



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:30 am GMT

PDB ID : 1KFL  
Title : Crystal structure of phenylalanine-regulated 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase (DAHP synthase) from E.coli complexed with Mn<sup>2+</sup>, PEP, and Phe  
Authors : Shumilin, I.A.; Zhao, C.; Bauerle, R.; Kretsinger, R.H.  
Deposited on : 2001-11-21  
Resolution : 2.80 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](mailto: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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

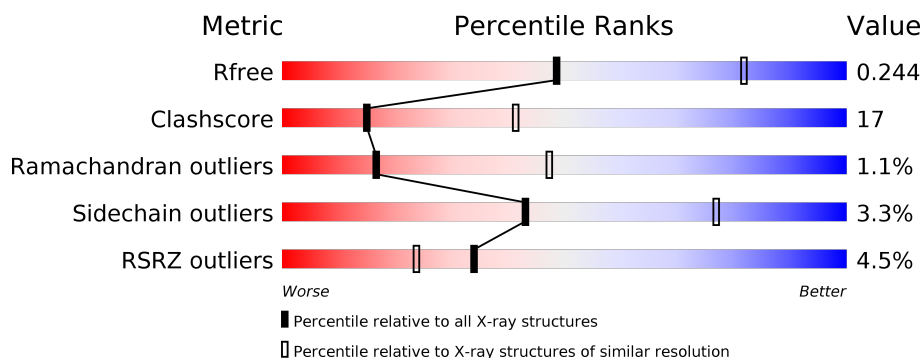
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	350	<div> <div>2%</div> <div>68% 30%</div> <div>.</div> </div>
1	B	350	<div> <div>5%</div> <div>67% 31%</div> <div>.</div> </div>
1	C	350	<div> <div>6%</div> <div>64% 33%</div> <div>.</div> </div>
1	D	350	<div> <div>3%</div> <div>62% 35%</div> <div>.</div> </div>
1	E	350	<div> <div>2%</div> <div>65% 33%</div> <div>..</div> </div>
1	F	350	<div> <div>7%</div> <div>71% 26%</div> <div>.</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	350	
1	H	350	

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
5	PEP	B	2352	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21675 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 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	Se	0	0	0
			2667	1672	474	506	7	8			
1	B	350	Total	C	N	O	S	Se	0	0	0
			2667	1672	474	506	7	8			
1	C	350	Total	C	N	O	S	Se	18	1	0
			2678	1678	478	507	7	8			
1	D	350	Total	C	N	O	S	Se	13	4	0
			2699	1691	481	512	7	8			
1	E	350	Total	C	N	O	S	Se	28	0	0
			2667	1672	474	506	7	8			
1	F	350	Total	C	N	O	S	Se	24	0	0
			2667	1672	474	506	7	8			
1	G	350	Total	C	N	O	S	Se	39	0	0
			2667	1672	474	506	7	8			
1	H	350	Total	C	N	O	S	Se	26	4	0
			2699	1691	481	512	7	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	CLONING ARTIFACT	UNP P00886
A	91	MSE	MET	CLONING ARTIFACT	UNP P00886
A	113	MSE	MET	CLONING ARTIFACT	UNP P00886
A	147	MSE	MET	CLONING ARTIFACT	UNP P00886
A	157	MSE	MET	CLONING ARTIFACT	UNP P00886
A	263	MSE	MET	CLONING ARTIFACT	UNP P00886
A	279	MSE	MET	CLONING ARTIFACT	UNP P00886
A	300	MSE	MET	CLONING ARTIFACT	UNP P00886
B	1	MSE	MET	CLONING ARTIFACT	UNP P00886
B	91	MSE	MET	CLONING ARTIFACT	UNP P00886
B	113	MSE	MET	CLONING ARTIFACT	UNP P00886
B	147	MSE	MET	CLONING ARTIFACT	UNP P00886
B	157	MSE	MET	CLONING ARTIFACT	UNP P00886

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	263	MSE	MET	CLONING ARTIFACT	UNP P00886
B	279	MSE	MET	CLONING ARTIFACT	UNP P00886
B	300	MSE	MET	CLONING ARTIFACT	UNP P00886
C	1	MSE	MET	CLONING ARTIFACT	UNP P00886
C	91	MSE	MET	CLONING ARTIFACT	UNP P00886
C	113	MSE	MET	CLONING ARTIFACT	UNP P00886
C	147	MSE	MET	CLONING ARTIFACT	UNP P00886
C	157	MSE	MET	CLONING ARTIFACT	UNP P00886
C	263	MSE	MET	CLONING ARTIFACT	UNP P00886
C	279	MSE	MET	CLONING ARTIFACT	UNP P00886
C	300	MSE	MET	CLONING ARTIFACT	UNP P00886
D	1	MSE	MET	CLONING ARTIFACT	UNP P00886
D	91	MSE	MET	CLONING ARTIFACT	UNP P00886
D	113	MSE	MET	CLONING ARTIFACT	UNP P00886
D	147	MSE	MET	CLONING ARTIFACT	UNP P00886
D	157	MSE	MET	CLONING ARTIFACT	UNP P00886
D	263	MSE	MET	CLONING ARTIFACT	UNP P00886
D	279	MSE	MET	CLONING ARTIFACT	UNP P00886
D	300	MSE	MET	CLONING ARTIFACT	UNP P00886
E	1	MSE	MET	CLONING ARTIFACT	UNP P00886
E	91	MSE	MET	CLONING ARTIFACT	UNP P00886
E	113	MSE	MET	CLONING ARTIFACT	UNP P00886
E	147	MSE	MET	CLONING ARTIFACT	UNP P00886
E	157	MSE	MET	CLONING ARTIFACT	UNP P00886
E	263	MSE	MET	CLONING ARTIFACT	UNP P00886
E	279	MSE	MET	CLONING ARTIFACT	UNP P00886
E	300	MSE	MET	CLONING ARTIFACT	UNP P00886
F	1	MSE	MET	CLONING ARTIFACT	UNP P00886
F	91	MSE	MET	CLONING ARTIFACT	UNP P00886
F	113	MSE	MET	CLONING ARTIFACT	UNP P00886
F	147	MSE	MET	CLONING ARTIFACT	UNP P00886
F	157	MSE	MET	CLONING ARTIFACT	UNP P00886
F	263	MSE	MET	CLONING ARTIFACT	UNP P00886
F	279	MSE	MET	CLONING ARTIFACT	UNP P00886
F	300	MSE	MET	CLONING ARTIFACT	UNP P00886
G	1	MSE	MET	CLONING ARTIFACT	UNP P00886
G	91	MSE	MET	CLONING ARTIFACT	UNP P00886
G	113	MSE	MET	CLONING ARTIFACT	UNP P00886
G	147	MSE	MET	CLONING ARTIFACT	UNP P00886
G	157	MSE	MET	CLONING ARTIFACT	UNP P00886
G	263	MSE	MET	CLONING ARTIFACT	UNP P00886
G	279	MSE	MET	CLONING ARTIFACT	UNP P00886

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	300	MSE	MET	CLONING ARTIFACT	UNP P00886
H	1	MSE	MET	CLONING ARTIFACT	UNP P00886
H	91	MSE	MET	CLONING ARTIFACT	UNP P00886
H	113	MSE	MET	CLONING ARTIFACT	UNP P00886
H	147	MSE	MET	CLONING ARTIFACT	UNP P00886
H	157	MSE	MET	CLONING ARTIFACT	UNP P00886
H	263	MSE	MET	CLONING ARTIFACT	UNP P00886
H	279	MSE	MET	CLONING ARTIFACT	UNP P00886
H	300	MSE	MET	CLONING ARTIFACT	UNP P00886

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



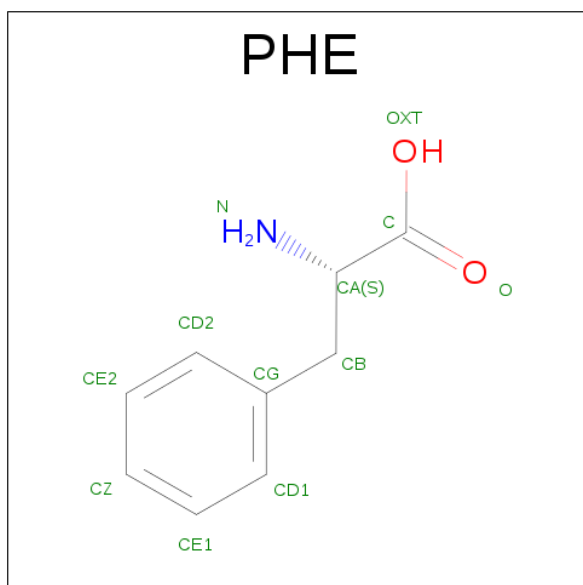
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

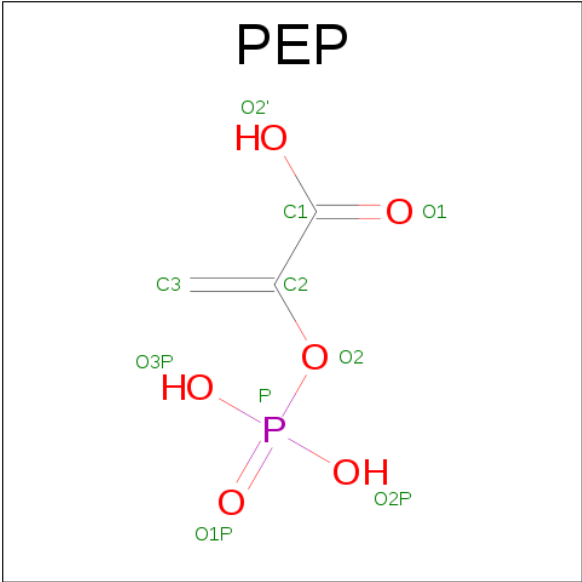
- Molecule 4 is PHENYLALANINE (three-letter code: PHE) (formula:  $C_9H_{11}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	9	1	2		
4	B	1	Total	C	N	O	0	0
			12	9	1	2		
4	C	1	Total	C	N	O	0	0
			12	9	1	2		
4	D	1	Total	C	N	O	0	0
			12	9	1	2		
4	E	1	Total	C	N	O	0	0
			12	9	1	2		
4	F	1	Total	C	N	O	0	0
			12	9	1	2		
4	G	1	Total	C	N	O	0	0
			12	9	1	2		
4	H	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 5 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula:  $C_3H_5O_6P$ ).



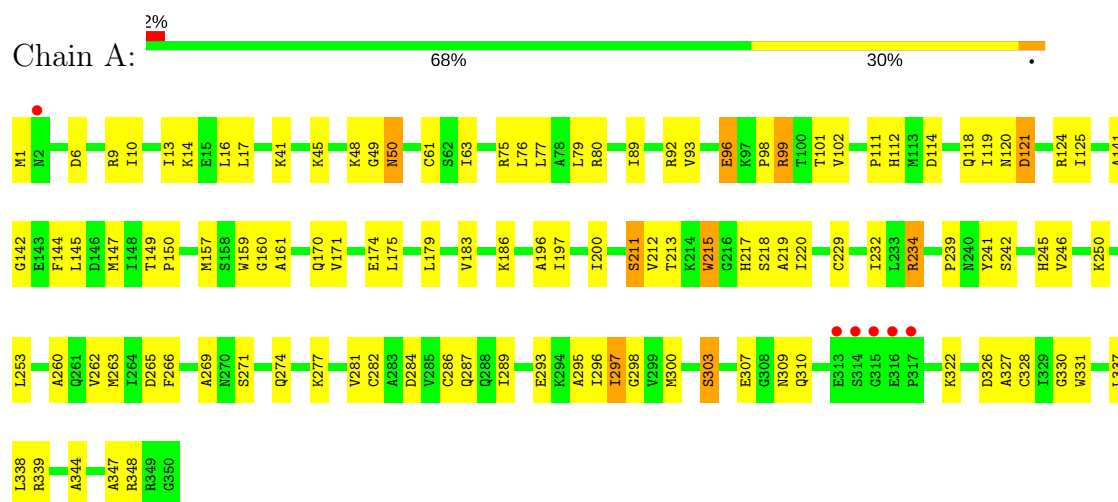


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			10	3	6	1		
5	B	1	Total	C	O	P	0	0
			10	3	6	1		
5	C	1	Total	C	O	P	0	0
			10	3	6	1		
5	D	1	Total	C	O	P	0	0
			10	3	6	1		
5	E	1	Total	C	O	P	0	0
			10	3	6	1		
5	F	1	Total	C	O	P	0	0
			10	3	6	1		
5	G	1	Total	C	O	P	0	0
			10	3	6	1		
5	H	1	Total	C	O	P	0	0
			10	3	6	1		

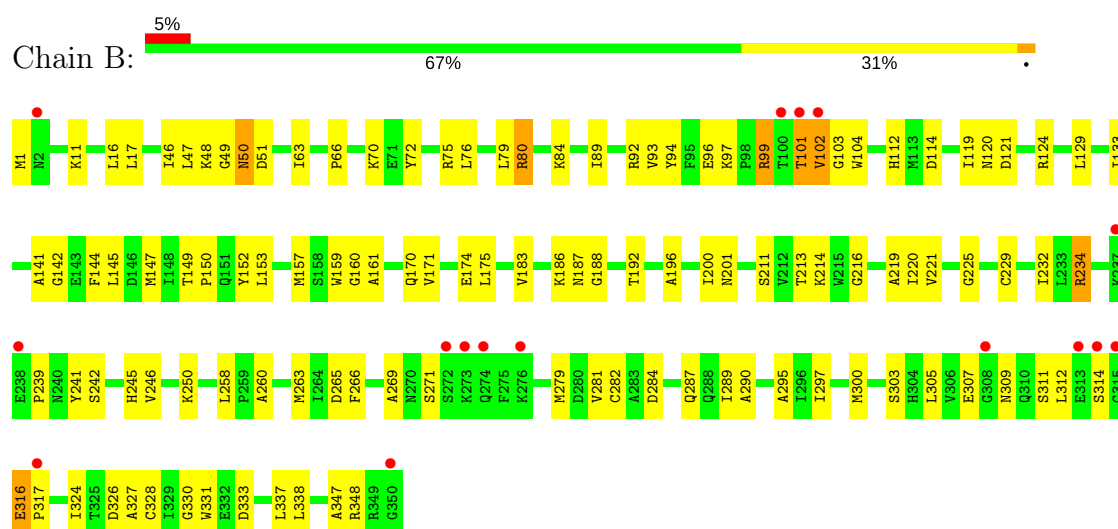
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase

