Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:35 PM GMT

PDB ID	:	1BKA
Title	:	OXALATE-SUBSTITUTED DIFERRIC LACTOFERRIN
Authors	:	Baker, H.M.; Smith, C.A.; Baker, E.N.
Deposited on	:	1996-04-15
Resolution	:	2.40 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

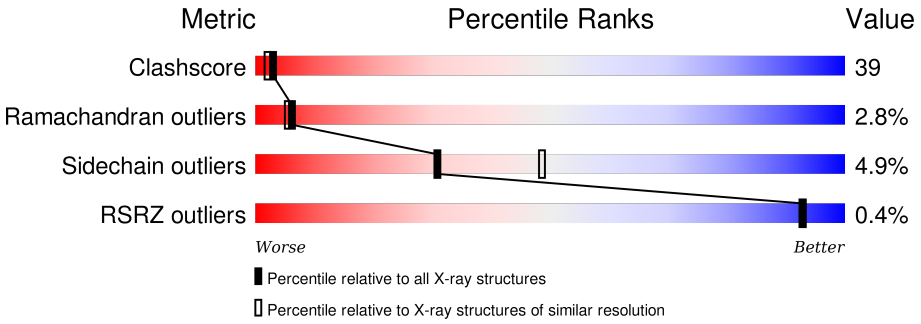
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	691	31% 46% 20% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5433 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 LACTOFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	688	Total	C	N	O	S	0	0	0
			5298	3314	941	1006	37			

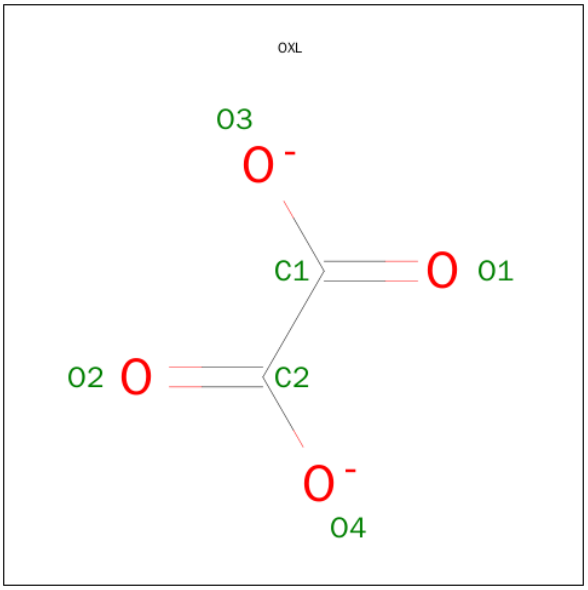
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	ARG	CONFLICT	UNP P02788

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 2 4	0	0
3	A	1	Total C O 6 2 4	0	0

- Molecule 4 is water.

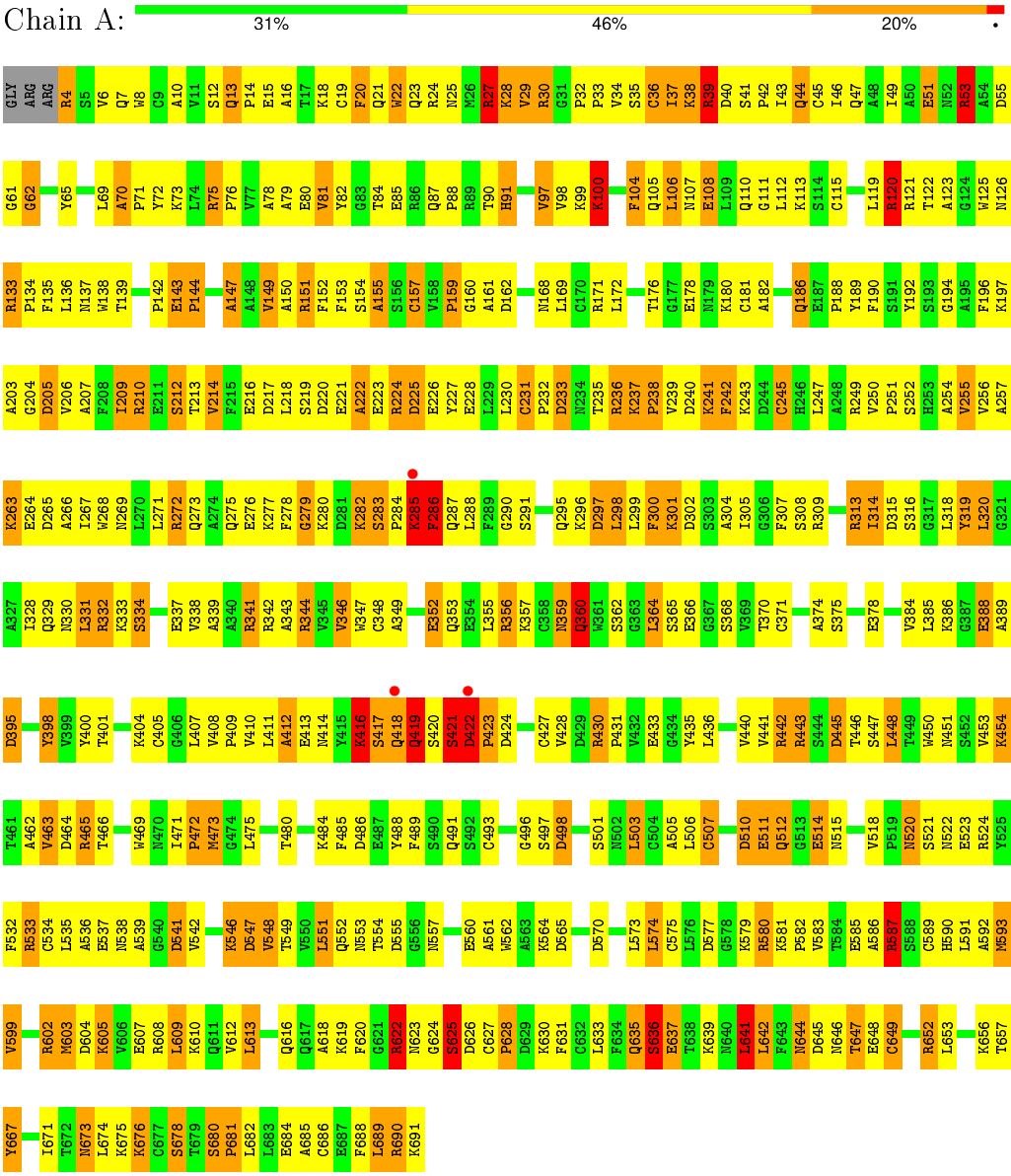
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	121	Total O 121 121	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: LACTOFERRIN

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	155.46Å 96.92Å 55.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 36.60 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.40) 88.1 (36.60-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.20Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available) 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 143.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 38454 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5433	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.15	8/5412 (0.1%)	2.63	384/7325 (5.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	PRO	CA-C	-16.70	1.19	1.52
1	A	286	PHE	C-O	-12.96	0.98	1.23
1	A	282	LYS	C-O	-8.90	1.06	1.23
1	A	79	ALA	C-O	-8.44	1.07	1.23
1	A	421	SER	C-N	-7.99	1.15	1.34
1	A	324	TYR	C-O	7.17	1.36	1.23
1	A	422	ASP	C-N	6.44	1.46	1.34
1	A	282	LYS	N-CA	-5.34	1.35	1.46

