HG2	1:F:28:ARG:HH11	1.72	0.55
1:H:68:ARG:HH21	1:H:94:VAL:HG23	1.70	0.55
1:K:70:VAL:HG13	1:K:78:ILE:HD11	1.88	0.55
1:E:182:ASP:HA	1:E:220:PHE:HB3	1.89	0.55
1:F:189:LEU:N	1:F:189:LEU:HD12	2.22	0.55
1:J:184:THR:CG2	1:J:222:GLU:H	2.13	0.55
1:C:11:ASN:ND2	1:C:232:SER:OG	2.39	0.55
1:H:198:GLY:HA2	1:H:235:PRO:HG3	1.88	0.55
1:L:87:GLN:O	1:L:91:VAL:HG23	2.05	0.55
1:B:182:ASP:HA	1:B:220:PHE:HB3	1.88	0.55
1:D:64:VAL:HG13	1:D:94:VAL:CG1	2.37	0.55
1:E:116:LYS:HB2	1:E:116:LYS:NZ	2.21	0.55
1:E:20:LEU:HD21	1:E:69:LYS:HG3	1.88	0.55
1:F:106:ARG:HG3	1:F:106:ARG:HH11	1.71	0.55
1:A:235:PRO:HA	5:A:436:HOH:O	2.07	0.54
1:B:49:ARG:NH2	1:B:231:LEU:O	2.40	0.54
1:B:41:LYS:HD3	1:B:41:LYS:C	2.32	0.54
1:K:63:GLY:O	1:K:67:LEU:HD13	2.08	0.54
1:K:128:PHE:HB3	5:L:282:HOH:O	2.06	0.54
1:B:151:LEU:HD13	1:B:173:MET:CE	2.37	0.54
1:F:138:VAL:HG11	1:F:176:TRP:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:227:PRO:HB3	1:K:237:ALA:CB	2.34	0.54
1:F:249:ALA:O	1:F:253:ILE:HD13	2.08	0.54
3:G:269:A5P:C5	1:H:106:ARG:HH22	2.20	0.54
1:D:19:LEU:HD22	1:D:40:PHE:HE2	1.73	0.54
1:E:130:ALA:HB3	1:E:133:ASP:OD2	2.07	0.54
1:F:243:LEU:O	1:F:247:ILE:HG13	2.08	0.54
1:G:183:ALA:HB2	1:G:208:ILE:HG12	1.90	0.54
1:H:68:ARG:HE	1:H:94:VAL:CG2	2.21	0.54
1:K:52:ILE:HG23	1:K:53:HIS:CD2	2.42	0.54
1:E:91:VAL:C	1:E:93:GLU:H	2.16	0.54
1:K:83:HIS:HD2	5:K:305:HOH:O	1.91	0.54
1:C:228:GLU:HG3	1:C:229:LYS:HG3	1.89	0.54
1:G:238:LEU:HD21	1:G:246:ILE:CD1	2.38	0.54
1:C:20:LEU:HB3	5:C:362:HOH:O	2.07	0.53
1:L:41:LYS:HD3	1:L:42:SER:N	2.23	0.53
1:E:87:GLN:O	1:E:91:VAL:HG22	2.09	0.53
1:E:239:PRO:HG2	1:E:242:GLN:NE2	2.24	0.53
1:L:11:ASN:ND2	1:L:46:LYS:HE3	2.22	0.53
1:D:264:ILE:HD12	5:D:342:HOH:O	2.07	0.53
1:J:184:THR:HB	5:J:399:HOH:O	2.06	0.53
1:D:41:LYS:HD3	1:D:41:LYS:C	2.33	0.53
1:K:41:LYS:HB2	1:K:79:THR:CG2	2.39	0.53
1:K:113:ALA:O	1:K:116:LYS:HG2	2.09	0.53
1:C:43:SER:HB2	1:C:46:LYS:NZ	2.20	0.53
1:H:68:ARG:HH21	1:H:94:VAL:CG2	2.21	0.53
1:C:60:LEU:C	1:C:60:LEU:HD23	2.34	0.53
1:C:234:ALA:HB3	1:C:235:PRO:HD3	1.90	0.53
1:F:219:VAL:HG11	1:F:221:MET:HE2	1.90	0.53
1:F:49:ARG:HE	3:F:269:A5P:H52	1.72	0.53
1:G:234:ALA:N	1:G:235:PRO:HD2	2.24	0.53
1:J:3:LYS:N	5:J:368:HOH:O	2.42	0.53
1:J:41:LYS:HG2	1:J:42:SER:N	2.24	0.53
1:L:49:ARG:HD2	3:L:269:A5P:O4	2.08	0.53
1:L:68:ARG:O	1:L:72:GLU:HG3	2.08	0.53
1:K:200:MET:HB3	1:K:203:PHE:HD2	1.74	0.53
1:L:46:LYS:HB2	1:L:56:ARG:HA	1.90	0.53
1:D:51:SER:HB2	1:D:195:ASP:HB2	1.90	0.52
1:F:113:ALA:O	1:F:117:THR:HG23	2.09	0.52
1:A:41:LYS:HB2	1:A:79:THR:HG23	1.92	0.52
1:F:7:ILE:H	1:F:7:ILE:CD1	2.21	0.52
1:H:68:ARG:HE	1:H:94:VAL:HG22	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:238:LEU:HD21	1:H:246:ILE:CD1	2.39	0.52
1:D:68:ARG:HH21	1:D:93:GLU:HB3	1.74	0.52
1:F:182:ASP:HA	1:F:220:PHE:HB3	1.92	0.52
1:I:247:ILE:O	1:I:250:ILE:HG13	2.09	0.52
1:K:41:LYS:HD3	1:K:41:LYS:C	2.34	0.52
1:B:151:LEU:CD1	1:B:173:MET:HE2	2.36	0.52
1:B:233:ASP:OD2	3:B:269:A5P:HC3	2.10	0.52
1:D:182:ASP:HA	1:D:220:PHE:HB3	1.92	0.52
1:G:60:LEU:C	1:G:60:LEU:HD23	2.35	0.52
1:A:60:LEU:C	1:A:60:LEU:HD23	2.35	0.52
1:A:136:ASN:HB3	1:B:50:SER:O	2.09	0.52
1:B:263:THR:HG22	1:B:264:ILE:HG13	1.91	0.52
1:C:20:LEU:HD12	5:C:359:HOH:O	2.07	0.52
1:K:91:VAL:O	1:K:94:VAL:HG12	2.09	0.52
1:L:182:ASP:HA	1:L:220:PHE:HB3	1.92	0.52
1:G:130:ALA:HB3	1:G:133:ASP:OD2	2.09	0.52
1:J:208:ILE:O	1:J:212:VAL:HG23	2.10	0.52
1:K:180:ILE:N	1:K:180:ILE:HD12	2.24	0.52
1:B:11:ASN:HD21	1:B:46:LYS:NZ	2.08	0.52
1:C:49:ARG:NE	3:C:269:A5P:H52	2.24	0.52
1:C:201:ARG:HG3	1:C:235:PRO:O	2.09	0.52
1:E:113:ALA:O	1:E:117:THR:HG23	2.10	0.52
1:H:247:ILE:O	1:H:250:ILE:HG12	2.10	0.52
1:L:60:LEU:C	1:L:60:LEU:HD23	2.35	0.52
1:K:238:LEU:HD21	1:K:246:ILE:HD12	1.92	0.52
1:A:11:ASN:HD21	1:A:46:LYS:NZ	2.08	0.51
1:E:78:ILE:HG22	1:E:79:THR:N	2.25	0.51
2:I:268:PEP:C1	3:I:269:A5P:H12	2.40	0.51
1:K:87:GLN:O	1:K:91:VAL:HG23	2.10	0.51
1:C:41:LYS:HD2	1:C:42:SER:H	1.75	0.51
1:D:20:LEU:HD21	1:D:69:LYS:HG3	1.91	0.51
1:K:45:ASP:HA	1:K:56:ARG:O	2.09	0.51
1:L:154:ARG:HH22	1:L:188:GLN:HE22	1.55	0.51
1:A:46:LYS:CE	3:A:269:A5P:H11	2.40	0.51
1:F:263:THR:HG22	1:F:264:ILE:N	2.26	0.51
1:H:4:PHE:CE2	1:H:250:ILE:HD12	2.44	0.51
1:H:233:ASP:OD2	3:H:269:A5P:HC3	2.09	0.51
1:K:113:ALA:HA	1:K:116:LYS:CD	2.40	0.51
1:C:13:ILE:HD12	1:C:44:PHE:HA	1.92	0.51
1:E:262:GLU:CD	1:H:209:ARG:HH22	2.19	0.51
1:K:40:PHE:HB3	1:K:78:ILE:HD13	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:154:ARG:HH22	1:L:188:GLN:HE21	1.55	0.51
1:I:205:PHE:HB3	1:I:206:PRO:HD3	1.93	0.51
1:K:19:LEU:HD12	1:K:19:LEU:H	1.75	0.51
1:K:67:LEU:HB3	1:K:78:ILE:HG21	1.92	0.51
1:B:151:LEU:CB	1:B:173:MET:HE2	2.39	0.51
1:D:60:LEU:HD23	1:D:60:LEU:O	2.10	0.51
1:K:16:GLU:O	1:K:20:LEU:HD13	2.10	0.51
1:G:136:ASN:HB3	1:H:50:SER:O	2.11	0.51
1:K:19:LEU:HD12	1:K:19:LEU:N	2.25	0.51
1:A:170:LEU:HB2	1:A:171:PRO:HD3	1.93	0.51
1:A:212:VAL:HG11	1:A:250:ILE:HG23	1.92	0.51
1:F:256:VAL:HG21	1:G:256:VAL:CG1	2.40	0.51
1:I:154:ARG:HD2	2:I:268:PEP:O3P	2.10	0.51
1:E:128:PHE:HB3	5:E:272:HOH:O	2.11	0.51
1:J:200:MET:HA	5:J:428:HOH:O	2.10	0.51
1:K:58:HIS:HB2	1:K:62:TYR:CD2	2.46	0.51
1:E:104:LEU:HD11	1:F:107:GLN:NE2	2.26	0.51
1:E:262:GLU:OE2	1:H:209:ARG:NH2	2.44	0.51
1:H:189:LEU:HD11	1:H:200:MET:CE	2.36	0.51
1:H:68:ARG:O	1:H:72:GLU:HG3	2.11	0.50
1:J:203:PHE:C	1:J:206:PRO:HD2	2.36	0.50
1:K:150:TYR:CD1	1:K:180:ILE:HD11	2.46	0.50
1:C:204:ILE:O	1:C:208:ILE:HG13	2.12	0.50
1:H:189:LEU:HD12	5:H:441:HOH:O	2.11	0.50
1:E:3:LYS:NZ	1:E:35:GLU:HA	2.27	0.50
5:E:272:HOH:O	1:F:128:PHE:HB3	2.11	0.50
1:L:258:SER:HA	1:L:261:TYR:CD2	2.46	0.50
1:G:83:HIS:HD2	5:H:341:HOH:O	1.93	0.50
1:E:205:PHE:HB3	1:E:206:PRO:HD3	1.94	0.50
1:F:78:ILE:HG22	1:F:79:THR:N	2.26	0.50
1:H:178:LYS:HD3	5:H:378:HOH:O	2.12	0.50
1:I:60:LEU:HD23	1:I:60:LEU:C	2.37	0.50