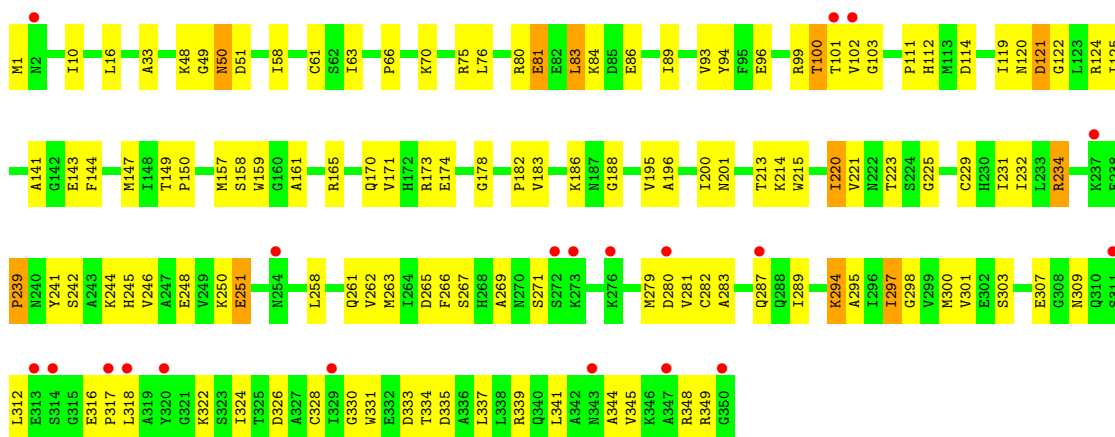


- Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase

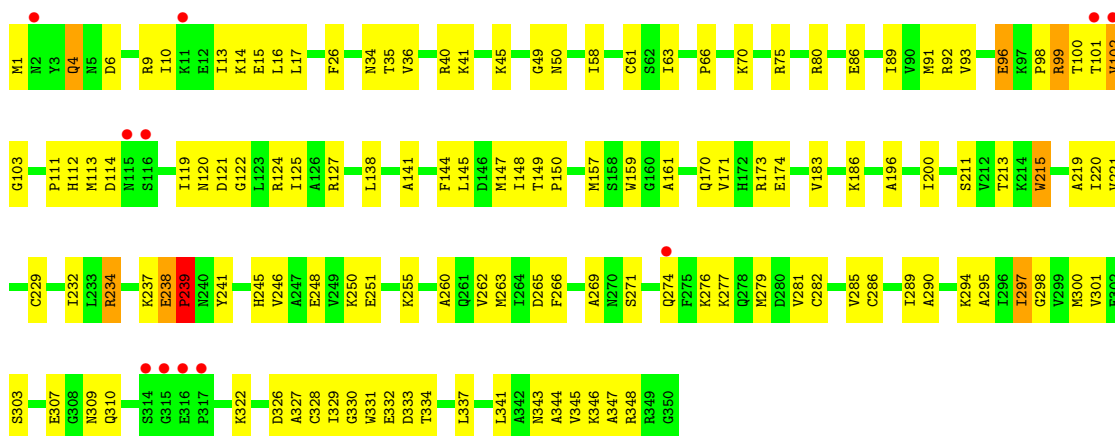


- Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase

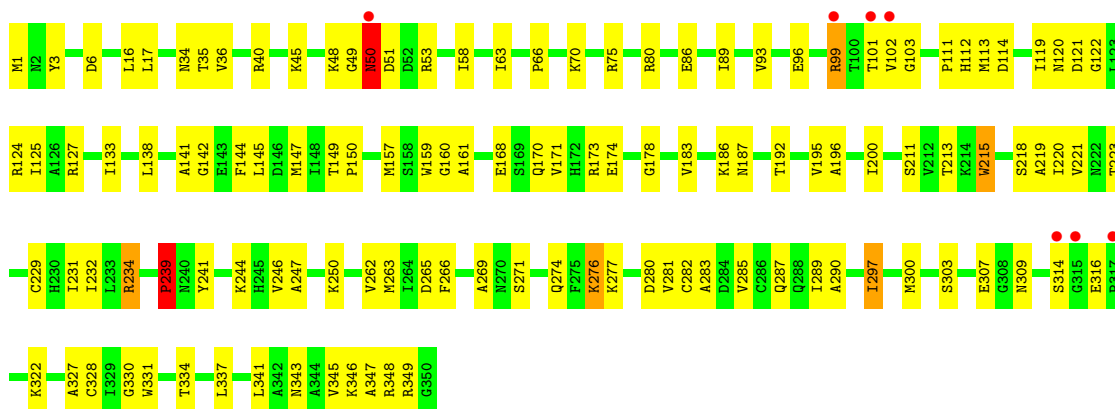




• Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase

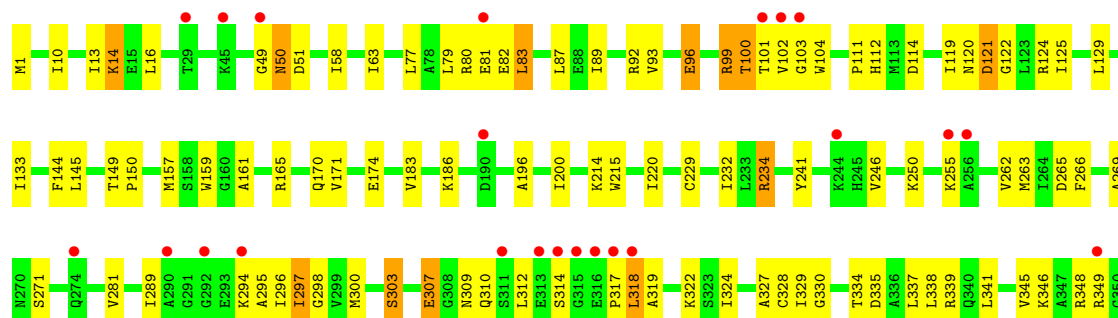


• Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase

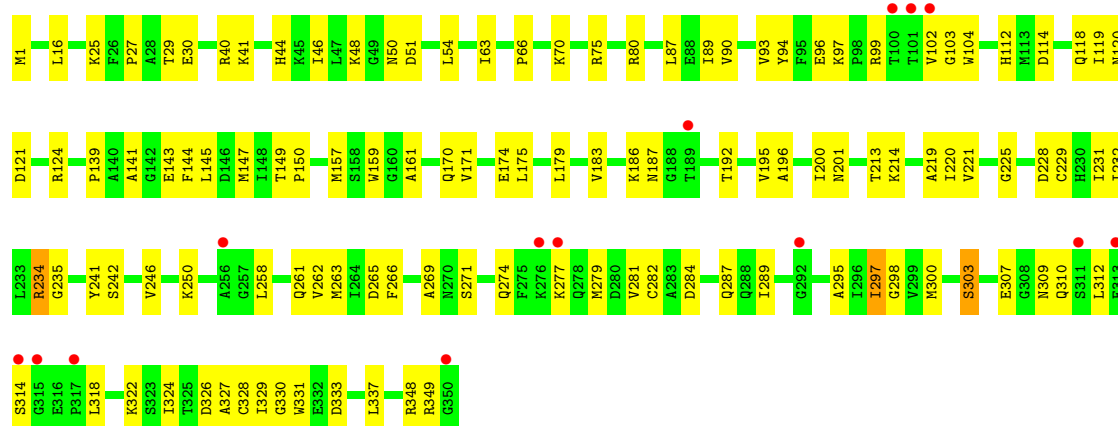


• Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase

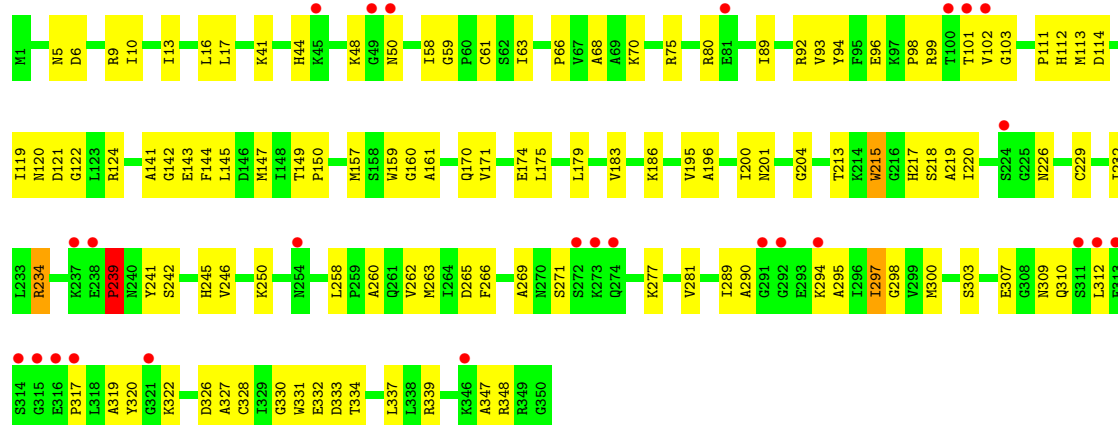




- Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase



- Molecule 1: 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	290.10Å 90.10Å 155.80Å 90.00° 120.77° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.80) 99.3 (20.00-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 2.79Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, $R_{free}$	0.218 , 0.246 0.215 , 0.244	Depositor DCC
$R_{free}$ test set	2598 reflections (3.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 67.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21675	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, PEP, SO4

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	0.44	0/2706	0.67	0/3647
1	B	0.44	0/2706	0.66	0/3647
1	C	0.39	0/2717	0.63	0/3661
1	D	0.43	0/2738	0.64	0/3691
1	E	0.37	0/2706	0.62	0/3647
1	F	0.37	0/2706	0.62	0/3647
1	G	0.36	0/2706	0.60	0/3647
1	H	0.34	0/2738	0.58	0/3691
All	All	0.39	0/21723	0.63	0/29278

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	2667	0	2684	107	0
1	B	2667	0	2684	104	0
1	C	2678	0	2696	121	0
1	D	2699	0	2718	128	0
1	E	2667	0	2684	94	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2667	0	2684	84	0
1	G	2667	0	2685	83	0
1	H	2699	0	2718	89	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
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
3	G	5	0	0	0	0
3	H	15	0	0	0	0
4	A	12	0	8	0	0
4	B	12	0	8	0	0
4	C	12	0	8	0	0
4	D	12	0	8	0	0
4	E	12	0	8	0	0
4	F	12	0	8	0	0
4	G	12	0	8	0	0
4	H	12	0	8	0	0
5	A	10	0	2	0	0
5	B	10	0	2	1	0
5	C	10	0	2	1	0
5	D	10	0	2	1	0
5	E	10	0	2	1	0
5	F	10	0	2	1	0
5	G	10	0	2	0	0
5	H	10	0	2	0	0
All	All	21675	0	21633	727	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 17.

All (727) 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:C:100:THR:HG23	1:C:165[A]:ARG:HH12	1.07	1.08
1:C:294:LYS:HD3	1:C:294:LYS:H	1.16	1.07
1:B:50:ASN:HD22	1:B:50:ASN:N	1.62	0.98
1:F:102:VAL:HG12	1:F:103:GLY:H	1.31	0.94
1:C:102:VAL:HG12	1:C:103:GLY:H	1.30	0.94
1:A:246:VAL:O	1:A:250:LYS:HG3	1.68	0.94
1:E:102:VAL:HG12	1:E:103:GLY:H	1.35	0.92
1:B:102:VAL:HG12	1:B:103:GLY:H	1.35	0.92
1:C:100:THR:HG23	1:C:165[A]:ARG:NH1	1.86	0.90
1:C:246:VAL:O	1:C:250:LYS:HG3	1.74	0.86
1:C:234:ARG:O	1:C:269:ALA:HB3	1.76	0.85
1:F:310:GLN:HE21	1:F:322:LYS:HB3	1.39	0.85
1:F:263:MSE:HE3	1:F:300:MSE:HB2	1.58	0.84
1:H:246:VAL:O	1:H:250:LYS:HG3	1.78	0.83
1:H:263:MSE:HE3	1:H:300:MSE:HB2	1.63	0.81
1:G:80:ARG:HA	1:G:89:ILE:HD12	1.63	0.81
1:C:16:LEU:HD11	1:C:119:ILE:HD13	1.64	0.80
1:F:246:VAL:O	1:F:250:LYS:HG3	1.81	0.80
1:D:250:LYS:HD3	1:D:295:ALA:CB	2.12	0.79
1:E:234:ARG:O	1:E:269:ALA:HB3	1.83	0.79
1:D:289:ILE:O	1:D:348:ARG:HB2	1.83	0.79
1:C:312:LEU:HD12	1:C:318:LEU:HD11	1.65	0.78
1:D:251:GLU:O	1:D:255:LYS:HG3	1.84	0.78
1:C:119:ILE:HD12	1:D:220:ILE:HD12	1.66	0.78
1:C:186:LYS:HD3	1:C:234:ARG:HG2	1.65	0.77
1:B:234:ARG:O	1:B:269:ALA:HB3	1.84	0.77
1:H:234:ARG:O	1:H:269:ALA:HB3	1.84	0.77
1:C:63:ILE:HD12	1:C:93:VAL:HG13	1.65	0.77
1:F:234:ARG:O	1:F:269:ALA:HB3	1.85	0.76
1:A:220:ILE:HD12	1:B:119:ILE:HD12	1.69	0.75
1:C:263:MSE:HE3	1:C:300:MSE:HB2	1.69	0.75
1:B:232:ILE:HG23	1:B:263:MSE:HE2	1.69	0.75
1:A:262:VAL:O	1:A:297:ILE:HD13	1.87	0.74
1:F:186:LYS:HD3	1:F:234:ARG:HG2	1.68	0.74
1:H:63:ILE:HD12	1:H:93:VAL:HG13	1.70	0.74
1:C:312:LEU:HD13	1:C:324:ILE:HD12	1.70	0.73
1:D:49:GLY:C	1:D:50:ASN:HD22	1.92	0.73
1:F:289:ILE:O	1:F:348:ARG:HB2	1.87	0.73
1:D:307:GLU:HB3	1:D:330:GLY:N	2.04	0.72
1:C:33:ALA:HB1	1:D:4:GLN:HG2	1.71	0.72
1:B:63:ILE:HD12	1:B:93:VAL:HG13	1.72	0.72
1:D:80:ARG:HA	1:D:89:ILE:HD12	1.71	0.72

