



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 07:54 AM EDT

PDB ID : 3EKM
Title : Crystal structure of diaminopimelate epimerase from arabidopsis thaliana in complex with irreversible inhibitor DL-AziDAP
Authors : Pillai, B.; Moorthie, V.A.; Cherney, M.M.; van Belkum, M.J.; Vederas, J.C.; James, M.N.G.
Deposited on : 2008-09-19
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

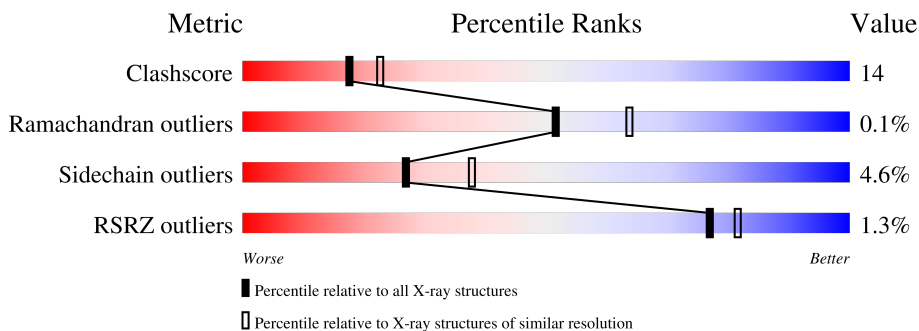
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	317	
1	B	317	
1	C	317	
1	D	317	
1	E	317	
1	F	317	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14519 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 Diaminopimelate epimerase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2169	1363	377	413	16	0	0	0
1	B	287	2169	1363	377	413	16	0	0	0
1	C	287	2169	1363	377	413	16	0	0	0
1	D	301	2273	1430	393	434	16	0	0	0
1	E	287	2169	1363	377	413	16	0	0	0
1	F	301	2273	1430	393	434	16	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

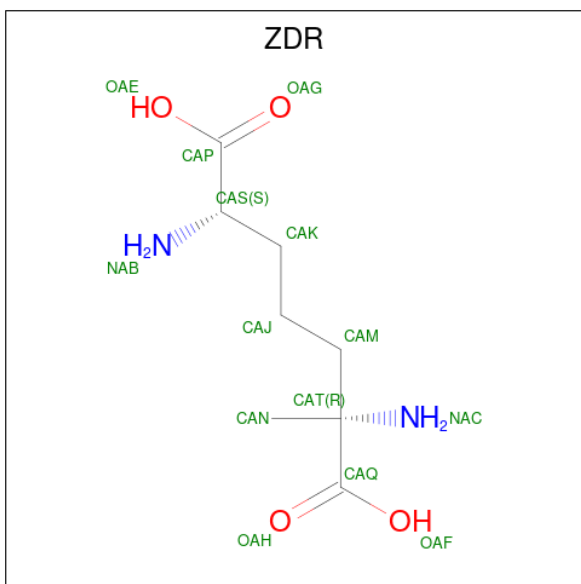
Chain	Residue	Modelled	Actual	Comment	Reference
A	312	HIS	-	expression tag	UNP Q9LFG2
A	313	HIS	-	expression tag	UNP Q9LFG2
A	314	HIS	-	expression tag	UNP Q9LFG2
A	315	HIS	-	expression tag	UNP Q9LFG2
A	316	HIS	-	expression tag	UNP Q9LFG2
A	317	HIS	-	expression tag	UNP Q9LFG2
B	312	HIS	-	expression tag	UNP Q9LFG2
B	313	HIS	-	expression tag	UNP Q9LFG2
B	314	HIS	-	expression tag	UNP Q9LFG2
B	315	HIS	-	expression tag	UNP Q9LFG2
B	316	HIS	-	expression tag	UNP Q9LFG2
B	317	HIS	-	expression tag	UNP Q9LFG2
C	312	HIS	-	expression tag	UNP Q9LFG2
C	313	HIS	-	expression tag	UNP Q9LFG2
C	314	HIS	-	expression tag	UNP Q9LFG2
C	315	HIS	-	expression tag	UNP Q9LFG2
C	316	HIS	-	expression tag	UNP Q9LFG2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	317	HIS	-	expression tag	UNP Q9LFG2
D	312	HIS	-	expression tag	UNP Q9LFG2
D	313	HIS	-	expression tag	UNP Q9LFG2
D	314	HIS	-	expression tag	UNP Q9LFG2
D	315	HIS	-	expression tag	UNP Q9LFG2
D	316	HIS	-	expression tag	UNP Q9LFG2
D	317	HIS	-	expression tag	UNP Q9LFG2
E	312	HIS	-	expression tag	UNP Q9LFG2
E	313	HIS	-	expression tag	UNP Q9LFG2
E	314	HIS	-	expression tag	UNP Q9LFG2
E	315	HIS	-	expression tag	UNP Q9LFG2
E	316	HIS	-	expression tag	UNP Q9LFG2
E	317	HIS	-	expression tag	UNP Q9LFG2
F	312	HIS	-	expression tag	UNP Q9LFG2
F	313	HIS	-	expression tag	UNP Q9LFG2
F	314	HIS	-	expression tag	UNP Q9LFG2
F	315	HIS	-	expression tag	UNP Q9LFG2
F	316	HIS	-	expression tag	UNP Q9LFG2
F	317	HIS	-	expression tag	UNP Q9LFG2

- Molecule 2 is (2R,6S)-2,6-DIAMINO-2-METHYLHEPTANEDIOIC ACID (three-letter code: ZDR) (formula: C₈H₁₆N₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
2	A	1	14	8	2	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	2	4		
2	C	1	Total	C	N	O	0	0
			14	8	2	4		
2	D	1	Total	C	N	O	0	0
			14	8	2	4		
2	E	1	Total	C	N	O	0	0
			14	8	2	4		
2	F	1	Total	C	N	O	0	0
			14	8	2	4		

- Molecule 3 is water.

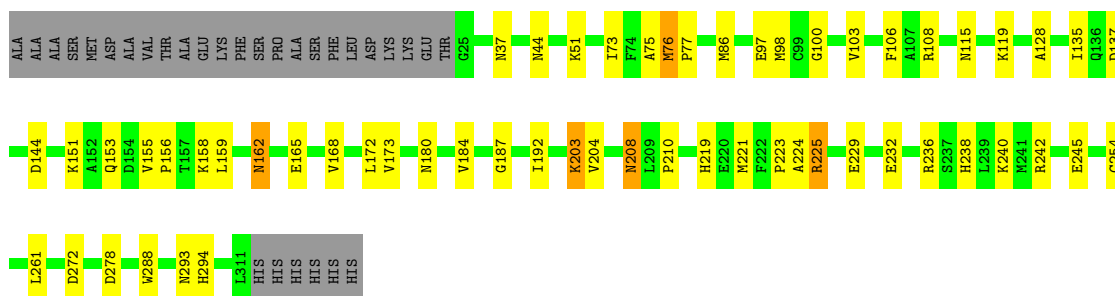
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	245	Total	O	0	0
			245	245		
3	B	228	Total	O	0	0
			228	228		
3	C	220	Total	O	0	0
			220	220		
3	D	189	Total	O	0	0
			189	189		
3	E	189	Total	O	0	0
			189	189		
3	F	142	Total	O	0	0
			142	142		

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.