All (384) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	ARG	CD-NE-CZ	27.71	162.39	123.60
1	A	24	ARG	NE-CZ-NH1	22.39	131.49	120.30
1	A	442	ARG	CD-NE-CZ	21.17	153.24	123.60
1	A	224	ARG	NE-CZ-NH2	-19.70	110.45	120.30
1	A	524	ARG	NE-CZ-NH1	19.26	129.93	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	580	ARG	NE-CZ-NH1	19.13	129.87	120.30
1	A	171	ARG	NE-CZ-NH1	19.01	129.80	120.30
1	A	430	ARG	NE-CZ-NH1	-18.66	110.97	120.30
1	A	465	ARG	NE-CZ-NH2	-18.03	111.29	120.30
1	A	560	GLU	CA-CB-CG	17.36	151.59	113.40
1	A	121	ARG	NE-CZ-NH2	-17.35	111.63	120.30
1	A	533	ARG	NE-CZ-NH2	-17.04	111.78	120.30
1	A	533	ARG	NE-CZ-NH1	16.17	128.38	120.30
1	A	442	ARG	NE-CZ-NH2	15.85	128.22	120.30
1	A	580	ARG	NE-CZ-NH2	-15.22	112.69	120.30
1	A	622	ARG	NE-CZ-NH1	15.03	127.81	120.30
1	A	27	ARG	NE-CZ-NH1	14.45	127.52	120.30
1	A	356	ARG	NE-CZ-NH1	13.93	127.26	120.30
1	A	448	LEU	CA-CB-CG	13.83	147.10	115.30
1	A	151	ARG	CD-NE-CZ	-13.57	104.61	123.60
1	A	272	ARG	NE-CZ-NH2	-13.56	113.52	120.30
1	A	486	ASP	CB-CG-OD1	13.12	130.11	118.30
1	A	210	ARG	NE-CZ-NH2	12.40	126.50	120.30
1	A	224	ARG	NH1-CZ-NH2	11.78	132.35	119.40
1	A	276	GLU	CA-CB-CG	11.74	139.22	113.40
1	A	24	ARG	CG-CD-NE	11.59	136.14	111.80
1	A	602	ARG	NE-CZ-NH2	-11.43	114.59	120.30
1	A	24	ARG	NH1-CZ-NH2	-11.24	107.03	119.40
1	A	421	SER	O-C-N	11.23	140.67	122.70
1	A	151	ARG	NE-CZ-NH1	-11.17	114.71	120.30
1	A	332	ARG	NE-CZ-NH1	11.15	125.88	120.30
1	A	401	THR	CA-CB-CG2	10.74	127.43	112.40
1	A	121	ARG	NH1-CZ-NH2	10.54	130.99	119.40
1	A	524	ARG	NE-CZ-NH2	-10.43	115.09	120.30
1	A	395	ASP	CB-CG-OD2	-10.37	108.97	118.30
1	A	604	ASP	CA-CB-CG	9.84	135.04	113.40
1	A	498	ASP	CB-CG-OD1	9.83	127.15	118.30
1	A	421	SER	CA-C-N	-9.80	95.65	117.20
1	A	570	ASP	O-C-N	9.69	138.20	122.70
1	A	391	ALA	CB-CA-C	-9.67	95.59	110.10
1	A	443	ARG	NE-CZ-NH2	9.58	125.09	120.30
1	A	660	GLU	OE1-CD-OE2	9.57	134.79	123.30
1	A	690	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	A	667	TYR	CB-CG-CD2	9.40	126.64	121.00
1	A	65	TYR	CB-CG-CD1	-9.38	115.37	121.00
1	A	236	ARG	NE-CZ-NH1	-9.38	115.61	120.30
1	A	422	ASP	O-C-N	-9.37	103.30	121.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	622	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	A	607	GLU	CB-CA-C	9.23	128.86	110.40
1	A	570	ASP	CB-CG-OD2	-9.22	110.00	118.30
1	A	81	VAL	O-C-N	9.22	137.45	122.70
1	A	133	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	430	ARG	NH1-CZ-NH2	9.05	129.36	119.40
1	A	65	TYR	CB-CG-CD2	9.00	126.40	121.00
1	A	548	VAL	CA-CB-CG2	8.99	124.39	110.90
1	A	171	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	A	541	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	A	641	LEU	CB-CG-CD2	-8.86	95.93	111.00
1	A	284	PRO	O-C-N	8.78	136.75	122.70
1	A	331	LEU	O-C-N	8.70	136.62	122.70
1	A	547	ASP	CB-CG-OD1	-8.66	110.50	118.30
1	A	297	ASP	CB-CG-OD1	8.62	126.06	118.30
1	A	324	TYR	CB-CG-CD2	8.58	126.15	121.00
1	A	645	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	A	237	LYS	CA-CB-CG	8.56	132.24	113.40
1	A	514	GLU	CG-CD-OE1	8.55	135.41	118.30
1	A	427	CYS	CA-CB-SG	8.53	129.36	114.00
1	A	690	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	366	GLU	OE1-CD-OE2	8.50	133.50	123.30
1	A	507	CYS	O-C-N	8.44	136.20	122.70
1	A	324	TYR	CB-CG-CD1	-8.43	115.94	121.00
1	A	216	GLU	CA-CB-CG	8.42	131.93	113.40
1	A	388	GLU	CB-CA-C	-8.38	93.64	110.40
1	A	300	PHE	C-N-CA	8.31	142.49	121.70
1	A	224	ARG	CD-NE-CZ	-8.25	112.05	123.60
1	A	642	LEU	CB-CG-CD1	-8.25	96.98	111.00
1	A	272	ARG	NH1-CZ-NH2	8.19	128.41	119.40
1	A	366	GLU	CG-CD-OE2	-8.17	101.96	118.30
1	A	286	PHE	CB-CA-C	-8.14	94.11	110.40
1	A	644	ASN	N-CA-CB	8.10	125.17	110.60
1	A	539	ALA	CB-CA-C	8.07	122.20	110.10
1	A	433	GLU	OE1-CD-OE2	7.91	132.79	123.30
1	A	313	ARG	CD-NE-CZ	-7.88	112.57	123.60
1	A	219	SER	N-CA-CB	-7.88	98.69	110.50
1	A	302	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	493	CYS	N-CA-CB	7.80	124.64	110.60
1	A	498	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	A	207	ALA	N-CA-CB	7.76	120.96	110.10
1	A	553	ASN	CA-CB-CG	7.76	130.47	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	652	ARG	CG-CD-NE	7.76	128.09	111.80
1	A	374	ALA	N-CA-CB	7.72	120.91	110.10
1	A	445	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	178	GLU	CB-CG-CD	7.70	134.98	114.20
1	A	607	GLU	OE1-CD-OE2	-7.66	114.10	123.30
1	A	388	GLU	OE1-CD-OE2	7.61	132.43	123.30
1	A	171	ARG	CG-CD-NE	7.60	127.76	111.80
1	A	599	VAL	CB-CA-C	7.60	125.83	111.40
1	A	551	LEU	CB-CA-C	7.59	124.62	110.20
1	A	30	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	155	ALA	O-C-N	7.54	134.77	122.70
1	A	265	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	206	VAL	CA-CB-CG2	7.51	122.16	110.90
1	A	356	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	276	GLU	CG-CD-OE1	7.33	132.96	118.30
1	A	548	VAL	CB-CA-C	7.33	125.32	111.40
1	A	120	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	636	SER	O-C-N	7.29	134.37	122.70
1	A	15	GLU	N-CA-CB	7.29	123.72	110.60
1	A	57	VAL	O-C-N	7.29	134.36	122.70
1	A	200	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	560	GLU	N-CA-C	-7.20	91.56	111.00
1	A	168	ASN	O-C-N	7.15	134.14	122.70
1	A	547	ASP	OD1-CG-OD2	7.12	136.82	123.30
1	A	236	ARG	NH1-CZ-NH2	7.08	127.19	119.40
1	A	171	ARG	CA-CB-CG	7.05	128.92	113.40
1	A	192	TYR	CA-CB-CG	7.05	126.79	113.40
1	A	27	ARG	NH1-CZ-NH2	-7.01	111.69	119.40
1	A	673	ASN	CA-CB-CG	-6.97	98.07	113.40
1	A	451	ASN	CB-CG-OD1	6.95	135.50	121.60
1	A	44	GLN	CB-CA-C	6.93	124.27	110.40
1	A	574	LEU	CB-CG-CD1	6.93	122.79	111.00
1	A	635	GLN	C-N-CA	6.93	139.02	121.70
1	A	87	GLN	CB-CA-C	6.92	124.24	110.40
1	A	459	CYS	CA-CB-SG	6.92	126.45	114.00
1	A	341	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	318	LEU	CA-CB-CG	6.86	131.07	115.30