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:ILE:HD12	1:F:93:VAL:HG13	1.71	0.72
1:D:348:ARG:O	1:D:348:ARG:HG2	1.87	0.72
1:E:63:ILE:HD12	1:E:93:VAL:HG13	1.72	0.72
1:A:310:GLN:NE2	1:A:322:LYS:HB3	2.05	0.71
1:C:232:ILE:HG23	1:C:263:MSE:HE2	1.70	0.71
1:H:196:ALA:O	1:H:200:ILE:HG13	1.90	0.71
1:B:232:ILE:CG2	1:B:263:MSE:HE2	2.22	0.70
1:H:102[B]:VAL:HG12	1:H:103:GLY:N	2.02	0.70
1:B:50:ASN:N	1:B:50:ASN:ND2	2.34	0.70
1:D:196:ALA:O	1:D:200:ILE:HG13	1.92	0.70
1:E:170:GLN:O	1:E:174:GLU:HG3	1.91	0.70
1:F:170:GLN:O	1:F:174:GLU:HG3	1.92	0.70
1:F:58:ILE:HD11	1:F:334:THR:HG23	1.72	0.70
1:C:1:MSE:HE2	1:D:215:TRP:HH2	1.55	0.70
1:G:263:MSE:HE3	1:G:300:MSE:HB2	1.73	0.70
1:B:186:LYS:HD3	1:B:234:ARG:HG2	1.72	0.69
1:E:307:GLU:HB3	1:E:330:GLY:N	2.06	0.69
1:B:49:GLY:C	1:B:50:ASN:HD22	1.96	0.69
1:B:16:LEU:HD11	1:B:119:ILE:HD13	1.75	0.69
1:G:201:ASN:OD1	1:G:258:LEU:HD21	1.93	0.69
1:H:309:ASN:HB3	1:H:327:ALA:HA	1.75	0.68
1:E:50:ASN:N	1:E:50:ASN:HD22	1.91	0.68
1:D:102[B]:VAL:HG12	1:D:103:GLY:N	2.08	0.68
1:H:307:GLU:HB3	1:H:330:GLY:N	2.08	0.68
1:B:80:ARG:HA	1:B:89:ILE:HD12	1.75	0.68
1:G:112:HIS:HB2	1:G:114:ASP:OD1	1.93	0.68
1:G:289:ILE:O	1:G:348:ARG:HB2	1.93	0.68
1:B:282:CYS:SG	1:B:337:LEU:HG	2.34	0.68
1:C:201:ASN:OD1	1:C:258:LEU:HD21	1.94	0.67
1:D:234:ARG:O	1:D:269:ALA:HB3	1.94	0.67
1:F:310:GLN:NE2	1:F:322:LYS:HB3	2.10	0.67
1:C:48:LYS:HE3	1:C:50:ASN:OD1	1.95	0.67
1:G:119:ILE:HD12	1:H:220:ILE:HD12	1.77	0.67
1:E:232:ILE:HG23	1:E:263:MSE:HE2	1.77	0.67
1:A:310:GLN:HE21	1:A:322:LYS:HB3	1.59	0.66
1:A:50:ASN:HD22	1:A:50:ASN:N	1.93	0.66
1:H:112:HIS:HB2	1:H:114:ASP:OD1	1.95	0.66
1:H:232:ILE:HG23	1:H:263:MSE:HE2	1.76	0.66
1:C:220:ILE:HG12	1:D:119:ILE:HG21	1.75	0.66
1:H:170:GLN:O	1:H:174:GLU:HG3	1.95	0.66
1:A:196:ALA:O	1:A:200:ILE:HG13	1.94	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:PRO:O	1:C:70:LYS:HG3	1.95	0.66
1:E:220:ILE:HD12	1:F:119:ILE:HD12	1.77	0.66
1:A:232:ILE:HG12	1:A:263:MSE:HE2	1.78	0.66
1:B:84:LYS:NZ	1:B:84:LYS:HB3	2.11	0.66
1:D:246:VAL:O	1:D:250:LYS:HG3	1.96	0.65
1:C:86:GLU:HG3	1:C:349:ARG:NH1	2.10	0.65
1:E:289:ILE:O	1:E:348:ARG:HB2	1.97	0.65
1:C:170:GLN:O	1:C:174:GLU:HG3	1.97	0.65
1:E:262:VAL:O	1:E:297:ILE:HD13	1.97	0.65
1:G:234:ARG:O	1:G:269:ALA:HB3	1.96	0.65
1:C:220:ILE:CD1	1:D:119:ILE:HG21	2.27	0.65
1:E:263:MSE:HE3	1:E:300:MSE:HB2	1.78	0.65
1:B:112:HIS:HB2	1:B:114:ASP:OD1	1.98	0.64
1:B:170:GLN:O	1:B:174:GLU:HG3	1.96	0.64
1:A:119:ILE:HG21	1:B:220:ILE:CD1	2.27	0.64
1:F:102:VAL:HG12	1:F:103:GLY:N	2.08	0.64
1:G:144:PHE:HZ	1:G:157:MSE:HG3	1.63	0.64
1:A:289:ILE:O	1:A:348:ARG:HB2	1.98	0.64
1:C:112:HIS:HB2	1:C:114:ASP:OD1	1.98	0.64
1:E:145:LEU:O	1:F:171:VAL:HG21	1.97	0.64
1:G:232:ILE:HG23	1:G:263:MSE:HE2	1.79	0.64
1:C:232:ILE:CG2	1:C:263:MSE:HE2	2.28	0.64
1:B:263:MSE:HE3	1:B:300:MSE:HB2	1.81	0.63
1:E:173:ARG:NH1	1:F:100:THR:HG22	2.14	0.63
1:C:294:LYS:N	1:C:294:LYS:HD3	2.00	0.63
1:C:220:ILE:CG1	1:D:16:LEU:HD13	2.29	0.63
1:A:16:LEU:HD13	1:B:220:ILE:CG1	2.29	0.62
1:A:234:ARG:O	1:A:269:ALA:HB3	1.99	0.62
1:G:63:ILE:HD12	1:G:93:VAL:HG13	1.81	0.62
1:A:80:ARG:HA	1:A:89:ILE:HD12	1.81	0.62
1:G:196:ALA:O	1:G:200:ILE:HG13	2.00	0.62
1:B:307:GLU:HB3	1:B:330:GLY:N	2.15	0.62
1:D:102[A]:VAL:HG12	1:D:103:GLY:N	2.15	0.61
1:B:186:LYS:NZ	1:B:300:MSE:HE1	2.15	0.61
1:B:316:GLU:HG3	1:B:317:PRO:HD2	1.82	0.61
1:E:232:ILE:CG2	1:E:263:MSE:HE2	2.31	0.61
1:F:13:ILE:O	1:F:14:LYS:HE2	2.00	0.61
1:E:119:ILE:HD12	1:F:220:ILE:HD12	1.81	0.61
1:D:120:ASN:O	1:D:124:ARG:HG3	2.00	0.61
1:A:147:MSE:HE3	1:A:171:VAL:HG11	1.81	0.61
1:A:339:ARG:HH11	1:A:339:ARG:HG2	1.65	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:VAL:HG12	1:C:103:GLY:N	2.09	0.61
1:C:80:ARG:HA	1:C:89:ILE:HD12	1.81	0.61
1:G:16:LEU:HD11	1:G:119:ILE:HD13	1.80	0.61
1:F:196:ALA:O	1:F:200:ILE:HG13	2.00	0.61
1:C:144:PHE:HZ	1:C:157:MSE:HG3	1.66	0.60
1:A:14:LYS:HE3	1:B:220:ILE:CD1	2.31	0.60
1:D:213:THR:HG23	1:D:219:ALA:HB2	1.82	0.60
1:D:250:LYS:HD3	1:D:295:ALA:HB2	1.82	0.60
1:D:63:ILE:HD12	1:D:93:VAL:HG13	1.82	0.60
1:E:102:VAL:HG12	1:E:103:GLY:N	2.12	0.60
1:D:232:ILE:HG23	1:D:263:MSE:HE2	1.83	0.60
1:A:265:ASP:CG	1:A:300:MSE:HE2	2.22	0.60
1:F:232:ILE:HG23	1:F:263:MSE:HE2	1.84	0.60
1:H:68:ALA:HA	1:H:320:TYR:OH	2.01	0.60
1:D:99:ARG:HG3	1:D:101[B]:THR:O	2.01	0.60
1:D:159:TRP:CH2	1:D:161:ALA:HB2	2.37	0.60
1:D:112:HIS:HB2	1:D:114:ASP:OD1	2.01	0.60
1:H:289:ILE:O	1:H:348:ARG:HB2	2.02	0.60
1:C:309:ASN:O	1:C:322:LYS:HE2	2.02	0.60
1:C:173:ARG:NH1	1:D:100[B]:THR:HG22	2.17	0.60
1:E:86:GLU:HA	1:E:349:ARG:HH22	1.67	0.60
1:B:147:MSE:HE3	1:B:171:VAL:HG11	1.83	0.59
1:C:215:TRP:HH2	1:D:1:MSE:HE2	1.67	0.59
1:B:303:SER:HA	1:B:328:CYS:HB3	1.83	0.59
1:A:14:LYS:HG3	1:B:220:ILE:HD12	1.83	0.59
1:D:307:GLU:HB3	1:D:330:GLY:H	1.66	0.59
1:C:279:MSE:SE	1:C:333:ASP:HB3	2.52	0.59
1:B:196:ALA:O	1:B:200:ILE:HG13	2.02	0.59
1:B:84:LYS:HZ3	1:B:84:LYS:HB3	1.67	0.59
1:G:46:ILE:HG12	1:G:51:ASP:HB3	1.84	0.59
1:G:66:PRO:O	1:G:70:LYS:HG3	2.03	0.59
1:H:250:LYS:HD2	1:H:295:ALA:CB	2.33	0.59
1:A:274:GLN:OE1	1:A:277:LYS:HE2	2.03	0.59
1:D:310:GLN:NE2	1:D:322:LYS:HB3	2.17	0.59
1:H:80:ARG:HA	1:H:89:ILE:HD12	1.84	0.59
1:C:81:GLU:O	1:C:84:LYS:HB3	2.03	0.59
1:E:48:LYS:HE3	1:E:50:ASN:OD1	2.03	0.59
1:F:144:PHE:HZ	1:F:157:MSE:HG3	1.67	0.59
1:F:80:ARG:HA	1:F:89:ILE:HD12	1.84	0.59
1:G:170:GLN:O	1:G:174:GLU:HG3	2.02	0.59
1:E:266:PHE:O	1:E:271:SER:HB2	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:ILE:CG2	1:G:263:MSE:HE2	2.33	0.58
1:C:196:ALA:O	1:C:200:ILE:HG13	2.04	0.58
1:H:186:LYS:HD3	1:H:234:ARG:HG2	1.83	0.58
1:G:262:VAL:O	1:G:297:ILE:HD13	2.03	0.58
1:B:144:PHE:HZ	1:B:157:MSE:HG3	1.69	0.58
1:A:309:ASN:HB3	1:A:327:ALA:HA	1.85	0.58
1:A:63:ILE:HD12	1:A:93:VAL:HG13	1.86	0.58
1:C:225:GLY:O	1:D:9:ARG:HD3	2.02	0.58
1:H:332:GLU:HG2	1:H:333:ASP:H	1.68	0.58
1:E:274:GLN:HB3	1:E:276:LYS:NZ	2.19	0.58
1:F:112:HIS:HB2	1:F:114:ASP:OD1	2.02	0.58
1:G:186:LYS:HD3	1:G:234:ARG:HG2	1.86	0.58
1:G:307:GLU:HB3	1:G:330:GLY:N	2.19	0.58
1:H:201:ASN:OD1	1:H:258:LEU:HD21	2.04	0.57
1:F:310:GLN:NE2	1:F:319:ALA:HB3	2.20	0.57
1:C:1:MSE:HE2	1:D:215:TRP:CH2	2.37	0.57
1:D:141:ALA:HB1	1:D:159:TRP:HE3	1.69	0.57
1:H:113:MSE:HB3	1:H:312:LEU:HD21	1.86	0.57
1:C:266:PHE:O	1:C:271:SER:HB2	2.04	0.57
1:E:49:GLY:O	1:E:51:ASP:N	2.36	0.57
1:A:76:LEU:HD11	1:A:89:ILE:HG21	1.84	0.57
1:B:246:VAL:O	1:B:250:LYS:HG3	2.04	0.57
1:H:262:VAL:O	1:H:297:ILE:HD13	2.05	0.57
1:G:274:GLN:OE1	1:G:277:LYS:HE2	2.04	0.57
1:C:220:ILE:HG13	1:D:16:LEU:HD13	1.86	0.57
1:D:144:PHE:HZ	1:D:157:MSE:HG3	1.69	0.57
1:H:266:PHE:O	1:H:271:SER:HB2	2.05	0.57
1:A:10:ILE:HD12	1:B:221:VAL:CG1	2.35	0.56
1:C:50:ASN:N	1:C:50:ASN:HD22	2.02	0.56
1:H:232:ILE:CG2	1:H:263:MSE:HE2	2.35	0.56
1:C:220:ILE:HD12	1:D:14:LYS:HG3	1.87	0.56
1:D:274:GLN:OE1	1:D:277:LYS:HE2	2.05	0.56
1:E:196:ALA:O	1:E:200:ILE:HG13	2.04	0.56
1:B:309:ASN:HB3	1:B:327:ALA:HA	1.87	0.56
1:E:348:ARG:O	1:E:348:ARG:HG2	2.05	0.56
1:E:50:ASN:N	1:E:50:ASN:ND2	2.53	0.56
1:C:294:LYS:H	1:C:294:LYS:CD	1.92	0.56
1:E:186:LYS:HZ1	1:E:300:MSE:HE1	1.71	0.56
1:E:173:ARG:HH12	1:F:100:THR:HG22	1.69	0.56
1:E:120:ASN:O	1:E:124:ARG:HG3	2.05	0.56
1:C:220:ILE:CG1	1:D:119:ILE:HG21	2.36	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:MSE:HE3	1:D:171:VAL:HG11	1.86	0.56
1:E:285:VAL:O	1:E:289:ILE:HG13	2.06	0.56
1:G:144:PHE:CZ	1:G:157:MSE:HG3	2.40	0.56
1:B:250:LYS:HD2	1:B:295:ALA:CB	2.36	0.56
1:G:159:TRP:CH2	1:G:161:ALA:HB2	2.41	0.56
1:A:112:HIS:HB2	1:A:114:ASP:OD1	2.05	0.56
1:G:40:ARG:NH1	1:H:5:ASN:HB3	2.20	0.56
1:H:310:GLN:HE21	1:H:322:LYS:HB3	1.71	0.56
1:A:9:ARG:HD3	1:B:225:GLY:O	2.06	0.56
1:A:49:GLY:C	1:A:50:ASN:HD22	2.10	0.55
1:D:66:PRO:O	1:D:70:LYS:HG3	2.06	0.55
1:E:265:ASP:CG	1:E:300:MSE:HE2	2.26	0.55
1:G:120:ASN:O	1:G:124:ARG:HG3	2.07	0.55
1:B:66:PRO:O	1:B:70:LYS:HG3	2.05	0.55
1:B:265:ASP:CG	1:B:300:MSE:HE2	2.27	0.55
1:G:186:LYS:NZ	1:G:300:MSE:HE1	2.21	0.55
1:B:129:LEU:O	1:B:133:ILE:HG13	2.07	0.55
1:E:246:VAL:O	1:E:250:LYS:HG3	2.06	0.55
1:C:248:GLU:O	1:C:251:GLU:HB2	2.06	0.55
1:C:147:MSE:HE3	1:C:171:VAL:HG11	1.88	0.55
1:E:1:MSE:HE2	1:F:215:TRP:HH2	1.72	0.55
1:D:50:ASN:HD22	1:D:50:ASN:N	2.00	0.55
1:C:220:ILE:HG12	1:D:119:ILE:HD13	1.88	0.55
1:A:101:THR:HG22	1:A:102:VAL:HG23	1.89	0.55
1:H:250:LYS:HD2	1:H:295:ALA:HB2	1.89	0.55
1:B:311:SER:HB3	1:B:314:SER:HB3	1.89	0.55
1:F:341:LEU:O	1:F:345:VAL:HG23	2.06	0.55
1:H:303:SER:HA	1:H:328:CYS:HB3	1.89	0.55
1:A:287:GLN:OE1	1:A:287:GLN:HA	2.07	0.54
1:C:283:ALA:O	1:C:287:GLN:HG3	2.07	0.54
1:C:289:ILE:O	1:C:348:ARG:HB2	2.07	0.54
1:D:238:GLU:N	1:D:238:GLU:CD	2.60	0.54
1:B:266:PHE:O	1:B:271:SER:HB2	2.05	0.54
1:C:173:ARG:HH12	1:D:100[B]:THR:HG22	1.73	0.54
1:D:262:VAL:O	1:D:297:ILE:HD13	2.08	0.54
1:B:120:ASN:O	1:B:124:ARG:HG3	2.07	0.54
1:E:186:LYS:HD3	1:E:234:ARG:HG2	1.88	0.54
1:H:141:ALA:HB1	1:H:159:TRP:HE3	1.71	0.54
1:H:307:GLU:HB3	1:H:330:GLY:H	1.71	0.54
1:A:215:TRP:HH2	1:B:1:MSE:HE2	1.72	0.54
1:D:237:LYS:HB2	1:D:238:GLU:OE1	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:PHE:HZ	1:E:157:MSE:HG3	1.73	0.54
1:A:307:GLU:HB3	1:A:330:GLY:H	1.73	0.54
1:G:75:ARG:HB3	1:G:331:TRP:CZ2	2.43	0.54
1:A:98:PRO:HA	1:B:170:GLN:NE2	2.23	0.54
1:B:250:LYS:HB3	1:B:260:ALA:HB1	1.90	0.54
1:E:149:THR:N	1:E:150:PRO:CD	2.71	0.54
1:F:79:LEU:O	1:F:83:LEU:HG	2.06	0.54
1:C:58:ILE:HD11	1:C:334:THR:HG23	1.89	0.54
1:E:112:HIS:HB2	1:E:114:ASP:OD1	2.08	0.54
1:C:341:LEU:O	1:C:345:VAL:HG23	2.08	0.54
1:B:337:LEU:C	1:B:337:LEU:HD23	2.29	0.53
1:B:72:TYR:HA	1:B:305:LEU:HD21	1.89	0.53
1:H:310:GLN:NE2	1:H:322:LYS:HB3	2.23	0.53
1:B:159:TRP:CH2	1:B:161:ALA:HB2	2.43	0.53
1:C:265:ASP:CG	1:C:300:MSE:HE2	2.29	0.53
1:D:341:LEU:O	1:D:345:VAL:HG23	2.09	0.53
1:B:99:ARG:HG3	1:B:101:THR:O	2.09	0.53
1:C:144:PHE:CZ	1:C:157:MSE:HG3	2.43	0.53
1:D:332:GLU:HG2	1:D:333:ASP:H	1.73	0.53
1:G:303:SER:HA	1:G:328:CYS:HB3	1.90	0.53
1:H:242:SER:OG	1:H:245:HIS:CD2	2.62	0.53