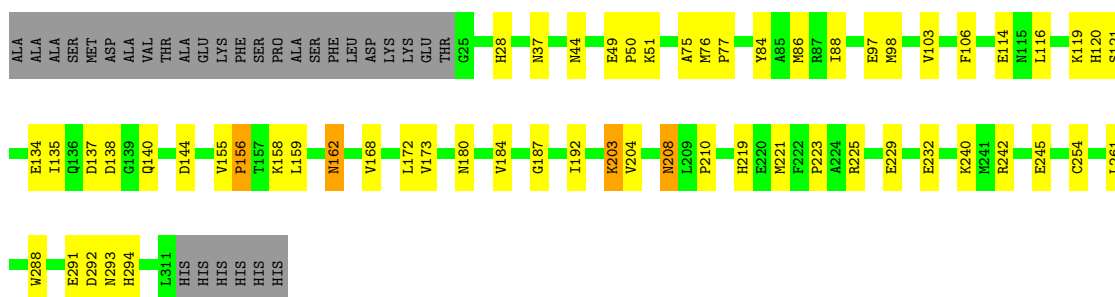
- Molecule 1: Diaminopimelate epimerase, chloroplastic

Chain A: 



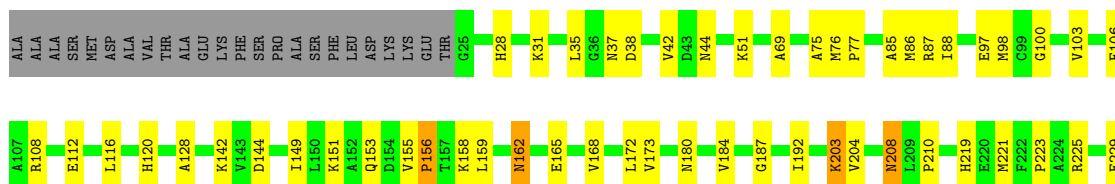
- Molecule 1: Diaminopimelate epimerase, chloroplastic

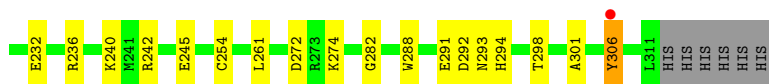
Chain B: 



- Molecule 1: Diaminopimelate epimerase, chloroplastic

Chain C: 

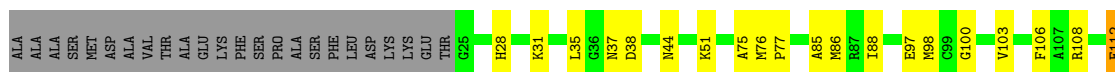




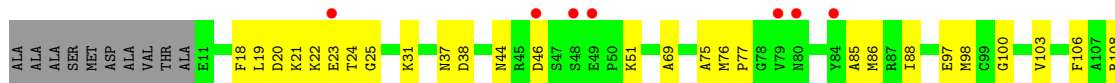
- Molecule 1: Diaminopimelate epimerase, chloroplastic



- Molecule 1: Diaminopimelate epimerase, chloroplastic



- Molecule 1: Diaminopimelate epimerase, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.36Å 136.61Å 102.56Å 90.00° 119.78° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 48.01 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.30) 99.7 (48.01-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.187 , 0.217 0.181 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h-l,k,h 0.003 for l,k,-h-l 0.014 for h,-k,-h-l 0.014 for -h-l,-k,l 0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14519	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	0.40	0/2214	0.70	2/2998 (0.1%)
1	B	0.39	0/2214	0.69	2/2998 (0.1%)
1	C	0.40	0/2214	0.69	2/2998 (0.1%)
1	D	0.39	0/2321	0.66	2/3141 (0.1%)
1	E	0.39	0/2214	0.69	3/2998 (0.1%)
1	F	0.38	0/2321	0.65	2/3141 (0.1%)
All	All	0.39	0/13498	0.68	13/18274 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	225	ARG	NE-CZ-NH1	-9.84	115.38	120.30
1	A	225	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	E	225	ARG	NE-CZ-NH2	9.13	124.87	120.30
1	A	225	ARG	NE-CZ-NH2	8.69	124.64	120.30
1	C	225	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	B	225	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	225	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	F	225	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	D	225	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	225	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	F	225	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	225	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	E	225	ARG	CD-NE-CZ	5.03	130.63	123.60

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	2169	0	2121	56	0
1	B	2169	0	2121	55	0
1	C	2169	0	2121	67	0
1	D	2273	0	2217	67	0
1	E	2169	0	2121	59	0
1	F	2273	0	2217	65	0
2	A	14	0	13	3	0
2	B	14	0	13	3	0
2	C	14	0	13	3	0
2	D	14	0	13	2	0
2	E	14	0	13	3	0
2	F	14	0	13	3	0
3	A	245	0	0	3	0
3	B	228	0	0	3	0
3	C	220	0	0	5	0
3	D	189	0	0	3	0
3	E	189	0	0	5	0
3	F	142	0	0	1	0
All	All	14519	0	12996	360	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 14.