1:E:61:GLU:HG2	1:E:62:TYR:N	2.27	0.50
1:F:10:PRO:HG3	1:F:22:VAL:HG21	1.94	0.50
1:I:204:ILE:HD13	1:I:238:LEU:HD11	1.94	0.50
1:A:83:HIS:HD2	5:B:282:HOH:O	1.94	0.50
1:B:234:ALA:HB3	1:B:235:PRO:HD3	1.92	0.50
1:D:201:ARG:NH1	1:D:235:PRO:HA	2.27	0.50
1:F:256:VAL:CG2	1:G:256:VAL:HG11	2.41	0.50
1:G:185:HIS:HB3	1:G:188:GLN:HE21	1.75	0.50
1:H:250:ILE:HG13	1:H:251:LEU:N	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ILE:HD12	1:D:40:PHE:CD1	2.46	0.49
1:F:156:THR:O	1:F:163:LEU:HA	2.12	0.49
1:F:170:LEU:O	1:F:174:LYS:HG3	2.11	0.49
1:F:201:ARG:HG3	1:F:204:ILE:HD12	1.93	0.49
1:H:61:GLU:HG3	5:H:410:HOH:O	2.11	0.49
1:K:14:GLU:HG2	1:K:231:LEU:HD12	1.93	0.49
1:E:136:ASN:HB3	1:F:50:SER:O	2.12	0.49
1:H:201:ARG:HH21	1:H:236:THR:N	2.10	0.49
1:J:201:ARG:HG3	1:J:204:ILE:HD12	1.93	0.49
1:F:101:PRO:CG	1:F:104:LEU:HD12	2.43	0.49
1:F:60:LEU:C	1:F:60:LEU:HD23	2.38	0.49
1:F:243:LEU:CD1	1:F:247:ILE:HD11	2.43	0.49
1:I:139:GLU:HB2	5:I:390:HOH:O	2.12	0.49
1:J:205:PHE:HB3	1:J:206:PRO:HD3	1.95	0.49
2:A:268:PEP:H32	2:A:268:PEP:O1P	2.13	0.49
1:F:87:GLN:O	1:F:91:VAL:HG23	2.13	0.49
1:G:212:VAL:HG11	1:G:250:ILE:HB	1.94	0.49
1:J:258:SER:HA	1:J:261:TYR:CE2	2.47	0.49
1:K:13:ILE:HG23	1:K:19:LEU:HD11	1.94	0.49
1:B:22:VAL:O	1:B:26:ILE:HG12	2.13	0.49
1:B:243:LEU:N	1:B:243:LEU:HD12	2.27	0.49
1:K:27:LYS:O	1:K:30:SER:HB3	2.13	0.49
1:K:89:GLU:HG2	5:K:309:HOH:O	2.13	0.49
1:B:243:LEU:O	1:B:247:ILE:HG12	2.13	0.49
1:F:13:ILE:HG13	1:F:43:SER:O	2.13	0.49
1:L:27:LYS:O	1:L:30:SER:HB3	2.12	0.49
2:L:268:PEP:O1P	2:L:268:PEP:H32	2.12	0.49
1:E:224:HIS:O	1:E:227:PRO:HD3	2.12	0.49
1:I:238:LEU:HD12	1:I:238:LEU:N	2.28	0.49
1:K:69:LYS:HG2	5:K:316:HOH:O	2.12	0.49
1:L:14:GLU:HG2	1:L:231:LEU:HD12	1.95	0.49
1:D:204:ILE:O	1:D:208:ILE:HG13	2.13	0.48
1:E:100:ILE:HD12	1:E:100:ILE:N	2.27	0.48
1:L:65:LYS:HG2	5:L:336:HOH:O	2.13	0.48
1:E:139:GLU:HA	1:E:142:LYS:NZ	2.28	0.48
5:I:409:HOH:O	1:J:83:HIS:HD2	1.95	0.48
1:K:25:GLU:OE1	1:K:28:ARG:HD3	2.13	0.48
1:L:61:GLU:HG3	5:L:319:HOH:O	2.12	0.48
1:B:261:TYR:HD1	1:C:209:ARG:HH12	1.60	0.48
1:G:189:LEU:HD21	1:G:200:MET:HE3	1.95	0.48
2:I:268:PEP:H32	2:I:268:PEP:O1P	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:SER:HA	1:K:38:PHE:CE2	2.48	0.48
1:F:49:ARG:NE	3:F:269:A5P:H52	2.28	0.48
1:D:124:LYS:HD3	1:D:152:THR:HB	1.95	0.48
1:F:41:LYS:HD3	1:F:41:LYS:C	2.38	0.48
2:F:268:PEP:O1P	2:F:268:PEP:H32	2.13	0.48
1:H:188:GLN:HA	1:H:199:GLY:HA2	1.95	0.48
1:L:14:GLU:HG2	1:L:231:LEU:CD1	2.44	0.48
1:D:26:ILE:HD12	1:D:40:PHE:HD1	1.78	0.48
1:E:233:ASP:HB3	1:E:236:THR:OG1	2.14	0.48
1:I:212:VAL:HG21	1:I:250:ILE:HB	1.95	0.48
1:K:234:ALA:HB3	1:K:235:PRO:HD3	1.94	0.48
1:L:116:LYS:HD3	5:L:348:HOH:O	2.14	0.48
1:B:49:ARG:HD2	3:B:269:A5P:O3P	2.14	0.48
1:C:107:GLN:OE1	1:D:48:ASN:HB3	2.13	0.48
1:D:96:ASP:HB2	1:D:97:ILE:HD12	1.95	0.48
1:H:201:ARG:HH21	1:H:235:PRO:C	2.22	0.48
1:J:25:GLU:HA	1:J:28:ARG:NH1	2.28	0.48
1:B:219:VAL:CG1	1:B:221:MET:HE2	2.44	0.48
1:C:47:ALA:HB1	5:C:287:HOH:O	2.14	0.48
1:K:5:LEU:HD12	1:K:37:GLU:O	2.13	0.48
1:C:43:SER:CB	1:C:46:LYS:HZ2	2.23	0.47
1:I:4:PHE:HZ	1:I:219:VAL:HG23	1.79	0.47
1:I:5:LEU:HD12	1:I:37:GLU:O	2.13	0.47
1:G:4:PHE:CE2	1:G:250:ILE:HD13	2.49	0.47
1:G:181:TYR:OH	1:G:207:LEU:HD23	2.13	0.47
1:B:17:GLU:HG3	5:B:454:HOH:O	2.13	0.47
1:D:193:LEU:HB2	1:D:196:LYS:O	2.14	0.47
1:E:83:HIS:HD2	5:E:308:HOH:O	1.96	0.47
1:H:238:LEU:HD21	1:H:246:ILE:HD12	1.96	0.47
1:K:249:ALA:O	1:K:253:ILE:HG12	2.14	0.47
1:D:19:LEU:HD22	1:D:40:PHE:CE2	2.49	0.47
1:F:262:GLU:HB2	5:F:317:HOH:O	2.14	0.47
1:I:201:ARG:HG3	1:I:204:ILE:HD12	1.97	0.47
1:K:223:THR:OG1	1:K:240:LEU:HA	2.14	0.47
1:F:228:GLU:OE1	1:F:228:GLU:N	2.44	0.47
1:G:147:LYS:NZ	5:G:300:HOH:O	2.47	0.47
1:K:3:LYS:HE3	1:K:3:LYS:CA	2.45	0.47
1:K:64:VAL:HG13	1:K:94:VAL:CG1	2.42	0.47
1:E:27:LYS:O	1:E:31:GLU:HG2	2.15	0.47
1:E:238:LEU:HD12	1:E:239:PRO:HD2	1.97	0.47
1:F:130:ALA:HB3	1:F:133:ASP:OD2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:PHE:CE2	1:I:250:ILE:HD13	2.49	0.47
1:K:200:MET:HB3	1:K:203:PHE:CD2	2.50	0.47
1:L:99:GLN:C	1:L:100:ILE:HD12	2.40	0.47
1:A:234:ALA:N	1:A:235:PRO:HD2	2.30	0.47
1:B:78:ILE:HG22	1:B:79:THR:N	2.28	0.47
1:B:154:ARG:HH21	1:B:163:LEU:CD1	2.28	0.47
1:B:263:THR:HA	5:B:448:HOH:O	2.15	0.47
1:F:41:LYS:HD3	1:F:42:SER:N	2.29	0.47
1:I:41:LYS:HD3	1:I:41:LYS:C	2.40	0.47
1:K:41:LYS:HB2	1:K:79:THR:HG23	1.96	0.47
1:K:154:ARG:HD2	2:K:268:PEP:O3P	2.14	0.47
1:K:188:GLN:HA	1:K:199:GLY:HA2	1.97	0.47
1:D:184:THR:HG21	1:D:222:GLU:H	1.80	0.47
1:L:168:ARG:O	1:L:172:ILE:HG13	2.15	0.47
1:E:12:ALA:HB1	5:E:310:HOH:O	2.13	0.47
1:E:49:ARG:NH1	1:E:232:SER:OG	2.47	0.47
1:K:130:ALA:HB3	1:K:133:ASP:OD2	2.15	0.47
1:C:195:ASP:OD1	1:C:196:LYS:HG2	2.15	0.47
1:J:201:ARG:HH11	1:J:201:ARG:CB	2.28	0.47
1:K:176:TRP:O	1:K:177:ALA:HB2	2.14	0.47
1:A:50:SER:O	1:B:136:ASN:HB3	2.15	0.46
1:A:129:LEU:HG	1:A:133:ASP:HB2	1.97	0.46
1:C:14:GLU:OE1	1:C:18:LEU:HD22	2.15	0.46
1:D:5:LEU:HD22	1:D:37:GLU:HB3	1.97	0.46
1:E:184:THR:HG23	1:E:221:MET:HA	1.97	0.46
1:F:176:TRP:O	1:F:177:ALA:HB2	2.14	0.46
1:K:184:THR:O	1:K:236:THR:HB	2.15	0.46
1:A:49:ARG:NH1	1:A:232:SER:HB3	2.30	0.46
1:B:61:GLU:HG3	5:B:335:HOH:O	2.16	0.46
1:E:11:ASN:ND2	1:E:232:SER:HB3	2.29	0.46
1:E:247:ILE:O	1:E:250:ILE:HG13	2.16	0.46
1:I:49:ARG:NH1	1:I:232:SER:HB3	2.29	0.46
1:I:195:ASP:HA	1:J:136:ASN:HD21	1.80	0.46
1:K:11:ASN:HD21	1:K:46:LYS:HE2	1.79	0.46
1:L:234:ALA:HB3	1:L:235:PRO:HD3	1.97	0.46
1:C:136:ASN:HB3	1:D:50:SER:O	2.15	0.46
1:D:154:ARG:HD2	4:D:268:1NT:O3P	2.15	0.46
1:E:4:PHE:CE2	1:E:250:ILE:HD13	2.50	0.46
1:G:258:SER:HA	1:G:261:TYR:CE2	2.49	0.46
1:H:212:VAL:HG11	1:H:250:ILE:HB	1.96	0.46
1:J:239:PRO:HG2	1:J:242:GLN:HE21	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LYS:NZ	1:B:259:LYS:HB3	2.30	0.46