1	A	337	GLU	CG-CD-OE1	6.85	132.00	118.30
1	A	222	ALA	CB-CA-C	6.82	120.33	110.10
1	A	613	LEU	CB-CA-C	6.81	123.14	110.20
1	A	412	ALA	N-CA-CB	-6.80	100.58	110.10
1	A	422	ASP	CA-C-N	6.80	136.14	117.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	241	LYS	CB-CG-CD	6.78	129.22	111.60
1	A	548	VAL	CG1-CB-CG2	-6.77	100.07	110.90
1	A	24	ARG	CB-CA-C	6.76	123.93	110.40
1	A	198	CYS	CA-CB-SG	6.75	126.14	114.00
1	A	149	VAL	CB-CA-C	6.74	124.20	111.40
1	A	443	ARG	CB-CG-CD	6.73	129.10	111.60
1	A	398	TYR	CB-CG-CD1	-6.70	116.98	121.00
1	A	522	ASN	CB-CA-C	6.69	123.79	110.40
1	A	604	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	62	GLY	O-C-N	6.69	133.40	122.70
1	A	599	VAL	CA-CB-CG1	6.67	120.90	110.90
1	A	249	ARG	CG-CD-NE	-6.64	97.85	111.80
1	A	258	ARG	CD-NE-CZ	6.63	132.88	123.60
1	A	106	LEU	CB-CG-CD1	-6.62	99.74	111.00
1	A	484	LYS	O-C-N	6.58	133.23	122.70
1	A	34	VAL	N-CA-CB	6.58	125.97	111.50
1	A	297	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	465	ARG	CA-CB-CG	-6.57	98.95	113.40
1	A	585	GLU	CG-CD-OE1	6.57	131.43	118.30
1	A	228	GLU	CA-CB-CG	6.55	127.81	113.40
1	A	602	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	A	435	TYR	CA-CB-CG	6.51	125.76	113.40
1	A	100	LYS	CG-CD-CE	6.49	131.37	111.90
1	A	537	GLU	CG-CD-OE2	-6.49	105.33	118.30
1	A	352	GLU	O-C-N	6.46	133.04	122.70
1	A	488	TYR	CB-CG-CD1	6.45	124.87	121.00
1	A	378	GLU	CA-CB-CG	6.45	127.58	113.40
1	A	488	TYR	CA-CB-CG	6.43	125.61	113.40
1	A	242	PHE	O-C-N	6.43	132.98	122.70
1	A	298	LEU	CA-CB-CG	6.41	130.05	115.30
1	A	22	TRP	CA-CB-CG	6.41	125.88	113.70
1	A	309	ARG	CA-CB-CG	6.40	127.48	113.40
1	A	139	THR	CA-CB-CG2	6.39	121.35	112.40
1	A	240	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	618	ALA	CB-CA-C	-6.39	100.52	110.10
1	A	38	LYS	CA-CB-CG	6.37	127.40	113.40
1	A	20	PHE	CB-CG-CD1	-6.36	116.35	120.80
1	A	39	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	205	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	A	514	GLU	CG-CD-OE2	-6.33	105.64	118.30
1	A	625	SER	N-CA-CB	-6.32	101.02	110.50
1	A	276	GLU	CG-CD-OE2	-6.32	105.66	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	217	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	201	ASP	O-C-N	6.30	133.91	123.20
1	A	259	SER	O-C-N	6.30	132.78	122.70
1	A	454	LYS	CA-CB-CG	6.29	127.25	113.40
1	A	239	VAL	CA-CB-CG1	6.29	120.33	110.90
1	A	186	GLN	CB-CA-C	6.27	122.95	110.40
1	A	417	SER	CA-C-N	-6.27	103.41	117.20
1	A	27	ARG	CB-CG-CD	6.25	127.86	111.60
1	A	547	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	610	LYS	CB-CG-CD	-6.24	95.38	111.60
1	A	236	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	649	CYS	O-C-N	6.23	132.66	122.70
1	A	53	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	A	224	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	A	314	ILE	CA-CB-CG1	-6.21	99.20	111.00
1	A	551	LEU	O-C-N	-6.20	112.78	122.70
1	A	463	VAL	CG1-CB-CG2	-6.18	101.01	110.90
1	A	560	GLU	CB-CA-C	6.18	122.76	110.40
1	A	104	PHE	N-CA-C	-6.17	94.33	111.00
1	A	171	ARG	CD-NE-CZ	6.17	132.23	123.60
1	A	261	ASN	N-CA-CB	6.16	121.68	110.60
1	A	546	LYS	CA-C-N	6.15	130.74	117.20
1	A	690	ARG	CD-NE-CZ	6.15	132.21	123.60
1	A	344	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	A	507	CYS	N-CA-CB	6.14	121.65	110.60
1	A	6	VAL	CA-C-N	-6.13	103.70	117.20
1	A	24	ARG	CA-CB-CG	6.13	126.90	113.40
1	A	143	GLU	CG-CD-OE1	6.12	130.54	118.30
1	A	315	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	603	MET	CB-CG-SD	-6.10	94.11	112.40
1	A	123	ALA	CB-CA-C	6.08	119.22	110.10
1	A	203	ALA	N-CA-CB	6.05	118.57	110.10
1	A	349	ALA	N-CA-CB	-6.04	101.64	110.10
1	A	322	SER	CA-CB-OG	6.03	127.49	111.20
1	A	657	THR	N-CA-CB	-6.03	98.85	110.30
1	A	531	ALA	CB-CA-C	6.02	119.13	110.10
1	A	121	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	190	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	A	532	PHE	CB-CG-CD1	-5.97	116.62	120.80
1	A	607	GLU	CB-CG-CD	5.96	130.31	114.20
1	A	684	GLU	OE1-CD-OE2	5.96	130.46	123.30
1	A	497	SER	CA-CB-OG	5.96	127.29	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	332	ARG	CD-NE-CZ	5.96	131.94	123.60
1	A	296	LYS	CA-CB-CG	5.95	126.48	113.40
1	A	657	THR	CA-CB-OG1	-5.95	96.51	109.00
1	A	127	VAL	CG1-CB-CG2	-5.92	101.42	110.90
1	A	258	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	465	ARG	NH1-CZ-NH2	5.92	125.91	119.40
1	A	233	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	24	ARG	CB-CG-CD	5.91	126.97	111.60
1	A	605	LYS	CA-C-O	-5.91	107.70	120.10
1	A	463	VAL	CA-CB-CG2	-5.90	102.06	110.90
1	A	36	CYS	CA-CB-SG	-5.88	103.41	114.00
1	A	217	ASP	CB-CG-OD1	5.88	123.60	118.30
1	A	235	THR	N-CA-CB	5.86	121.44	110.30
1	A	120	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	593	MET	CA-CB-CG	-5.84	103.37	113.30
1	A	510	ASP	CA-C-N	-5.82	104.39	117.20
1	A	570	ASP	CB-CA-C	-5.81	98.77	110.40
1	A	518	VAL	N-CA-CB	-5.81	98.71	111.50
1	A	334	SER	N-CA-CB	-5.81	101.78	110.50
1	A	609	LEU	O-C-N	5.81	131.99	122.70
1	A	160	GLY	CA-C-O	-5.79	110.17	120.60
1	A	201	ASP	CB-CA-C	-5.79	98.82	110.40
1	A	171	ARG	N-CA-CB	5.79	121.02	110.60
1	A	325	PHE	CB-CG-CD1	-5.77	116.76	120.80
1	A	91	HIS	O-C-N	5.76	131.92	122.70
1	A	520	ASN	N-CA-CB	5.76	120.97	110.60
1	A	241	LYS	O-C-N	-5.76	113.48	122.70
1	A	689	LEU	CB-CG-CD2	-5.74	101.23	111.00
1	A	680	SER	N-CA-CB	5.72	119.08	110.50
1	A	421	SER	CB-CA-C	-5.72	99.24	110.10
1	A	503	LEU	CB-CA-C	5.71	121.05	110.20
1	A	15	GLU	CG-CD-OE2	-5.70	106.90	118.30
1	A	245	CYS	N-CA-CB	-5.70	100.35	110.60
1	A	70	ALA	N-CA-C	-5.69	95.64	111.00
1	A	605	LYS	CB-CA-C	-5.68	99.03	110.40
1	A	442	ARG	NH1-CZ-NH2	-5.68	113.15	119.40
1	A	81	VAL	N-CA-C	-5.66	95.71	111.00
1	A	510	ASP	O-C-N	5.66	131.76	122.70
1	A	36	CYS	CB-CA-C	-5.65	99.09	110.40