All (360) 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:F:162:ASN:HD21	1:F:168:VAL:H	1.04	1.00
1:A:162:ASN:HD22	1:A:162:ASN:H	1.10	0.98
1:D:162:ASN:HD21	1:D:168:VAL:H	1.11	0.95
1:B:162:ASN:H	1:B:162:ASN:HD22	1.10	0.91
1:E:162:ASN:HD22	1:E:162:ASN:H	1.17	0.91
1:E:162:ASN:HD21	1:E:168:VAL:H	1.16	0.91
1:B:162:ASN:HD21	1:B:168:VAL:H	1.17	0.89
1:A:162:ASN:HD21	1:A:168:VAL:H	1.15	0.89
1:A:219:HIS:HD2	1:A:221:MET:H	1.23	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:ASN:HD22	1:F:162:ASN:H	1.22	0.86
1:C:162:ASN:HD22	1:C:162:ASN:H	1.24	0.85
1:C:162:ASN:HD21	1:C:168:VAL:H	1.21	0.85
1:E:219:HIS:HD2	1:E:221:MET:H	1.24	0.85
1:D:219:HIS:HD2	1:D:221:MET:H	1.26	0.84
1:C:219:HIS:HD2	1:C:221:MET:H	1.26	0.84
1:D:162:ASN:H	1:D:162:ASN:HD22	1.26	0.80
1:B:219:HIS:HD2	1:B:221:MET:H	1.24	0.80
1:F:219:HIS:HD2	1:F:221:MET:H	1.30	0.78
1:A:137:ASP:HB3	1:B:28:HIS:CD2	2.18	0.77
1:B:162:ASN:HD22	1:B:162:ASN:N	1.81	0.77
1:A:204:VAL:CG1	1:A:242:ARG:HG3	2.17	0.74
1:B:44:ASN:HD21	1:B:51:LYS:H	1.33	0.74
1:D:204:VAL:CG1	1:D:242:ARG:HG3	2.19	0.73
1:C:204:VAL:CG1	1:C:242:ARG:HG3	2.19	0.73
1:C:112:GLU:HG2	3:C:889:HOH:O	1.88	0.73
1:A:162:ASN:HD22	1:A:162:ASN:N	1.81	0.73
1:B:204:VAL:CG1	1:B:242:ARG:HG3	2.19	0.72
1:E:204:VAL:CG1	1:E:242:ARG:HG3	2.20	0.71
1:F:204:VAL:CG1	1:F:242:ARG:HG3	2.20	0.71
1:F:44:ASN:HD21	1:F:51:LYS:H	1.38	0.71
1:A:44:ASN:HD21	1:A:51:LYS:H	1.38	0.71
1:D:158:LYS:HE3	1:D:223:PRO:HG3	1.75	0.69
1:A:119:LYS:NZ	1:A:119:LYS:HB2	2.08	0.69
1:C:108:ARG:HH11	1:C:108:ARG:HG2	1.58	0.68
1:E:108:ARG:HD2	1:E:301:ALA:HB3	1.74	0.68
1:E:219:HIS:CD2	1:E:221:MET:H	2.11	0.68
1:D:151:LYS:HE2	1:D:153:GLN:HE21	1.59	0.67
1:D:108:ARG:HD2	1:D:301:ALA:HB3	1.76	0.67
1:E:153:GLN:HG2	3:E:686:HOH:O	1.92	0.67
1:A:158:LYS:HE3	1:A:223:PRO:HG3	1.77	0.66
1:D:44:ASN:HD21	1:D:51:LYS:H	1.41	0.66
1:C:219:HIS:CD2	1:C:221:MET:H	2.12	0.66
1:D:242:ARG:HD2	3:D:715:HOH:O	1.96	0.65
1:D:18:PHE:CZ	1:D:22:LYS:HD2	2.31	0.65
1:C:44:ASN:HD21	1:C:51:LYS:H	1.44	0.65
1:E:203:LYS:HE3	1:E:203:LYS:HA	1.79	0.65
1:C:158:LYS:HE3	1:C:223:PRO:HG3	1.78	0.65
1:B:219:HIS:CD2	1:B:221:MET:H	2.11	0.64
1:D:113:LEU:HD21	1:F:19:LEU:HD12	1.79	0.64
1:D:219:HIS:CD2	1:D:221:MET:H	2.13	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:GLU:HG3	1:C:187:GLY:O	1.97	0.64
1:D:162:ASN:HD22	1:D:162:ASN:N	1.94	0.64
1:F:162:ASN:ND2	1:F:168:VAL:H	1.87	0.64
1:A:203:LYS:HA	1:A:203:LYS:HE3	1.80	0.63
1:A:219:HIS:CD2	1:A:221:MET:H	2.11	0.63
1:A:173:VAL:O	1:A:219:HIS:HE1	1.83	0.62
1:C:162:ASN:HD22	1:C:162:ASN:N	1.92	0.62
1:D:203:LYS:HE3	1:D:203:LYS:HA	1.81	0.62
1:B:203:LYS:HE3	1:B:203:LYS:HA	1.81	0.62
1:F:119:LYS:HB2	1:F:119:LYS:HZ2	1.65	0.62
1:A:204:VAL:HG12	1:A:242:ARG:HG3	1.83	0.61
1:C:151:LYS:HE3	1:C:165:GLU:HG2	1.80	0.61
1:B:44:ASN:HD21	1:B:51:LYS:N	1.98	0.61
1:B:162:ASN:H	1:B:162:ASN:ND2	1.92	0.61
1:E:44:ASN:HD21	1:E:51:LYS:H	1.47	0.61
1:F:203:LYS:HE3	1:F:203:LYS:HA	1.81	0.61
1:B:44:ASN:ND2	1:B:51:LYS:H	1.98	0.61
1:C:203:LYS:HA	1:C:203:LYS:HE3	1.81	0.61
1:F:162:ASN:HD22	1:F:162:ASN:N	1.92	0.60
1:B:173:VAL:O	1:B:219:HIS:HE1	1.84	0.60
1:F:219:HIS:CD2	1:F:221:MET:H	2.15	0.60
1:D:18:PHE:CE1	1:D:22:LYS:HD2	2.37	0.60
1:F:44:ASN:HD21	1:F:51:LYS:N	2.00	0.60
1:B:137:ASP:HB3	1:C:28:HIS:CD2	2.36	0.60
1:E:173:VAL:O	1:E:219:HIS:HE1	1.85	0.60
1:C:144:ASP:OD1	1:C:294:HIS:HD2	1.85	0.59
1:A:44:ASN:HD21	1:A:51:LYS:N	2.01	0.59
1:D:242:ARG:HD3	3:D:630:HOH:O	2.01	0.59
1:B:116:LEU:HD13	1:B:120:HIS:CD2	2.38	0.59
1:A:97:GLU:HG3	1:A:187:GLY:O	2.03	0.59
1:C:173:VAL:O	1:C:219:HIS:HE1	1.85	0.59
1:D:204:VAL:HG12	1:D:242:ARG:HG3	1.85	0.59
1:B:119:LYS:HB2	1:B:119:LYS:NZ	2.17	0.59
1:C:291:GLU:CD	1:C:291:GLU:H	2.06	0.59
1:E:162:ASN:HD22	1:E:162:ASN:N	1.88	0.59
1:B:204:VAL:HG12	1:B:242:ARG:HG3	1.85	0.58
1:C:108:ARG:HD3	1:C:301:ALA:HB3	1.84	0.58
1:B:144:ASP:OD1	1:B:294:HIS:HD2	1.87	0.58
1:C:204:VAL:HG12	1:C:242:ARG:HG3	1.86	0.58
1:B:291:GLU:CD	1:B:291:GLU:H	2.06	0.57
1:F:44:ASN:ND2	1:F:51:LYS:H	2.02	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:LYS:HE3	1:F:223:PRO:HG3	1.85	0.57
1:F:173:VAL:O	1:F:219:HIS:HE1	1.86	0.57
1:D:44:ASN:HD21	1:D:51:LYS:N	2.03	0.57
1:B:121:SER:HB3	1:B:134:GLU:HG3	1.86	0.57
1:B:97:GLU:HG3	1:B:187:GLY:O	2.05	0.57
1:E:144:ASP:OD1	1:E:294:HIS:HD2	1.87	0.56
1:E:242:ARG:HD3	3:E:674:HOH:O	2.04	0.56
1:B:162:ASN:N	1:B:162:ASN:ND2	2.52	0.56
1:E:204:VAL:HG12	1:E:242:ARG:HG3	1.86	0.56
1:F:204:VAL:HG12	1:F:242:ARG:HG3	1.87	0.56
1:C:108:ARG:HG2	1:C:108:ARG:NH1	2.19	0.56
1:D:22:LYS:HD3	1:E:28:HIS:ND1	2.20	0.56
1:D:44:ASN:ND2	1:D:51:LYS:H	2.04	0.56
1:A:44:ASN:ND2	1:A:51:LYS:HG3	2.22	0.55
1:B:158:LYS:HE3	1:B:223:PRO:HG3	1.89	0.55
1:B:84:TYR:OH	1:B:114:GLU:OE1	2.23	0.54
1:F:242:ARG:HD2	3:F:689:HOH:O	2.06	0.54
1:B:203:LYS:NZ	3:B:877:HOH:O	2.40	0.54
1:D:173:VAL:O	1:D:219:HIS:HE1	1.89	0.54
1:C:44:ASN:HD21	1:C:51:LYS:N	2.05	0.54
1:F:44:ASN:ND2	1:F:51:LYS:HG3	2.22	0.54
1:F:151:LYS:HE2	1:F:153:GLN:HE21	1.72	0.54
1:C:236:ARG:NH1	1:C:272:ASP:OD1	2.40	0.54
1:C:162:ASN:H	1:C:162:ASN:ND2	1.99	0.54
1:A:159:LEU:HD23	1:A:221:MET:HE2	1.90	0.54
1:D:116:LEU:HB3	1:D:120:HIS:CD2	2.43	0.54
1:E:238:HIS:CE1	1:E:278:ASP:OD2	2.61	0.54
1:F:147:THR:HG22	1:F:293:ASN:O	2.08	0.54
1:A:208:ASN:HD21	1:A:210:PRO:HG2	1.73	0.53
1:B:76:MET:HB3	1:B:77:PRO:HD2	1.89	0.53
1:D:28:HIS:CE1	1:F:22:LYS:HD2	2.43	0.53
1:E:97:GLU:HG3	1:E:187:GLY:O	2.08	0.53