1:C:100:THR:HG22	1:D:173:ARG:NH1	2.23	0.53
1:E:183:VAL:O	1:E:229:CYS:HA	2.09	0.53
1:B:102:VAL:HG12	1:B:103:GLY:N	2.14	0.53
1:D:265:ASP:CG	1:D:300:MSE:HE2	2.30	0.53
1:F:310:GLN:HG3	1:F:324:ILE:HG22	1.91	0.53
1:A:303:SER:HA	1:A:328:CYS:HB3	1.91	0.52
1:C:63:ILE:CD1	1:C:93:VAL:HG13	2.39	0.52
1:E:170:GLN:OE1	1:F:165:ARG:NH2	2.35	0.52
1:F:266:PHE:O	1:F:271:SER:HB2	2.08	0.52
1:C:75:ARG:HB3	1:C:331:TRP:CZ2	2.45	0.52
1:F:144:PHE:CZ	1:F:157:MSE:HG3	2.45	0.52
1:H:144:PHE:HZ	1:H:157:MSE:HG3	1.73	0.52
1:D:232:ILE:CG2	1:D:263:MSE:HE2	2.40	0.52
1:A:274:GLN:CD	1:A:277:LYS:HE2	2.30	0.52
1:C:241:TYR:CG	1:C:281:VAL:HG13	2.45	0.52
1:D:144:PHE:CZ	1:D:157:MSE:HG3	2.44	0.52
1:C:171:VAL:HG21	1:D:145:LEU:O	2.10	0.52
1:E:274:GLN:HB3	1:E:276:LYS:HD2	1.92	0.52
1:G:266:PHE:O	1:G:271:SER:HB2	2.10	0.52
1:A:41:LYS:HE2	1:A:45:LYS:HE3	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LYS:HD3	1:C:295:ALA:CB	2.39	0.52
1:G:1:MSE:HE2	1:H:215:TRP:HH2	1.75	0.52
1:H:175:LEU:HD11	1:H:179:LEU:HD21	1.90	0.52
1:B:242:SER:OG	1:B:245:HIS:CD2	2.63	0.52
1:C:159:TRP:CH2	1:C:161:ALA:HB2	2.45	0.52
1:F:50:ASN:HD22	1:F:50:ASN:N	2.07	0.52
1:B:232:ILE:HG12	1:B:263:MSE:HE2	1.90	0.52
1:A:141:ALA:HB1	1:A:159:TRP:HE3	1.75	0.51
1:D:285:VAL:O	1:D:289:ILE:HG13	2.09	0.51
1:F:309:ASN:HB3	1:F:327:ALA:HA	1.92	0.51
1:C:76:LEU:HD11	1:C:89:ILE:HG21	1.92	0.51
1:E:341:LEU:O	1:E:345:VAL:HG23	2.10	0.51
1:E:171:VAL:HG21	1:F:145:LEU:O	2.10	0.51
1:G:145:LEU:O	1:H:171:VAL:HG21	2.10	0.51
1:A:186:LYS:HD3	1:A:234:ARG:HG2	1.91	0.51
1:H:102[A]:VAL:HG12	1:H:103:GLY:N	2.24	0.51
1:H:149:THR:N	1:H:150:PRO:CD	2.73	0.51
1:H:213:THR:HG23	1:H:219:ALA:HB2	1.92	0.51
1:B:284:ASP:O	1:B:287:GLN:HB3	2.09	0.51
1:D:241:TYR:CG	1:D:281:VAL:HG13	2.46	0.51
1:H:307:GLU:HB3	1:H:330:GLY:CA	2.41	0.51
1:E:213:THR:HG23	1:E:219:ALA:HB2	1.93	0.51
1:F:232:ILE:CG2	1:F:263:MSE:HE2	2.39	0.51
1:H:239:PRO:HB3	1:H:241:TYR:CE2	2.46	0.51
1:B:76:LEU:HD11	1:B:89:ILE:HG21	1.92	0.51
1:E:186:LYS:NZ	1:E:300:MSE:HE1	2.25	0.51
1:F:294:LYS:HG2	1:F:348:ARG:HD3	1.92	0.51
1:D:282:CYS:SG	1:D:337:LEU:HG	2.51	0.51
1:E:159:TRP:CH2	1:E:161:ALA:HB2	2.46	0.51
1:G:309:ASN:O	1:G:322:LYS:HE2	2.11	0.51
1:C:282:CYS:SG	1:C:337:LEU:HD12	2.51	0.51
1:D:337:LEU:C	1:D:337:LEU:HD23	2.31	0.51
1:E:119:ILE:CD1	1:F:220:ILE:HD12	2.40	0.51
1:G:90:VAL:HG22	1:G:139:PRO:HB2	1.93	0.51
1:G:147:MSE:HE3	1:G:171:VAL:HG11	1.93	0.51
1:G:41:LYS:O	1:G:44:HIS:HB3	2.10	0.51
1:A:282:CYS:O	1:A:286:CYS:SG	2.68	0.51
1:B:75:ARG:HB3	1:B:331:TRP:CZ2	2.46	0.51
1:C:170:GLN:NE2	1:D:98:PRO:HB3	2.26	0.51
1:E:147:MSE:HE3	1:E:171:VAL:HG11	1.93	0.51
1:G:29:THR:O	1:G:30:GLU:C	2.49	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:241:TYR:CG	1:H:281:VAL:HG13	2.46	0.51
1:C:183:VAL:O	1:C:229:CYS:HA	2.11	0.50
1:D:213:THR:CG2	1:D:219:ALA:HB2	2.41	0.50
1:H:215:TRP:HB3	1:H:217:HIS:CE1	2.46	0.50
1:A:149:THR:N	1:A:150:PRO:CD	2.74	0.50
1:A:98:PRO:HA	1:B:170:GLN:HE22	1.76	0.50
1:D:266:PHE:O	1:D:271:SER:HB2	2.11	0.50
1:E:303:SER:HA	1:E:328:CYS:HB3	1.94	0.50
1:H:120:ASN:O	1:H:124:ARG:HG3	2.11	0.50
1:H:204:GLY:HA2	1:H:226:ASN:O	2.12	0.50
1:C:297:ILE:HD13	1:C:297:ILE:H	1.77	0.50
1:G:231:ILE:CG2	1:G:262:VAL:HG12	2.42	0.50
1:A:183:VAL:O	1:A:229:CYS:HA	2.12	0.50
1:A:50:ASN:N	1:A:50:ASN:ND2	2.60	0.50
1:D:186:LYS:HD3	1:D:234:ARG:HG2	1.93	0.50
1:D:303:SER:HB2	1:D:329:ILE:HG13	1.93	0.50
1:E:66:PRO:O	1:E:70:LYS:HG3	2.12	0.50
1:F:129:LEU:O	1:F:133:ILE:HG13	2.10	0.50
1:H:144:PHE:CZ	1:H:157:MSE:HG3	2.46	0.50
1:A:170:GLN:O	1:A:174:GLU:HG3	2.12	0.50
1:C:120:ASN:O	1:C:124:ARG:HG3	2.11	0.50
1:C:262:VAL:O	1:C:297:ILE:HD13	2.12	0.50
1:G:102:VAL:HG12	1:G:103:GLY:N	2.27	0.50
1:A:48:LYS:HE3	1:A:50:ASN:OD1	2.11	0.50
1:D:300:MSE:HE1	5:D:4352:PEP:O1P	2.12	0.50
1:E:141:ALA:HB1	1:E:159:TRP:HE3	1.77	0.50
1:G:159:TRP:CZ3	1:G:161:ALA:HB2	2.47	0.50
1:C:50:ASN:N	1:C:50:ASN:ND2	2.60	0.50
1:F:300:MSE:HE1	5:F:6352:PEP:O1P	2.12	0.50
1:D:297:ILE:H	1:D:297:ILE:HD13	1.76	0.50
1:F:144:PHE:CZ	1:F:157:MSE:HE3	2.47	0.50
1:A:337:LEU:C	1:A:337:LEU:HD23	2.32	0.49
1:D:309:ASN:HB3	1:D:327:ALA:HA	1.93	0.49
1:A:61:CYS:SG	1:A:326:ASP:HB2	2.52	0.49
1:A:120:ASN:O	1:A:124:ARG:HG3	2.13	0.49
1:D:343:ASN:HA	1:D:346:LYS:HD2	1.93	0.49
1:E:244:LYS:O	1:E:247:ALA:HB3	2.12	0.49
1:F:310:GLN:HE22	1:F:319:ALA:HB3	1.77	0.49
1:H:297:ILE:HD13	1:H:297:ILE:H	1.76	0.49
1:A:232:ILE:HG23	1:A:263:MSE:HE2	1.94	0.49
1:A:16:LEU:HD13	1:B:220:ILE:HG12	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ILE:O	1:B:348:ARG:HB2	2.12	0.49
1:D:149:THR:N	1:D:150:PRO:CD	2.75	0.49
1:C:220:ILE:CD1	1:D:14:LYS:HE3	2.42	0.49
1:D:41:LYS:HE2	1:D:45:LYS:HE3	1.92	0.49
1:E:282:CYS:SG	1:E:337:LEU:HG	2.53	0.49
1:B:144:PHE:CZ	1:B:157:MSE:HG3	2.48	0.49
1:A:213:THR:HG23	1:A:219:ALA:HB2	1.95	0.49
1:B:144:PHE:CZ	1:B:157:MSE:HE3	2.48	0.49
1:F:297:ILE:H	1:F:297:ILE:HD13	1.78	0.49
1:G:186:LYS:HZ2	1:G:300:MSE:HE1	1.78	0.49
1:H:58:ILE:HD11	1:H:334:THR:HG23	1.94	0.49
1:A:215:TRP:HB3	1:A:217:HIS:CE1	2.48	0.49
1:B:186:LYS:HZ1	1:B:300:MSE:HE1	1.76	0.49
1:H:147:MSE:HE3	1:H:171:VAL:HG11	1.93	0.49
1:C:220:ILE:HD13	1:D:14:LYS:HE3	1.95	0.49
1:A:266:PHE:O	1:A:271:SER:HB2	2.13	0.48
1:A:79:LEU:HD13	1:A:338:LEU:HD12	1.95	0.48
1:E:309:ASN:O	1:E:322:LYS:HE2	2.14	0.48
1:E:75:ARG:HB3	1:E:331:TRP:CZ2	2.47	0.48
1:C:294:LYS:N	1:C:294:LYS:CD	2.69	0.48
1:C:94:TYR:CE2	1:C:143:GLU:HB2	2.49	0.48
1:G:225:GLY:O	1:H:9:ARG:HD3	2.12	0.48
1:A:232:ILE:CG1	1:A:263:MSE:HE2	2.43	0.48
1:E:144:PHE:CZ	1:E:157:MSE:HG3	2.48	0.48
1:G:265:ASP:CG	1:G:300:MSE:HE2	2.34	0.48
1:A:186:LYS:NZ	1:A:300:MSE:HE1	2.28	0.48
1:A:265:ASP:OD2	1:A:300:MSE:HE2	2.14	0.48
1:F:159:TRP:CH2	1:F:161:ALA:HB2	2.48	0.48
1:E:215:TRP:HH2	1:F:1:MSE:HE2	1.77	0.48
1:E:195:VAL:HG23	1:E:196:ALA:N	2.28	0.48
1:E:6:ASP:OD1	1:F:214:LYS:NZ	2.46	0.48
1:A:6:ASP:OD1	1:B:214:LYS:NZ	2.44	0.48
1:C:49:GLY:C	1:C:51:ASP:H	2.17	0.48
1:G:171:VAL:HG21	1:H:145:LEU:O	2.14	0.48
1:G:246:VAL:O	1:G:250:LYS:HG3	2.13	0.48
1:A:159:TRP:CH2	1:A:161:ALA:HB2	2.49	0.48
1:A:144:PHE:HZ	1:A:157:MSE:HG3	1.79	0.47
1:C:303:SER:HB2	1:C:334:THR:OG1	2.14	0.47
1:C:49:GLY:O	1:C:51:ASP:N	2.42	0.47
1:D:263:MSE:HA	1:D:298:GLY:O	2.13	0.47
1:E:50:ASN:ND2	1:E:50:ASN:H	2.12	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:ILE:HD11	1:E:334:THR:HG23	1.95	0.47
1:B:265:ASP:OD2	1:B:300:MSE:HE2	2.15	0.47
1:C:215:TRP:CH2	1:D:1:MSE:HE2	2.48	0.47
1:F:149:THR:N	1:F:150:PRO:CD	2.77	0.47
1:F:250:LYS:HD2	1:F:295:ALA:HB2	1.96	0.47
1:A:250:LYS:HB3	1:A:260:ALA:HB1	1.96	0.47
1:B:187:ASN:HB2	1:B:192:THR:O	2.14	0.47
1:B:279:MSE:SE	1:B:333:ASP:HB3	2.65	0.47
1:D:232:ILE:HG12	1:D:263:MSE:HE2	1.95	0.47
1:A:112:HIS:CD2	1:A:118:GLN:HG3	2.49	0.47
1:B:183:VAL:O	1:B:229:CYS:HA	2.14	0.47
1:E:80:ARG:HA	1:E:89:ILE:HD12	1.96	0.47
1:B:201:ASN:OD1	1:B:258:LEU:HD21	2.14	0.47
1:D:183:VAL:O	1:D:229:CYS:HA	2.14	0.47
1:F:82:GLU:C	1:F:83:LEU:HD23	2.34	0.47
1:B:104:TRP:HB2	1:B:312:LEU:CD2	2.44	0.47
1:B:79:LEU:HD13	1:B:338:LEU:HD12	1.95	0.47
1:D:262:VAL:N	1:D:295:ALA:O	2.42	0.47
1:F:337:LEU:C	1:F:337:LEU:HD23	2.35	0.47
1:C:303:SER:HA	1:C:328:CYS:HB3	1.97	0.47
1:C:221:VAL:CG1	1:D:10:ILE:HD12	2.45	0.47
1:E:337:LEU:HD23	1:E:337:LEU:C	2.34	0.47
1:F:120:ASN:O	1:F:124:ARG:HG3	2.14	0.47
1:G:149:THR:N	1:G:150:PRO:CD	2.78	0.47
1:G:187:ASN:HB2	1:G:192:THR:O	2.15	0.47
1:H:61:CYS:SG	1:H:326:ASP:HB2	2.54	0.47
1:D:263:MSE:HE3	1:D:300:MSE:HB2	1.95	0.47
1:F:263:MSE:HA	1:F:298:GLY:O	2.14	0.47
1:C:83:LEU:N	1:C:83:LEU:HD23	2.30	0.47
1:A:239:PRO:HB3	1:A:241:TYR:CE2	2.50	0.47
1:F:241:TYR:CG	1:F:281:VAL:HG13	2.49	0.47
1:F:50:ASN:ND2	1:F:50:ASN:N	2.63	0.47
1:D:250:LYS:HB3	1:D:260:ALA:HB1	1.97	0.47
1:G:241:TYR:CG	1:G:281:VAL:HG13	2.49	0.47
1:A:241:TYR:CG	1:A:281:VAL:HG13	2.50	0.46
1:C:339:ARG:HG2	1:C:339:ARG:HH11	1.78	0.46
1:C:220:ILE:CD1	1:D:119:ILE:CG2	2.93	0.46
1:D:282:CYS:O	1:D:286:CYS:SG	2.74	0.46
1:C:33:ALA:CB	1:D:4:GLN:HG2	2.44	0.46
1:A:119:ILE:CG2	1:B:220:ILE:CD1	2.92	0.46
1:C:335:ASP:O	1:C:339:ARG:HG3	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:213:THR:HG23	1:G:219:ALA:HB2	1.97	0.46
1:H:94:TYR:CE2	1:H:143:GLU:HB2	2.50	0.46
1:A:75:ARG:HB3	1:A:331:TRP:CZ2	2.51	0.46
1:G:170:GLN:NE2	1:H:98:PRO:HB3	2.31	0.46
1:H:265:ASP:CG	1:H:300:MSE:HE2	2.35	0.46
1:A:307:GLU:HB3	1:A:330:GLY:N	2.30	0.46
1:B:232:ILE:CG1	1:B:263:MSE:HE2	2.46	0.46
1:B:250:LYS:HD2	1:B:295:ALA:HB2	1.96	0.46
1:B:11:LYS:HB3	1:B:11:LYS:HE2	1.57	0.46
1:C:149:THR:N	1:C:150:PRO:CD	2.79	0.46
1:C:195:VAL:HG23	1:C:196:ALA:N	2.30	0.46
1:C:170:GLN:NE2	1:D:98:PRO:HA	2.30	0.46
1:F:121:ASP:O	1:F:125:ILE:HG13	2.15	0.46
1:G:297:ILE:HD13	1:G:297:ILE:H	1.79	0.46
1:A:16:LEU:HD13	1:B:220:ILE:HG13	1.98	0.46
1:A:339:ARG:HG2	1:A:339:ARG:NH1	2.30	0.46
1:A:96:GLU:OE2	1:A:99:ARG:NH2	2.49	0.46
1:A:101:THR:HG22	1:A:102:VAL:N	2.31	0.46
1:B:97:LYS:NZ	1:B:326:ASP:OD2	2.48	0.46
1:H:263:MSE:HA	1:H:298:GLY:O	2.16	0.46
1:A:13:ILE:O	1:A:13:ILE:HG23	2.15	0.46
1:C:141:ALA:HB1	1:C:159:TRP:HE3	1.81	0.46
1:D:238:GLU:CD	1:D:238:GLU:H	2.19	0.46
1:E:1:MSE:HE2	1:F:215:TRP:CH2	2.50	0.46
1:F:16:LEU:HD11	1:F:119:ILE:HD13	1.97	0.46
1:A:242:SER:OG	1:A:245:HIS:CD2	2.69	0.46
1:A:263:MSE:HA	1:A:298:GLY:O	2.16	0.46
1:D:13:ILE:O	1:D:13:ILE:HG23	2.16	0.46
1:E:111:PRO:HG3	1:E:122:GLY:CA	2.46	0.46
1:G:94:TYR:CE2	1:G:143:GLU:HB2	2.51	0.46
1:G:220:ILE:O	1:G:220:ILE:HG23	2.16	0.46
1:G:309:ASN:HB3	1:G:327:ALA:HA	1.98	0.46
1:H:294:LYS:HG2	1:H:348:ARG:HD3	1.98	0.46
1:D:111:PRO:HB3	1:D:125:ILE:HD12	1.98	0.45
1:F:310:GLN:OE1	1:F:318:LEU:HD22	2.16	0.45
1:A:175:LEU:HD11	1:A:179:LEU:HD21	1.98	0.45
1:A:16:LEU:O	1:A:17:LEU:C	2.54	0.45
1:E:49:GLY:C	1:E:51:ASP:H	2.19	0.45
1:H:48:LYS:HB2	1:H:50:ASN:ND2	2.29	0.45
1:B:141:ALA:HB1	1:B:159:TRP:HE3	1.81	0.45
1:B:213:THR:HG23	1:B:219:ALA:HB2	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:GLU:HB3	1:E:330:GLY:H	1.79	0.45
1:H:111:PRO:HG3	1:H:122:GLY:CA	2.46	0.45
1:H:75:ARG:HB3	1:H:331:TRP:CZ2	2.51	0.45