1:D:259:LYS:N	5:D:337:HOH:O	2.42	0.46
1:I:3:LYS:N	5:I:451:HOH:O	2.48	0.46
1:K:122:ASN:HA	1:K:150:TYR:HB2	1.96	0.46
1:K:206:PRO:HA	1:K:209:ARG:HH21	1.80	0.46
1:K:206:PRO:HA	1:K:209:ARG:HE	1.81	0.46
5:G:294:HOH:O	1:J:139:GLU:HB2	2.15	0.46
1:C:239:PRO:HG2	1:C:242:GLN:NE2	2.30	0.46
1:F:248:GLU:HG3	1:F:252:GLU:OE2	2.16	0.46
1:E:85:SER:O	1:E:87:GLN:N	2.49	0.46
1:B:184:THR:CG2	1:B:221:MET:HA	2.46	0.46
1:B:185:HIS:NE2	3:B:269:A5P:H11	2.31	0.46
1:C:246:ILE:O	1:C:250:ILE:HG12	2.15	0.46
1:F:20:LEU:HD21	1:F:69:LYS:HG3	1.97	0.46
1:F:106:ARG:HG3	1:F:106:ARG:NH1	2.30	0.46
1:G:205:PHE:N	1:G:206:PRO:HD2	2.30	0.46
1:J:129:LEU:HG	1:J:133:ASP:HB2	1.97	0.46
1:D:19:LEU:HD12	1:D:66:ALA:CB	2.46	0.46
1:B:150:TYR:CE1	1:B:178:LYS:HD3	2.51	0.46
1:C:41:LYS:HE3	1:C:220:PHE:HZ	1.81	0.46
1:C:78:ILE:HG22	1:C:79:THR:N	2.31	0.46
1:E:81:ASP:HA	1:E:99:GLN:O	2.16	0.46
1:J:201:ARG:NH1	1:J:201:ARG:CB	2.78	0.46
1:K:92:ALA:HB2	1:K:117:THR:HB	1.98	0.46
1:L:128:PHE:HB3	5:L:282:HOH:O	2.15	0.46
1:E:30:SER:HA	1:E:38:PHE:CE2	2.51	0.45
1:E:113:ALA:O	1:E:116:LYS:HG2	2.15	0.45
1:J:212:VAL:HG21	1:J:250:ILE:HB	1.98	0.45
1:L:14:GLU:CD	1:L:231:LEU:HG	2.41	0.45
2:B:268:PEP:C1	3:B:269:A5P:H12	2.46	0.45
1:D:52:ILE:HG23	1:D:53:HIS:CD2	2.51	0.45
1:F:28:ARG:HG2	1:F:28:ARG:NH1	2.32	0.45
1:F:213:ALA:HB2	1:G:213:ALA:HB2	1.98	0.45
1:H:3:LYS:N	5:H:369:HOH:O	2.48	0.45
1:K:230:ALA:HB3	1:K:234:ALA:HA	1.98	0.45
1:C:30:SER:HA	1:C:38:PHE:CE2	2.52	0.45
1:G:195:ASP:HA	1:H:136:ASN:HD21	1.82	0.45
1:H:5:LEU:HD12	1:H:37:GLU:O	2.15	0.45
1:B:234:ALA:HA	5:B:301:HOH:O	2.17	0.45
1:D:60:LEU:HD23	1:D:60:LEU:C	2.42	0.45
1:F:35:GLU:OE1	1:F:35:GLU:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:131:PRO:HG3	5:L:293:HOH:O	2.16	0.45
1:E:227:PRO:HB3	1:E:237:ALA:CB	2.44	0.45
1:G:239:PRO:HG2	1:G:242:GLN:NE2	2.32	0.45
1:I:228:GLU:HG2	5:I:459:HOH:O	2.16	0.45
1:K:27:LYS:HD3	1:K:74:PHE:O	2.17	0.45
1:K:40:PHE:O	1:K:79:THR:HG22	2.16	0.45
1:B:25:GLU:HG2	1:B:240:LEU:HD22	1.99	0.45
1:B:65:LYS:NZ	1:B:68:ARG:NH1	2.65	0.45
1:B:93:GLU:HG3	5:B:303:HOH:O	2.17	0.45
1:B:219:VAL:HG11	1:B:221:MET:HE2	1.98	0.45
1:D:10:PRO:HG3	1:D:22:VAL:HG21	1.97	0.45
1:L:254:ARG:HD2	5:L:362:HOH:O	2.17	0.45
1:D:66:ALA:O	1:D:70:VAL:HG23	2.17	0.45
1:F:141:LEU:HD12	1:F:149:ILE:HG23	1.98	0.45
1:J:61:GLU:HG2	5:J:347:HOH:O	2.17	0.45
1:C:223:THR:OG1	1:C:240:LEU:HA	2.17	0.45
1:D:29:LEU:HD13	1:D:247:ILE:HD12	1.99	0.45
1:D:96:ASP:CB	1:D:97:ILE:HD12	2.47	0.45
1:I:184:THR:CG2	1:I:222:GLU:H	2.30	0.45
1:C:8:ALA:HA	1:C:221:MET:O	2.17	0.45
1:D:201:ARG:NH2	1:D:234:ALA:O	2.49	0.45
1:D:260:TYR:O	1:D:261:TYR:C	2.59	0.45
1:K:216:CYS:HA	5:K:325:HOH:O	2.17	0.45
1:I:30:SER:HA	1:I:38:PHE:CE2	2.52	0.44
1:D:248:GLU:HB3	5:D:324:HOH:O	2.17	0.44
1:F:239:PRO:HG2	1:F:242:GLN:NE2	2.31	0.44
1:J:10:PRO:HD3	1:J:22:VAL:HG11	1.99	0.44
1:J:250:ILE:C	1:J:250:ILE:HD12	2.43	0.44
1:K:49:ARG:HD2	3:K:269:A5P:O4	2.17	0.44
1:K:92:ALA:CB	1:K:117:THR:HB	2.47	0.44
1:C:184:THR:HG21	1:C:222:GLU:H	1.82	0.44
1:D:3:LYS:HB2	1:D:35:GLU:O	2.17	0.44
1:D:200:MET:HB2	1:D:202:GLU:HG2	1.99	0.44
1:I:140:LYS:HG2	1:J:52:ILE:HB	2.00	0.44
1:K:60:LEU:O	1:K:64:VAL:HG23	2.18	0.44
1:K:150:TYR:HB3	1:K:180:ILE:HD13	1.98	0.44
1:K:193:LEU:HD12	1:K:197:SER:O	2.17	0.44
1:L:258:SER:HA	1:L:261:TYR:CE2	2.51	0.44
4:D:268:1NT:O2P	4:D:268:1NT:CI3	2.66	0.44
1:H:102:ALA:HB2	1:H:154:ARG:HD3	1.97	0.44
1:H:207:LEU:HB2	5:H:276:HOH:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:227:PRO:C	1:L:229:LYS:H	2.25	0.44
1:E:193:LEU:HB2	1:E:196:LYS:O	2.17	0.44
1:G:22:VAL:O	1:G:26:ILE:HG12	2.17	0.44
1:H:234:ALA:N	1:H:235:PRO:HD2	2.32	0.44
2:H:268:PEP:C3	3:H:269:A5P:H12	2.48	0.44
1:A:232:SER:HA	5:A:335:HOH:O	2.18	0.44
1:E:250:ILE:HD12	1:E:251:LEU:N	2.32	0.44
1:K:82:ILE:O	1:K:82:ILE:HG13	2.17	0.44
1:L:247:ILE:HA	1:L:250:ILE:HD11	2.00	0.44
1:I:246:ILE:O	1:I:250:ILE:HG23	2.18	0.44
1:A:156:THR:HG21	1:D:158:PHE:HZ	1.82	0.44
1:B:68:ARG:O	1:B:72:GLU:HG3	2.18	0.44
1:D:46:LYS:CB	1:D:49:ARG:HD3	2.48	0.44
1:F:41:LYS:HB2	1:F:79:THR:CG2	2.47	0.44
1:F:201:ARG:NH1	1:F:237:ALA:O	2.51	0.44
1:K:89:GLU:N	1:K:90:PRO:HD2	2.33	0.44
1:L:205:PHE:HB3	1:L:206:PRO:HD3	1.99	0.44
1:F:89:GLU:HB3	1:F:90:PRO:CD	2.48	0.43
1:K:69:LYS:HA	1:K:72:GLU:HG2	2.00	0.43
1:F:11:ASN:HD22	1:F:232:SER:HB3	1.83	0.43
1:B:3:LYS:N	5:B:381:HOH:O	2.50	0.43
1:C:4:PHE:HZ	1:C:219:VAL:HG13	1.82	0.43
1:D:239:PRO:HB2	1:D:242:GLN:HG3	2.00	0.43
1:E:182:ASP:CG	1:E:185:HIS:HD1	2.25	0.43
1:H:154:ARG:HH21	1:H:163:LEU:CD1	2.32	0.43
1:I:68:ARG:NH2	5:I:369:HOH:O	2.50	0.43
1:K:106:ARG:O	1:L:48:ASN:HA	2.18	0.43
1:L:189:LEU:HD21	1:L:200:MET:CE	2.48	0.43
1:B:88:ALA:HB3	5:B:293:HOH:O	2.17	0.43
2:E:268:PEP:O1P	2:E:268:PEP:H32	2.17	0.43
1:F:97:ILE:HG12	1:F:120:ALA:CB	2.48	0.43
1:J:184:THR:HG22	1:J:221:MET:HA	2.01	0.43
1:J:261:TYR:HA	1:K:209:ARG:HH12	1.83	0.43
1:L:30:SER:HA	1:L:38:PHE:CD2	2.53	0.43
1:E:49:ARG:NE	1:E:54:SER:HB3	2.26	0.43
1:F:51:SER:HB2	1:F:195:ASP:HB2	2.00	0.43
1:I:203:PHE:C	1:I:206:PRO:HD2	2.44	0.43
1:I:238:LEU:N	1:I:238:LEU:CD1	2.82	0.43
1:K:206:PRO:HG3	1:K:209:ARG:HH21	1.84	0.43
1:F:78:ILE:CG2	1:F:79:THR:N	2.82	0.43
1:F:227:PRO:HB3	1:F:237:ALA:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:219:VAL:HG12	1:I:221:MET:HG3	2.00	0.43
3:F:269:A5P:O4	3:F:269:A5P:C1	2.66	0.43
1:K:238:LEU:HD21	1:K:246:ILE:CD1	2.48	0.43
1:L:100:ILE:HD12	1:L:100:ILE:N	2.33	0.43
1:L:154:ARG:NH2	1:L:188:GLN:NE2	2.56	0.43
1:A:170:LEU:CB	1:A:171:PRO:HD3	2.49	0.43
1:B:78:ILE:CG2	1:B:79:THR:N	2.82	0.43
1:C:4:PHE:CE1	1:C:218:GLY:HA2	2.54	0.43
1:C:46:LYS:HD3	5:C:323:HOH:O	2.18	0.43
1:D:5:LEU:HD13	1:D:6:VAL:N	2.33	0.43
1:E:13:ILE:HD12	1:E:44:PHE:HA	2.00	0.43
1:F:30:SER:HA	1:F:38:PHE:CD2	2.53	0.43
1:G:185:HIS:O	1:G:188:GLN:HG2	2.19	0.43
