



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 2PP1 / pdb\_00002pp1  
Title : Crystal structure of L-talarate/galactarate dehydratase from Salmonella typhimurium LT2 liganded with Mg and L-lyxarohydroxamate  
Authors : Fedorov, A.A.; Fedorov, E.V.; Yew, W.S.; Gerlt, J.A.; Almo, S.C.  
Deposited on : 2007-04-27  
Resolution : 2.20 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

<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  
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

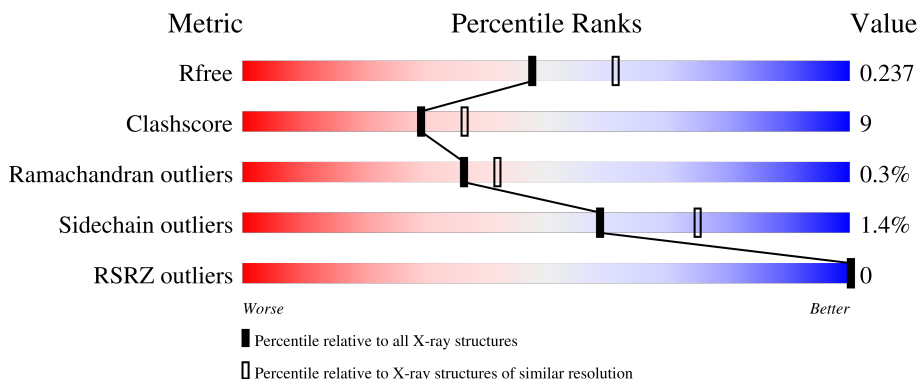
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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  $\geq 3$ , 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	398	78% 20% ..
1	B	398	80% 18% ..
1	C	398	79% 18% ..
1	D	398	78% 19% ..
1	E	398	78% 19% ..

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	398	 79% 18% ..

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19057 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.

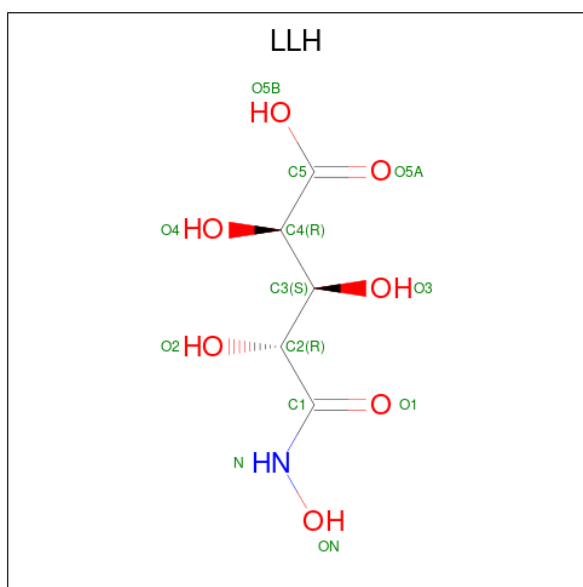
- Molecule 1 is a protein called L-talarate/galactarate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	395	3081	1951	548	570	12	0	0	0
1	B	395	3081	1951	548	570	12	0	0	0
1	C	391	3056	1937	543	564	12	0	0	0
1	D	391	3056	1937	543	564	12	0	0	0
1	E	391	3056	1937	543	564	12	0	0	0
1	F	391	3056	1937	543	564	12	0	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is (2R,3S,4R)-2,3,4-TRIHYDROXY-5-(HYDROXYAMINO)-5-OXOPENTANOIC ACID (CCD ID: LLH) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	13	5	1	7	0	0
3	B	1	13	5	1	7	0	0
3	C	1	13	5	1	7	0	0
3	D	1	13	5	1	7	0	0
3	E	1	13	5	1	7	0	0
3	F	1	13	5	1	7	0	0

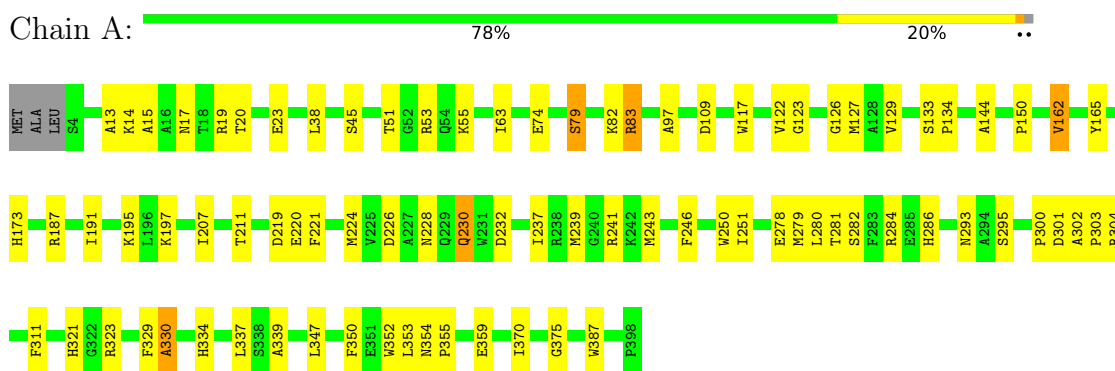
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total 143	O 143	0	0
4	B	137	Total 137	O 137	0	0
4	C	71	Total 71	O 71	0	0
4	D	65	Total 65	O 65	0	0
4	E	90	Total 90	O 90	0	0
4	F	85	Total 85	O 85	0	0

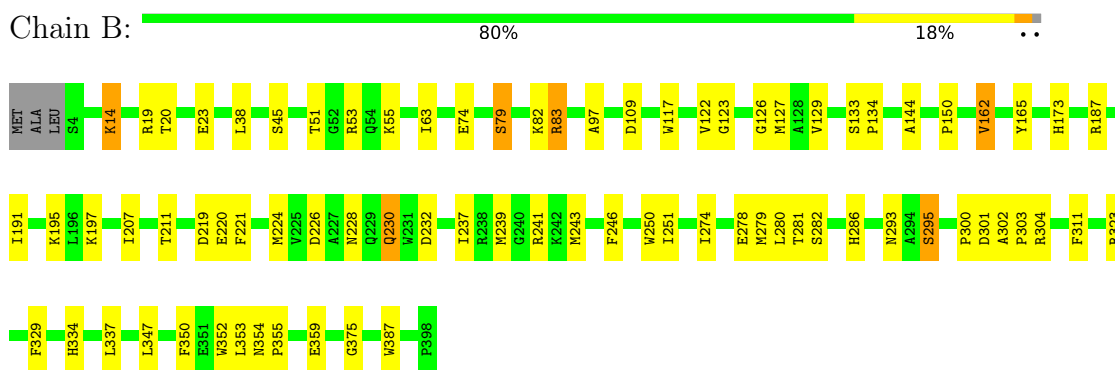
### 3 Residue-property plots [i](#)

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.