1:E:238:HIS:HE1	1:E:278:ASP:OD2	1.91	0.53
1:F:155:VAL:N	1:F:156:PRO:HA	2.24	0.53
1:D:151:LYS:CE	1:D:153:GLN:HE21	2.22	0.53
1:F:76:MET:HB3	1:F:77:PRO:HD2	1.90	0.53
1:A:144:ASP:OD1	1:A:294:HIS:HD2	1.91	0.53
1:D:97:GLU:HG3	1:D:187:GLY:O	2.09	0.53
1:B:86:MET:HE3	1:B:103:VAL:HA	1.91	0.53
1:F:288:TRP:HE1	1:F:293:ASN:ND2	2.06	0.53
1:F:162:ASN:H	1:F:162:ASN:ND2	2.01	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:TYR:CE1	1:E:308:SER:HB2	2.45	0.52
1:E:149:ILE:HB	1:E:185:SER:HB3	1.92	0.52
1:E:162:ASN:H	1:E:162:ASN:ND2	1.97	0.52
1:C:44:ASN:ND2	1:C:51:LYS:H	2.07	0.52
1:B:44:ASN:ND2	1:B:51:LYS:HG3	2.25	0.52
1:D:44:ASN:ND2	1:D:51:LYS:HG3	2.25	0.52
1:B:155:VAL:N	1:B:156:PRO:HA	2.25	0.52
1:C:242:ARG:HD2	3:C:909:HOH:O	2.09	0.52
1:A:162:ASN:N	1:A:162:ASN:ND2	2.53	0.51
1:D:144:ASP:OD1	1:D:294:HIS:HD2	1.93	0.51
1:F:119:LYS:HB2	1:F:119:LYS:NZ	2.24	0.51
1:D:238:HIS:HE1	1:D:278:ASP:OD2	1.93	0.51
1:E:232:GLU:HG2	1:E:240:LYS:HB3	1.92	0.51
1:A:44:ASN:ND2	1:A:51:LYS:H	2.05	0.51
1:A:162:ASN:H	1:A:162:ASN:ND2	1.92	0.51
1:C:291:GLU:CD	1:C:291:GLU:N	2.64	0.51
1:D:159:LEU:HD23	1:D:221:MET:HE2	1.92	0.51
1:E:208:ASN:HD21	1:E:210:PRO:HG2	1.76	0.51
1:F:151:LYS:HE2	1:F:153:GLN:NE2	2.26	0.51
1:A:76:MET:HB3	1:A:77:PRO:HD2	1.93	0.51
1:C:75:ALA:HA	1:C:106:PHE:CE2	2.45	0.51
1:B:245:GLU:CD	2:B:500:ZDR:HAN3	2.31	0.51
1:C:288:TRP:HE1	1:C:293:ASN:ND2	2.09	0.50
1:E:274:LYS:HG3	3:E:697:HOH:O	2.09	0.50
1:C:155:VAL:N	1:C:156:PRO:HA	2.26	0.50
1:B:51:LYS:NZ	3:B:815:HOH:O	2.42	0.50
1:D:192:ILE:HG13	1:D:229:GLU:HG2	1.93	0.50
1:A:245:GLU:CD	2:A:500:ZDR:HAN3	2.32	0.50
1:D:236:ARG:NH1	1:D:272:ASP:OD1	2.44	0.50
1:F:292:ASP:OD2	1:F:294:HIS:HB2	2.11	0.50
1:D:159:LEU:HD23	1:D:221:MET:CE	2.42	0.50
1:E:76:MET:HB3	1:E:77:PRO:HD2	1.92	0.50
1:A:153:GLN:HG2	3:A:597:HOH:O	2.12	0.50
1:F:159:LEU:HD23	1:F:221:MET:CE	2.42	0.50
1:B:208:ASN:HD21	1:B:210:PRO:HG2	1.77	0.49
1:E:192:ILE:HG13	1:E:229:GLU:HG2	1.95	0.49
1:E:203:LYS:HG3	3:E:654:HOH:O	2.12	0.49
1:C:76:MET:HB3	1:C:77:PRO:HD2	1.94	0.49
1:E:44:ASN:HD21	1:E:51:LYS:N	2.09	0.49
1:A:75:ALA:HA	1:A:106:PHE:CE2	2.47	0.49
1:E:155:VAL:N	1:E:156:PRO:HA	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:ASN:HD21	1:F:210:PRO:HG2	1.77	0.49
1:A:151:LYS:HE3	1:A:165:GLU:OE1	2.12	0.49
1:F:108:ARG:HG2	1:F:108:ARG:HH11	1.77	0.49
1:E:44:ASN:ND2	1:E:51:LYS:H	2.11	0.49
1:B:242:ARG:HD2	3:B:814:HOH:O	2.13	0.49
1:D:238:HIS:CE1	1:D:278:ASP:OD2	2.66	0.49
1:E:245:GLU:CD	2:E:500:ZDR:HAN3	2.34	0.49
1:A:245:GLU:OE1	2:A:500:ZDR:HAN3	2.13	0.49
1:B:159:LEU:HD23	1:B:221:MET:HE2	1.95	0.49
1:F:232:GLU:HG2	1:F:240:LYS:HB3	1.95	0.49
1:F:245:GLU:OE1	2:F:500:ZDR:HAN3	2.12	0.49
1:B:114:GLU:OE2	1:B:116:LEU:HD11	2.12	0.48
1:C:44:ASN:ND2	1:C:51:LYS:HG3	2.28	0.48
1:C:232:GLU:HG2	1:C:240:LYS:HB3	1.94	0.48
1:C:159:LEU:HD23	1:C:221:MET:CE	2.43	0.48
1:C:142:LYS:HG3	1:C:298:THR:OG1	2.13	0.48
1:C:208:ASN:HD21	1:C:210:PRO:HG2	1.78	0.48
1:F:192:ILE:HD12	1:F:192:ILE:N	2.28	0.48
1:A:119:LYS:HB2	1:A:119:LYS:HZ3	1.77	0.48
1:D:192:ILE:N	1:D:192:ILE:HD12	2.29	0.48
1:B:75:ALA:HA	1:B:106:PHE:CE2	2.48	0.48
1:F:119:LYS:HA	1:F:135:ILE:O	2.13	0.48
1:C:292:ASP:O	1:C:293:ASN:HB3	2.14	0.48
1:A:192:ILE:HG13	1:A:229:GLU:HG2	1.96	0.48
1:D:76:MET:HB2	1:D:85:ALA:HB3	1.95	0.48
1:D:76:MET:HB3	1:D:77:PRO:HD2	1.95	0.47
1:D:208:ASN:HD21	1:D:210:PRO:HG2	1.79	0.47
1:A:236:ARG:NH1	1:A:272:ASP:OD1	2.47	0.47
1:B:192:ILE:HG13	1:B:229:GLU:HG2	1.96	0.47
1:A:86:MET:HE3	1:A:103:VAL:HA	1.96	0.47
1:D:245:GLU:CD	2:D:500:ZDR:HAN3	2.34	0.47
1:E:245:GLU:OE1	2:E:500:ZDR:HAN3	2.15	0.47
1:D:19:LEU:HD12	1:E:113:LEU:HD21	1.96	0.47
1:D:245:GLU:OE1	2:D:500:ZDR:HAN3	2.13	0.47
1:E:236:ARG:NH1	1:E:272:ASP:OD1	2.47	0.47
1:B:138:ASP:OD1	1:B:140:GLN:HB2	2.15	0.47
1:B:159:LEU:HD23	1:B:221:MET:CE	2.44	0.47
1:C:192:ILE:HG13	1:C:229:GLU:HG2	1.96	0.47
1:D:232:GLU:HG2	1:D:240:LYS:HB3	1.96	0.47
1:E:254:CYS:HA	2:E:500:ZDR:HAN2	1.52	0.47
1:F:122:PHE:O	1:F:133:PRO:HD2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:245:GLU:CD	2:F:500:ZDR:HAN3	2.35	0.47
1:A:232:GLU:HG2	1:A:240:LYS:HB3	1.97	0.47
1:C:86:MET:HE3	1:C:103:VAL:HA	1.96	0.47
1:C:151:LYS:HE2	1:C:153:GLN:HE21	1.80	0.47
1:C:31:LYS:HE2	1:C:38:ASP:HB2	1.96	0.47
1:C:159:LEU:HD23	1:C:221:MET:HE2	1.97	0.47
1:A:119:LYS:HG3	1:A:135:ILE:O	2.14	0.47
1:F:97:GLU:HG3	1:F:187:GLY:O	2.14	0.46
1:F:162:ASN:ND2	1:F:162:ASN:N	2.62	0.46
1:A:208:ASN:ND2	1:A:210:PRO:HG2	2.30	0.46
1:E:31:LYS:HE2	1:E:38:ASP:HB2	1.98	0.46
1:F:151:LYS:HE3	1:F:165:GLU:OE1	2.15	0.46
1:A:155:VAL:N	1:A:156:PRO:HA	2.31	0.46
1:B:180:ASN:HD22	1:B:180:ASN:HA	1.58	0.46
1:C:245:GLU:CD	2:C:500:ZDR:HAN3	2.36	0.46
1:D:149:ILE:HB	1:D:185:SER:HB3	1.97	0.46
1:F:192:ILE:HG12	1:F:261:LEU:HA	1.98	0.46
1:B:208:ASN:ND2	1:B:210:PRO:HG2	2.31	0.46
1:B:292:ASP:O	1:B:293:ASN:HB3	2.16	0.46
1:A:254:CYS:HA	2:A:500:ZDR:HAN2	1.52	0.45
1:C:245:GLU:OE1	2:C:500:ZDR:HAN3	2.16	0.45
1:E:86:MET:HE3	1:E:103:VAL:HA	1.97	0.45
1:C:162:ASN:N	1:C:162:ASN:ND2	2.61	0.45
1:A:192:ILE:HG12	1:A:261:LEU:HA	1.98	0.45
1:F:192:ILE:HG13	1:F:229:GLU:HG2	1.98	0.45
1:B:232:GLU:HG2	1:B:240:LYS:HB3	1.97	0.45
1:C:192:ILE:HG12	1:C:261:LEU:HA	1.99	0.45
1:D:219:HIS:HD2	1:D:221:MET:N	2.05	0.45
1:E:208:ASN:ND2	1:E:210:PRO:HG2	2.30	0.45
1:F:159:LEU:HD23	1:F:221:MET:HE2	1.99	0.45
1:F:208:ASN:ND2	1:F:210:PRO:HG2	2.32	0.45
1:A:242:ARG:HD2	3:A:615:HOH:O	2.16	0.45
1:D:155:VAL:N	1:D:156:PRO:HA	2.31	0.45