1	A	254	ALA	CB-CA-C	-5.64	101.64	110.10
1	A	368	SER	N-CA-CB	5.62	118.93	110.50
1	A	298	LEU	CB-CA-C	5.62	120.87	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	337	GLU	CG-CD-OE2	-5.61	107.07	118.30
1	A	360	GLN	N-CA-CB	-5.61	100.50	110.60
1	A	511	GLU	OE1-CD-OE2	5.61	130.03	123.30
1	A	667	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	A	104	PHE	CB-CA-C	5.60	121.60	110.40
1	A	155	ALA	CA-C-O	-5.59	108.36	120.10
1	A	673	ASN	CB-CG-OD1	-5.59	110.42	121.60
1	A	20	PHE	N-CA-CB	5.58	120.64	110.60
1	A	30	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	554	THR	CA-CB-CG2	5.58	120.21	112.40
1	A	56	ALA	N-CA-CB	-5.58	102.29	110.10
1	A	390	ASP	N-CA-CB	-5.57	100.57	110.60
1	A	90	THR	CA-CB-CG2	-5.57	104.60	112.40
1	A	637	GLU	O-C-N	5.57	131.61	122.70
1	A	69	LEU	N-CA-CB	-5.56	99.28	110.40
1	A	249	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	265	ASP	CA-C-N	-5.56	104.97	117.20
1	A	97	VAL	CA-CB-CG2	5.56	119.23	110.90
1	A	674	LEU	CB-CG-CD1	-5.55	101.56	111.00
1	A	599	VAL	CG1-CB-CG2	-5.55	102.02	110.90
1	A	386	LYS	CD-CE-NZ	-5.53	98.98	111.70
1	A	265	ASP	O-C-N	5.52	131.53	122.70
1	A	314	ILE	N-CA-C	5.51	125.88	111.00
1	A	182	ALA	CA-C-N	-5.51	105.08	117.20
1	A	249	ARG	O-C-N	5.51	131.52	122.70
1	A	349	ALA	CB-CA-C	5.50	118.34	110.10
1	A	51	GLU	O-C-N	5.49	131.48	122.70
1	A	405	CYS	C-N-CA	-5.49	110.78	122.30
1	A	6	VAL	CA-C-O	5.48	131.61	120.10
1	A	133	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	420	SER	O-C-N	5.48	131.47	122.70
1	A	143	GLU	CG-CD-OE2	-5.47	107.35	118.30
1	A	635	GLN	O-C-N	-5.47	113.95	122.70
1	A	59	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	A	78	ALA	N-CA-CB	5.45	117.73	110.10
1	A	217	ASP	CA-CB-CG	5.45	125.39	113.40
1	A	286	PHE	CA-C-N	-5.45	105.21	117.20
1	A	132	LEU	N-CA-CB	-5.42	99.56	110.40
1	A	15	GLU	CA-CB-CG	5.42	125.32	113.40
1	A	511	GLU	C-N-CA	5.42	135.25	121.70
1	A	59	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	135	PHE	CB-CA-C	-5.41	99.58	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	388	GLU	CG-CD-OE2	-5.41	107.48	118.30
1	A	147	ALA	CB-CA-C	5.40	118.19	110.10
1	A	302	ASP	CB-CG-OD1	5.39	123.16	118.30
1	A	392	MET	N-CA-CB	-5.39	100.89	110.60
1	A	450	TRP	CA-CB-CG	-5.39	103.46	113.70
1	A	416	LYS	CA-C-O	5.39	131.41	120.10
1	A	319	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	A	537	GLU	CG-CD-OE1	5.38	129.06	118.30
1	A	290	GLY	N-CA-C	-5.38	99.66	113.10
1	A	384	VAL	CA-CB-CG2	5.38	118.96	110.90
1	A	392	MET	CA-CB-CG	-5.38	104.16	113.30
1	A	237	LYS	CB-CG-CD	5.38	125.58	111.60
1	A	451	ASN	CA-CB-CG	5.37	125.22	113.40
1	A	460	HIS	CB-CA-C	-5.37	99.67	110.40
1	A	587	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	212	SER	CA-CB-OG	5.36	125.66	111.20
1	A	524	ARG	CG-CD-NE	5.36	123.05	111.80
1	A	684	GLU	CG-CD-OE2	-5.35	107.60	118.30
1	A	308	SER	CA-CB-OG	-5.34	96.79	111.20
1	A	243	LYS	CA-CB-CG	5.33	125.12	113.40
1	A	676	LYS	CA-CB-CG	5.32	125.10	113.40
1	A	120	ARG	CD-NE-CZ	5.32	131.04	123.60
1	A	4	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	A	127	VAL	CA-CB-CG2	5.31	118.86	110.90
1	A	419	GLN	N-CA-CB	5.31	120.16	110.60
1	A	85	GLU	CB-CG-CD	5.30	128.52	114.20
1	A	180	LYS	CA-C-O	5.30	131.23	120.10
1	A	607	GLU	CG-CD-OE1	5.30	128.90	118.30
1	A	647	THR	O-C-N	5.30	131.18	122.70
1	A	225	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	594	ALA	O-C-N	5.29	131.16	121.10
1	A	339	ALA	N-CA-CB	-5.29	102.70	110.10
1	A	357	LYS	CD-CE-NZ	-5.28	99.55	111.70
1	A	309	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	512	GLN	CB-CA-C	-5.27	99.85	110.40
1	A	450	TRP	C-N-CA	5.26	134.86	121.70
1	A	157	CYS	N-CA-CB	5.25	120.05	110.60
1	A	691	LYS	CA-C-O	-5.25	109.08	120.10
1	A	346	VAL	O-C-N	5.24	131.08	122.70
1	A	580	ARG	N-CA-CB	5.23	120.02	110.60
1	A	69	LEU	CA-C-O	5.23	131.09	120.10
1	A	421	SER	C-N-CA	5.23	134.78	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	239	VAL	CA-CB-CG2	-5.22	103.06	110.90
1	A	580	ARG	CD-NE-CZ	5.22	130.90	123.60
1	A	108	GLU	CG-CD-OE2	-5.19	107.91	118.30
1	A	238	PRO	C-N-CA	5.19	134.68	121.70
1	A	681	PRO	O-C-N	5.19	131.00	122.70
1	A	126	ASN	CB-CG-ND2	5.18	129.14	116.70
1	A	371	CYS	CA-CB-SG	-5.18	104.67	114.00
1	A	389	ALA	N-CA-CB	5.18	117.35	110.10
1	A	320	LEU	CB-CG-CD2	-5.17	102.20	111.00
1	A	375	SER	O-C-N	5.17	130.98	122.70
1	A	511	GLU	CG-CD-OE2	-5.17	107.97	118.30
1	A	231	CYS	CA-CB-SG	-5.16	104.70	114.00
1	A	249	ARG	CA-CB-CG	-5.16	102.04	113.40
1	A	272	ARG	CD-NE-CZ	-5.16	116.38	123.60
1	A	570	ASP	OD1-CG-OD2	5.16	133.10	123.30
1	A	85	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	A	304	ALA	N-CA-C	-5.15	97.09	111.00
1	A	485	PHE	N-CA-CB	5.15	119.86	110.60
1	A	12	SER	CA-C-N	-5.14	105.89	117.20
1	A	411	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	465	ARG	N-CA-CB	-5.12	101.38	110.60
1	A	602	ARG	CA-CB-CG	5.12	124.67	113.40
1	A	624	GLY	C-N-CA	5.12	134.50	121.70
1	A	691	LYS	CG-CD-CE	5.12	127.27	111.90
1	A	144	PRO	O-C-N	5.12	130.89	122.70
1	A	673	ASN	OD1-CG-ND2	5.12	133.67	121.90
1	A	391	ALA	N-CA-CB	-5.11	102.94	110.10
1	A	296	LYS	N-CA-CB	5.10	119.79	110.60
1	A	85	GLU	CA-CB-CG	5.10	124.63	113.40
1	A	348	CYS	N-CA-CB	5.10	119.78	110.60
1	A	161	ALA	N-CA-CB	5.10	117.24	110.10
1	A	636	SER	CA-C-N	-5.09	105.99	117.20
1	A	359	ASN	CA-C-N	-5.09	106.00	117.20
1	A	137	ASN	CA-C-N	-5.06	106.06	117.20
1	A	180	LYS	CA-C-N	-5.06	106.06	117.20
1	A	359	ASN	O-C-N	5.05	130.79	122.70
1	A	258	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
1	A	610	LYS	CA-C-O	5.03	130.65	120.10
1	A	496	GLY	O-C-N	5.02	130.74	122.70
1	A	255	VAL	CB-CA-C	5.02	120.94	111.40
1	A	417	SER	CA-C-O	5.02	130.64	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	249	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	LYS	Mainchain
1	A	587	ARG	Sidechain