1:G:252:GLU:O	1:G:255:GLU:HB3	2.18	0.43
1:K:161:ASN:HD21	1:L:132:TRP:NE1	2.00	0.43
1:A:258:SER:HA	1:A:261:TYR:CE2	2.54	0.43
1:D:62:TYR:O	1:D:65:LYS:HB3	2.19	0.43
1:F:252:GLU:O	1:F:255:GLU:HB3	2.18	0.43
1:H:87:GLN:O	1:H:90:PRO:HG2	2.19	0.43
1:H:237:ALA:CB	5:H:274:HOH:O	2.65	0.43
1:D:36:VAL:HB	1:D:38:PHE:CE2	2.54	0.43
1:H:122:ASN:HA	1:H:150:TYR:HB2	2.00	0.43
1:B:30:SER:HA	1:B:38:PHE:CE2	2.54	0.42
1:D:255:GLU:HB3	5:D:304:HOH:O	2.19	0.42
1:E:139:GLU:HA	1:E:142:LYS:HZ3	1.84	0.42
1:F:141:LEU:CD1	1:F:149:ILE:HG23	2.48	0.42
1:J:228:GLU:HG2	1:J:229:LYS:N	2.34	0.42
1:G:89:GLU:HB3	1:G:90:PRO:CD	2.49	0.42
1:K:41:LYS:HA	1:K:79:THR:O	2.19	0.42
1:L:78:ILE:HG22	1:L:79:THR:N	2.33	0.42
1:C:49:ARG:HD2	3:C:269:A5P:C5	2.49	0.42
1:C:136:ASN:ND2	1:D:195:ASP:HA	2.33	0.42
1:B:11:ASN:HD21	1:B:46:LYS:CE	2.31	0.42
1:C:189:LEU:HD11	1:C:200:MET:HE2	2.02	0.42
1:D:41:LYS:HE2	1:D:220:PHE:HZ	1.84	0.42
1:D:64:VAL:HG13	1:D:94:VAL:HG12	2.01	0.42
1:G:247:ILE:O	1:G:250:ILE:HG13	2.19	0.42
1:K:99:GLN:NE2	1:K:124:LYS:HE2	2.34	0.42
1:D:78:ILE:HG22	1:D:79:THR:N	2.34	0.42
1:F:195:ASP:OD1	1:F:196:LYS:HG3	2.19	0.42
1:F:256:VAL:HG22	5:F:315:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:ASN:ND2	5:G:387:HOH:O	2.51	0.42
2:K:268:PEP:O1P	2:K:268:PEP:H32	2.15	0.42
3:A:269:A5P:HC4	3:A:269:A5P:H12	1.81	0.42
1:B:99:GLN:NE2	1:B:124:LYS:HE3	2.34	0.42
1:D:106:ARG:HA	5:D:297:HOH:O	2.18	0.42
1:F:179:VAL:C	1:F:180:ILE:HD12	2.44	0.42
1:J:25:GLU:HA	1:J:28:ARG:HH11	1.85	0.42
1:J:247:ILE:O	1:J:250:ILE:HG13	2.20	0.42
1:J:256:VAL:HG12	1:J:256:VAL:O	2.19	0.42
1:F:84:GLU:HG3	5:F:307:HOH:O	2.20	0.42
1:F:243:LEU:HD12	1:F:247:ILE:HD11	2.01	0.42
1:I:154:ARG:HH21	1:I:163:LEU:CD1	2.32	0.42
1:J:22:VAL:O	1:J:26:ILE:HG12	2.19	0.42
1:L:212:VAL:HG23	1:L:253:ILE:HG21	2.01	0.42
1:C:16:GLU:O	1:C:20:LEU:HG	2.19	0.42
1:D:87:GLN:O	1:D:91:VAL:HB	2.19	0.42
1:H:89:GLU:HB3	1:H:90:PRO:CD	2.49	0.42
1:J:111:LEU:HD22	1:J:141:LEU:HD21	2.02	0.42
1:K:200:MET:HE2	1:K:203:PHE:CE2	2.52	0.42
1:L:193:LEU:HB2	1:L:196:LYS:HG3	2.02	0.42
1:D:5:LEU:HD12	1:D:7:ILE:HG13	2.02	0.42
1:D:91:VAL:C	1:D:93:GLU:H	2.27	0.42
1:F:19:LEU:HD12	1:F:66:ALA:HB1	2.02	0.42
1:G:154:ARG:HH21	1:G:163:LEU:CD1	2.33	0.42
1:J:41:LYS:C	1:J:41:LYS:HE2	2.45	0.42
1:L:176:TRP:O	1:L:177:ALA:HB2	2.20	0.42
1:B:263:THR:HG22	1:B:264:ILE:N	2.35	0.42
1:D:46:LYS:HB3	1:D:49:ARG:HD3	2.01	0.42
1:E:210:ALA:HB2	1:H:214:VAL:HG23	2.02	0.42
1:H:154:ARG:CD	2:H:268:PEP:O3P	2.66	0.42
1:J:234:ALA:N	1:J:235:PRO:CD	2.82	0.42
1:K:179:VAL:C	1:K:180:ILE:HD12	2.45	0.42
1:L:246:ILE:O	1:L:250:ILE:HG12	2.19	0.42
1:A:202:GLU:H	1:A:202:GLU:CD	2.25	0.41
1:E:60:LEU:HD23	1:E:60:LEU:O	2.20	0.41
1:F:187:VAL:HG21	1:F:204:ILE:HG12	2.02	0.41
1:G:201:ARG:HD3	1:G:204:ILE:HD12	2.01	0.41
1:K:86:TRP:HD1	5:K:302:HOH:O	2.02	0.41
1:C:4:PHE:CZ	1:C:219:VAL:HG13	2.55	0.41
1:C:140:LYS:HG2	1:D:52:ILE:HB	2.02	0.41
1:H:78:ILE:HG22	1:H:79:THR:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:201:ARG:HB2	1:J:201:ARG:CZ	2.50	0.41
1:J:254:ARG:O	1:J:258:SER:HB3	2.21	0.41
1:A:12:ALA:HB2	1:A:46:LYS:HD3	2.03	0.41
1:C:107:GLN:NE2	1:D:104:LEU:HD11	2.35	0.41
1:C:128:PHE:HB3	5:D:272:HOH:O	2.19	0.41
1:E:10:PRO:HG3	1:E:22:VAL:HG21	2.02	0.41
1:G:5:LEU:HD12	1:G:37:GLU:HB3	2.02	0.41
2:H:268:PEP:O1P	2:H:268:PEP:H32	2.16	0.41
1:L:14:GLU:HB2	1:L:18:LEU:HD22	2.03	0.41
1:B:201:ARG:HA	1:B:204:ILE:HG13	2.02	0.41
1:H:184:THR:CG2	1:H:221:MET:HA	2.47	0.41
1:L:87:GLN:O	1:L:90:PRO:HG2	2.20	0.41
1:C:47:ALA:HB3	1:C:83:HIS:CD2	2.54	0.41
1:E:126:GLY:C	1:E:128:PHE:H	2.27	0.41
1:I:4:PHE:CE2	1:I:219:VAL:HG23	2.55	0.41
1:I:222:GLU:O	1:I:238:LEU:HD13	2.21	0.41
1:J:52:ILE:O	1:J:52:ILE:HG13	2.19	0.41
1:K:13:ILE:HD11	1:K:67:LEU:HD11	2.03	0.41
1:K:169:SER:O	1:K:173:MET:HG3	2.21	0.41
1:L:44:PHE:CD1	1:L:44:PHE:C	2.99	0.41
1:A:132:TRP:HA	1:A:176:TRP:CH2	2.56	0.41
1:C:3:LYS:HD2	1:C:35:GLU:O	2.21	0.41
1:D:55:PHE:CZ	1:D:57:GLY:HA2	2.55	0.41
1:E:71:LYS:HE3	5:E:339:HOH:O	2.20	0.41
1:F:14:GLU:OE1	1:F:231:LEU:HG	2.20	0.41
1:F:60:LEU:O	1:F:64:VAL:HG23	2.21	0.41
1:I:244:GLU:C	1:I:244:GLU:CD	2.89	0.41
1:J:5:LEU:HD12	1:J:37:GLU:O	2.20	0.41
1:K:264:ILE:H	1:K:264:ILE:HG13	1.74	0.41
1:B:228:GLU:CD	1:B:228:GLU:N	2.77	0.41
1:J:3:LYS:N	5:J:453:HOH:O	2.54	0.41
1:C:124:LYS:NZ	1:C:182:ASP:OD2	2.50	0.41
1:E:5:LEU:HD22	1:E:7:ILE:HG13	2.03	0.41
1:E:116:LYS:HG3	1:E:117:THR:N	2.35	0.41
1:K:19:LEU:H	1:K:19:LEU:CD1	2.34	0.41
1:K:201:ARG:NH1	1:K:237:ALA:O	2.52	0.41
1:L:201:ARG:NH2	1:L:234:ALA:O	2.54	0.41
1:D:161:ASN:HA	1:D:190:PRO:HG2	2.03	0.41
1:E:180:ILE:HG22	1:E:181:TYR:N	2.36	0.41
1:K:67:LEU:HD21	1:K:80:THR:HB	2.03	0.41
1:K:207:LEU:HB2	5:K:278:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:187:VAL:HG21	1:L:204:ILE:HG12	2.03	0.41
1:E:219:VAL:HG12	1:E:221:MET:HG3	2.03	0.41
1:F:13:ILE:HD12	1:F:44:PHE:HA	2.03	0.41
1:G:89:GLU:HG3	5:G:404:HOH:O	2.19	0.41
1:H:226:GLU:HA	1:H:227:PRO:HD2	1.90	0.41
1:I:237:ALA:HB2	5:I:403:HOH:O	2.21	0.41
1:K:50:SER:O	1:L:136:ASN:HB3	2.21	0.41
1:K:96:ASP:HB3	5:K:311:HOH:O	2.21	0.41
1:L:89:GLU:N	1:L:90:PRO:HD2	2.36	0.41
1:C:5:LEU:HD12	1:C:37:GLU:O	2.21	0.40
1:C:34:LYS:HG2	5:C:353:HOH:O	2.19	0.40
1:C:97:ILE:HG12	1:C:120:ALA:HB3	2.02	0.40
2:C:268:PEP:O1P	2:C:268:PEP:H32	2.21	0.40
1:D:11:ASN:HD22	1:D:232:SER:HB3	1.85	0.40
1:D:96:ASP:C	1:D:97:ILE:HD12	2.45	0.40
1:F:89:GLU:HB3	1:F:90:PRO:HD3	2.03	0.40
1:F:89:GLU:N	1:F:90:PRO:HD2	2.36	0.40
1:B:60:LEU:HD23	1:B:60:LEU:C	2.46	0.40
1:I:44:PHE:CD1	1:I:60:LEU:HA	2.56	0.40
1:J:60:LEU:HD23	1:J:60:LEU:C	2.46	0.40
1:J:184:THR:CG2	1:J:221:MET:HA	2.51	0.40
1:C:13:ILE:HG13	1:C:43:SER:O	2.21	0.40
1:E:52:ILE:HG23	1:E:53:HIS:HD2	1.82	0.40
1:I:165:VAL:CG2	1:I:186:SER:HB3	2.51	0.40
1:K:11:ASN:HD21	1:K:46:LYS:CE	2.35	0.40