1:D:115:ASN:ND2	1:D:117:GLN:OE1	2.49	0.45
1:A:159:LEU:HD23	1:A:221:MET:CE	2.46	0.45
1:B:192:ILE:HG12	1:B:261:LEU:HA	1.99	0.45
1:C:76:MET:CE	1:C:87:ARG:HD3	2.47	0.45
1:C:180:ASN:HD22	1:C:180:ASN:HA	1.59	0.45
1:F:180:ASN:HD22	1:F:180:ASN:HA	1.61	0.45
1:D:288:TRP:HE1	1:D:293:ASN:ND2	2.15	0.44
1:F:108:ARG:HG2	1:F:108:ARG:NH1	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLU:OE1	2:B:500:ZDR:HAN3	2.16	0.44
1:C:116:LEU:HB3	1:C:120:HIS:CD2	2.53	0.44
1:A:219:HIS:HD2	1:A:221:MET:N	2.04	0.44
1:C:128:ALA:HB2	1:C:187:GLY:HA3	1.99	0.44
1:F:18:PHE:O	1:F:22:LYS:HG2	2.17	0.44
1:F:86:MET:CE	1:F:103:VAL:HA	2.47	0.44
1:D:151:LYS:HD3	1:D:154:ASP:OD2	2.17	0.44
1:D:180:ASN:HD22	1:D:180:ASN:HA	1.59	0.44
1:D:192:ILE:HG12	1:D:261:LEU:HA	1.99	0.44
1:F:100:GLY:O	1:F:103:VAL:HG12	2.18	0.44
1:A:224:ALA:O	1:A:225:ARG:HB2	2.17	0.44
1:C:208:ASN:ND2	1:C:210:PRO:HG2	2.33	0.44
1:D:46:ASP:HB3	3:D:746:HOH:O	2.17	0.44
1:E:44:ASN:ND2	1:E:51:LYS:HG3	2.31	0.44
1:D:31:LYS:HE2	1:D:38:ASP:HB2	2.00	0.44
1:D:208:ASN:ND2	1:D:210:PRO:HG2	2.33	0.43
1:E:100:GLY:O	1:E:103:VAL:HG12	2.18	0.43
1:D:16:ALA:HB2	1:E:112:GLU:OE2	2.18	0.43
1:D:22:LYS:HD3	1:E:28:HIS:CE1	2.53	0.43
1:E:180:ASN:HD22	1:E:180:ASN:HA	1.60	0.43
1:F:254:CYS:HA	2:F:500:ZDR:HAN2	1.51	0.43
1:A:76:MET:HE2	3:A:685:HOH:O	2.17	0.43
1:C:97:GLU:HG3	1:C:187:GLY:C	2.38	0.43
1:C:108:ARG:CD	1:C:301:ALA:HB3	2.48	0.43
1:D:162:ASN:N	1:D:162:ASN:ND2	2.64	0.43
1:E:35:LEU:HD22	1:E:282:GLY:HA3	2.00	0.43
1:F:149:ILE:HB	1:F:185:SER:HB3	1.99	0.43
1:B:86:MET:HE2	1:B:106:PHE:HD2	1.83	0.43
1:D:241:MET:HG2	1:D:261:LEU:HD21	2.00	0.43
1:C:274:LYS:HG3	3:C:884:HOH:O	2.19	0.43
1:D:86:MET:HE2	1:D:106:PHE:HD2	1.84	0.43
1:E:86:MET:HE2	1:E:106:PHE:HD2	1.83	0.43
1:F:86:MET:HE2	1:F:106:PHE:CD2	2.54	0.43
1:B:86:MET:CE	1:B:103:VAL:HA	2.49	0.43
1:C:151:LYS:HE2	1:C:153:GLN:NE2	2.34	0.43
1:D:100:GLY:O	1:D:103:VAL:HG12	2.19	0.43
1:E:192:ILE:HG12	1:E:261:LEU:HA	2.01	0.43
1:C:76:MET:HE2	1:C:87:ARG:HD3	2.00	0.42
1:E:86:MET:HE2	1:E:106:PHE:CD2	2.54	0.42
1:E:224:ALA:O	1:E:225:ARG:HB2	2.19	0.42
1:F:86:MET:HE2	1:F:106:PHE:HD2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:MET:CE	1:A:103:VAL:HA	2.49	0.42
1:B:86:MET:HE2	1:B:106:PHE:CD2	2.53	0.42
1:D:86:MET:HE3	1:D:103:VAL:HA	2.01	0.42
1:D:117:GLN:HE21	1:D:117:GLN:HA	1.84	0.42
1:E:86:MET:CE	1:E:106:PHE:HB2	2.49	0.42
1:F:20:ASP:C	1:F:22:LYS:H	2.22	0.42
1:F:86:MET:HE3	1:F:103:VAL:HA	1.99	0.42
1:A:86:MET:HE2	1:A:106:PHE:HD2	1.83	0.42
1:A:180:ASN:HD22	1:A:180:ASN:HA	1.60	0.42
1:E:163:LYS:HE3	1:E:163:LYS:HB2	1.92	0.42
1:F:31:LYS:HE2	1:F:38:ASP:HB2	2.01	0.42
1:C:31:LYS:HE3	1:C:69:ALA:HB2	2.01	0.42
1:F:31:LYS:HE3	1:F:69:ALA:HB2	2.01	0.42
1:F:75:ALA:HA	1:F:106:PHE:CE2	2.54	0.42
1:F:207:LEU:O	1:F:242:ARG:NH2	2.52	0.42
1:E:75:ALA:HA	1:E:106:PHE:CE2	2.55	0.42
1:B:86:MET:CE	1:B:106:PHE:HB2	2.50	0.42
1:C:151:LYS:HG3	1:C:165:GLU:HB3	2.01	0.42
1:D:128:ALA:HB2	1:D:187:GLY:HA3	2.01	0.42
1:E:86:MET:CE	1:E:103:VAL:HA	2.49	0.42
1:B:254:CYS:HA	2:B:500:ZDR:HAN2	1.52	0.42
1:D:86:MET:CE	1:D:103:VAL:HA	2.50	0.42
1:C:76:MET:HB2	1:C:85:ALA:HB3	2.01	0.41
1:E:162:ASN:N	1:E:162:ASN:ND2	2.59	0.41
1:C:149:ILE:HD13	3:C:789:HOH:O	2.19	0.41
1:C:192:ILE:HD12	1:C:192:ILE:N	2.35	0.41
1:E:134:GLU:HG2	1:E:136:GLN:NE2	2.36	0.41
1:E:192:ILE:HD12	1:E:192:ILE:N	2.34	0.41
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.84	0.41
1:B:49:GLU:HA	1:B:50:PRO:HD3	1.90	0.41
1:B:288:TRP:HE1	1:B:293:ASN:ND2	2.18	0.41
1:E:242:ARG:HD2	3:E:679:HOH:O	2.19	0.41
1:A:108:ARG:HG2	1:A:108:ARG:NH1	2.35	0.41
1:C:242:ARG:HD3	3:C:922:HOH:O	2.20	0.41
1:E:277:VAL:O	1:E:283:PRO:HA	2.21	0.41
1:F:86:MET:CE	1:F:106:PHE:HB2	2.51	0.41
1:F:137:ASP:C	1:F:139:GLY:H	2.24	0.41
1:A:192:ILE:N	1:A:192:ILE:HD12	2.36	0.41
1:B:119:LYS:HG3	1:B:135:ILE:O	2.20	0.41
1:C:254:CYS:HA	2:C:500:ZDR:HAN2	1.52	0.41
1:A:100:GLY:O	1:A:103:VAL:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:ARG:NH1	1:D:139:GLY:O	2.49	0.41
1:E:76:MET:HB2	1:E:85:ALA:HB3	2.02	0.41
1:F:24:THR:CG2	1:F:25:GLY:N	2.84	0.41
1:F:151:LYS:HD3	1:F:154:ASP:OD2	2.21	0.41
1:A:86:MET:HE2	1:A:106:PHE:CD2	2.56	0.41
1:A:238:HIS:CE1	1:A:278:ASP:OD2	2.73	0.41
1:C:86:MET:HE2	1:C:106:PHE:HD2	1.86	0.41
1:C:100:GLY:O	1:C:103:VAL:HG12	2.21	0.41
1:F:241:MET:HG2	1:F:261:LEU:HD21	2.03	0.41
1:A:128:ALA:HB2	1:A:187:GLY:HA3	2.03	0.40
1:D:151:LYS:HE2	1:D:153:GLN:HG2	2.03	0.40
1:A:86:MET:CE	1:A:106:PHE:HB2	2.51	0.40
1:F:76:MET:HB2	1:F:85:ALA:HB3	2.03	0.40
1:B:192:ILE:N	1:B:192:ILE:HD12	2.36	0.40
1:C:35:LEU:HD22	1:C:282:GLY:HA3	2.02	0.40
1:E:159:LEU:HD23	1:E:221:MET:CE	2.51	0.40
1:A:288:TRP:HE1	1:A:293:ASN:ND2	2.20	0.40
1:C:86:MET:CE	1:C:103:VAL:HA	2.51	0.40
1:D:73:ILE:HG21	1:D:86:MET:HE2	2.02	0.40
1:D:134:GLU:HG2	1:D:136:GLN:NE2	2.36	0.40
1:A:73:ILE:HG21	1:A:86:MET:HE2	2.02	0.40
1:B:292:ASP:O	1:B:293:ASN:CB	2.70	0.40
1:D:106:PHE:O	1:D:110:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	285/317 (90%)	277 (97%)	8 (3%)	0	100 100
1	B	285/317 (90%)	274 (96%)	11 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	285/317 (90%)	277 (97%)	8 (3%)	0	100	100
1	D	299/317 (94%)	288 (96%)	11 (4%)	0	100	100
1	E	285/317 (90%)	273 (96%)	12 (4%)	0	100	100
1	F	299/317 (94%)	287 (96%)	10 (3%)	2 (1%)	22	26
All	All	1738/1902 (91%)	1676 (96%)	60 (4%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	21	LYS
1	F	23	GLU