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	5298	0	5140	408	0
2	A	2	0	0	0	0
3	A	12	0	0	0	0
4	A	121	0	0	31	0
All	All	5433	0	5140	408	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 39.

All (408) 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:A:291:SER:HB3	1:A:298:LEU:HD23	1.19	1.19
1:A:462:ALA:HB3	1:A:465:ARG:HD2	1.31	1.08
1:A:417:SER:C	1:A:419:GLN:H	1.42	1.08
1:A:119:LEU:HG	1:A:120:ARG:HD3	1.30	1.05
1:A:13:GLN:HB3	1:A:14:PRO:HD3	1.35	1.05
1:A:100:LYS:HD2	1:A:225:ASP:O	1.59	1.03
1:A:295:GLN:HB3	1:A:298:LEU:HD21	1.33	1.03
1:A:231:CYS:SG	1:A:237:LYS:HD3	2.00	1.02
1:A:220:ASP:OD1	1:A:221:GLU:N	2.00	0.95
1:A:283:SER:OG	1:A:285:LYS:NZ	2.00	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ASP:HB3	1:A:630:LYS:HB2	1.51	0.93
1:A:257:ALA:HB1	4:A:713:HOH:O	1.67	0.93
1:A:686:CYS:O	1:A:690:ARG:HG2	1.69	0.92
1:A:259:SER:O	4:A:835:HOH:O	1.88	0.92
1:A:417:SER:C	1:A:419:GLN:N	2.24	0.91
1:A:422:ASP:O	1:A:424:ASP:N	2.04	0.90
1:A:13:GLN:HB3	1:A:14:PRO:CD	2.02	0.90
1:A:113:LYS:O	1:A:205:ASP:HB2	1.71	0.89
1:A:658:THR:HG21	1:A:661:LYS:HG3	1.52	0.89
1:A:291:SER:HB3	1:A:298:LEU:CD2	2.02	0.89
1:A:443:ARG:CD	4:A:868:HOH:O	2.21	0.88
1:A:238:PRO:HD2	1:A:241:LYS:HG3	1.54	0.87
1:A:36:CYS:C	1:A:37:ILE:HD12	1.96	0.87
1:A:647:THR:HG22	1:A:649:CYS:O	1.75	0.85
1:A:138:TRP:NE1	1:A:143:GLU:O	2.09	0.85
1:A:58:THR:HG23	4:A:704:HOH:O	1.76	0.84
1:A:295:GLN:HB3	1:A:298:LEU:CD2	2.06	0.84
1:A:214:VAL:HG12	4:A:934:HOH:O	1.77	0.84
1:A:646:ASN:OD1	4:A:886:HOH:O	1.95	0.83
1:A:622:ARG:HD3	1:A:622:ARG:O	1.76	0.82
1:A:443:ARG:HD2	4:A:868:HOH:O	1.77	0.82
1:A:561:ALA:HA	1:A:564:LYS:HD3	1.61	0.82
1:A:41:SER:HB2	1:A:42:PRO:HD2	1.62	0.82
1:A:70:ALA:HA	1:A:73:LYS:HE3	1.62	0.82
1:A:295:GLN:CB	1:A:298:LEU:HD21	2.10	0.82
1:A:176:THR:HG22	1:A:176:THR:O	1.77	0.81
1:A:446:THR:N	4:A:784:HOH:O	2.12	0.81
1:A:680:SER:HB2	1:A:681:PRO:HD2	1.62	0.81
1:A:322:SER:HB3	1:A:385:LEU:O	1.78	0.81
1:A:647:THR:CG2	1:A:649:CYS:O	2.29	0.81
1:A:658:THR:CG2	1:A:661:LYS:HG3	2.10	0.81
1:A:291:SER:CB	1:A:298:LEU:HD23	2.09	0.81
1:A:443:ARG:NE	4:A:868:HOH:O	2.13	0.81
1:A:658:THR:HG23	1:A:661:LYS:H	1.45	0.80
1:A:39:ARG:CG	1:A:39:ARG:HH11	1.94	0.80
1:A:27:ARG:HD2	1:A:28:LYS:N	1.96	0.80
1:A:430:ARG:HG2	1:A:431:PRO:HD2	1.63	0.79
1:A:446:THR:CA	4:A:784:HOH:O	2.31	0.79
1:A:385:LEU:HD23	1:A:407:LEU:HD21	1.64	0.78
1:A:104:PHE:HA	1:A:108:GLU:OE1	1.84	0.78
1:A:352:GLU:H	1:A:352:GLU:CD	1.87	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:TYR:CE2	1:A:671:ILE:HD11	2.20	0.76
1:A:115:CYS:SG	1:A:204:GLY:HA3	2.26	0.76
1:A:4:ARG:HG3	1:A:4:ARG:HH11	1.48	0.76
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.49	0.76
1:A:214:VAL:O	1:A:218:LEU:HB2	1.86	0.75
1:A:99:LYS:HG2	1:A:227:TYR:CE1	2.22	0.74
1:A:359:ASN:O	1:A:362:SER:HB3	1.87	0.74
1:A:326:THR:HG22	1:A:329:GLN:HE22	1.52	0.73
1:A:595:PRO:O	4:A:918:HOH:O	2.05	0.73
1:A:40:ASP:HB2	1:A:44:GLN:OE1	1.87	0.73
1:A:447:SER:N	4:A:784:HOH:O	2.20	0.73
1:A:385:LEU:CD2	1:A:407:LEU:HD21	2.17	0.73
1:A:417:SER:O	1:A:419:GLN:N	2.19	0.73
1:A:4:ARG:NH1	1:A:263:LYS:HE3	2.05	0.72
1:A:533:ARG:NH1	4:A:914:HOH:O	2.17	0.72
1:A:462:ALA:HB3	1:A:465:ARG:CD	2.17	0.72
1:A:220:ASP:HB3	1:A:223:GLU:HG3	1.72	0.71
1:A:186:GLN:O	1:A:188:PRO:HD3	1.91	0.70
1:A:47:GLN:HG2	1:A:72:TYR:CE1	2.26	0.70
1:A:573:LEU:HD11	1:A:586:ALA:HB2	1.72	0.70
1:A:344:ARG:HD3	1:A:370:THR:HG21	1.73	0.70
1:A:612:VAL:O	1:A:616:GLN:HG2	1.90	0.70
1:A:446:THR:CB	4:A:784:HOH:O	2.40	0.69
1:A:7:GLN:HG2	1:A:35:SER:OG	1.92	0.69
1:A:282:LYS:O	1:A:283:SER:HB2	1.91	0.69
1:A:413:GLU:OE2	4:A:774:HOH:O	2.11	0.69
1:A:38:LYS:O	1:A:39:ARG:HG2	1.93	0.69
1:A:13:GLN:CB	1:A:14:PRO:CD	2.69	0.68
1:A:352:GLU:O	1:A:355:LEU:HB3	1.93	0.68
1:A:119:LEU:HG	1:A:120:ARG:CD	2.19	0.67
1:A:223:GLU:HB3	4:A:921:HOH:O	1.94	0.67
1:A:98:VAL:HG11	1:A:230:LEU:HD21	1.76	0.67
1:A:445:ASP:O	1:A:580:ARG:NH2	2.28	0.67
1:A:18:LYS:O	1:A:22:TRP:N	2.17	0.66
1:A:622:ARG:C	1:A:622:ARG:HD3	2.15	0.66
1:A:480:THR:HG21	4:A:936:HOH:O	1.94	0.66
1:A:547:ASP:OD1	1:A:547:ASP:N	2.28	0.66
1:A:133:ARG:N	1:A:134:PRO:CD	2.59	0.66
1:A:4:ARG:HH22	1:A:266:ALA:HB2	1.59	0.65
1:A:107:ASN:OD1	1:A:107:ASN:N	2.15	0.65
1:A:29:VAL:O	1:A:30:ARG:HB2	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:HG3	1:A:4:ARG:NH1	2.12	0.65
1:A:441:VAL:HG13	1:A:574:LEU:HD13	1.79	0.64
1:A:658:THR:CG2	1:A:661:LYS:CG	2.76	0.64
1:A:288:LEU:HD11	1:A:300:PHE:CE2	2.33	0.64
1:A:122:THR:HG21	1:A:250:VAL:HG21	1.79	0.64
1:A:422:ASP:O	1:A:423:PRO:C	2.32	0.63
1:A:409:PRO:HB2	1:A:653:LEU:HD11	1.81	0.63
1:A:430:ARG:HG2	1:A:431:PRO:CD	2.28	0.63
1:A:220:ASP:OD1	1:A:220:ASP:C	2.36	0.63
1:A:359:ASN:O	1:A:362:SER:CB	2.47	0.63
1:A:13:GLN:CB	1:A:14:PRO:HD3	2.20	0.63
1:A:250:VAL:HB	1:A:251:PRO:HD2	1.80	0.63
1:A:258:ARG:NH1	1:A:261:ASN:O	2.33	0.62
1:A:622:ARG:C	1:A:622:ARG:CD	2.68	0.62
1:A:132:LEU:O	1:A:136:LEU:HG	1.99	0.62
1:A:456:LYS:HD2	1:A:456:LYS:N	2.15	0.61
1:A:51:GLU:HG3	1:A:53:ARG:CG	2.30	0.61
1:A:442:ARG:HD3	1:A:538:ASN:OD1	2.01	0.61
1:A:360:GLN:NE2	1:A:631:PHE:HE1	1.98	0.61
1:A:644:ASN:HB3	4:A:886:HOH:O	2.01	0.61
1:A:42:PRO:O	1:A:46:ILE:HG13	2.01	0.60
1:A:436:LEU:HD21	1:A:593:MET:CE	2.30	0.60
1:A:448:LEU:HD11	1:A:456:LYS:HG2	1.83	0.60
1:A:330:ASN:C	1:A:332:ARG:H	2.05	0.60
1:A:430:ARG:HH22	1:A:648:GLU:CD	2.04	0.60
1:A:636:SER:HB3	1:A:641:LEU:HD22	1.83	0.60
1:A:346:VAL:HG22	1:A:370:THR:CG2	2.32	0.60
1:A:133:ARG:HB3	1:A:134:PRO:HD3	1.83	0.60
1:A:446:THR:HB	4:A:784:HOH:O	2.00	0.60
1:A:36:CYS:O	1:A:37:ILE:HD12	2.02	0.60
1:A:247:LEU:HD12	1:A:247:LEU:N	2.17	0.60
1:A:181:CYS:SG	1:A:181:CYS:O	2.61	0.59
1:A:288:LEU:HD11	1:A:300:PHE:HE2	1.68	0.59
1:A:4:ARG:NH2	1:A:266:ALA:HB2	2.18	0.59
1:A:88:PRO:HB3	1:A:305:ILE:HD11	1.85	0.59
1:A:581:LYS:HB3	1:A:582:PRO:CD	2.33	0.58
1:A:76:PRO:HA	1:A:256:VAL:HA	1.86	0.58
1:A:20:PHE:O	1:A:23:GLN:HB3	2.03	0.58
1:A:313:ARG:NH1	1:A:313:ARG:HG3	2.18	0.58
1:A:410:VAL:HG21	1:A:609:LEU:HD23	1.85	0.58