1:K:95:ALA:O	1:K:119:ARG:HD2	2.21	0.40
1:L:193:LEU:HB2	1:L:196:LYS:O	2.21	0.40
1:L:234:ALA:N	1:L:235:PRO:CD	2.84	0.40
1:F:210:ALA:O	1:F:214:VAL:HG23	2.21	0.40
1:I:89:GLU:HB3	1:I:90:PRO:CD	2.51	0.40
1:I:201:ARG:NH1	5:I:450:HOH:O	2.55	0.40
1:J:41:LYS:HE3	1:J:42:SER:HA	2.04	0.40
1:J:83:HIS:HE1	5:J:270:HOH:O	2.03	0.40
1:K:70:VAL:HA	5:K:316:HOH:O	2.21	0.40
1:L:154:ARG:NH2	1:L:188:GLN:HE21	2.17	0.40
1:C:52:ILE:O	1:C:52:ILE:HG13	2.21	0.40
1:F:5:LEU:HD12	1:F:5:LEU:N	2.37	0.40
1:F:91:VAL:C	1:F:93:GLU:N	2.75	0.40
1:F:91:VAL:O	1:F:93:GLU:N	2.55	0.40
1:F:227:PRO:CB	1:F:237:ALA:HB3	2.51	0.40
1:H:25:GLU:O	1:H:29:LEU:HG	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:190:PRO:O	1:L:191:GLY:C	2.64	0.40
1:L:242:GLN:O	1:L:246:ILE:HG12	2.22	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	260/267 (97%)	253 (97%)	7 (3%)	0	100	100
1	B	260/267 (97%)	253 (97%)	7 (3%)	0	100	100
1	C	260/267 (97%)	245 (94%)	15 (6%)	0	100	100
1	D	260/267 (97%)	246 (95%)	14 (5%)	0	100	100
1	E	260/267 (97%)	241 (93%)	15 (6%)	4 (2%)	8	4
1	F	260/267 (97%)	235 (90%)	22 (8%)	3 (1%)	10	7
1	G	260/267 (97%)	253 (97%)	7 (3%)	0	100	100
1	H	260/267 (97%)	251 (96%)	9 (4%)	0	100	100
1	I	260/267 (97%)	252 (97%)	8 (3%)	0	100	100
1	J	260/267 (97%)	249 (96%)	10 (4%)	1 (0%)	30	28
1	K	260/267 (97%)	237 (91%)	22 (8%)	1 (0%)	30	28
1	L	260/267 (97%)	246 (95%)	14 (5%)	0	100	100
All	All	3120/3204 (97%)	2961 (95%)	150 (5%)	9 (0%)	36	36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	86	TRP
1	E	92	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	92	ALA
1	K	94	VAL
1	F	105	CYS
1	F	262	GLU
1	E	85	SER
1	E	190	PRO
1	J	235	PRO

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	218/223 (98%)	217 (100%)	1 (0%)	81	88
1	B	218/223 (98%)	214 (98%)	4 (2%)	51	60
1	C	218/223 (98%)	216 (99%)	2 (1%)	70	78
1	D	218/223 (98%)	215 (99%)	3 (1%)	59	67
1	E	218/223 (98%)	214 (98%)	4 (2%)	51	60
1	F	218/223 (98%)	213 (98%)	5 (2%)	44	51
1	G	218/223 (98%)	215 (99%)	3 (1%)	59	67
1	H	218/223 (98%)	217 (100%)	1 (0%)	81	88
1	I	218/223 (98%)	216 (99%)	2 (1%)	70	78
1	J	218/223 (98%)	215 (99%)	3 (1%)	59	67
1	K	218/223 (98%)	217 (100%)	1 (0%)	81	88
1	L	218/223 (98%)	217 (100%)	1 (0%)	81	88
All	All	2616/2676 (98%)	2586 (99%)	30 (1%)	65	74

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	B	65	LYS
1	B	184	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	188	GLN
1	B	259	LYS
1	C	112	LEU
1	C	250	ILE
1	D	5	LEU
1	D	200	MET
1	D	201	ARG
1	E	35	GLU
1	E	116	LYS
1	E	125	LYS
1	E	250	ILE
1	F	7	ILE
1	F	35	GLU
1	F	69	LYS
1	F	208	ILE
1	F	243	LEU
1	G	228	GLU
1	G	243	LEU
1	G	250	ILE
1	H	21	LYS
1	I	208	ILE
1	I	222	GLU
1	J	184	THR
1	J	243	LEU
1	J	250	ILE
1	K	3	LYS
1	L	69	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	53	HIS
1	A	83	HIS
1	A	136	ASN
1	A	242	GLN
1	B	11	ASN
1	B	83	HIS
1	B	99	GLN
1	B	107	GLN
1	B	136	ASN
1	B	175	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	188	GLN
1	C	11	ASN
1	C	83	HIS
1	C	99	GLN
1	C	136	ASN
1	C	242	GLN
1	D	11	ASN
1	D	53	HIS
1	D	83	HIS
1	D	175	GLN
1	D	188	GLN
1	E	53	HIS
1	E	122	ASN
1	E	136	ASN
1	E	161	ASN
1	E	188	GLN
1	E	242	GLN
1	F	53	HIS
1	F	83	HIS
1	F	99	GLN
1	F	185	HIS
1	G	83	HIS
1	G	136	ASN
1	G	188	GLN
1	H	11	ASN
1	H	53	HIS
1	H	136	ASN
1	H	175	GLN
1	H	188	GLN
1	I	11	ASN
1	I	53	HIS
1	I	83	HIS
1	I	188	GLN
1	I	242	GLN
1	J	11	ASN
1	J	83	HIS
1	J	136	ASN
1	J	175	GLN
1	J	242	GLN
1	K	11	ASN
1	K	53	HIS
1	K	83	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	107	GLN
1	K	136	ASN
1	K	161	ASN
1	K	188	GLN
1	L	83	HIS
1	L	136	ASN
1	L	175	GLN
1	L	188	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	A5P	C	269	-	13,13,13	1.78	2 (15%)	17,18,18	1.53	3 (17%)
2	PEP	K	268	-	9,9,9	2.10	2 (22%)	11,13,13	1.38	2 (18%)
3	A5P	A	269	-	13,13,13	1.78	2 (15%)	17,18,18	1.47	2 (11%)
4	1NT	D	268	-	23,24,24	1.30	2 (8%)	27,37,37	1.30	3 (11%)
2	PEP	C	268	-	9,9,9	2.11	2 (22%)	11,13,13	1.38	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEP	H	268	-	9,9,9	2.13	2 (22%)	11,13,13	1.41	2 (18%)
2	PEP	B	268	-	9,9,9	2.09	2 (22%)	11,13,13	1.28	2 (18%)
3	A5P	G	269	-	13,13,13	1.77	2 (15%)	17,18,18	1.55	3 (17%)
3	A5P	B	269	-	13,13,13	1.77	2 (15%)	17,18,18	1.45	2 (11%)
2	PEP	J	268	-	9,9,9	2.12	2 (22%)	11,13,13	1.33	2 (18%)
3	A5P	H	269	-	13,13,13	1.77	2 (15%)	17,18,18	1.45	3 (17%)
2	PEP	E	268	-	9,9,9	2.09	2 (22%)	11,13,13	1.42	2 (18%)
3	A5P	L	269	-	13,13,13	1.78	2 (15%)	17,18,18	1.49	3 (17%)
3	A5P	J	269	-	13,13,13	1.77	2 (15%)	17,18,18	1.47	3 (17%)
2	PEP	I	268	-	9,9,9	2.09	2 (22%)	11,13,13	1.34	2 (18%)
2	PEP	F	268	-	9,9,9	2.13	2 (22%)	11,13,13	1.42	2 (18%)
3	A5P	E	269	-	13,13,13	1.77	2 (15%)	17,18,18	1.46	2 (11%)
2	PEP	A	268	-	9,9,9	2.13	2 (22%)	11,13,13	1.44	2 (18%)
3	A5P	K	269	-	13,13,13	1.77	2 (15%)	17,18,18	1.50	3 (17%)
3	A5P	I	269	-	13,13,13	1.77	2 (15%)	17,18,18	1.54	3 (17%)
2	PEP	L	268	-	9,9,9	2.09	2 (22%)	11,13,13	1.39	2 (18%)
3	A5P	F	269	-	13,13,13	1.77	2 (15%)	17,18,18	1.43	2 (11%)
2	PEP	G	268	-	9,9,9	2.13	2 (22%)	11,13,13	1.41	2 (18%)

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	A5P	C	269	-	-	4/16/16/16	-
2	PEP	K	268	-	-	0/9/9/9	-
3	A5P	A	269	-	-	6/16/16/16	-
4	1NT	D	268	-	-	9/30/35/35	-
2	PEP	C	268	-	-	0/9/9/9	-
2	PEP	H	268	-	-	0/9/9/9	-
2	PEP	B	268	-	-	0/9/9/9	-
3	A5P	G	269	-	-	5/16/16/16	-
3	A5P	B	269	-	-	5/16/16/16	-
2	PEP	J	268	-	-	0/9/9/9	-
3	A5P	H	269	-	-	5/16/16/16	-
2	PEP	E	268	-	-	0/9/9/9	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A5P	L	269	-	-	5/16/16/16	-
3	A5P	J	269	-	-	3/16/16/16	-
2	PEP	I	268	-	-	0/9/9/9	-
2	PEP	F	268	-	-	0/9/9/9	-
3	A5P	E	269	-	-	5/16/16/16	-
2	PEP	A	268	-	-	0/9/9/9	-
3	A5P	K	269	-	-	5/16/16/16	-
3	A5P	I	269	-	-	3/16/16/16	-
2	PEP	L	268	-	-	0/9/9/9	-
3	A5P	F	269	-	-	5/16/16/16	-