1:H:63:ILE:CD1	1:H:93:VAL:HG13	2.44	0.45
1:A:215:TRP:CH2	1:B:1:MSE:HE2	2.52	0.45
1:A:197:ILE:HG12	1:A:253:LEU:HD23	1.97	0.45
1:E:280:ASP:O	1:E:283:ALA:HB3	2.17	0.45
1:G:284:ASP:O	1:G:287:GLN:HB3	2.16	0.45
1:G:337:LEU:HD23	1:G:337:LEU:C	2.37	0.45
1:A:111:PRO:HB3	1:A:125:ILE:HD12	1.98	0.45
1:D:245:HIS:O	1:D:248:GLU:N	2.50	0.45
1:E:187:ASN:HB2	1:E:192:THR:O	2.17	0.45
1:F:111:PRO:HG3	1:F:122:GLY:CA	2.47	0.45
1:G:263:MSE:HA	1:G:298:GLY:O	2.17	0.45
1:A:41:LYS:HE2	1:A:45:LYS:CE	2.47	0.45
1:D:61:CYS:SG	1:D:326:ASP:HB2	2.56	0.45
1:A:284:ASP:O	1:A:287:GLN:HB3	2.16	0.45
1:D:303:SER:HA	1:D:328:CYS:HB3	1.98	0.45
1:H:337:LEU:HD23	1:H:337:LEU:C	2.36	0.45
1:C:282:CYS:SG	1:C:337:LEU:CD1	3.05	0.45
1:C:10:ILE:HD12	1:D:221:VAL:CG1	2.47	0.45
1:G:221:VAL:CG1	1:H:10:ILE:HD12	2.46	0.45
1:G:279:MSE:SE	1:G:333:ASP:HB3	2.67	0.45
1:C:294:LYS:HE2	1:C:295:ALA:N	2.31	0.45
1:F:303:SER:HB2	1:F:329:ILE:HG13	1.98	0.45
1:G:16:LEU:CD1	1:G:119:ILE:HD13	2.47	0.45
1:G:54:LEU:HB3	1:G:87:LEU:CD2	2.47	0.45
1:H:16:LEU:O	1:H:17:LEU:C	2.54	0.45
1:D:310:GLN:HE21	1:D:322:LYS:HB3	1.80	0.44
1:F:262:VAL:O	1:F:297:ILE:HD13	2.17	0.44
1:G:141:ALA:HB1	1:G:159:TRP:HE3	1.82	0.44
1:H:332:GLU:HG2	1:H:333:ASP:N	2.32	0.44
1:A:13:ILE:HD12	1:B:221:VAL:HG22	2.00	0.44
1:C:261:GLN:HA	1:C:295:ALA:O	2.18	0.44
1:G:183:VAL:O	1:G:229:CYS:HA	2.17	0.44
1:A:171:VAL:HG21	1:B:145:LEU:O	2.17	0.44
1:B:290:ALA:HA	1:B:347:ALA:HB3	1.98	0.44
1:B:104:TRP:CE3	1:B:324:ILE:HD11	2.53	0.44
1:D:170:GLN:O	1:D:174:GLU:HG3	2.18	0.44
1:F:183:VAL:O	1:F:229:CYS:HA	2.17	0.44
1:A:1:MSE:HE1	1:D:120:ASN:ND2	2.32	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:GLU:HA	1:C:328:CYS:O	2.17	0.44
1:E:168:GLU:HG2	1:F:165:ARG:HB3	1.99	0.44
1:H:13:ILE:HG23	1:H:13:ILE:O	2.17	0.44
1:H:142:GLY:O	1:H:160:GLY:HA2	2.17	0.44
1:C:178:GLY:HA3	1:C:223:THR:HG22	1.99	0.44
1:D:111:PRO:HG3	1:D:122:GLY:CA	2.47	0.44
1:D:294:LYS:HB2	1:D:294:LYS:HE3	1.75	0.44
1:F:289:ILE:HG23	1:F:348:ARG:HE	1.83	0.44
1:A:282:CYS:SG	1:A:337:LEU:HG	2.58	0.44
1:A:344:ALA:O	1:A:347:ALA:HB3	2.18	0.44
1:B:46:ILE:HG12	1:B:51:ASP:HB3	2.00	0.44
1:G:175:LEU:HD11	1:G:179:LEU:HD21	1.99	0.44
1:H:234:ARG:HA	1:H:265:ASP:HB3	1.99	0.44
1:C:316:GLU:HA	1:C:317:PRO:HD3	1.86	0.44
1:C:121:ASP:O	1:C:125:ILE:HG13	2.18	0.44
1:D:147:MSE:SE	1:D:171:VAL:HG12	2.68	0.44
1:A:121:ASP:O	1:A:125:ILE:HG13	2.18	0.44
1:A:141:ALA:HB1	1:A:159:TRP:CE3	2.53	0.44
1:A:293:GLU:HG2	1:A:296:ILE:HD12	2.00	0.44
1:D:58:ILE:HD11	1:D:334:THR:HG23	2.00	0.44
1:B:152:TYR:O	1:B:153:LEU:HD23	2.18	0.43
1:B:84:LYS:NZ	1:B:84:LYS:CB	2.80	0.43
1:C:231:ILE:HG12	1:C:232:ILE:N	2.33	0.43
1:C:244:LYS:O	1:C:248:GLU:HG3	2.18	0.43
1:D:279:MSE:SE	1:D:333:ASP:HB3	2.68	0.43
1:F:335:ASP:O	1:F:339:ARG:HG3	2.17	0.43
1:H:183:VAL:O	1:H:229:CYS:HA	2.18	0.43
1:H:289:ILE:HG23	1:H:348:ARG:HE	1.83	0.43
1:A:14:LYS:HE3	1:B:220:ILE:HD12	2.00	0.43
1:B:303:SER:CA	1:B:328:CYS:HB3	2.46	0.43
1:C:119:ILE:CD1	1:D:220:ILE:HD12	2.43	0.43
1:D:96:GLU:OE2	1:D:99:ARG:NH2	2.52	0.43
1:F:312:LEU:C	1:F:314:SER:H	2.21	0.43
1:F:77:LEU:O	1:F:81:GLU:HG2	2.18	0.43
1:G:234:ARG:HD3	1:G:235:GLY:O	2.18	0.43
1:A:211:SER:OG	1:A:212:VAL:N	2.50	0.43
1:D:290:ALA:HA	1:D:347:ALA:HB3	2.00	0.43
1:E:297:ILE:H	1:E:297:ILE:HD13	1.83	0.43
1:F:265:ASP:CG	1:F:300:MSE:HE2	2.39	0.43
1:F:49:GLY:C	1:F:51:ASP:H	2.21	0.43
1:A:297:ILE:H	1:A:297:ILE:HD13	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:TRP:HB2	1:B:312:LEU:HD23	2.00	0.43
1:C:170:GLN:HE22	1:D:98:PRO:HA	1.83	0.43
1:D:75:ARG:HB3	1:D:331:TRP:CZ2	2.54	0.43
1:H:277:LYS:O	1:H:281:VAL:HG23	2.18	0.43
1:C:100:THR:CG2	1:D:173:ARG:HH12	2.32	0.43
1:D:147:MSE:N	1:D:147:MSE:SE	3.02	0.43
1:E:274:GLN:HB3	1:E:276:LYS:CD	2.47	0.43
1:H:250:LYS:HB3	1:H:260:ALA:HB1	2.00	0.43
1:B:314:SER:C	1:B:316:GLU:H	2.22	0.43
1:E:290:ALA:HA	1:E:347:ALA:HB3	2.00	0.43
1:H:339:ARG:HG2	1:H:339:ARG:HH11	1.83	0.43
1:A:144:PHE:CZ	1:A:157:MSE:HG3	2.52	0.43
1:B:149:THR:N	1:B:150:PRO:CD	2.82	0.43
1:C:58:ILE:CD1	1:C:334:THR:HG23	2.49	0.43
1:D:343:ASN:O	1:D:346:LYS:N	2.52	0.43
1:E:99:ARG:HG2	1:E:99:ARG:O	2.17	0.43
1:F:63:ILE:CD1	1:F:93:VAL:HG13	2.45	0.43
1:G:312:LEU:HD12	1:G:318:LEU:HD11	2.01	0.43
1:H:111:PRO:HG3	1:H:122:GLY:HA2	2.00	0.43
1:H:290:ALA:HA	1:H:347:ALA:HB3	2.01	0.43
1:A:217:HIS:HA	1:B:216:GLY:O	2.18	0.43
1:B:142:GLY:O	1:B:160:GLY:HA2	2.19	0.43
1:C:289:ILE:HG22	1:C:344:ALA:O	2.19	0.43
1:C:279:MSE:SE	1:C:337:LEU:HD13	2.69	0.43
1:E:86:GLU:HG2	1:E:346:LYS:HG3	2.00	0.43
1:A:77:LEU:O	1:A:80:ARG:HB3	2.18	0.43
1:A:145:LEU:O	1:B:171:VAL:HG21	2.19	0.43
1:D:276:LYS:HA	1:D:276:LYS:HD2	1.83	0.43
1:E:274:GLN:OE1	1:E:277:LYS:HE2	2.19	0.43
1:E:34:ASN:O	1:E:35:THR:C	2.56	0.43
1:E:221:VAL:CG1	1:F:10:ILE:HD12	2.49	0.43
1:G:310:GLN:NE2	1:G:322:LYS:HB3	2.34	0.43
1:C:242:SER:OG	1:C:245:HIS:ND1	2.46	0.42
1:D:91:MSE:HB2	1:D:138:LEU:HD21	2.01	0.42
1:E:239:PRO:HB3	1:E:241:TYR:CE2	2.54	0.42
1:G:242:SER:O	1:G:246:VAL:HG23	2.19	0.42
1:G:282:CYS:SG	1:G:337:LEU:HG	2.59	0.42
1:H:159:TRP:CH2	1:H:161:ALA:HB2	2.54	0.42
1:E:213:THR:CG2	1:E:219:ALA:HB2	2.49	0.42
1:E:53:ARG:HB3	1:E:86:GLU:O	2.18	0.42
1:F:346:LYS:O	1:F:349:ARG:HB3	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:ILE:CD1	1:H:334:THR:HG23	2.49	0.42
1:C:300:MSE:HE1	5:C:3352:PEP:O1P	2.18	0.42
1:E:178:GLY:HA3	1:E:223:THR:HG22	2.01	0.42
1:E:220:ILE:O	1:E:220:ILE:HG23	2.19	0.42
1:G:44:HIS:ND1	1:G:228:ASP:OD1	2.48	0.42
1:A:119:ILE:CG2	1:B:220:ILE:HD11	2.50	0.42
1:C:158:SER:O	1:C:182:PRO:HD2	2.19	0.42
1:D:186:LYS:NZ	1:D:300:MSE:HE1	2.34	0.42
1:D:332:GLU:HG2	1:D:333:ASP:N	2.34	0.42
1:D:92:ARG:NH1	1:D:300:MSE:HE3	2.33	0.42
1:A:14:LYS:HE3	1:B:220:ILE:HD13	2.02	0.42
1:B:266:PHE:CD1	1:B:266:PHE:N	2.88	0.42
1:D:239:PRO:HB3	1:D:241:TYR:CE2	2.54	0.42
1:D:343:ASN:O	1:D:344:ALA:C	2.58	0.42
1:D:50:ASN:ND2	1:D:50:ASN:N	2.68	0.42
1:F:83:LEU:HD12	1:F:87:LEU:HD12	2.02	0.42
1:D:26:PHE:HB2	1:D:127:ARG:HD3	2.01	0.42
1:E:300:MSE:HE1	5:E:5352:PEP:O1P	2.19	0.42
1:F:104:TRP:HB2	1:F:312:LEU:CD2	2.50	0.42
1:C:213:THR:HG21	1:D:15:GLU:OE2	2.20	0.42
1:F:92:ARG:NH1	1:F:300:MSE:HE3	2.35	0.42
1:G:220:ILE:HD12	1:H:119:ILE:HD12	2.00	0.42
1:H:147:MSE:N	1:H:147:MSE:SE	3.03	0.42
1:B:289:ILE:HG23	1:B:348:ARG:HE	1.84	0.42
1:H:195:VAL:HG23	1:H:196:ALA:N	2.34	0.42
1:B:92:ARG:HG3	1:B:94:TYR:CE1	2.54	0.42
1:G:303:SER:HB2	1:G:329:ILE:HG13	2.01	0.42
1:C:239:PRO:HB3	1:C:241:TYR:CE2	2.55	0.42
1:E:16:LEU:O	1:E:17:LEU:C	2.57	0.42
1:G:232:ILE:HG12	1:G:263:MSE:HE2	2.01	0.42
1:A:175:LEU:O	1:A:175:LEU:HD12	2.20	0.41
1:A:92:ARG:NH1	1:A:300:MSE:HE3	2.35	0.41
1:F:303:SER:HA	1:F:328:CYS:HB3	2.01	0.41
1:G:104:TRP:CE3	1:G:324:ILE:HD11	2.55	0.41
1:C:266:PHE:N	1:C:266:PHE:CD1	2.87	0.41
1:C:267:SER:HA	1:C:271:SER:HB2	2.01	0.41
1:D:232:ILE:CG1	1:D:263:MSE:HE2	2.51	0.41
1:E:309:ASN:HB3	1:E:327:ALA:HA	2.01	0.41
1:G:261:GLN:HA	1:G:295:ALA:O	2.20	0.41
1:G:97:LYS:NZ	1:G:326:ASP:OD2	2.51	0.41
1:A:250:LYS:HD2	1:A:295:ALA:CB	2.50	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:HD21	1:C:1:MSE:HE3	2.02	0.41
1:B:300:MSE:HE1	5:B:2352:PEP:O1P	2.20	0.41
1:D:220:ILE:O	1:D:220:ILE:HG23	2.21	0.41
1:D:36:VAL:O	1:D:40:ARG:HG3	2.19	0.41
1:F:102:VAL:CG1	1:F:103:GLY:H	2.14	0.41
1:F:96:GLU:OE2	1:F:99:ARG:NH2	2.54	0.41
1:G:221:VAL:HG22	1:H:13:ILE:HD12	2.02	0.41
1:A:147:MSE:HE3	1:A:171:VAL:CG1	2.49	0.41
1:A:348:ARG:HG2	1:A:348:ARG:O	2.21	0.41
1:G:25:LYS:C	1:G:27:PRO:HD3	2.40	0.41
1:G:312:LEU:CD1	1:G:318:LEU:HD11	2.50	0.41
1:G:48:LYS:HD3	1:G:50:ASN:OD1	2.20	0.41
1:D:34:ASN:O	1:D:35:THR:C	2.58	0.41
1:E:343:ASN:O	1:E:346:LYS:HB2	2.20	0.41
1:G:266:PHE:CD1	1:G:266:PHE:N	2.87	0.41
1:H:310:GLN:NE2	1:H:319:ALA:HB3	2.36	0.41
1:B:104:TRP:CZ3	1:B:324:ILE:HD11	2.55	0.41
1:C:111:PRO:HG3	1:C:122:GLY:CA	2.50	0.41
1:F:49:GLY:O	1:F:51:ASP:N	2.45	0.41
1:H:66:PRO:O	1:H:70:LYS:HG3	2.19	0.41
1:C:307:GLU:HB3	1:C:330:GLY:N	2.36	0.41
1:D:16:LEU:O	1:D:17:LEU:C	2.59	0.41
1:E:220:ILE:HD12	1:F:119:ILE:CD1	2.49	0.41
1:E:274:GLN:HB3	1:E:276:LYS:HZ2	1.84	0.41
1:H:41:LYS:O	1:H:44:HIS:HB3	2.21	0.41
1:H:59:GLY:O	1:H:92:ARG:HD3	2.21	0.41
1:D:58:ILE:HG13	1:D:301:VAL:HB	2.02	0.41
1:E:111:PRO:HB3	1:E:125:ILE:HD12	2.02	0.41
1:E:133:ILE:HG22	1:E:138:LEU:O	2.21	0.41
1:G:119:ILE:CD1	1:H:220:ILE:HD12	2.46	0.41
1:B:241:TYR:CG	1:B:281:VAL:HG13	2.55	0.41
1:D:148:ILE:C	1:D:150:PRO:HD2	2.41	0.41
1:E:127:ARG:HG2	1:E:127:ARG:O	2.21	0.41
1:G:214:LYS:NZ	1:H:6:ASP:OD1	2.47	0.41
1:A:142:GLY:O	1:A:160:GLY:HA2	2.20	0.41
1:A:263:MSE:HE3	1:A:300:MSE:HB2	2.02	0.41
1:C:86:GLU:HG3	1:C:349:ARG:HH11	1.83	0.41
1:E:231:ILE:HG12	1:E:232:ILE:N	2.36	0.41
1:H:310:GLN:HE22	1:H:319:ALA:HB3	1.85	0.41
1:D:309:ASN:O	1:D:322:LYS:HE2	2.21	0.41
1:E:142:GLY:O	1:E:160:GLY:HA2	2.20	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:LYS:O	1:E:281:VAL:HG23	2.21	0.41
1:F:337:LEU:HD23	1:F:338:LEU:N	2.36	0.41
1:A:234:ARG:C	1:A:234:ARG:HD3	2.41	0.40
1:F:255:LYS:HB2	1:F:255:LYS:NZ	2.36	0.40
1:A:246:VAL:O	1:A:250:LYS:CG	2.54	0.40
1:B:147:MSE:SE	1:B:175:LEU:HD22	2.71	0.40
1:B:234:ARG:HA	1:B:265:ASP:HB3	2.03	0.40
1:F:266:PHE:N	1:F:266:PHE:CD1	2.89	0.40
1:F:339:ARG:NH1	1:F:339:ARG:HG2	2.36	0.40
1:A:232:ILE:CG2	1:A:263:MSE:HE2	2.50	0.40
1:A:337:LEU:O	1:A:337:LEU:HD23	2.22	0.40
1:B:48:LYS:HD3	1:B:50:ASN:OD1	2.22	0.40
1:C:280:ASP:O	1:C:283:ALA:HB3	2.20	0.40
1:C:301:VAL:HG21	1:C:337:LEU:HD21	2.03	0.40
1:C:61:CYS:SG	1:C:326:ASP:HB2	2.61	0.40
1:D:144:PHE:CZ	1:D:157:MSE:HE3	2.56	0.40
1:C:214:LYS:NZ	1:D:6:ASP:OD1	2.48	0.40
1:E:1:MSE:HG2	1:E:3:TYR:OH	2.21	0.40
1:E:36:VAL:O	1:E:40:ARG:HG3	2.22	0.40
1:F:307:GLU:HB2	1:F:330:GLY:N	2.36	0.40
1:G:195:VAL:HG23	1:G:196:ALA:N	2.35	0.40
1:B:47:LEU:HD23	1:B:297:ILE:HD12	2.03	0.40
1:C:263:MSE:HA	1:C:298:GLY:O	2.21	0.40
1:C:165[B]:ARG:NH2	1:D:170:GLN:OE1	2.52	0.40
1:G:112:HIS:CD2	1:G:118:GLN:HG3	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	348/350 (99%)	322 (92%)	25 (7%)	1 (0%)	44 77