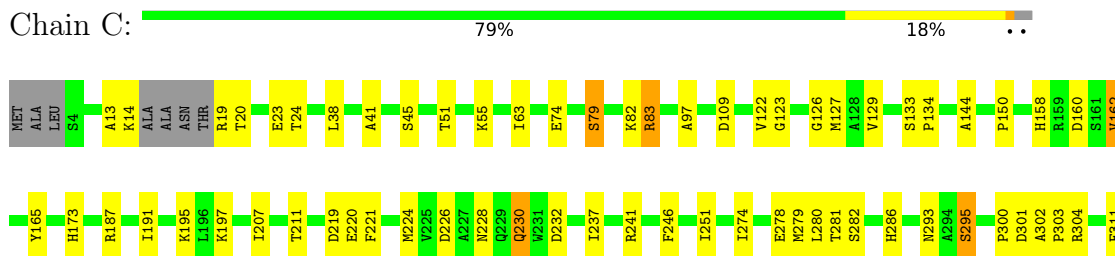
- Molecule 1: L-tartrate/galactarate dehydratase



- Molecule 1: L-tartrate/galactarate dehydratase



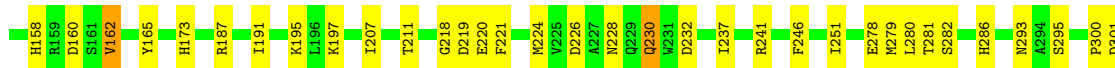
- Molecule 1: L-tartrate/galactarate dehydratase





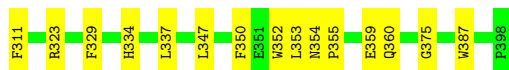
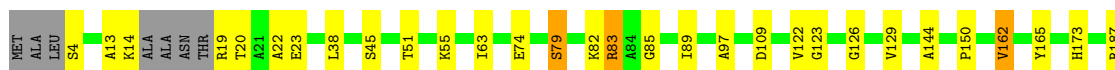
- Molecule 1: L-talarate/galactarate dehydratase

Chain D: 78% 19% ..



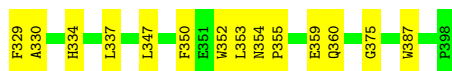
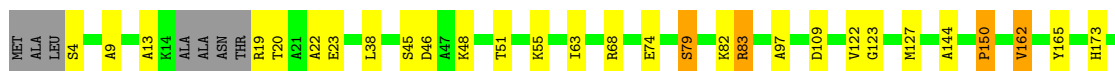
- Molecule 1: L-talarate/galactarate dehydratase

Chain E: 78% 19% ..



- Molecule 1: L-talarate/galactarate dehydratase

Chain F: 79% 18% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.19Å 173.83Å 173.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.87 – 2.20 24.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.8 (24.87-2.20) 86.8 (24.87-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.223 , 0.237 0.224 , 0.237	Depositor DCC
$R_{free}$ test set	9480 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtrriage
Anisotropy	0.528	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 16.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.487 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: LLH, MG

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	0/3149	0.94	14/4266 (0.3%)
1	B	0.44	0/3149	0.94	13/4266 (0.3%)
1	C	0.40	0/3123	0.93	15/4228 (0.4%)
1	D	0.39	0/3123	0.93	16/4228 (0.4%)
1	E	0.41	0/3123	0.92	13/4228 (0.3%)
1	F	0.41	0/3123	0.93	15/4228 (0.4%)
All	All	0.41	0/18790	0.93	86/25444 (0.3%)

There are no bond length outliers.

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	GLN	N-CA-C	7.95	122.82	113.20
1	C	230	GLN	N-CA-C	7.85	122.49	113.15
1	D	230	GLN	N-CA-C	7.84	122.69	113.20
1	B	230	GLN	N-CA-C	7.83	122.67	113.20
1	E	230	GLN	N-CA-C	7.74	122.36	113.15
1	F	230	GLN	N-CA-C	7.64	122.45	113.20
1	F	220	GLU	N-CA-C	6.86	120.13	111.69
1	D	220	GLU	N-CA-C	6.82	120.08	111.69
1	C	220	GLU	N-CA-C	6.79	120.04	111.69
1	E	220	GLU	N-CA-C	6.76	120.01	111.69
1	C	150	PRO	N-CA-C	-6.63	100.83	111.38
1	D	150	PRO	N-CA-C	-6.63	100.84	111.38
1	A	220	GLU	N-CA-C	6.61	119.82	111.69
1	A	150	PRO	N-CA-C	-6.59	100.90	111.38
1	B	220	GLU	N-CA-C	6.57	119.77	111.69
1	B	150	PRO	N-CA-C	-6.54	100.98	111.38
1	E	150	PRO	N-CA-C	-6.50	101.05	111.38
1	E	123	GLY	N-CA-C	6.46	123.82	112.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ASP	N-CA-C	6.45	119.12	111.71
1	F	123	GLY	N-CA-C	6.43	123.76	112.83
1	F	150	PRO	N-CA-C	-6.39	101.21	111.38
1	D	123	GLY	N-CA-C	6.35	123.63	112.83
1	B	219	ASP	N-CA-C	6.32	118.97	111.71
1	D	219	ASP	N-CA-C	6.32	118.97	111.71
1	B	122	VAL	N-CA-C	6.29	117.50	111.91
1	E	219	ASP	N-CA-C	6.28	118.93	111.71
1	C	219	ASP	N-CA-C	6.27	118.92	111.71
1	F	219	ASP	N-CA-C	6.26	118.91	111.71
1	C	123	GLY	N-CA-C	6.23	123.42	112.83
1	C	232	ASP	N-CA-C	-6.23	101.56	110.59
1	A	122	VAL	N-CA-C	6.17	117.40	111.91
1	A	232	ASP	N-CA-C	-6.12	101.71	110.59
1	F	232	ASP	N-CA-C	-6.10	101.74	110.59
1	C	122	VAL	N-CA-C	6.09	117.33	111.91
1	D	232	ASP	N-CA-C	-6.09	101.45	110.46
1	E	122	VAL	N-CA-C	6.06	117.30	111.91
1	E	232	ASP	N-CA-C	-6.06	101.81	110.59
1	D	122	VAL	N-CA-C	6.03	117.27	111.91
1	F	122	VAL	N-CA-C	5.98	117.23	111.91
1	A	123	GLY	N-CA-C	5.96	122.97	112.83
1	A	350	PHE	N-CA-C	-5.93	100.03	109.23
1	B	232	ASP	N-CA-C	-5.92	102.00	110.59
1	B	350	PHE	N-CA-C	-5.82	100.21	109.23
1	B	123	GLY	N-CA-C	5.81	122.71	112.83
1	E	350	PHE	N-CA-C	-5.78	100.27	109.23
1	C	79	SER	N-CA-C	-5.74	101.03	109.18
1	D	79	SER	N-CA-C	-5.67	101.13	109.18
1	B	79	SER	N-CA-C	-5.66	101.14	109.18
1	F	350	PHE	N-CA-C	-5.63	100.51	109.23
1	E	79	SER	N-CA-C	-5.62	101.19	109.18
1	A	79	SER	N-CA-C	-5.55	101.30	109.18
1	D	350	PHE	N-CA-C	-5.54	100.64	109.23
1	C	350	PHE	N-CA-C	-5.54	100.65	109.23
1	F	79	SER	N-CA-C	-5.52	101.34	109.18
1	C	295	SER	N-CA-C	5.47	117.39	109.07
1	A	295	SER	N-CA-C	5.47	117.38	109.07
1	A	251	ILE	N-CA-C	-5.46	99.78	107.75
1	D	218	GLY	N-CA-C	-5.45	105.81	112.68
1	A	97	ALA	N-CA-C	5.45	117.92	111.33
1	E	221	PHE	N-CA-C	5.43	116.25	109.57