1:A:272:ARG:O	1:A:275:GLN:HB3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ASN:O	1:A:362:SER:N	2.37	0.57
1:A:58:THR:HG21	1:A:300:PHE:CD1	2.39	0.57
1:A:551:LEU:HD11	1:A:583:VAL:HG12	1.84	0.57
1:A:58:THR:HB	1:A:255:VAL:HG22	1.87	0.57
1:A:122:THR:HA	1:A:324:TYR:OH	2.04	0.57
1:A:577:ASP:OD1	1:A:579:LYS:N	2.30	0.57
1:A:41:SER:HB2	1:A:42:PRO:CD	2.33	0.57
1:A:220:ASP:OD1	1:A:222:ALA:N	2.37	0.57
1:A:221:GLU:HG3	4:A:761:HOH:O	2.04	0.57
1:A:271:LEU:O	1:A:275:GLN:HB2	2.05	0.57
1:A:413:GLU:HB3	1:A:647:THR:HG23	1.85	0.57
1:A:440:VAL:HG12	1:A:535:LEU:CD2	2.35	0.57
1:A:346:VAL:HG22	1:A:370:THR:HG23	1.87	0.57
1:A:471:ILE:HD13	1:A:592:ALA:HB3	1.87	0.57
1:A:442:ARG:HH12	1:A:541:ASP:HA	1.69	0.57
1:A:605:LYS:HG3	1:A:605:LYS:O	2.05	0.56
1:A:47:GLN:HG2	1:A:72:TYR:HE1	1.67	0.56
1:A:81:VAL:HG11	1:A:88:PRO:HB2	1.88	0.56
1:A:271:LEU:HB3	1:A:307:PHE:CD2	2.41	0.56
1:A:334:SER:HA	4:A:705:HOH:O	2.04	0.56
1:A:352:GLU:CD	1:A:352:GLU:N	2.58	0.56
1:A:580:ARG:O	1:A:581:LYS:HG3	2.06	0.56
1:A:196:PHE:O	1:A:200:ARG:HB2	2.06	0.56
1:A:360:GLN:HE21	1:A:631:PHE:HE1	1.54	0.56
1:A:25:ASN:HA	1:A:28:LYS:HB2	1.87	0.55
1:A:37:ILE:HD12	1:A:37:ILE:N	2.19	0.55
1:A:514:GLU:O	1:A:515:ASN:HB2	2.07	0.55
1:A:71:PRO:C	1:A:73:LYS:HD2	2.26	0.55
1:A:445:ASP:HB3	1:A:448:LEU:HD23	1.87	0.55
1:A:324:TYR:O	1:A:328:ILE:HG13	2.06	0.55
1:A:286:PHE:CG	1:A:287:GLN:N	2.74	0.55
1:A:416:LYS:HD2	1:A:416:LYS:C	2.27	0.55
1:A:129:ILE:O	1:A:129:ILE:HG22	2.06	0.55
1:A:417:SER:OG	1:A:418:GLN:N	2.38	0.55
1:A:268:TRP:HA	1:A:268:TRP:CE3	2.43	0.55
1:A:214:VAL:CG1	4:A:934:HOH:O	2.46	0.54
1:A:297:ASP:OD2	4:A:768:HOH:O	2.18	0.54
1:A:221:GLU:O	1:A:224:ARG:HB2	2.07	0.54
1:A:436:LEU:HD22	1:A:590:HIS:ND1	2.23	0.54
1:A:680:SER:HB2	1:A:681:PRO:CD	2.35	0.54
1:A:362:SER:O	1:A:365:SER:OG	2.26	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:NH1	1:A:330:ASN:O	2.40	0.54
1:A:346:VAL:O	1:A:390:ASP:HB2	2.08	0.54
1:A:81:VAL:CG1	1:A:88:PRO:HB2	2.38	0.54
1:A:100:LYS:HG3	1:A:226:GLU:O	2.08	0.54
1:A:42:PRO:O	1:A:46:ILE:N	2.35	0.54
1:A:510:ASP:N	1:A:514:GLU:O	2.35	0.53
1:A:129:ILE:HD13	1:A:129:ILE:N	2.22	0.53
1:A:231:CYS:HB2	1:A:233:ASP:OD1	2.09	0.53
1:A:47:GLN:O	1:A:51:GLU:HG2	2.08	0.53
1:A:344:ARG:HD3	1:A:370:THR:CG2	2.39	0.53
1:A:330:ASN:C	1:A:332:ARG:N	2.62	0.53
1:A:551:LEU:HD11	1:A:583:VAL:CG1	2.39	0.53
1:A:97:VAL:O	1:A:199:LEU:HD22	2.09	0.53
1:A:352:GLU:OE1	1:A:352:GLU:N	2.22	0.52
1:A:436:LEU:HD22	1:A:590:HIS:CG	2.44	0.52
1:A:680:SER:HB2	4:A:820:HOH:O	2.08	0.52
1:A:639:LYS:HB2	1:A:641:LEU:HD13	1.92	0.52
1:A:575:CYS:HB2	1:A:577:ASP:OD1	2.08	0.52
1:A:111:GLY:N	1:A:152:PHE:O	2.32	0.52
1:A:10:ALA:HB3	1:A:37:ILE:O	2.09	0.52
1:A:75:ARG:NH1	1:A:314:ILE:O	2.42	0.52
1:A:436:LEU:HD21	1:A:593:MET:HE2	1.92	0.52
1:A:97:VAL:HG23	1:A:209:ILE:HD13	1.92	0.52
1:A:71:PRO:O	1:A:73:LYS:HD2	2.10	0.52
1:A:360:GLN:NE2	1:A:631:PHE:CE1	2.78	0.52
1:A:343:ALA:O	1:A:608:ARG:NE	2.41	0.52
1:A:231:CYS:SG	1:A:237:LYS:CD	2.88	0.51
1:A:40:ASP:O	1:A:41:SER:HB3	2.11	0.51
1:A:133:ARG:N	1:A:134:PRO:HD2	2.24	0.51
1:A:580:ARG:NH1	4:A:785:HOH:O	1.94	0.51
1:A:316:SER:O	1:A:320:LEU:HG	2.11	0.51
1:A:100:LYS:HG3	1:A:226:GLU:C	2.30	0.51
1:A:51:GLU:HG3	1:A:53:ARG:HG3	1.93	0.51
1:A:577:ASP:OD1	1:A:579:LYS:HB2	2.10	0.51
1:A:581:LYS:CB	1:A:582:PRO:CD	2.89	0.51
1:A:247:LEU:CD1	1:A:247:LEU:N	2.73	0.51
1:A:400:TYR:O	1:A:404:LYS:HG2	2.10	0.51
1:A:313:ARG:HB3	1:A:685:ALA:HB2	1.91	0.51
1:A:301:LYS:C	1:A:301:LYS:HD3	2.31	0.51
1:A:332:ARG:C	1:A:333:LYS:HG2	2.31	0.50
1:A:466:THR:HG21	1:A:594:ALA:HB1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:O	1:A:39:ARG:CG	2.58	0.50
1:A:128:PRO:HG2	1:A:129:ILE:H	1.76	0.50
1:A:91:HIS:HA	1:A:250:VAL:O	2.11	0.50
1:A:13:GLN:N	1:A:38:LYS:HE2	2.26	0.50
1:A:70:ALA:CA	1:A:73:LYS:HE3	2.37	0.50
1:A:51:GLU:CD	1:A:53:ARG:HH11	2.14	0.50
1:A:70:ALA:CB	1:A:73:LYS:HE3	2.42	0.49
1:A:491:GLN:HB2	1:A:505:ALA:HB3	1.94	0.49
1:A:347:TRP:CH2	1:A:613:LEU:HD11	2.47	0.49
1:A:620:PHE:CE1	1:A:626:ASP:HB2	2.47	0.49
1:A:507:CYS:HB3	1:A:523:GLU:CD	2.33	0.49
1:A:221:GLU:HA	1:A:224:ARG:HD2	1.94	0.49
1:A:72:TYR:HE2	4:A:714:HOH:O	1.95	0.49
1:A:528:TYR:O	1:A:549:THR:HG21	2.12	0.49
1:A:18:LYS:NZ	1:A:288:LEU:O	2.39	0.49
1:A:581:LYS:HD2	1:A:589:CYS:HB2	1.93	0.48
1:A:341:ARG:HG3	1:A:341:ARG:O	2.12	0.48
1:A:491:GLN:HG3	1:A:506:LEU:HD21	1.95	0.48
1:A:104:PHE:H	1:A:236:ARG:HH11	1.60	0.48
1:A:441:VAL:HG11	1:A:574:LEU:HD11	1.96	0.48
1:A:471:ILE:N	1:A:472:PRO:CD	2.76	0.48
1:A:210:ARG:HD2	1:A:212:SER:OG	2.12	0.48
1:A:27:ARG:HD2	1:A:28:LYS:CA	2.44	0.48
1:A:264:GLU:HA	1:A:267:ILE:HD12	1.94	0.48
1:A:4:ARG:HH11	1:A:4:ARG:CG	2.16	0.48
1:A:313:ARG:HH11	1:A:313:ARG:HG3	1.78	0.48
1:A:469:TRP:O	1:A:472:PRO:HD2	2.13	0.48
1:A:428:VAL:HG12	1:A:652:ARG:HG3	1.95	0.48
1:A:43:ILE:HD12	1:A:43:ILE:HG23	1.64	0.48
1:A:619:LYS:HA	1:A:625:SER:HB3	1.95	0.47
1:A:436:LEU:CD2	1:A:593:MET:CE	2.91	0.47
1:A:194:GLY:O	1:A:197:LYS:N	2.47	0.47
1:A:644:ASN:O	1:A:647:THR:OG1	2.26	0.47
1:A:275:GLN:O	1:A:279:GLY:HA3	2.14	0.47
1:A:147:ALA:O	1:A:151:ARG:HG3	2.13	0.47
1:A:220:ASP:CB	1:A:223:GLU:HG3	2.40	0.47
1:A:37:ILE:N	1:A:37:ILE:CD1	2.76	0.47
1:A:332:ARG:O	1:A:333:LYS:HG2	2.13	0.47
1:A:353:GLN:HG2	1:A:356:ARG:NH1	2.29	0.47
1:A:653:LEU:HD13	1:A:656:LYS:O	2.15	0.47
1:A:326:THR:HG22	1:A:329:GLN:NE2	2.25	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ASN:O	1:A:676:LYS:HB2	2.14	0.47
1:A:38:LYS:O	1:A:39:ARG:NH1	2.46	0.47
1:A:241:LYS:O	1:A:245:CYS:N	2.47	0.47
1:A:110:GLN:HA	1:A:152:PHE:CZ	2.50	0.47
1:A:586:ALA:O	1:A:590:HIS:ND1	2.33	0.47
1:A:639:LYS:CB	1:A:641:LEU:HD13	2.45	0.47
1:A:440:VAL:O	1:A:542:VAL:HA	2.14	0.47
1:A:105:GLN:HE21	1:A:105:GLN:HB3	1.40	0.47
1:A:680:SER:CB	1:A:681:PRO:HD2	2.36	0.47
1:A:189:TYR:C	1:A:194:GLY:HA3	2.35	0.47
1:A:498:ASP:HB3	1:A:501:SER:HB3	1.95	0.47
1:A:463:VAL:O	1:A:464:ASP:HB2	2.14	0.47
1:A:220:ASP:HB3	1:A:223:GLU:CG	2.43	0.46
1:A:364:LEU:HB3	1:A:620:PHE:CZ	2.50	0.46
1:A:97:VAL:HG23	1:A:209:ILE:CD1	2.44	0.46
1:A:21:GLN:HG3	1:A:286:PHE:CE1	2.51	0.46