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	348/350 (99%)	326 (94%)	17 (5%)	5 (1%)	13	39
1	C	349/350 (100%)	323 (93%)	22 (6%)	4 (1%)	17	47
1	D	352/350 (101%)	323 (92%)	24 (7%)	5 (1%)	13	39
1	E	348/350 (99%)	323 (93%)	19 (6%)	6 (2%)	11	34
1	F	348/350 (99%)	318 (91%)	25 (7%)	5 (1%)	13	39
1	G	348/350 (99%)	327 (94%)	19 (6%)	2 (1%)	28	62
1	H	352/350 (101%)	319 (91%)	29 (8%)	4 (1%)	17	47
All	All	2793/2800 (100%)	2581 (92%)	180 (6%)	32 (1%)	17	47

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	50	ASN
1	F	318	LEU
1	H	101[A]	THR
1	H	101[B]	THR
1	C	50	ASN
1	E	101	THR
1	E	314	SER
1	F	50	ASN
1	B	101	THR
1	C	101	THR
1	F	101	THR
1	F	317	PRO
1	H	239	PRO
1	H	317	PRO
1	A	211	SER
1	C	239	PRO
1	G	349	ARG
1	B	239	PRO
1	D	113	MSE
1	E	113	MSE
1	E	211	SER
1	G	314	SER
1	B	211	SER
1	D	211	SER
1	D	239	PRO
1	C	188	GLY
1	E	239	PRO
1	B	102	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	296	ILE
1	B	188	GLY
1	D	102[A]	VAL
1	D	102[B]	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/275 (103%)	274 (97%)	9 (3%)	44	78
1	B	283/275 (103%)	276 (98%)	7 (2%)	53	84
1	C	284/275 (103%)	273 (96%)	11 (4%)	37	71
1	D	287/275 (104%)	277 (96%)	10 (4%)	41	75
1	E	283/275 (103%)	270 (95%)	13 (5%)	31	65
1	F	283/275 (103%)	273 (96%)	10 (4%)	41	75
1	G	283/275 (103%)	277 (98%)	6 (2%)	59	88
1	H	287/275 (104%)	279 (97%)	8 (3%)	49	82
All	All	2273/2200 (103%)	2199 (97%)	74 (3%)	43	77