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	SER	N-CA-C	5.42	117.31	109.07
1	F	221	PHE	N-CA-C	5.42	116.23	109.57
1	E	97	ALA	N-CA-C	5.39	117.86	111.33
1	D	295	SER	N-CA-C	5.39	117.27	109.07
1	F	97	ALA	N-CA-C	5.39	117.85	111.33
1	B	97	ALA	N-CA-C	5.37	117.82	111.33
1	C	127	MET	N-CA-C	5.32	117.50	111.11
1	D	221	PHE	N-CA-C	5.32	116.11	109.57
1	D	127	MET	N-CA-C	5.29	117.46	111.11
1	D	97	ALA	N-CA-C	5.27	117.71	111.33
1	D	158	HIS	N-CA-C	-5.25	106.90	113.72
1	C	221	PHE	N-CA-C	5.24	116.02	109.57
1	B	221	PHE	N-CA-C	5.23	116.00	109.57
1	A	15	ALA	N-CA-C	5.22	116.82	108.41
1	B	251	ILE	N-CA-C	-5.22	100.13	107.75
1	C	158	HIS	N-CA-C	-5.21	106.94	113.72
1	D	251	ILE	N-CA-C	-5.19	100.17	107.75
1	C	251	ILE	N-CA-C	-5.18	100.19	107.75
1	E	251	ILE	N-CA-C	-5.18	100.19	107.75
1	C	97	ALA	N-CA-C	5.17	117.58	111.33
1	F	251	ILE	N-CA-C	-5.17	100.20	107.75
1	A	221	PHE	N-CA-C	5.15	115.91	109.57
1	E	295	SER	N-CA-C	5.15	116.89	109.07
1	F	295	SER	N-CA-C	5.12	116.85	109.07
1	F	9	ALA	CA-C-O	5.11	120.90	117.94
1	F	127	MET	N-CA-C	5.01	117.12	111.11

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	3081	0	3064	58	0
1	B	3081	0	3064	52	0
1	C	3056	0	3040	51	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3056	0	3040	53	0
1	E	3056	0	3040	58	0
1	F	3056	0	3040	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	8	0	0
3	B	13	0	8	0	0
3	C	13	0	8	0	0
3	D	13	0	8	0	0
3	E	13	0	8	0	0
3	F	13	0	8	0	0
4	A	143	0	0	4	0
4	B	137	0	0	0	0
4	C	71	0	0	2	0
4	D	65	0	0	0	0
4	E	90	0	0	3	1
4	F	85	0	0	6	0
All	All	19057	0	18336	318	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (318) 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:B:302:ALA:H	1:B:334:HIS:HE1	1.24	0.86
1:D:302:ALA:H	1:D:334:HIS:HE1	1.24	0.85
1:F:302:ALA:H	1:F:334:HIS:HE1	1.26	0.84
1:A:302:ALA:H	1:A:334:HIS:HE1	1.24	0.84
1:C:14:LYS:HA	1:C:14:LYS:HE2	1.59	0.83
1:C:302:ALA:H	1:C:334:HIS:HE1	1.24	0.82
1:E:302:ALA:H	1:E:334:HIS:HE1	1.25	0.82
1:E:19:ARG:HG3	1:E:19:ARG:HH11	1.45	0.80
1:B:207:ILE:O	1:B:211:THR:HG23	1.84	0.77
1:A:284:ARG:CZ	4:A:936:HOH:O	2.34	0.76
1:A:207:ILE:O	1:A:211:THR:HG23	1.85	0.76
1:D:207:ILE:O	1:D:211:THR:HG23	1.86	0.75
1:A:19:ARG:HG3	1:A:19:ARG:HH11	1.50	0.75
1:C:207:ILE:O	1:C:211:THR:HG23	1.87	0.74
1:F:207:ILE:O	1:F:211:THR:HG23	1.87	0.74
1:F:293:ASN:HD22	1:F:323:ARG:HH21	1.37	0.73