2	PEP	G	268	-	-	0/9/9/9	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	269	A5P	O1-C1	-4.54	1.23	1.42
3	I	269	A5P	O1-C1	-4.54	1.23	1.42
3	C	269	A5P	O1-C1	-4.53	1.23	1.42
3	F	269	A5P	O1-C1	-4.53	1.23	1.42
3	J	269	A5P	O1-C1	-4.53	1.23	1.42
3	E	269	A5P	O1-C1	-4.52	1.23	1.42
3	B	269	A5P	O1-C1	-4.51	1.23	1.42
3	K	269	A5P	O1-C1	-4.51	1.23	1.42
3	A	269	A5P	O1-C1	-4.51	1.23	1.42
3	G	269	A5P	O1-C1	-4.51	1.23	1.42
3	H	269	A5P	O1-C1	-4.50	1.23	1.42
2	G	268	PEP	C2-C1	4.39	1.53	1.49
2	H	268	PEP	C2-C1	4.36	1.53	1.49
2	A	268	PEP	C2-C1	4.35	1.53	1.49
2	F	268	PEP	C2-C1	4.35	1.53	1.49
2	J	268	PEP	C2-C1	4.31	1.53	1.49
2	C	268	PEP	C2-C1	4.25	1.53	1.49
2	L	268	PEP	C2-C1	4.22	1.53	1.49
2	K	268	PEP	C2-C1	4.22	1.53	1.49
2	E	268	PEP	C2-C1	4.20	1.53	1.49
2	I	268	PEP	C2-C1	4.13	1.53	1.49
2	B	268	PEP	C2-C1	4.12	1.53	1.49
3	C	269	A5P	P-O1P	3.53	1.61	1.50
3	H	269	A5P	P-O1P	3.53	1.61	1.50
4	D	268	1NT	P-O3P	3.53	1.61	1.50
3	G	269	A5P	P-O1P	3.52	1.61	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	269	A5P	P-O1P	3.52	1.61	1.50
3	E	269	A5P	P-O1P	3.52	1.61	1.50
3	F	269	A5P	P-O1P	3.52	1.61	1.50
3	L	269	A5P	P-O1P	3.52	1.61	1.50
3	J	269	A5P	P-O1P	3.51	1.61	1.50
3	K	269	A5P	P-O1P	3.51	1.61	1.50
3	A	269	A5P	P-O1P	3.50	1.61	1.50
3	I	269	A5P	P-O1P	3.49	1.61	1.50
2	B	268	PEP	C3-C2	2.91	1.39	1.31
2	I	268	PEP	C3-C2	2.89	1.39	1.31
2	J	268	PEP	C3-C2	2.88	1.39	1.31
2	L	268	PEP	C3-C2	2.87	1.39	1.31
2	K	268	PEP	C3-C2	2.86	1.39	1.31
2	C	268	PEP	C3-C2	2.85	1.39	1.31
2	A	268	PEP	C3-C2	2.85	1.39	1.31
2	G	268	PEP	C3-C2	2.85	1.39	1.31
2	H	268	PEP	C3-C2	2.84	1.39	1.31
2	E	268	PEP	C3-C2	2.84	1.39	1.31
2	F	268	PEP	C3-C2	2.81	1.39	1.31
4	D	268	1NT	O3-C2	2.69	1.43	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	269	A5P	O1-C1-C2	4.80	121.24	111.16
3	E	269	A5P	O1-C1-C2	4.74	121.11	111.16
3	G	269	A5P	O1-C1-C2	4.72	121.07	111.16
3	L	269	A5P	O1-C1-C2	4.64	120.89	111.16
3	K	269	A5P	O1-C1-C2	4.62	120.87	111.16
3	B	269	A5P	O1-C1-C2	4.58	120.78	111.16
3	C	269	A5P	O1-C1-C2	4.58	120.77	111.16
3	F	269	A5P	O1-C1-C2	4.53	120.66	111.16
3	H	269	A5P	O1-C1-C2	4.52	120.65	111.16
3	J	269	A5P	O1-C1-C2	4.43	120.46	111.16
3	I	269	A5P	O1-C1-C2	4.38	120.36	111.16
4	D	268	1NT	O2'-C1-C2	-4.03	117.13	123.85
4	D	268	1NT	CI3-CA1-CA2	-3.21	108.88	113.97
3	I	269	A5P	O3P-P-O5	2.88	114.18	106.67
3	C	269	A5P	O3P-P-O5	2.69	113.68	106.67
3	F	269	A5P	O3P-P-O5	2.68	113.66	106.67
3	K	269	A5P	O3P-P-O5	2.64	113.56	106.67
2	A	268	PEP	O1-C1-C2	-2.63	117.83	121.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	268	PEP	O1-C1-C2	-2.61	117.86	121.79
2	E	268	PEP	O1-C1-C2	-2.59	117.89	121.79
3	L	269	A5P	O3P-P-O5	2.57	113.37	106.67
2	F	268	PEP	O1-C1-C2	-2.56	117.92	121.79
2	H	268	PEP	O1-C1-C2	-2.56	117.92	121.79
3	E	269	A5P	O3P-P-O5	2.54	113.30	106.67
2	A	268	PEP	O2'-C1-C2	2.54	118.25	113.91
2	C	268	PEP	O1-C1-C2	-2.51	118.01	121.79
3	G	269	A5P	C4-C3-C2	-2.51	109.40	113.57
2	E	268	PEP	O2'-C1-C2	2.48	118.14	113.91
2	H	268	PEP	O2'-C1-C2	2.47	118.13	113.91
2	I	268	PEP	O1-C1-C2	-2.45	118.09	121.79
2	L	268	PEP	O1-C1-C2	-2.45	118.10	121.79
2	F	268	PEP	O2'-C1-C2	2.44	118.07	113.91
2	K	268	PEP	O1-C1-C2	-2.44	118.11	121.79
3	G	269	A5P	O3P-P-O5	2.41	112.96	106.67
3	A	269	A5P	O3P-P-O5	2.41	112.96	106.67
2	L	268	PEP	O2'-C1-C2	2.41	118.02	113.91
2	G	268	PEP	O2'-C1-C2	2.40	118.01	113.91
2	C	268	PEP	O2'-C1-C2	2.34	117.91	113.91
2	K	268	PEP	O2'-C1-C2	2.32	117.87	113.91
2	J	268	PEP	O1-C1-C2	-2.27	118.37	121.79
2	J	268	PEP	O2'-C1-C2	2.26	117.77	113.91
4	D	268	1NT	OP4-PA-OP2	2.26	112.54	106.44
2	I	268	PEP	O2'-C1-C2	2.19	117.64	113.91
2	B	268	PEP	O1-C1-C2	-2.19	118.49	121.79
3	B	269	A5P	O3P-P-O5	2.13	112.23	106.67
3	H	269	A5P	C4-C3-C2	-2.13	110.03	113.57
3	J	269	A5P	O3P-P-O5	2.12	112.19	106.67
3	K	269	A5P	C4-C3-C2	-2.11	110.06	113.57
2	B	268	PEP	O2'-C1-C2	2.09	117.48	113.91
3	H	269	A5P	O3P-P-O5	2.04	112.00	106.67
3	J	269	A5P	C1-C2-C3	-2.03	108.03	112.17
3	L	269	A5P	C4-C3-C2	-2.02	110.20	113.57
3	C	269	A5P	C4-C3-C2	-2.02	110.20	113.57
3	I	269	A5P	C1-C2-C3	-2.01	108.08	112.17

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	269	A5P	C5-O5-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	269	A5P	C5-O5-P-O1P
3	B	269	A5P	C5-O5-P-O2P
3	B	269	A5P	C5-O5-P-O3P
3	C	269	A5P	C5-O5-P-O2P
3	C	269	A5P	C5-O5-P-O3P
3	E	269	A5P	O1-C1-C2-O2
3	E	269	A5P	C5-O5-P-O1P
3	E	269	A5P	C5-O5-P-O2P
3	E	269	A5P	C5-O5-P-O3P
3	F	269	A5P	C5-O5-P-O2P
3	F	269	A5P	C5-O5-P-O3P
3	G	269	A5P	O1-C1-C2-O2
3	G	269	A5P	O1-C1-C2-C3
3	G	269	A5P	C5-O5-P-O2P
3	G	269	A5P	C5-O5-P-O3P
3	H	269	A5P	O1-C1-C2-C3
3	H	269	A5P	C5-O5-P-O1P
3	H	269	A5P	C5-O5-P-O2P
3	H	269	A5P	C5-O5-P-O3P
3	I	269	A5P	C5-O5-P-O1P
3	I	269	A5P	C5-O5-P-O2P
3	I	269	A5P	C5-O5-P-O3P
3	J	269	A5P	C5-O5-P-O2P
3	J	269	A5P	C5-O5-P-O3P
3	K	269	A5P	C5-O5-P-O1P
3	K	269	A5P	C5-O5-P-O2P
3	K	269	A5P	C5-O5-P-O3P
3	L	269	A5P	O1-C1-C2-C3
3	L	269	A5P	C5-O5-P-O1P
3	L	269	A5P	C5-O5-P-O2P
3	L	269	A5P	C5-O5-P-O3P
4	D	268	1NT	O1-C1-C2-CI3
4	D	268	1NT	O2'-C1-C2-CI3
4	D	268	1NT	O2-C2-CI3-CA1
4	D	268	1NT	C1-C2-CI3-CA1
4	D	268	1NT	O3-C2-CI3-CA1
4	D	268	1NT	CA5-OP4-PA-OP3
4	D	268	1NT	CA5-OP4-PA-OP1
4	D	268	1NT	CA5-OP4-PA-OP2
3	H	269	A5P	O1-C1-C2-O2
3	K	269	A5P	O1-C1-C2-O2
3	L	269	A5P	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	269	A5P	O1-C1-C2-C3
3	F	269	A5P	O1-C1-C2-C3
3	K	269	A5P	O1-C1-C2-C3
3	F	269	A5P	O1-C1-C2-O2
3	A	269	A5P	O1-C1-C2-O2
3	C	269	A5P	O1-C1-C2-O2
3	C	269	A5P	O1-C1-C2-C3
3	A	269	A5P	C5-O5-P-O1P
3	G	269	A5P	C5-O5-P-O1P
3	J	269	A5P	C5-O5-P-O1P
3	B	269	A5P	O1-C1-C2-O2
4	D	268	1NT	C2-O2-P-O3P
3	A	269	A5P	C5-O5-P-O2P
3	A	269	A5P	O1-C1-C2-C3
3	B	269	A5P	O1-C1-C2-C3
3	F	269	A5P	C5-O5-P-O1P
3	A	269	A5P	C1-C2-C3-C4

There are no ring outliers.