1:A:332:ARG:C	1:A:333:LYS:CG	2.84	0.46
1:A:627:CYS:HA	1:A:628:PRO:HA	1.57	0.46
1:A:680:SER:OG	4:A:792:HOH:O	2.21	0.46
1:A:220:ASP:HB3	1:A:223:GLU:OE2	2.15	0.46
1:A:80:GLU:OE1	1:A:301:LYS:HB2	2.15	0.46
1:A:441:VAL:CG1	1:A:574:LEU:HD13	2.45	0.46
1:A:58:THR:HG23	1:A:299:LEU:O	2.15	0.46
1:A:40:ASP:CB	1:A:44:GLN:OE1	2.59	0.46
1:A:347:TRP:CZ3	1:A:613:LEU:HD11	2.50	0.46
1:A:119:LEU:O	1:A:120:ARG:HB2	2.14	0.46
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.77	0.46
1:A:466:THR:HG21	1:A:594:ALA:CB	2.46	0.46
1:A:453:VAL:CG1	1:A:454:LYS:N	2.79	0.46
1:A:656:LYS:HA	1:A:661:LYS:HB3	1.98	0.46
1:A:41:SER:CB	1:A:42:PRO:CD	2.94	0.45
1:A:619:LYS:HB3	1:A:619:LYS:HE2	1.58	0.45
1:A:20:PHE:HD1	1:A:23:GLN:OE1	1.99	0.45
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.69	0.45
1:A:688:PHE:CD1	1:A:689:LEU:HD23	2.50	0.45
1:A:97:VAL:CG2	1:A:209:ILE:HD11	2.46	0.45
1:A:682:LEU:O	1:A:682:LEU:HG	2.16	0.45
1:A:546:LYS:HE3	1:A:548:VAL:CG2	2.47	0.45
1:A:385:LEU:HD21	1:A:407:LEU:HD21	1.96	0.45
1:A:512:GLN:HG3	4:A:907:HOH:O	2.15	0.45
1:A:561:ALA:CA	1:A:564:LYS:HD3	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ALA:HA	1:A:73:LYS:CE	2.39	0.45
1:A:636:SER:HB3	1:A:641:LEU:HB2	1.99	0.45
1:A:39:ARG:NH1	1:A:39:ARG:HG2	2.24	0.45
1:A:286:PHE:CD1	1:A:287:GLN:N	2.84	0.45
1:A:688:PHE:HD1	1:A:689:LEU:HD23	1.82	0.45
1:A:456:LYS:O	1:A:489:PHE:HB3	2.17	0.45
1:A:271:LEU:O	1:A:275:GLN:CB	2.65	0.45
1:A:111:GLY:O	1:A:154:SER:OG	2.24	0.45
1:A:62:GLY:HA3	1:A:120:ARG:O	2.17	0.44
1:A:441:VAL:CG1	1:A:574:LEU:CD1	2.95	0.44
1:A:548:VAL:O	1:A:552:GLN:HG3	2.17	0.44
1:A:97:VAL:HG21	1:A:209:ILE:HD11	1.99	0.44
1:A:40:ASP:N	1:A:44:GLN:OE1	2.50	0.44
1:A:688:PHE:HD1	1:A:689:LEU:CD2	2.30	0.44
1:A:440:VAL:HG12	1:A:535:LEU:HD21	1.99	0.44
1:A:125:TRP:O	1:A:128:PRO:HG2	2.18	0.44
1:A:112:LEU:O	1:A:153:PHE:HB3	2.18	0.44
1:A:45:CYS:O	1:A:49:ILE:HG13	2.18	0.44
1:A:690:ARG:HD2	1:A:690:ARG:HA	1.72	0.44
1:A:241:LYS:O	1:A:242:PHE:C	2.53	0.44
1:A:573:LEU:CD2	1:A:583:VAL:HG22	2.48	0.44
1:A:507:CYS:HB3	1:A:523:GLU:OE1	2.17	0.44
1:A:587:ARG:O	1:A:590:HIS:CE1	2.70	0.44
1:A:593:MET:HB2	1:A:593:MET:HE3	1.87	0.44
1:A:637:GLU:O	1:A:639:LYS:HG2	2.18	0.44
1:A:150:ALA:HB2	1:A:169:LEU:HG	2.00	0.44
1:A:285:LYS:HB3	1:A:285:LYS:NZ	2.33	0.44
1:A:142:PRO:O	1:A:144:PRO:HD3	2.18	0.44
1:A:29:VAL:HG11	1:A:277:LYS:HD3	2.00	0.44
1:A:51:GLU:O	1:A:53:ARG:HG2	2.18	0.44
1:A:498:ASP:HB3	1:A:501:SER:CB	2.48	0.44
1:A:520:ASN:HB2	4:A:727:HOH:O	2.17	0.43
1:A:503:LEU:HA	1:A:503:LEU:HD23	1.76	0.43
1:A:551:LEU:CD1	1:A:583:VAL:HG11	2.48	0.43
1:A:591:LEU:N	1:A:591:LEU:HD23	2.32	0.43
1:A:32:PRO:HA	1:A:33:PRO:HD3	1.82	0.43
1:A:555:ASP:C	1:A:557:ASN:H	2.20	0.43
1:A:22:TRP:O	1:A:23:GLN:C	2.56	0.43
1:A:43:ILE:HD13	1:A:46:ILE:HD12	2.01	0.43
1:A:143:GLU:HA	1:A:144:PRO:HD2	1.75	0.43
1:A:263:LYS:O	1:A:267:ILE:HG13	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:LYS:CG	1:A:605:LYS:O	2.63	0.43
1:A:129:ILE:O	1:A:129:ILE:CG2	2.65	0.43
1:A:633:LEU:HD12	1:A:633:LEU:HA	1.78	0.43
1:A:564:LYS:NZ	1:A:565:ASP:OD2	2.44	0.43
1:A:680:SER:CB	1:A:681:PRO:CD	2.97	0.43
1:A:390:ASP:OD1	1:A:602:ARG:NH2	2.43	0.43
1:A:394:LEU:HB3	1:A:398:TYR:HB2	1.99	0.43
1:A:82:TYR:CE2	1:A:252:SER:HB2	2.53	0.43
1:A:404:LYS:HE3	1:A:404:LYS:HB3	1.69	0.43
1:A:603:MET:HE2	1:A:603:MET:HB2	1.54	0.43
1:A:162:ASP:OD1	1:A:162:ASP:C	2.56	0.43
1:A:395:ASP:OD2	1:A:465:ARG:HA	2.18	0.43
1:A:125:TRP:O	1:A:129:ILE:HG12	2.19	0.42
1:A:675:LYS:O	1:A:678:SER:O	2.37	0.42
1:A:231:CYS:HB3	1:A:232:PRO:HD2	2.00	0.42
1:A:28:LYS:HB3	1:A:29:VAL:H	1.37	0.42
1:A:91:HIS:CA	1:A:250:VAL:O	2.66	0.42
1:A:531:ALA:O	1:A:534:CYS:HB3	2.20	0.42
1:A:30:ARG:HD3	1:A:30:ARG:HA	1.77	0.42
1:A:51:GLU:CG	1:A:53:ARG:HH11	2.33	0.42
1:A:430:ARG:NH2	1:A:648:GLU:OE2	2.53	0.42
1:A:526:TYR:CG	1:A:527:GLY:N	2.87	0.42
1:A:8:TRP:CD1	1:A:299:LEU:HD22	2.54	0.42
1:A:112:LEU:N	1:A:112:LEU:CD1	2.82	0.42
1:A:412:ALA:HA	1:A:598:ALA:HA	2.01	0.42
1:A:419:GLN:C	1:A:421:SER:N	2.72	0.42
1:A:18:LYS:HA	1:A:21:GLN:HG2	2.02	0.42
1:A:110:GLN:HB2	1:A:152:PHE:CE1	2.54	0.42
1:A:314:ILE:HD13	1:A:689:LEU:HD21	2.01	0.42
1:A:430:ARG:HA	1:A:431:PRO:HD3	1.77	0.41
1:A:251:PRO:HB2	1:A:319:TYR:CE2	2.55	0.41
1:A:105:GLN:NE2	4:A:928:HOH:O	2.53	0.41
1:A:408:VAL:HG12	4:A:778:HOH:O	2.19	0.41
1:A:658:THR:HG23	1:A:661:LYS:N	2.25	0.41
1:A:16:ALA:O	1:A:19:CYS:HB3	2.19	0.41
1:A:561:ALA:O	1:A:564:LYS:HG2	2.19	0.41
1:A:43:ILE:HA	1:A:43:ILE:HD13	1.86	0.41
1:A:269:ASN:O	1:A:273:GLN:HG2	2.18	0.41
1:A:510:ASP:HB2	1:A:511:GLU:H	1.55	0.41
1:A:128:PRO:HG2	1:A:129:ILE:N	2.36	0.41
1:A:110:GLN:N	1:A:152:PHE:CZ	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LEU:HA	1:A:331:LEU:HD23	1.83	0.41
1:A:338:VAL:O	1:A:342:ARG:HG3	2.20	0.41
1:A:231:CYS:HB3	1:A:232:PRO:CD	2.51	0.41
1:A:533:ARG:HB2	1:A:562:TRP:CH2	2.56	0.41
1:A:581:LYS:CB	1:A:582:PRO:HD3	2.50	0.41
1:A:75:ARG:HA	1:A:76:PRO:HD3	1.82	0.41
1:A:472:PRO:O	1:A:475:LEU:N	2.50	0.41
1:A:111:GLY:O	1:A:154:SER:CB	2.69	0.41
1:A:84:THR:O	1:A:88:PRO:N	2.54	0.41
1:A:157:CYS:C	1:A:159:PRO:HD3	2.40	0.41
1:A:596:ASN:N	1:A:596:ASN:OD1	2.54	0.41
1:A:25:ASN:ND2	1:A:25:ASN:H	2.18	0.41
1:A:414:ASN:O	1:A:648:GLU:N	2.42	0.41
1:A:82:TYR:O	1:A:88:PRO:HA	2.21	0.41
1:A:19:CYS:O	1:A:36:CYS:SG	2.79	0.40
1:A:214:VAL:HG12	1:A:214:VAL:H	1.38	0.40
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.35	0.40
1:A:104:PHE:H	1:A:236:ARG:NH1	2.19	0.40
1:A:106:LEU:HD12	1:A:230:LEU:HD13	2.03	0.40
1:A:60:ASP:CG	1:A:61:GLY:N	2.75	0.40
1:A:625:SER:OG	1:A:626:ASP:OD1	2.35	0.40
1:A:551:LEU:CD1	1:A:583:VAL:CG1	2.99	0.40
1:A:436:LEU:CD2	1:A:593:MET:HE2	2.51	0.40
1:A:475:LEU:HA	1:A:475:LEU:HD23	1.89	0.40
1:A:155:ALA:CB	1:A:172:LEU:HD21	2.51	0.40
1:A:329:GLN:HB2	1:A:329:GLN:HE21	1.27	0.40
1:A:280:LYS:O	1:A:282:LYS:HG3	2.21	0.40
1:A:277:LYS:HB2	1:A:278:PHE:CE2	2.56	0.40
1:A:268:TRP:HE3	1:A:268:TRP:HA	1.86	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	686/691 (99%)	594 (87%)	73 (11%)	19 (3%)	6 5