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:GLU:OE1	4:C:874:HOH:O	2.05	0.73
1:E:293:ASN:HD22	1:E:323:ARG:HH21	1.35	0.73
1:F:45:SER:H	1:F:173:HIS:HD2	1.36	0.73
1:F:19:ARG:HG3	1:F:19:ARG:HH11	1.52	0.73
1:E:207:ILE:O	1:E:211:THR:HG23	1.88	0.73
1:B:19:ARG:HG3	1:B:19:ARG:HH11	1.54	0.72
1:D:293:ASN:HD22	1:D:323:ARG:HH21	1.36	0.72
1:D:45:SER:H	1:D:173:HIS:HD2	1.37	0.72
1:B:293:ASN:HD22	1:B:323:ARG:HH21	1.36	0.71
1:C:45:SER:H	1:C:173:HIS:HD2	1.37	0.71
1:C:41:ALA:HB2	1:E:4:SER:N	2.06	0.70
1:B:45:SER:H	1:B:173:HIS:HD2	1.38	0.70
1:A:293:ASN:HD22	1:A:323:ARG:HH21	1.38	0.69
1:C:293:ASN:HD22	1:C:323:ARG:HH21	1.37	0.69
1:E:45:SER:H	1:E:173:HIS:HD2	1.36	0.69
1:A:45:SER:H	1:A:173:HIS:HD2	1.39	0.68
1:A:45:SER:H	1:A:173:HIS:CD2	2.13	0.67
1:E:278:GLU:OE1	4:E:895:HOH:O	2.12	0.67
1:E:45:SER:H	1:E:173:HIS:CD2	2.13	0.67
1:B:197:LYS:NZ	1:B:228:ASN:HD21	1.93	0.66
1:F:211:THR:HG22	1:F:246:PHE:CZ	2.30	0.66
1:F:165:TYR:CE1	1:F:195:LYS:HE3	2.31	0.66
1:A:197:LYS:NZ	1:A:228:ASN:HD21	1.94	0.66
1:E:302:ALA:H	1:E:334:HIS:CE1	2.12	0.66
1:D:45:SER:H	1:D:173:HIS:CD2	2.13	0.66
1:F:45:SER:H	1:F:173:HIS:CD2	2.12	0.66
1:E:165:TYR:CE1	1:E:195:LYS:HE3	2.30	0.66
1:A:321:HIS:HD2	4:A:841:HOH:O	1.79	0.66
1:B:45:SER:H	1:B:173:HIS:CD2	2.12	0.66
1:B:211:THR:HG22	1:B:246:PHE:CZ	2.31	0.66
1:D:14:LYS:HA	1:D:14:LYS:HE3	1.77	0.66
1:B:302:ALA:H	1:B:334:HIS:CE1	2.11	0.66
1:C:45:SER:H	1:C:173:HIS:CD2	2.13	0.66
1:E:19:ARG:HG3	1:E:19:ARG:NH1	2.10	0.66
1:C:211:THR:HG22	1:C:246:PHE:CZ	2.32	0.65
1:E:211:THR:HG22	1:E:246:PHE:CZ	2.30	0.65
1:A:302:ALA:HB3	1:A:303:PRO:HD3	1.78	0.65
1:A:211:THR:HG22	1:A:246:PHE:CZ	2.31	0.65
1:A:302:ALA:H	1:A:334:HIS:CE1	2.11	0.65
1:F:278:GLU:OE1	4:F:891:HOH:O	2.14	0.65
1:D:211:THR:HG22	1:D:246:PHE:CZ	2.32	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:THR:HG22	1:E:246:PHE:HZ	1.62	0.64
1:F:302:ALA:H	1:F:334:HIS:CE1	2.13	0.64
1:F:302:ALA:HB3	1:F:303:PRO:HD3	1.80	0.64
1:D:165:TYR:CE1	1:D:195:LYS:HE3	2.33	0.64
1:C:302:ALA:H	1:C:334:HIS:CE1	2.11	0.64
1:D:302:ALA:HB3	1:D:303:PRO:HD3	1.80	0.64
1:C:165:TYR:CE1	1:C:195:LYS:HE3	2.33	0.63
1:D:302:ALA:H	1:D:334:HIS:CE1	2.11	0.63
1:F:211:THR:HG22	1:F:246:PHE:HZ	1.63	0.63
1:C:302:ALA:HB3	1:C:303:PRO:HD3	1.81	0.63
1:B:329:PHE:O	1:B:334:HIS:HD2	1.82	0.63
1:C:197:LYS:NZ	1:C:228:ASN:HD21	1.96	0.63
1:E:197:LYS:NZ	1:E:228:ASN:HD21	1.97	0.62
1:B:302:ALA:HB3	1:B:303:PRO:HD3	1.80	0.62
1:E:302:ALA:HB3	1:E:303:PRO:HD3	1.81	0.62
1:C:329:PHE:O	1:C:334:HIS:HD2	1.82	0.62
1:A:329:PHE:O	1:A:334:HIS:HD2	1.82	0.62
1:B:211:THR:HG22	1:B:246:PHE:HZ	1.64	0.62
1:C:211:THR:HG22	1:C:246:PHE:HZ	1.64	0.62
1:D:211:THR:HG22	1:D:246:PHE:HZ	1.64	0.62
1:D:197:LYS:NZ	1:D:228:ASN:HD21	1.97	0.62
1:A:165:TYR:CE1	1:A:195:LYS:HE3	2.35	0.62
1:E:55:LYS:HE2	1:E:55:LYS:HA	1.82	0.61
1:A:211:THR:HG22	1:A:246:PHE:HZ	1.64	0.61
1:B:165:TYR:CE1	1:B:195:LYS:HE3	2.34	0.61
1:D:329:PHE:O	1:D:334:HIS:HD2	1.83	0.61
1:F:197:LYS:NZ	1:F:228:ASN:HD21	1.98	0.61
1:F:329:PHE:O	1:F:334:HIS:HD2	1.83	0.61
1:C:55:LYS:HE2	1:C:55:LYS:HA	1.83	0.61
1:A:53:ARG:HD2	1:B:117:TRP:NE1	2.16	0.60
1:E:329:PHE:O	1:E:334:HIS:HD2	1.83	0.60
1:F:55:LYS:HA	1:F:55:LYS:HE2	1.83	0.60
1:E:195:LYS:HD3	1:E:226:ASP:HB2	1.84	0.60
1:A:117:TRP:NE1	1:B:53:ARG:HD2	2.17	0.60
1:D:55:LYS:HE2	1:D:55:LYS:HA	1.83	0.59
1:A:55:LYS:HA	1:A:55:LYS:HE2	1.83	0.59
1:A:127:MET:HB3	1:B:127:MET:HB3	1.84	0.58
1:B:55:LYS:HE2	1:B:55:LYS:HA	1.84	0.58
1:F:19:ARG:HG3	1:F:19:ARG:NH1	2.18	0.58
1:C:195:LYS:HD3	1:C:226:ASP:HB2	1.86	0.58
1:F:195:LYS:HD3	1:F:226:ASP:HB2	1.85	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ARG:HG3	1:A:19:ARG:NH1	2.19	0.57
1:F:82:LYS:O	1:F:83:ARG:HB2	2.05	0.57
1:B:195:LYS:HD3	1:B:226:ASP:HB2	1.87	0.57
1:D:195:LYS:HD3	1:D:226:ASP:HB2	1.87	0.57
1:E:293:ASN:HD22	1:E:323:ARG:NH2	2.03	0.56
1:D:197:LYS:HZ2	1:D:228:ASN:HD21	1.54	0.56
1:F:284:ARG:HG2	4:F:872:HOH:O	2.06	0.56
1:C:197:LYS:HZ2	1:C:228:ASN:HD21	1.54	0.55
1:A:195:LYS:HD3	1:A:226:ASP:HB2	1.89	0.55
1:C:82:LYS:O	1:C:83:ARG:HB2	2.07	0.55
1:D:41:ALA:HB2	1:F:4:SER:CB	2.36	0.55
1:B:82:LYS:O	1:B:83:ARG:HB2	2.07	0.55
1:D:82:LYS:O	1:D:83:ARG:HB2	2.06	0.55
1:B:19:ARG:HG3	1:B:19:ARG:NH1	2.21	0.54
1:B:197:LYS:HZ2	1:B:228:ASN:HD21	1.55	0.54
1:B:293:ASN:HD22	1:B:323:ARG:NH2	2.05	0.54
1:F:293:ASN:HD22	1:F:323:ARG:NH2	2.05	0.54
1:D:360:GLN:HG3	1:F:13:ALA:HB1	1.89	0.54
1:E:284:ARG:HG2	4:E:878:HOH:O	2.06	0.54