22 monomers are involved in 50 short contacts:

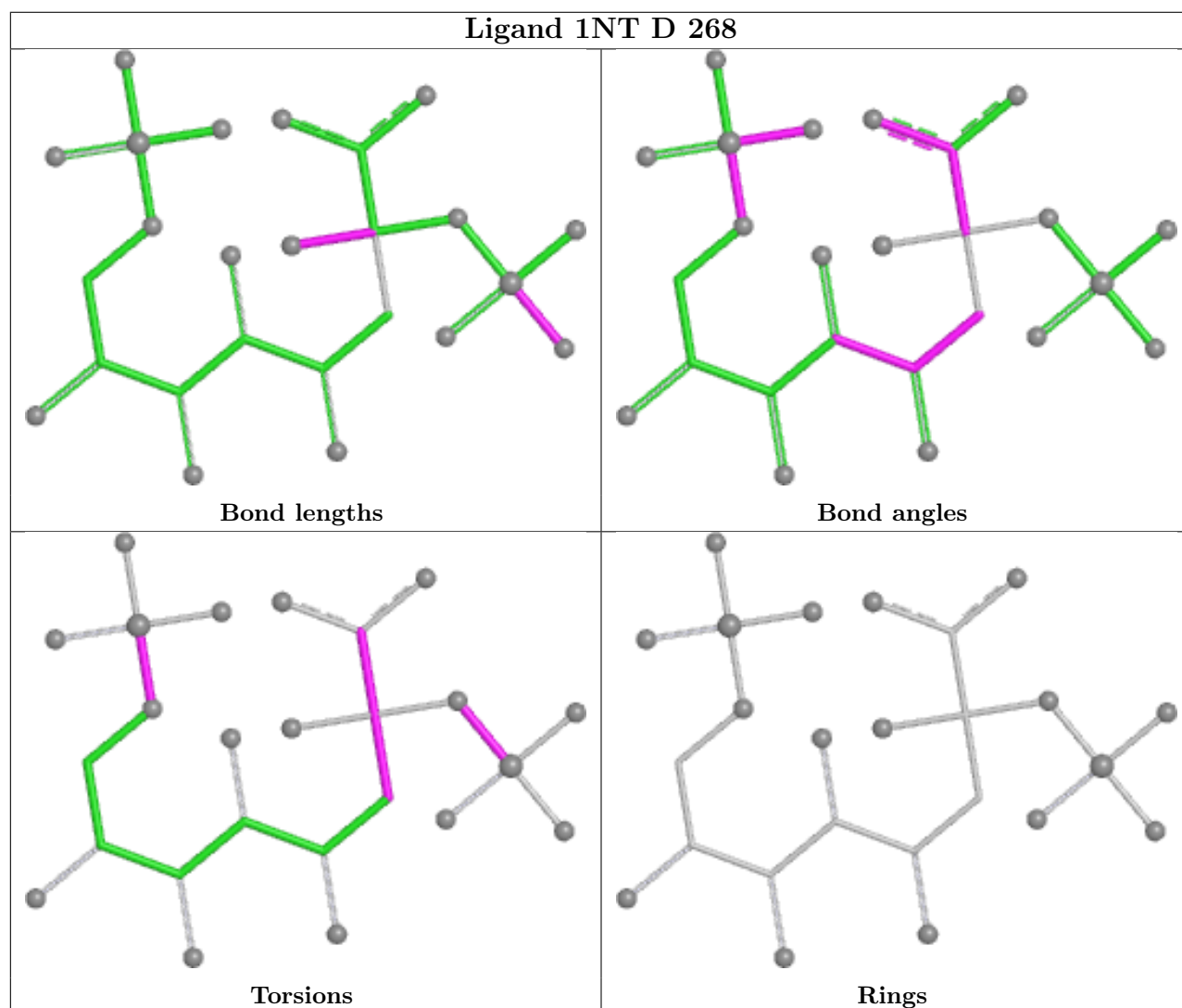
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	269	A5P	3	0
2	K	268	PEP	2	0
3	A	269	A5P	2	0
4	D	268	1NT	3	0
2	C	268	PEP	2	0
2	H	268	PEP	5	0
2	B	268	PEP	4	0
3	G	269	A5P	3	0
3	B	269	A5P	6	0
2	J	268	PEP	3	0
3	H	269	A5P	3	0
2	E	268	PEP	1	0
3	L	269	A5P	1	0
3	J	269	A5P	2	0
2	I	268	PEP	5	0
2	F	268	PEP	2	0
2	A	268	PEP	2	0
3	K	269	A5P	1	0
3	I	269	A5P	3	0
2	L	268	PEP	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	269	A5P	4	0
2	G	268	PEP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	262/267 (98%)	-0.15	6 (2%) 61 64	16, 27, 50, 74	0
1	B	262/267 (98%)	-0.10	10 (3%) 44 46	16, 28, 49, 71	0
1	C	262/267 (98%)	0.76	25 (9%) 14 14	23, 47, 65, 72	0
1	D	262/267 (98%)	1.16	46 (17%) 4 4	24, 52, 72, 79	0
1	E	262/267 (98%)	1.20	56 (21%) 2 2	26, 58, 82, 90	0
1	F	262/267 (98%)	1.44	63 (24%) 2 2	30, 60, 78, 89	0
1	G	262/267 (98%)	0.14	10 (3%) 44 46	19, 32, 61, 86	0
1	H	262/267 (98%)	0.06	12 (4%) 37 39	19, 31, 56, 75	0
1	I	262/267 (98%)	-0.10	7 (2%) 56 59	19, 29, 48, 69	0
1	J	262/267 (98%)	-0.02	13 (4%) 34 36	19, 30, 59, 79	0
1	K	262/267 (98%)	1.42	63 (24%) 2 2	30, 62, 82, 87	0
1	L	262/267 (98%)	0.88	30 (11%) 9 10	26, 50, 68, 86	0
All	All	3144/3204 (98%)	0.56	341 (10%) 11 11	16, 40, 74, 90	0

All (341) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	235	PRO	5.1
1	J	264	ILE	4.7
1	G	194	GLY	4.7
1	H	235	PRO	4.6
1	E	264	ILE	4.5
1	G	264	ILE	4.5
1	H	264	ILE	4.5
1	C	264	ILE	4.4
1	L	264	ILE	4.4
1	E	22	VAL	4.3
1	L	195	ASP	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	67	LEU	4.1
1	F	150	TYR	4.1
1	K	62	TYR	4.1
1	B	264	ILE	4.1
1	H	192	GLY	4.0
1	F	264	ILE	4.0
1	A	264	ILE	3.9
1	B	197	SER	3.9
1	F	191	GLY	3.8
1	L	193	LEU	3.8
1	K	63	GLY	3.8
1	F	94	VAL	3.6
1	E	55	PHE	3.6
1	D	70	VAL	3.6
1	K	18	LEU	3.6
1	I	264	ILE	3.5
1	D	19	LEU	3.5
1	L	235	PRO	3.5
1	B	195	ASP	3.5
1	D	264	ILE	3.5
1	E	191	GLY	3.5
1	D	235	PRO	3.4
1	K	198	GLY	3.4
1	G	196	LYS	3.4
1	F	22	VAL	3.3
1	B	235	PRO	3.3
1	E	90	PRO	3.3
1	F	198	GLY	3.3
1	F	6	VAL	3.3
1	F	70	VAL	3.3
1	D	193	LEU	3.3
1	F	193	LEU	3.3
1	F	196	LYS	3.3
1	A	199	GLY	3.2
1	C	194	GLY	3.2
1	L	55	PHE	3.2
1	D	195	ASP	3.2
1	K	194	GLY	3.2
1	E	86	TRP	3.2
1	D	92	ALA	3.2
1	D	76	LEU	3.2
1	K	195	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	193	LEU	3.1
1	K	243	LEU	3.1
1	H	197	SER	3.1
1	F	195	ASP	3.1
1	L	95	ALA	3.1
1	K	264	ILE	3.1
1	D	196	LYS	3.1
1	K	200	MET	3.1
1	E	64	VAL	3.1
1	K	64	VAL	3.1
1	E	20	LEU	3.1
1	F	26	ILE	3.1
1	H	198	GLY	3.0
1	E	60	LEU	3.0
1	F	141	LEU	3.0
1	J	194	GLY	3.0
1	F	263	THR	3.0
1	H	195	ASP	3.0
1	D	230	ALA	3.0
1	K	19	LEU	3.0
1	K	59	GLY	3.0
1	E	196	LYS	3.0
1	F	55	PHE	3.0
1	F	13	ILE	2.9
1	F	62	TYR	2.9
1	F	249	ALA	2.9
1	A	193	LEU	2.9
1	E	76	LEU	2.9
1	F	194	GLY	2.9
1	K	39	VAL	2.9
1	K	70	VAL	2.9
1	F	220	PHE	2.9
1	C	193	LEU	2.9
1	K	29	LEU	2.9
1	E	70	VAL	2.9
1	K	13	ILE	2.9
1	H	191	GLY	2.9
1	J	198	GLY	2.9
1	E	91	VAL	2.8
1	K	55	PHE	2.8
1	C	195	ASP	2.8
1	L	191	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	67	LEU	2.8
1	F	19	LEU	2.8
1	K	91	VAL	2.8
1	F	149	ILE	2.8
1	E	195	ASP	2.8
1	K	143	PHE	2.8
1	K	220	PHE	2.8
1	E	12	ALA	2.8
1	E	193	LEU	2.8
1	K	20	LEU	2.8
1	K	76	LEU	2.8
1	D	94	VAL	2.8
1	L	197	SER	2.8
1	E	57	GLY	2.8
1	K	74	PHE	2.8
1	D	18	LEU	2.8
1	K	60	LEU	2.8
1	H	190	PRO	2.8
1	D	97	ILE	2.8
1	D	197	SER	2.7
1	D	74	PHE	2.7
1	E	190	PRO	2.7
1	L	39	VAL	2.7
1	D	100	ILE	2.7
1	E	10	PRO	2.7
1	E	52	ILE	2.7
1	L	100	ILE	2.7
1	K	196	LYS	2.7
1	L	196	LYS	2.7
1	I	194	GLY	2.7
1	K	118	GLY	2.7
1	C	234	ALA	2.7
1	K	256	VAL	2.7
1	L	70	VAL	2.7
1	F	176	TRP	2.7
1	E	13	ILE	2.6
1	F	7	ILE	2.6
1	C	86	TRP	2.6
1	D	176	TRP	2.6
1	K	86	TRP	2.6
1	E	47	ALA	2.6
1	D	238	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	189	LEU	2.6
1	G	193	LEU	2.6
1	G	195	ASP	2.6
1	K	197	SER	2.6
1	D	190	PRO	2.6
1	H	193	LEU	2.6
1	J	196	LYS	2.6
1	E	220	PHE	2.6
1	K	38	PHE	2.6
1	D	26	ILE	2.6
1	E	26	ILE	2.6
1	J	235	PRO	2.6
1	C	141	LEU	2.6
1	E	243	LEU	2.6
1	I	193	LEU	2.6
1	J	28	ARG	2.5
1	D	95	ALA	2.5
1	F	235	PRO	2.5
1	F	18	LEU	2.5
1	K	193	LEU	2.5
1	D	200	MET	2.5
1	B	192	GLY	2.5
1	B	198	GLY	2.5
1	C	94	VAL	2.5
1	D	247	ILE	2.5
1	F	91	VAL	2.5
1	I	198	GLY	2.5
1	A	235	PRO	2.5
1	L	146	ALA	2.5
1	D	141	LEU	2.5
1	K	238	LEU	2.5