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	SER
1	A	418	GLN
1	A	421	SER
1	A	279	GLY
1	A	286	PHE
1	A	472	PRO
1	A	625	SER
1	A	678	SER
1	A	473	MET
1	A	521	SER
1	A	642	LEU
1	A	28	LYS
1	A	29	VAL
1	A	213	THR
1	A	263	LYS
1	A	360	GLN
1	A	422	ASP
1	A	536	ALA
1	A	423	PRO

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	568/574 (99%)	540 (95%)	28 (5%)	31 48

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	27	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	37	ILE
1	A	39	ARG
1	A	53	ARG
1	A	58	THR
1	A	75	ARG
1	A	100	LYS
1	A	120	ARG
1	A	149	VAL
1	A	159	PRO
1	A	209	ILE
1	A	214	VAL
1	A	285	LYS
1	A	301	LYS
1	A	364	LEU
1	A	388	GLU
1	A	416	LYS
1	A	419	GLN
1	A	422	ASP
1	A	473	MET
1	A	599	VAL
1	A	622	ARG
1	A	623	ASN
1	A	628	PRO
1	A	635	GLN
1	A	636	SER
1	A	641	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	25	ASN
1	A	47	GLN
1	A	105	GLN
1	A	261	ASN
1	A	329	GLN
1	A	330	ASN
1	A	360	GLN
1	A	491	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	OXL	A	695	2	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	A	696	2	0,5,5	0.00	-	0,6,6	0.00	-

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	OXL	A	695	2	-	0/0/4/4	0/0/0/0
3	OXL	A	696	2	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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^{th} 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	688/691 (99%)	-0.70	3 (0%)	93	93	23, 45, 80, 99	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	LYS	2.3
1	A	422	ASP	2.2
1	A	418	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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^{th} 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(Å^2)	Q<0.9
3	OXL	A	695	6/6	0.98	0.14	0.59	37,40,43,46	0
2	FE	A	693	1/1	1.00	0.10	-0.25	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FE	A	694	1/1	1.00	0.10	-0.98	35,35,35,35	0
3	OXL	A	696	6/6	0.99	0.09	-1.28	19,22,31,33	0

6.5 Other polymers (i)

There are no such residues in this entry.