1:E:82:LYS:O	1:E:83:ARG:HB2	2.06	0.54
1:B:14:LYS:HA	1:B:14:LYS:HZ3	1.73	0.53
1:D:301:ASP:OD1	1:D:303:PRO:HD2	2.09	0.52
1:B:301:ASP:OD1	1:B:303:PRO:HD2	2.09	0.52
1:C:301:ASP:OD1	1:C:303:PRO:HD2	2.08	0.52
1:A:82:LYS:O	1:A:83:ARG:HB2	2.09	0.52
1:D:293:ASN:HD22	1:D:323:ARG:NH2	2.05	0.52
1:F:68:ARG:CZ	4:F:828:HOH:O	2.58	0.52
1:A:301:ASP:OD1	1:A:303:PRO:HD2	2.09	0.52
1:F:197:LYS:HZ2	1:F:228:ASN:HD21	1.58	0.51
1:C:293:ASN:HD22	1:C:323:ARG:NH2	2.07	0.51
1:E:79:SER:HA	1:E:303:PRO:HB3	1.92	0.51
1:A:79:SER:HA	1:A:303:PRO:HB3	1.93	0.51
1:B:79:SER:HA	1:B:303:PRO:HB3	1.91	0.51
1:E:301:ASP:OD1	1:E:303:PRO:HD2	2.11	0.51
1:F:45:SER:HB2	1:F:173:HIS:HB3	1.93	0.51
1:D:79:SER:HA	1:D:303:PRO:HB3	1.92	0.51
1:D:41:ALA:HB2	1:F:4:SER:HB2	1.93	0.50
1:A:280:LEU:HB2	1:A:286:HIS:CE1	2.47	0.50
1:E:45:SER:HB2	1:E:173:HIS:HB3	1.94	0.50
1:E:280:LEU:HB2	1:E:286:HIS:CE1	2.46	0.50
1:F:301:ASP:OD1	1:F:303:PRO:HD2	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:ALA:HB3	1:F:375:GLY:HA2	1.94	0.50
1:B:38:LEU:HD21	1:B:352:TRP:O	2.12	0.50
1:C:79:SER:HA	1:C:303:PRO:HB3	1.93	0.49
1:E:286:HIS:HE1	4:E:807:HOH:O	1.94	0.49
1:F:79:SER:HA	1:F:303:PRO:HB3	1.93	0.49
1:C:45:SER:HB2	1:C:173:HIS:HB3	1.94	0.49
1:D:41:ALA:HB2	1:F:4:SER:OG	2.12	0.49
1:E:144:ALA:HB3	1:E:375:GLY:HA2	1.93	0.49
1:B:45:SER:HB2	1:B:173:HIS:HB3	1.94	0.49
1:F:280:LEU:HB2	1:F:286:HIS:CE1	2.47	0.49
1:C:19:ARG:HD3	1:C:24:THR:HG21	1.94	0.49
1:E:20:THR:OG1	1:E:23:GLU:HG2	2.13	0.49
1:C:20:THR:OG1	1:C:23:GLU:HG2	2.13	0.49
1:A:144:ALA:HB3	1:A:375:GLY:HA2	1.94	0.48
1:C:311:PHE:CD2	1:C:337:LEU:HD13	2.48	0.48
1:A:45:SER:HB2	1:A:173:HIS:HB3	1.95	0.48
1:A:284:ARG:NH2	4:A:936:HOH:O	2.45	0.48
1:B:14:LYS:HA	1:B:14:LYS:NZ	2.28	0.48
1:C:280:LEU:HB2	1:C:286:HIS:CE1	2.47	0.48
1:D:311:PHE:CD2	1:D:337:LEU:HD13	2.48	0.48
1:A:63:ILE:N	1:A:63:ILE:HD12	2.29	0.48
1:A:237:ILE:O	1:A:241:ARG:HG2	2.13	0.48
1:B:280:LEU:HB2	1:B:286:HIS:CE1	2.49	0.48
1:D:38:LEU:HD21	1:D:352:TRP:O	2.14	0.48
1:D:45:SER:HB2	1:D:173:HIS:HB3	1.95	0.48
1:D:278:GLU:HG3	1:D:279:MET:N	2.28	0.48
1:A:38:LEU:HD21	1:A:352:TRP:O	2.14	0.48
1:C:278:GLU:HG3	1:C:279:MET:N	2.29	0.48
1:E:311:PHE:CD2	1:E:337:LEU:HD13	2.49	0.48
1:B:63:ILE:HD12	1:B:63:ILE:N	2.29	0.48
1:A:293:ASN:HD22	1:A:323:ARG:NH2	2.07	0.48
1:D:13:ALA:HB1	1:F:360:GLN:HG3	1.95	0.48
1:F:20:THR:OG1	1:F:23:GLU:HG2	2.14	0.48
1:B:237:ILE:O	1:B:241:ARG:HG2	2.14	0.48
1:D:280:LEU:HB2	1:D:286:HIS:CE1	2.48	0.48
1:F:354:ASN:HB2	1:F:355:PRO:HD3	1.96	0.48
1:C:237:ILE:O	1:C:241:ARG:HG2	2.14	0.47
1:C:144:ALA:HB3	1:C:375:GLY:HA2	1.96	0.47
1:D:20:THR:OG1	1:D:23:GLU:HG2	2.13	0.47
1:D:144:ALA:HB3	1:D:375:GLY:HA2	1.95	0.47
1:F:68:ARG:NE	4:F:828:HOH:O	2.46	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:GLU:HG3	1:F:279:MET:N	2.29	0.47
1:B:144:ALA:HB3	1:B:375:GLY:HA2	1.95	0.47
1:C:38:LEU:HD21	1:C:352:TRP:O	2.15	0.47
1:C:360:GLN:HG3	1:E:13:ALA:HB1	1.97	0.47
1:F:311:PHE:CD2	1:F:337:LEU:HD13	2.50	0.47
1:F:150:PRO:HB3	4:F:837:HOH:O	2.14	0.47
1:B:281:THR:O	1:B:282:SER:HB3	2.14	0.47
1:D:237:ILE:O	1:D:241:ARG:HG2	2.15	0.47
1:A:278:GLU:HG3	1:A:279:MET:N	2.30	0.46
1:B:311:PHE:CD2	1:B:337:LEU:HD13	2.50	0.46
1:F:286:HIS:HE1	4:F:810:HOH:O	1.98	0.46
1:E:38:LEU:CD2	1:E:353:LEU:HD23	2.45	0.46
1:B:354:ASN:HB2	1:B:355:PRO:HD3	1.97	0.46
1:D:293:ASN:ND2	1:D:323:ARG:HH21	2.09	0.46
1:F:38:LEU:CD2	1:F:353:LEU:HD23	2.46	0.46
1:C:38:LEU:CD2	1:C:353:LEU:HD23	2.46	0.46
1:E:278:GLU:HG3	1:E:279:MET:N	2.29	0.46
1:E:354:ASN:HB2	1:E:355:PRO:HD3	1.97	0.46
1:F:187:ARG:HA	1:F:191:ILE:HG22	1.98	0.46
1:F:237:ILE:O	1:F:241:ARG:HG2	2.16	0.46
1:A:311:PHE:CD2	1:A:337:LEU:HD13	2.51	0.46
1:A:354:ASN:HB2	1:A:355:PRO:HD3	1.97	0.46
1:B:278:GLU:HG3	1:B:279:MET:N	2.31	0.45
1:D:38:LEU:CD2	1:D:353:LEU:HD23	2.46	0.45
1:F:38:LEU:HD21	1:F:352:TRP:O	2.16	0.45
1:C:13:ALA:HB1	1:E:360:GLN:HG3	1.98	0.45
1:B:20:THR:OG1	1:B:23:GLU:HG2	2.16	0.45
1:E:38:LEU:HD21	1:E:352:TRP:O	2.16	0.45
1:D:160:ASP:CB	1:F:22:ALA:HB2	2.47	0.45
1:E:187:ARG:HA	1:E:191:ILE:HG22	1.98	0.45
1:A:301:ASP:HB3	1:A:304:ARG:HB2	1.99	0.45
1:C:301:ASP:HB3	1:C:304:ARG:HB2	1.99	0.45
1:E:281:THR:O	1:E:282:SER:HB3	2.16	0.45
1:B:301:ASP:HB3	1:B:304:ARG:HB2	1.98	0.45
1:E:237:ILE:O	1:E:241:ARG:HG2	2.16	0.45
1:A:187:ARG:HA	1:A:191:ILE:HG22	1.99	0.44
1:D:63:ILE:N	1:D:63:ILE:HD12	2.31	0.44
1:A:281:THR:O	1:A:282:SER:HB3	2.17	0.44
1:F:293:ASN:ND2	1:F:323:ARG:HH21	2.09	0.44