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	231/255 (91%)	222 (96%)	9 (4%)	32	46
1	B	231/255 (91%)	222 (96%)	9 (4%)	32	46
1	C	231/255 (91%)	220 (95%)	11 (5%)	25	36
1	D	242/255 (95%)	231 (96%)	11 (4%)	27	39
1	E	231/255 (91%)	216 (94%)	15 (6%)	17	23
1	F	242/255 (95%)	232 (96%)	10 (4%)	30	43
All	All	1408/1530 (92%)	1343 (95%)	65 (5%)	27	38

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	76	MET
1	A	98	MET
1	A	115	ASN
1	A	162	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	172	LEU
1	A	184	VAL
1	A	203	LYS
1	A	208	ASN
1	B	37	ASN
1	B	88	ILE
1	B	98	MET
1	B	156	PRO
1	B	162	ASN
1	B	172	LEU
1	B	184	VAL
1	B	203	LYS
1	B	208	ASN
1	C	37	ASN
1	C	42	VAL
1	C	88	ILE
1	C	98	MET
1	C	156	PRO
1	C	162	ASN
1	C	172	LEU
1	C	184	VAL
1	C	203	LYS
1	C	208	ASN
1	C	306	TYR
1	D	22	LYS
1	D	37	ASN
1	D	88	ILE
1	D	98	MET
1	D	115	ASN
1	D	137	ASP
1	D	162	ASN
1	D	172	LEU
1	D	184	VAL
1	D	203	LYS
1	D	208	ASN
1	E	37	ASN
1	E	88	ILE
1	E	98	MET
1	E	112	GLU
1	E	115	ASN
1	E	122	PHE
1	E	137	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	162	ASN
1	E	165	GLU
1	E	172	LEU
1	E	180	ASN
1	E	184	VAL
1	E	203	LYS
1	E	208	ASN
1	E	283	PRO
1	F	37	ASN
1	F	46	ASP
1	F	88	ILE
1	F	98	MET
1	F	115	ASN
1	F	162	ASN
1	F	172	LEU
1	F	184	VAL
1	F	203	LYS
1	F	208	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	54	GLN
1	A	115	ASN
1	A	117	GLN
1	A	153	GLN
1	A	162	ASN
1	A	180	ASN
1	A	208	ASN
1	A	219	HIS
1	A	238	HIS
1	A	290	GLN
1	A	293	ASN
1	A	294	HIS
1	B	44	ASN
1	B	54	GLN
1	B	115	ASN
1	B	117	GLN
1	B	120	HIS
1	B	153	GLN
1	B	162	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	180	ASN
1	B	208	ASN
1	B	219	HIS
1	B	238	HIS
1	B	290	GLN
1	B	293	ASN
1	B	294	HIS
1	C	44	ASN
1	C	54	GLN
1	C	80	ASN
1	C	117	GLN
1	C	153	GLN
1	C	162	ASN
1	C	180	ASN
1	C	208	ASN
1	C	219	HIS
1	C	238	HIS
1	C	290	GLN
1	C	293	ASN
1	C	294	HIS
1	D	44	ASN
1	D	54	GLN
1	D	115	ASN
1	D	117	GLN
1	D	120	HIS
1	D	153	GLN
1	D	162	ASN
1	D	180	ASN
1	D	208	ASN
1	D	219	HIS
1	D	238	HIS
1	D	290	GLN
1	D	293	ASN
1	D	294	HIS
1	E	44	ASN
1	E	54	GLN
1	E	115	ASN
1	E	117	GLN
1	E	162	ASN
1	E	180	ASN
1	E	208	ASN
1	E	219	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	238	HIS
1	E	293	ASN
1	E	294	HIS
1	F	44	ASN
1	F	54	GLN
1	F	80	ASN
1	F	115	ASN
1	F	117	GLN
1	F	153	GLN
1	F	162	ASN
1	F	180	ASN
1	F	208	ASN
1	F	219	HIS
1	F	238	HIS
1	F	290	GLN
1	F	293	ASN
1	F	294	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ZDR	B	500	-	9,13,13	1.68	1 (11%)	9,18,18	1.02	1 (11%)
2	ZDR	D	500	-	9,13,13	1.69	1 (11%)	9,18,18	0.96	1 (11%)
2	ZDR	F	500	-	9,13,13	1.70	1 (11%)	9,18,18	0.91	0
2	ZDR	A	500	-	9,13,13	1.63	1 (11%)	9,18,18	0.91	0
2	ZDR	C	500	-	9,13,13	1.56	1 (11%)	9,18,18	0.97	1 (11%)
2	ZDR	E	500	-	9,13,13	1.61	1 (11%)	9,18,18	0.98	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
2	ZDR	B	500	-	-	5/17/17/17	-
2	ZDR	D	500	-	-	5/17/17/17	-
2	ZDR	F	500	-	-	5/17/17/17	-
2	ZDR	A	500	-	-	5/17/17/17	-
2	ZDR	C	500	-	-	5/17/17/17	-
2	ZDR	E	500	-	-	5/17/17/17	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	ZDR	CAM-CAT	-4.03	1.50	1.55
2	B	500	ZDR	CAM-CAT	-4.03	1.50	1.55
2	F	500	ZDR	CAM-CAT	-3.94	1.50	1.55
2	E	500	ZDR	CAM-CAT	-3.72	1.50	1.55
2	A	500	ZDR	CAM-CAT	-3.65	1.50	1.55
2	C	500	ZDR	CAM-CAT	-3.60	1.51	1.55