1	F	200	MET	2.5
1	K	40	PHE	2.5
1	D	86	TRP	2.5
1	H	194	GLY	2.5
1	L	190	PRO	2.5
1	D	20	LEU	2.5
1	D	231	LEU	2.5
1	H	189	LEU	2.5
1	K	121	VAL	2.4
1	G	263	THR	2.4
1	F	67	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	38	PHE	2.4
1	K	33	PHE	2.4
1	L	194	GLY	2.4
1	C	15	SER	2.4
1	G	190	PRO	2.4
1	E	116	LYS	2.4
1	F	115	ALA	2.4
1	I	234	ALA	2.4
1	K	114	ALA	2.4
1	C	19	LEU	2.4
1	D	67	LEU	2.4
1	K	199	GLY	2.4
1	L	198	GLY	2.4
1	K	94	VAL	2.4
1	D	227	PRO	2.4
1	F	234	ALA	2.4
1	K	66	ALA	2.4
1	E	189	LEU	2.4
1	F	222	GLU	2.4
1	A	195	ASP	2.4
1	F	74	PHE	2.4
1	E	97	ILE	2.4
1	L	26	ILE	2.4
1	F	190	PRO	2.4
1	J	190	PRO	2.4
1	D	72	GLU	2.3
1	K	47	ALA	2.3
1	E	231	LEU	2.3
1	J	192	GLY	2.3
1	I	195	ASP	2.3
1	D	64	VAL	2.3
1	F	79	THR	2.3
1	D	16	GLU	2.3
1	K	222	GLU	2.3
1	F	230	ALA	2.3
1	F	111	LEU	2.3
1	F	145	GLY	2.3
1	K	231	LEU	2.3
1	L	60	LEU	2.3
1	C	221	MET	2.3
1	H	196	LYS	2.3
1	F	15	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	22	VAL	2.3
1	D	22	VAL	2.3
1	F	187	VAL	2.3
1	K	138	VAL	2.3
1	E	48	ASN	2.3
1	G	192	GLY	2.3
1	J	193	LEU	2.3
1	K	57	GLY	2.3
1	C	44	PHE	2.3
1	F	250	ILE	2.3
1	D	6	VAL	2.3
1	D	10	PRO	2.3
1	E	113	ALA	2.3
1	K	12	ALA	2.3
1	C	18	LEU	2.3
1	C	20	LEU	2.3
1	F	29	LEU	2.3
1	F	231	LEU	2.3
1	D	55	PHE	2.2
1	E	40	PHE	2.2
1	E	143	PHE	2.2
1	D	138	VAL	2.2
1	F	137	VAL	2.2
1	K	90	PRO	2.2
1	C	198	GLY	2.2
1	E	95	ALA	2.2
1	E	194	GLY	2.2
1	F	192	GLY	2.2
1	L	189	LEU	2.2
1	L	176	TRP	2.2
1	E	51	SER	2.2
1	E	44	PHE	2.2
1	F	143	PHE	2.2
1	C	52	ILE	2.2
1	F	82	ILE	2.2
1	F	122	ASN	2.2
1	K	82	ILE	2.2
1	K	149	ILE	2.2
1	E	94	VAL	2.2
1	K	22	VAL	2.2
1	L	94	VAL	2.2
1	L	145	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	88	ALA	2.2
1	D	189	LEU	2.2
1	L	54	SER	2.2
1	F	132	TRP	2.2
1	D	38	PHE	2.2
1	E	74	PHE	2.2
1	E	100	ILE	2.2
1	E	250	ILE	2.2
1	I	235	PRO	2.2
1	K	239	PRO	2.2
1	C	70	VAL	2.2
1	B	191	GLY	2.2
1	L	192	GLY	2.2
1	E	115	ALA	2.2
1	K	111	LEU	2.2
1	L	20	LEU	2.2
1	C	232	SER	2.2
1	E	46	LYS	2.2
1	F	11	ASN	2.2
1	D	220	PHE	2.1
1	F	121	VAL	2.1
1	D	188	GLN	2.1
1	D	243	LEU	2.1
1	E	19	LEU	2.1
1	K	85	SER	2.1
1	D	40	PHE	2.1
1	F	151	LEU	2.1
1	L	231	LEU	2.1
1	E	236	THR	2.1
1	E	185	HIS	2.1
1	F	180	ILE	2.1
1	L	59	GLY	2.1
1	K	36	VAL	2.1
1	B	196	LYS	2.1
1	K	41	LYS	2.1
1	K	116	LYS	2.1
1	C	47	ALA	2.1
1	E	237	ALA	2.1
1	J	234	ALA	2.1
1	F	20	LEU	2.1
1	L	110	LEU	2.1
1	F	14	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	62	TYR	2.1
1	G	235	PRO	2.1
1	A	198	GLY	2.1
1	E	192	GLY	2.1
1	K	98	ILE	2.1
1	L	250	ILE	2.1
1	D	36	VAL	2.1
1	F	88	ALA	2.1
1	K	42	SER	2.1
1	K	72	GLU	2.0
1	K	92	ALA	2.1
1	K	230	ALA	2.1
1	L	200	MET	2.0
1	C	238	LEU	2.0
1	C	243	LEU	2.0
1	D	29	LEU	2.0
1	E	111	LEU	2.0
1	F	110	LEU	2.0
1	J	195	ASP	2.0
1	B	194	GLY	2.0
1	E	62	TYR	2.0
1	F	144	GLY	2.0
1	G	198	GLY	2.0
1	J	191	GLY	2.0
1	F	98	ILE	2.0
1	E	39	VAL	2.0
1	F	219	VAL	2.0
1	E	15	SER	2.0
1	F	42	SER	2.0
1	J	200	MET	2.0
1	K	241	SER	2.0
1	D	115	ALA	2.0
1	C	231	LEU	2.0
1	E	110	LEU	2.0
1	F	60	LEU	2.0
1	E	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

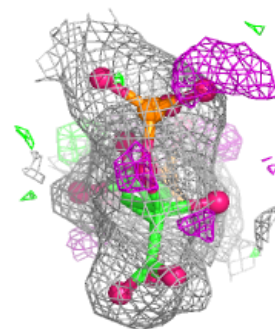
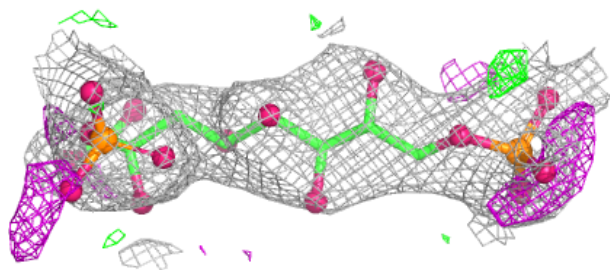
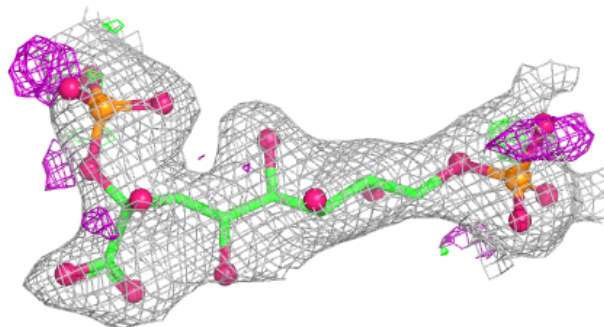
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A5P	L	269	14/14	0.79	0.15	77,78,79,79	0
3	A5P	F	269	14/14	0.81	0.15	77,81,84,85	0
3	A5P	K	269	14/14	0.82	0.13	72,74,75,75	0
3	A5P	E	269	14/14	0.83	0.13	70,72,73,74	0
2	PEP	F	268	10/10	0.85	0.15	62,66,71,72	0
2	PEP	L	268	10/10	0.85	0.16	61,65,66,66	0
4	1NT	D	268	25/25	0.85	0.14	59,64,67,68	0
2	PEP	E	268	10/10	0.88	0.14	63,66,67,67	0
2	PEP	C	268	10/10	0.88	0.14	52,58,65,65	0
2	PEP	K	268	10/10	0.88	0.15	67,70,74,74	0
3	A5P	C	269	14/14	0.90	0.12	53,61,64,65	0
3	A5P	G	269	14/14	0.91	0.12	38,45,48,51	0
2	PEP	J	268	10/10	0.92	0.11	36,39,40,42	0
3	A5P	I	269	14/14	0.92	0.11	35,40,47,47	0
3	A5P	J	269	14/14	0.92	0.11	35,42,47,48	0
2	PEP	H	268	10/10	0.93	0.10	41,46,48,49	0
3	A5P	H	269	14/14	0.94	0.10	41,49,56,58	0
2	PEP	I	268	10/10	0.94	0.10	32,41,45,45	0
3	A5P	A	269	14/14	0.94	0.11	36,46,51,54	0
2	PEP	G	268	10/10	0.95	0.09	35,39,43,43	0
3	A5P	B	269	14/14	0.95	0.08	35,40,45,47	0
2	PEP	B	268	10/10	0.95	0.09	31,37,39,40	0
2	PEP	A	268	10/10	0.96	0.08	30,34,35,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1NT D 268:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.