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	96	GLU
1	A	99	ARG
1	A	121	ASP
1	A	215	TRP
1	A	218	SER
1	A	234	ARG
1	A	297	ILE
1	A	303	SER
1	B	50	ASN
1	B	80	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	96	GLU
1	B	99	ARG
1	B	121	ASP
1	B	234	ARG
1	B	316	GLU
1	C	81	GLU
1	C	83	LEU
1	C	96	GLU
1	C	99	ARG
1	C	100	THR
1	C	121	ASP
1	C	220	ILE
1	C	234	ARG
1	C	251	GLU
1	C	294	LYS
1	C	297	ILE
1	D	4	GLN
1	D	86	GLU
1	D	96	GLU
1	D	99	ARG
1	D	121	ASP
1	D	215	TRP
1	D	234	ARG
1	D	238	GLU
1	D	239	PRO
1	D	297	ILE
1	E	45	LYS
1	E	50	ASN
1	E	96	GLU
1	E	99	ARG
1	E	121	ASP
1	E	215	TRP
1	E	218	SER
1	E	234	ARG
1	E	239	PRO
1	E	276	LYS
1	E	287	GLN
1	E	297	ILE
1	E	316	GLU
1	F	14	LYS
1	F	83	LEU
1	F	96	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	99	ARG
1	F	100	THR
1	F	121	ASP
1	F	234	ARG
1	F	297	ILE
1	F	303	SER
1	F	307	GLU
1	G	96	GLU
1	G	99	ARG
1	G	121	ASP
1	G	234	ARG
1	G	297	ILE
1	G	303	SER
1	H	96	GLU
1	H	99	ARG
1	H	121	ASP
1	H	215	TRP
1	H	218	SER
1	H	234	ARG
1	H	239	PRO
1	H	297	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	112	HIS
1	A	240	ASN
1	A	245	HIS
1	A	254	ASN
1	B	50	ASN
1	B	112	HIS
1	B	170	GLN
1	B	240	ASN
1	B	245	HIS
1	B	288	GLN
1	C	50	ASN
1	C	112	HIS
1	C	170	GLN
1	C	240	ASN
1	C	254	ASN
1	D	50	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	240	ASN
1	D	245	HIS
1	D	254	ASN
1	D	261	GLN
1	E	50	ASN
1	E	240	ASN
1	E	245	HIS
1	E	254	ASN
1	F	50	ASN
1	F	112	HIS
1	F	240	ASN
1	F	245	HIS
1	F	254	ASN
1	F	310	GLN
1	G	170	GLN
1	G	217	HIS
1	G	240	ASN
1	G	245	HIS
1	G	254	ASN
1	H	50	ASN
1	H	112	HIS
1	H	217	HIS
1	H	240	ASN
1	H	245	HIS
1	H	254	ASN
1	H	261	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 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$
5	PEP	A	1352	-	6,9,9	1.16	0	9,13,13	2.22	4 (44%)
4	PHE	A	1354	-	8,12,12	1.63	2 (25%)	10,15,15	1.56	1 (10%)
3	SO4	A	1355	-	4,4,4	0.46	0	6,6,6	0.30	0
3	SO4	A	1356	-	4,4,4	0.32	0	6,6,6	0.17	0
5	PEP	B	2352	-	6,9,9	1.16	0	9,13,13	2.16	3 (33%)
4	PHE	B	2354	-	8,12,12	1.71	2 (25%)	10,15,15	1.40	1 (10%)
3	SO4	B	2355	-	4,4,4	0.34	0	6,6,6	0.21	0
3	SO4	B	2356	-	4,4,4	0.36	0	6,6,6	0.23	0
5	PEP	C	3352	-	6,9,9	1.11	0	9,13,13	2.21	3 (33%)
4	PHE	C	3354	-	8,12,12	1.61	2 (25%)	10,15,15	1.26	1 (10%)
3	SO4	C	3355	-	4,4,4	0.40	0	6,6,6	0.19	0
3	SO4	C	3356	-	4,4,4	0.35	0	6,6,6	0.24	0
5	PEP	D	4352	-	6,9,9	1.23	0	9,13,13	2.26	4 (44%)
4	PHE	D	4354	-	8,12,12	1.81	4 (50%)	10,15,15	1.49	1 (10%)
3	SO4	D	4355	-	4,4,4	0.38	0	6,6,6	0.19	0
3	SO4	D	4356	-	4,4,4	0.32	0	6,6,6	0.21	0
5	PEP	E	5352	-	6,9,9	1.27	0	9,13,13	2.31	4 (44%)
4	PHE	E	5354	-	8,12,12	1.81	4 (50%)	10,15,15	1.49	1 (10%)
3	SO4	E	5355	-	4,4,4	0.36	0	6,6,6	0.11	0
3	SO4	E	5356	-	4,4,4	0.35	0	6,6,6	0.13	0
5	PEP	F	6352	-	6,9,9	1.26	1 (16%)	9,13,13	2.30	3 (33%)
4	PHE	F	6354	-	8,12,12	1.64	2 (25%)	10,15,15	1.24	1 (10%)
3	SO4	F	6355	-	4,4,4	0.37	0	6,6,6	0.15	0
3	SO4	F	6356	-	4,4,4	0.34	0	6,6,6	0.16	0
5	PEP	G	7352	-	6,9,9	1.20	0	9,13,13	2.26	3 (33%)
4	PHE	G	7354	-	8,12,12	1.80	4 (50%)	10,15,15	1.41	1 (10%)
3	SO4	G	7356	-	4,4,4	0.34	0	6,6,6	0.14	0
3	SO4	H	7355	-	4,4,4	0.35	0	6,6,6	0.11	0
5	PEP	H	8352	-	6,9,9	1.16	0	9,13,13	2.24	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PHE	H	8354	-	8,12,12	1.71	2 (25%)	10,15,15	1.38	1 (10%)
3	SO4	H	8355	-	4,4,4	0.42	0	6,6,6	0.15	0
3	SO4	H	8356	-	4,4,4	0.34	0	6,6,6	0.15	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
5	PEP	A	1352	-	-	0/5/9/9	0/0/0/0
4	PHE	A	1354	-	-	0/4/8/8	0/1/1/1
3	SO4	A	1355	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1356	-	-	0/0/0/0	0/0/0/0
5	PEP	B	2352	-	-	0/5/9/9	0/0/0/0
4	PHE	B	2354	-	-	0/4/8/8	0/1/1/1
3	SO4	B	2355	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2356	-	-	0/0/0/0	0/0/0/0
5	PEP	C	3352	-	-	0/5/9/9	0/0/0/0
4	PHE	C	3354	-	-	0/4/8/8	0/1/1/1
3	SO4	C	3355	-	-	0/0/0/0	0/0/0/0
3	SO4	C	3356	-	-	0/0/0/0	0/0/0/0
5	PEP	D	4352	-	-	0/5/9/9	0/0/0/0
4	PHE	D	4354	-	-	0/4/8/8	0/1/1/1
3	SO4	D	4355	-	-	0/0/0/0	0/0/0/0
3	SO4	D	4356	-	-	0/0/0/0	0/0/0/0
5	PEP	E	5352	-	-	0/5/9/9	0/0/0/0
4	PHE	E	5354	-	-	0/4/8/8	0/1/1/1
3	SO4	E	5355	-	-	0/0/0/0	0/0/0/0
3	SO4	E	5356	-	-	0/0/0/0	0/0/0/0
5	PEP	F	6352	-	-	0/5/9/9	0/0/0/0
4	PHE	F	6354	-	-	0/4/8/8	0/1/1/1
3	SO4	F	6355	-	-	0/0/0/0	0/0/0/0
3	SO4	F	6356	-	-	0/0/0/0	0/0/0/0
5	PEP	G	7352	-	-	0/5/9/9	0/0/0/0
4	PHE	G	7354	-	-	0/4/8/8	0/1/1/1
3	SO4	G	7356	-	-	0/0/0/0	0/0/0/0
3	SO4	H	7355	-	-	0/0/0/0	0/0/0/0
5	PEP	H	8352	-	-	0/5/9/9	0/0/0/0
4	PHE	H	8354	-	-	0/4/8/8	0/1/1/1
3	SO4	H	8355	-	-	0/0/0/0	0/0/0/0
3	SO4	H	8356	-	-	0/0/0/0	0/0/0/0