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	ZDR	CAN-CAT-CAM	-2.16	107.19	111.00
2	D	500	ZDR	CAN-CAT-CAM	-2.07	107.35	111.00
2	C	500	ZDR	CAN-CAT-CAM	-2.06	107.37	111.00

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	ZDR	OAF-CAQ-CAT-CAM
2	A	500	ZDR	CAJ-CAM-CAT-CAN
2	A	500	ZDR	CAJ-CAM-CAT-NAC
2	A	500	ZDR	CAJ-CAM-CAT-CAQ
2	B	500	ZDR	OAF-CAQ-CAT-CAM
2	B	500	ZDR	CAJ-CAM-CAT-CAN
2	B	500	ZDR	CAJ-CAM-CAT-NAC
2	B	500	ZDR	CAJ-CAM-CAT-CAQ
2	C	500	ZDR	CAJ-CAM-CAT-CAN
2	C	500	ZDR	CAJ-CAM-CAT-NAC
2	C	500	ZDR	CAJ-CAM-CAT-CAQ
2	D	500	ZDR	OAF-CAQ-CAT-CAM
2	D	500	ZDR	CAJ-CAM-CAT-CAN
2	D	500	ZDR	CAJ-CAM-CAT-NAC
2	D	500	ZDR	CAJ-CAM-CAT-CAQ
2	E	500	ZDR	OAF-CAQ-CAT-CAM
2	E	500	ZDR	CAJ-CAM-CAT-CAN
2	E	500	ZDR	CAJ-CAM-CAT-NAC
2	E	500	ZDR	CAJ-CAM-CAT-CAQ
2	F	500	ZDR	OAF-CAQ-CAT-CAM
2	F	500	ZDR	CAJ-CAM-CAT-CAN
2	F	500	ZDR	CAJ-CAM-CAT-NAC
2	F	500	ZDR	CAJ-CAM-CAT-CAQ
2	A	500	ZDR	OAH-CAQ-CAT-CAM
2	B	500	ZDR	OAH-CAQ-CAT-CAM
2	C	500	ZDR	OAF-CAQ-CAT-CAM
2	C	500	ZDR	OAH-CAQ-CAT-CAM
2	D	500	ZDR	OAH-CAQ-CAT-CAM
2	E	500	ZDR	OAH-CAQ-CAT-CAM
2	F	500	ZDR	OAH-CAQ-CAT-CAM