1:C:160:ASP:CB	1:E:22:ALA:HB2	2.48	0.44
1:D:38:LEU:HD12	1:D:387:TRP:CZ3	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:ASP:HB3	1:E:304:ARG:HB2	1.99	0.44
1:E:293:ASN:ND2	1:E:323:ARG:HH21	2.09	0.44
1:A:20:THR:OG1	1:A:23:GLU:HG2	2.16	0.44
1:B:359:GLU:OE1	1:B:359:GLU:N	2.51	0.44
1:B:187:ARG:HA	1:B:191:ILE:HG22	2.00	0.44
1:C:133:SER:HB2	1:C:134:PRO:HD3	1.99	0.44
1:C:162:VAL:CG2	1:C:347:LEU:HB2	2.47	0.44
1:A:38:LEU:CD2	1:A:353:LEU:HD23	2.48	0.44
1:F:51:THR:OG1	1:F:230:GLN:NE2	2.51	0.44
1:F:63:ILE:N	1:F:63:ILE:HD12	2.33	0.44
1:C:187:ARG:HA	1:C:191:ILE:HG22	1.99	0.44
1:D:301:ASP:HB3	1:D:304:ARG:HB2	2.00	0.44
1:F:301:ASP:HB3	1:F:304:ARG:HB2	2.00	0.43
1:A:162:VAL:CG2	1:A:347:LEU:HB2	2.47	0.43
1:A:300:PRO:HB2	1:A:311:PHE:CE1	2.53	0.43
1:B:38:LEU:CD2	1:B:353:LEU:HD23	2.47	0.43
1:D:133:SER:HB2	1:D:134:PRO:HD3	2.00	0.43
1:D:187:ARG:HA	1:D:191:ILE:HG22	1.99	0.43
1:D:354:ASN:HB2	1:D:355:PRO:HD3	1.99	0.43
1:F:281:THR:O	1:F:282:SER:HB3	2.18	0.43
1:D:162:VAL:CG2	1:D:347:LEU:HB2	2.47	0.43
1:A:13:ALA:C	1:A:14:LYS:HD2	2.43	0.43
1:B:239:MET:O	1:B:243:MET:HG3	2.18	0.43
1:C:38:LEU:HD22	1:C:353:LEU:HD23	2.01	0.43
1:E:38:LEU:HD12	1:E:387:TRP:CZ3	2.53	0.43
1:A:126:GLY:O	1:A:129:VAL:HG22	2.17	0.43
1:B:162:VAL:CG2	1:B:347:LEU:HB2	2.48	0.43
1:C:63:ILE:N	1:C:63:ILE:HD12	2.32	0.43
1:C:354:ASN:HB2	1:C:355:PRO:HD3	1.99	0.43
1:E:162:VAL:CG2	1:E:347:LEU:HB2	2.48	0.43
1:F:38:LEU:HD12	1:F:387:TRP:CZ3	2.54	0.43
1:F:162:VAL:CG2	1:F:347:LEU:HB2	2.48	0.43
1:A:197:LYS:HZ1	1:A:228:ASN:HD21	1.64	0.43
1:C:281:THR:O	1:C:282:SER:HB3	2.19	0.43
1:E:63:ILE:HD12	1:E:63:ILE:N	2.33	0.43
1:B:38:LEU:HD12	1:B:387:TRP:CZ3	2.54	0.43
1:C:38:LEU:HD12	1:C:387:TRP:CZ3	2.53	0.43
1:B:51:THR:OG1	1:B:230:GLN:NE2	2.52	0.42
1:D:38:LEU:HD22	1:D:353:LEU:HD23	2.00	0.42
1:D:300:PRO:HB2	1:D:311:PHE:CE1	2.54	0.42
1:E:274:ILE:O	1:E:295:SER:HB2	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:GLY:O	1:B:129:VAL:HG22	2.19	0.42
1:B:300:PRO:HB2	1:B:311:PHE:CE1	2.55	0.42
1:C:300:PRO:HB2	1:C:311:PHE:CE1	2.54	0.42
1:E:293:ASN:ND2	1:E:323:ARG:NH2	2.67	0.42
1:E:300:PRO:HB2	1:E:311:PHE:CE1	2.54	0.42
1:D:51:THR:OG1	1:D:230:GLN:NE2	2.52	0.42
1:D:41:ALA:CB	1:F:4:SER:OG	2.67	0.42
1:D:281:THR:O	1:D:282:SER:HB3	2.19	0.42
1:F:274:ILE:O	1:F:295:SER:HB2	2.20	0.42
1:A:38:LEU:HD12	1:A:387:TRP:CZ3	2.54	0.42
1:A:239:MET:O	1:A:243:MET:HG3	2.20	0.42
1:A:293:ASN:ND2	1:A:323:ARG:HH21	2.11	0.42
1:B:293:ASN:ND2	1:B:323:ARG:HH21	2.10	0.42
1:C:51:THR:OG1	1:C:230:GLN:NE2	2.53	0.42
1:C:286:HIS:HE1	4:C:817:HOH:O	2.03	0.42
1:D:126:GLY:O	1:D:129:VAL:HG22	2.19	0.42
1:E:14:LYS:HA	1:E:14:LYS:HD3	1.93	0.42
1:A:197:LYS:HG2	4:A:807:HOH:O	2.20	0.42
1:C:293:ASN:ND2	1:C:323:ARG:HH21	2.10	0.42
1:F:165:TYR:HE1	1:F:195:LYS:HE3	1.83	0.42
1:A:359:GLU:OE1	1:A:359:GLU:N	2.50	0.42
1:B:38:LEU:HD22	1:B:353:LEU:HD23	2.02	0.41
1:C:126:GLY:O	1:C:129:VAL:HG22	2.19	0.41
1:E:165:TYR:HE1	1:E:195:LYS:HE3	1.81	0.41
1:E:221:PHE:HA	1:E:222:PRO:HD3	1.94	0.41
1:A:51:THR:OG1	1:A:230:GLN:NE2	2.53	0.41
1:D:293:ASN:ND2	1:D:323:ARG:NH2	2.68	0.41
1:E:51:THR:OG1	1:E:230:GLN:NE2	2.53	0.41
1:A:133:SER:HB2	1:A:134:PRO:HD3	2.02	0.41
1:B:133:SER:HB2	1:B:134:PRO:HD3	2.02	0.41
1:F:359:GLU:OE1	1:F:359:GLU:N	2.52	0.41
1:D:46:ASP:CG	1:D:48:LYS:HZ2	2.29	0.41
1:E:359:GLU:OE1	1:E:359:GLU:N	2.53	0.41
1:F:293:ASN:ND2	1:F:323:ARG:NH2	2.67	0.41
1:F:300:PRO:HB2	1:F:311:PHE:CE1	2.55	0.41
1:A:250:TRP:CD1	1:A:250:TRP:C	2.98	0.41
1:E:38:LEU:HD22	1:E:353:LEU:HD23	2.03	0.41
1:A:284:ARG:HG2	1:A:284:ARG:HH11	1.86	0.41
1:A:17:ASN:OD1	1:A:19:ARG:HB2	2.22	0.40
1:D:85:GLY:O	1:D:89:ILE:HG13	2.21	0.40
1:F:38:LEU:HD22	1:F:353:LEU:HD23	2.02	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:ASP:CG	1:F:48:LYS:HZ2	2.29	0.40
1:A:38:LEU:HD22	1:A:353:LEU:HD23	2.02	0.40
1:A:339:ALA:CB	1:A:370:ILE:HD11	2.52	0.40
1:C:274:ILE:O	1:C:295:SER:HB2	2.20	0.40
1:C:293:ASN:ND2	1:C:323:ARG:NH2	2.68	0.40
1:E:85:GLY:O	1:E:89:ILE:HG13	2.21	0.40
1:E:197:LYS:HZ3	1:E:228:ASN:HD21	1.69	0.40
1:F:329:PHE:CG	1:F:330:ALA:N	2.89	0.40
1:A:329:PHE:CG	1:A:330:ALA:N	2.88	0.40
1:B:274:ILE:O	1:B:295:SER:HB2	2.22	0.40
1:D:160:ASP:HB3	1:F:22:ALA:HB2	2.04	0.40
1:E:126:GLY:O	1:E:129:VAL:HG22	2.21	0.40
1:E:239:MET:O	1:E:243:MET:HG3	2.22	0.40
1:E:354:ASN:N	1:E:355:PRO:CD	2.85	0.40
1:B:250:TRP:CD1	1:B:250:TRP:C	2.99	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:871:HOH:O	4:E:887:HOH:O[3_455]	2.18	0.02