All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	6354	PHE	CE1-CD1	2.01	1.42	1.38
4	D	4354	PHE	CE1-CD1	2.02	1.42	1.38
4	C	3354	PHE	CD2-CG	2.02	1.43	1.38
4	F	6354	PHE	CZ-CE1	2.02	1.43	1.38
5	F	6352	PEP	C3-C2	2.04	1.37	1.33
4	H	8354	PHE	CZ-CE1	2.04	1.43	1.38
4	G	7354	PHE	CD1-CG	2.06	1.43	1.38
4	H	8354	PHE	CD1-CG	2.10	1.43	1.38
4	G	7354	PHE	CE2-CD2	2.12	1.43	1.38
4	E	5354	PHE	CZ-CE2	2.15	1.43	1.38
4	D	4354	PHE	CZ-CE2	2.16	1.43	1.38
4	E	5354	PHE	CD1-CG	2.17	1.43	1.38
4	D	4354	PHE	CE2-CD2	2.18	1.43	1.38
4	C	3354	PHE	CZ-CE1	2.18	1.43	1.38
4	E	5354	PHE	CE1-CD1	2.19	1.43	1.38
4	G	7354	PHE	CZ-CE2	2.19	1.43	1.38
4	E	5354	PHE	CZ-CE1	2.20	1.43	1.38
4	B	2354	PHE	CZ-CE1	2.20	1.43	1.38
4	B	2354	PHE	CE1-CD1	2.20	1.43	1.38
4	D	4354	PHE	CZ-CE1	2.21	1.43	1.38
4	A	1354	PHE	CE1-CD1	2.28	1.43	1.38
4	A	1354	PHE	CZ-CE1	2.32	1.43	1.38
4	G	7354	PHE	CE1-CD1	2.49	1.43	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6352	PEP	O2-C2-C3	-4.15	116.87	124.87
5	E	5352	PEP	O2-C2-C3	-4.01	117.15	124.87
5	G	7352	PEP	O2-C2-C3	-3.98	117.20	124.87
5	D	4352	PEP	O2-C2-C3	-3.92	117.33	124.87
5	H	8352	PEP	O2-C2-C3	-3.90	117.36	124.87
5	C	3352	PEP	O2-C2-C3	-3.80	117.55	124.87
5	A	1352	PEP	O2-C2-C3	-3.73	117.69	124.87
5	B	2352	PEP	O2-C2-C3	-3.69	117.77	124.87
5	D	4352	PEP	P-O2-C2	2.08	127.71	123.13
5	F	6352	PEP	O3P-P-O2P	2.15	116.29	107.61
5	A	1352	PEP	P-O2-C2	2.18	127.94	123.13
5	H	8352	PEP	P-O2-C2	2.19	127.96	123.13
4	C	3354	PHE	CG-CB-CA	2.20	118.98	114.43
5	C	3352	PEP	O3P-P-O2P	2.21	116.55	107.61
5	G	7352	PEP	O3P-P-O2P	2.24	116.65	107.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2352	PEP	O3P-P-O2P	2.27	116.78	107.61
5	H	8352	PEP	O3P-P-O2P	2.30	116.90	107.61
5	A	1352	PEP	O3P-P-O2P	2.31	116.95	107.61
5	D	4352	PEP	O3P-P-O2P	2.32	116.95	107.61
5	E	5352	PEP	P-O2-C2	2.33	128.27	123.13
4	F	6354	PHE	CG-CB-CA	2.34	119.26	114.43
5	E	5352	PEP	O3P-P-O2P	2.36	117.13	107.61
4	B	2354	PHE	CG-CB-CA	2.73	120.07	114.43
4	G	7354	PHE	CG-CB-CA	2.87	120.36	114.43
4	H	8354	PHE	CG-CB-CA	2.93	120.48	114.43
4	A	1354	PHE	CG-CB-CA	3.25	121.14	114.43
4	D	4354	PHE	CG-CB-CA	3.25	121.14	114.43
4	E	5354	PHE	CG-CB-CA	3.31	121.28	114.43
5	B	2352	PEP	C1-C2-C3	3.98	128.50	121.07
5	H	8352	PEP	C1-C2-C3	4.13	128.78	121.07
5	C	3352	PEP	C1-C2-C3	4.20	128.93	121.07
5	F	6352	PEP	C1-C2-C3	4.26	129.03	121.07
5	G	7352	PEP	C1-C2-C3	4.29	129.08	121.07
5	E	5352	PEP	C1-C2-C3	4.32	129.14	121.07
5	D	4352	PEP	C1-C2-C3	4.32	129.14	121.07
5	A	1352	PEP	C1-C2-C3	4.40	129.28	121.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2352	PEP	1	0
5	C	3352	PEP	1	0
5	D	4352	PEP	1	0
5	E	5352	PEP	1	0
5	F	6352	PEP	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	342/350 (97%)	-0.55	6 (1%) 69 60	8, 29, 55, 111	0
1	B	342/350 (97%)	-0.28	16 (4%) 32 22	11, 37, 79, 104	0
1	C	342/350 (97%)	0.04	20 (5%) 24 15	14, 55, 92, 118	4 (1%)
1	D	342/350 (97%)	-0.34	11 (3%) 48 37	10, 40, 79, 118	3 (0%)
1	E	341/350 (97%)	-0.15	7 (2%) 64 54	27, 50, 78, 132	5 (1%)
1	F	341/350 (97%)	0.04	23 (6%) 19 11	20, 57, 90, 126	5 (1%)
1	G	341/350 (97%)	-0.04	14 (4%) 38 27	27, 57, 91, 127	6 (1%)
1	H	341/350 (97%)	0.13	26 (7%) 15 8	23, 65, 91, 125	5 (1%)
All	All	2732/2800 (97%)	-0.15	123 (4%) 34 24	8, 50, 88, 132	28 (1%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	350	GLY	11.9
1	G	314	SER	7.0
1	G	101	THR	7.0
1	B	350	GLY	7.0
1	C	350	GLY	6.1
1	E	315	GLY	5.6
1	E	314	SER	5.1
1	C	272	SER	4.8
1	E	101	THR	4.8
1	F	49	GLY	4.8
1	H	315	GLY	4.7
1	D	317	PRO	4.7
1	F	314	SER	4.6
1	D	316	GLU	4.5
1	B	102	VAL	4.4
1	H	272	SER	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	276	LYS	4.3
1	C	101	THR	4.3
1	F	102	VAL	4.2
1	G	317	PRO	4.2
1	B	101	THR	4.1
1	C	102	VAL	4.1
1	G	292	GLY	4.1
1	D	274	GLN	4.1
1	B	314	SER	4.0
1	G	102	VAL	3.9
1	C	314	SER	3.7
1	H	224	SER	3.7
1	D	315	GLY	3.7
1	G	315	GLY	3.7
1	C	276	LYS	3.6
1	A	316	GLU	3.6
1	F	292	GLY	3.6
1	E	102	VAL	3.5
1	F	317	PRO	3.5
1	D	314	SER	3.4
1	F	103	GLY	3.4
1	H	292	GLY	3.4
1	F	315	GLY	3.3
1	H	317	PRO	3.2
1	F	318	LEU	3.2
1	F	101	THR	3.2
1	B	273	LYS	3.1
1	B	315	GLY	3.1
1	H	237	LYS	3.0
1	A	314	SER	3.0
1	A	313	GLU	3.0
1	E	317	PRO	2.9
1	B	2	ASN	2.9
1	B	272	SER	2.9
1	G	100	THR	2.9
1	H	294	LYS	2.9
1	D	115	ASN	2.9
1	H	316	GLU	2.9
1	H	101[A]	THR	2.9
1	D	2	ASN	2.8
1	F	290	ALA	2.8
1	H	273	LYS	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	313	GLU	2.8
1	H	314	SER	2.8
1	F	81	GLU	2.7
1	C	318	LEU	2.7
1	H	102[A]	VAL	2.7
1	H	49	GLY	2.7
1	C	254	ASN	2.7
1	F	313	GLU	2.7
1	C	237	LYS	2.7
1	A	2	ASN	2.7
1	D	102[A]	VAL	2.6
1	F	316	GLU	2.6
1	B	308	GLY	2.5
1	A	317	PRO	2.5
1	D	116	SER	2.5
1	A	315	GLY	2.5
1	C	280	ASP	2.5
1	C	287	GLN	2.5
1	B	317	PRO	2.5
1	H	274	GLN	2.5
1	H	45	LYS	2.5
1	F	274	GLN	2.5
1	G	313	GLU	2.5
1	C	317	PRO	2.4
1	H	254	ASN	2.4
1	E	99	ARG	2.4
1	H	50	ASN	2.4
1	H	311	SER	2.4
1	G	311	SER	2.4
1	F	244	LYS	2.3
1	F	255	LYS	2.3
1	D	101[A]	THR	2.3
1	H	312	LEU	2.3
1	B	276	LYS	2.3
1	C	329	ILE	2.3
1	B	274	GLN	2.3
1	H	346	LYS	2.3
1	C	2	ASN	2.2
1	G	277	LYS	2.2
1	F	311	SER	2.2
1	B	237	LYS	2.2
1	H	100[A]	THR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	238	GLU	2.2
1	F	349	ARG	2.2
1	B	238	GLU	2.2
1	G	189	THR	2.2
1	F	294	LYS	2.2
1	H	291	GLY	2.1
1	C	320	TYR	2.1
1	B	313	GLU	2.1
1	C	313	GLU	2.1
1	F	29	THR	2.1
1	H	81	GLU	2.1
1	E	50	ASN	2.1
1	C	311	SER	2.1
1	F	256	ALA	2.1
1	H	321	GLY	2.1
1	C	273	LYS	2.1
1	F	45	LYS	2.1
1	B	100	THR	2.0
1	C	343	ASN	2.0
1	F	190	ASP	2.0
1	G	256	ALA	2.0
1	D	11	LYS	2.0
1	C	347	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PEP	B	2352	10/10	0.90	0.21	2.47	55,71,80,81	0
3	SO4	E	5355	5/5	0.92	0.19	1.11	74,81,82,86	0
4	PHE	B	2354	12/12	0.97	0.16	1.07	7,16,34,39	0
4	PHE	F	6354	12/12	0.94	0.18	0.98	28,36,41,47	0
4	PHE	H	8354	12/12	0.93	0.21	0.81	44,54,72,80	0
5	PEP	F	6352	10/10	0.93	0.19	0.42	54,76,91,103	0
4	PHE	D	4354	12/12	0.98	0.14	0.41	11,24,34,36	0
5	PEP	C	3352	10/10	0.90	0.20	0.28	68,88,102,106	0
5	PEP	H	8352	10/10	0.93	0.21	0.18	84,94,97,99	0
4	PHE	A	1354	12/12	0.97	0.14	0.18	1,15,32,33	0
4	PHE	G	7354	12/12	0.95	0.15	0.01	19,25,48,49	0
4	PHE	E	5354	12/12	0.96	0.15	-0.07	25,39,50,54	0
5	PEP	A	1352	10/10	0.97	0.14	-0.08	29,47,60,69	0
5	PEP	E	5352	10/10	0.94	0.18	-0.14	71,76,77,85	0
5	PEP	G	7352	10/10	0.93	0.18	-0.22	85,93,99,100	0
3	SO4	D	4355	5/5	0.96	0.14	-0.39	60,65,77,80	0
3	SO4	F	6355	5/5	0.97	0.11	-0.66	63,66,71,84	0
3	SO4	B	2355	5/5	1.00	0.09	-0.68	25,34,58,59	0
4	PHE	C	3354	12/12	0.98	0.12	-0.75	15,26,37,51	0
5	PEP	D	4352	10/10	0.96	0.14	-0.85	56,69,77,78	0
3	SO4	C	3355	5/5	0.99	0.09	-1.13	26,33,44,46	0
2	MN	E	5351	1/1	0.97	0.03	-2.21	64,64,64,64	0
2	MN	G	7351	1/1	0.94	0.07	-2.92	77,77,77,77	0
2	MN	H	8351	1/1	0.96	0.04	-2.99	68,68,68,68	0
2	MN	B	2351	1/1	0.98	0.07	-3.30	57,57,57,57	0
2	MN	C	3351	1/1	0.97	0.04	-3.61	71,71,71,71	0
2	MN	A	1351	1/1	0.98	0.06	-3.77	33,33,33,33	0
2	MN	D	4351	1/1	0.98	0.03	-3.90	47,47,47,47	0
2	MN	F	6351	1/1	0.97	0.04	-4.64	61,61,61,61	0
3	SO4	F	6356	5/5	0.90	0.21	-	82,93,94,107	0
3	SO4	D	4356	5/5	0.96	0.16	-	60,65,75,90	0
3	SO4	H	8355	5/5	0.96	0.17	-	49,62,73,74	0
3	SO4	H	8356	5/5	0.88	0.19	-	102,102,110,113	0
3	SO4	E	5356	5/5	0.91	0.17	-	68,74,78,88	0
3	SO4	G	7356	5/5	0.93	0.26	-	87,88,90,103	0
3	SO4	C	3356	5/5	0.90	0.26	-	75,77,85,97	0
3	SO4	A	1355	5/5	0.96	0.17	-	42,56,59,68	0
3	SO4	A	1356	5/5	0.97	0.13	-	60,63,70,79	0
3	SO4	B	2356	5/5	0.95	0.16	-	62,69,73,88	0
3	SO4	H	7355	5/5	0.97	0.18	-	85,95,98,99	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.