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	ZDR	3	0
2	D	500	ZDR	2	0
2	F	500	ZDR	3	0
2	A	500	ZDR	3	0
2	C	500	ZDR	3	0
2	E	500	ZDR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	287/317 (90%)	-0.41	0 100 100	15, 22, 36, 46	0
1	B	287/317 (90%)	-0.51	0 100 100	15, 23, 39, 48	0
1	C	287/317 (90%)	-0.50	1 (0%) 94 96	15, 22, 37, 48	0
1	D	301/317 (94%)	-0.37	4 (1%) 77 81	17, 25, 50, 67	0
1	E	287/317 (90%)	-0.44	2 (0%) 87 91	16, 24, 45, 59	0
1	F	301/317 (94%)	-0.03	16 (5%) 26 33	17, 30, 57, 70	0
All	All	1750/1902 (92%)	-0.37	23 (1%) 77 81	15, 24, 46, 70	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	116	LEU	4.1
1	F	46	ASP	3.6
1	F	23	GLU	3.6
1	D	137	ASP	3.6
1	F	117	GLN	3.5
1	F	137	ASP	3.3
1	F	49	GLU	3.0
1	F	79	VAL	3.0
1	D	12	LYS	3.0
1	C	306	TYR	2.9
1	E	117	GLN	2.8
1	E	137	ASP	2.7
1	F	115	ASN	2.7
1	D	117	GLN	2.6
1	F	48	SER	2.5
1	F	139	GLY	2.4
1	F	272	ASP	2.4
1	D	138	ASP	2.3
1	F	84	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	306	TYR	2.1
1	F	163	LYS	2.1
1	F	290	GLN	2.1
1	F	80	ASN	2.1

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 monosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZDR	A	500	14/14	0.95	0.14	17,19,21,22	0
2	ZDR	B	500	14/14	0.95	0.10	16,20,25,25	0
2	ZDR	C	500	14/14	0.95	0.11	16,21,24,24	0
2	ZDR	E	500	14/14	0.95	0.11	21,23,27,27	0
2	ZDR	F	500	14/14	0.95	0.12	20,24,26,28	0
2	ZDR	D	500	14/14	0.97	0.10	18,22,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.