## 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	393/398 (99%)	383 (98%)	8 (2%)	2 (0%)	24 27
1	B	393/398 (99%)	383 (98%)	9 (2%)	1 (0%)	36 42
1	C	387/398 (97%)	377 (97%)	9 (2%)	1 (0%)	36 42
1	D	387/398 (97%)	377 (97%)	9 (2%)	1 (0%)	36 42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	387/398 (97%)	376 (97%)	10 (3%)	1 (0%)	36	42
1	F	387/398 (97%)	377 (97%)	9 (2%)	1 (0%)	36	42
All	All	2334/2388 (98%)	2273 (97%)	54 (2%)	7 (0%)	36	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	B	83	ARG
1	C	83	ARG
1	D	83	ARG
1	E	83	ARG
1	F	83	ARG
1	A	330	ALA

### 5.3.2 Protein sidechains [i](#)

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	318/320 (99%)	314 (99%)	4 (1%)	61	76
1	B	318/320 (99%)	313 (98%)	5 (2%)	55	71
1	C	316/320 (99%)	312 (99%)	4 (1%)	61	76
1	D	316/320 (99%)	311 (98%)	5 (2%)	55	71
1	E	316/320 (99%)	312 (99%)	4 (1%)	61	76
1	F	316/320 (99%)	312 (99%)	4 (1%)	61	76
All	All	1900/1920 (99%)	1874 (99%)	26 (1%)	59	75

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLU
1	A	109	ASP
1	A	162	VAL

Continued on next page...

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	224	MET
1	B	14	LYS
1	B	74	GLU
1	B	109	ASP
1	B	162	VAL
1	B	224	MET
1	C	74	GLU
1	C	109	ASP
1	C	162	VAL
1	C	224	MET
1	D	14	LYS
1	D	74	GLU
1	D	109	ASP
1	D	162	VAL
1	D	224	MET
1	E	74	GLU
1	E	109	ASP
1	E	162	VAL
1	E	224	MET
1	F	74	GLU
1	F	109	ASP
1	F	162	VAL
1	F	224	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	106	ASN
1	A	163	GLN
1	A	173	HIS
1	A	178	GLN
1	A	228	ASN
1	A	230	GLN
1	A	263	HIS
1	A	286	HIS
1	A	293	ASN
1	A	321	HIS
1	A	334	HIS
1	A	358	ASN
1	B	106	ASN
1	B	163	GLN
1	B	173	HIS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	178	GLN
1	B	228	ASN
1	B	230	GLN
1	B	263	HIS
1	B	286	HIS
1	B	293	ASN
1	B	334	HIS
1	B	358	ASN
1	C	106	ASN
1	C	163	GLN
1	C	173	HIS
1	C	178	GLN
1	C	228	ASN
1	C	230	GLN
1	C	263	HIS
1	C	286	HIS
1	C	293	ASN
1	C	334	HIS
1	C	358	ASN
1	D	106	ASN
1	D	163	GLN
1	D	173	HIS
1	D	178	GLN
1	D	228	ASN
1	D	230	GLN
1	D	263	HIS
1	D	286	HIS
1	D	293	ASN
1	D	334	HIS
1	D	358	ASN
1	E	106	ASN
1	E	163	GLN
1	E	173	HIS
1	E	178	GLN
1	E	228	ASN
1	E	230	GLN
1	E	263	HIS
1	E	286	HIS
1	E	293	ASN
1	E	334	HIS
1	E	358	ASN
1	F	106	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	163	GLN
1	F	173	HIS
1	F	178	GLN
1	F	228	ASN
1	F	230	GLN
1	F	263	HIS
1	F	286	HIS
1	F	293	ASN
1	F	334	HIS
1	F	358	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	LLH	C	803	-	11,12,12	1.04	0	13,16,16	1.16	2 (15%)
3	LLH	A	801	2	11,12,12	0.80	0	13,16,16	1.12	2 (15%)
3	LLH	B	802	2	11,12,12	0.81	0	13,16,16	1.14	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LLH	F	806	-	11,12,12	0.98	0	13,16,16	1.23	2 (15%)
3	LLH	E	805	-	11,12,12	1.18	1 (9%)	13,16,16	1.35	2 (15%)
3	LLH	D	804	-	11,12,12	1.23	2 (18%)	13,16,16	1.21	1 (7%)

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	LLH	C	803	-	-	4/18/18/18	-
3	LLH	A	801	2	-	2/18/18/18	-
3	LLH	B	802	2	-	3/18/18/18	-
3	LLH	F	806	-	-	4/18/18/18	-
3	LLH	E	805	-	-	4/18/18/18	-
3	LLH	D	804	-	-	4/18/18/18	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	805	LLH	C2-C1	2.40	1.57	1.52
3	D	804	LLH	C2-C1	2.09	1.57	1.52
3	D	804	LLH	C4-C5	2.09	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	805	LLH	C3-C2-C1	2.83	116.61	109.78
3	E	805	LLH	O2-C2-C3	-2.48	104.99	110.38
3	B	802	LLH	C3-C2-C1	2.46	115.70	109.78
3	C	803	LLH	C3-C2-C1	2.45	115.69	109.78
3	D	804	LLH	C3-C2-C1	2.44	115.67	109.78
3	A	801	LLH	O2-C2-C3	-2.37	105.23	110.38
3	F	806	LLH	O2-C2-C3	-2.35	105.28	110.38
3	A	801	LLH	C3-C2-C1	2.26	115.24	109.78
3	F	806	LLH	C3-C2-C1	2.18	115.04	109.78
3	B	802	LLH	O2-C2-C3	-2.16	105.70	110.38
3	C	803	LLH	O2-C2-C3	-2.15	105.70	110.38

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	LLH	O1-C1-C2-O2
3	A	801	LLH	N-C1-C2-O2
3	B	802	LLH	O1-C1-C2-O2
3	B	802	LLH	N-C1-C2-O2
3	C	803	LLH	C2-C1-N-ON
3	C	803	LLH	O1-C1-N-ON
3	D	804	LLH	C2-C1-N-ON
3	D	804	LLH	O1-C1-N-ON
3	E	805	LLH	O1-C1-C2-O2
3	E	805	LLH	N-C1-C2-O2
3	F	806	LLH	C2-C1-N-ON
3	F	806	LLH	O1-C1-N-ON
3	C	803	LLH	O1-C1-C2-O2
3	C	803	LLH	N-C1-C2-O2
3	D	804	LLH	O1-C1-C2-O2
3	D	804	LLH	N-C1-C2-O2
3	F	806	LLH	O1-C1-C2-O2
3	F	806	LLH	N-C1-C2-O2
3	E	805	LLH	O1-C1-C2-C3
3	E	805	LLH	N-C1-C2-C3
3	B	802	LLH	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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	395/398 (99%)	-1.51	0 100 100	21, 30, 43, 57	0
1	B	395/398 (99%)	-1.52	0 100 100	22, 30, 43, 58	0
1	C	391/398 (98%)	-1.39	0 100 100	23, 37, 56, 68	0
1	D	391/398 (98%)	-1.42	0 100 100	26, 38, 56, 68	0
1	E	391/398 (98%)	-1.40	0 100 100	23, 35, 55, 71	0
1	F	391/398 (98%)	-1.45	0 100 100	23, 36, 55, 72	0
All	All	2354/2388 (98%)	-1.45	0 100 100	21, 34, 55, 72	0

There are no RSRZ outliers to report.

### 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 oligosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	444	1/1	0.99	0.02	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LLH	A	801	13/13	0.99	0.03	29,32,35,36	0
3	LLH	B	802	13/13	0.99	0.03	30,33,36,38	0
3	LLH	C	803	13/13	0.99	0.03	38,40,49,49	0
3	LLH	D	804	13/13	0.99	0.03	38,41,48,49	0
3	LLH	E	805	13/13	0.99	0.04	38,39,46,46	0
3	LLH	F	806	13/13	0.99	0.03	37,39,49,51	0
2	MG	A	399	1/1	1.00	0.01	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.