Full wwPDB X-ray Structure Validation Report

Aug 3, 2023 – 04:46 AM EDT

PDB ID	:	1I6Q
Title	:	Formation of a protein intermediate and its trapping by the simultaneous crystallization process: Crystal structure of an iron-saturated intermediate in the FE3+ binding pathway of camel lactoferrin at 2.7 resolution
Authors	:	Khan, J.A.; Kumar, P.; Srinivasan, A.; Singh, T.P.
Deposited on	:	2001-03-03
Resolution	:	2.70 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:

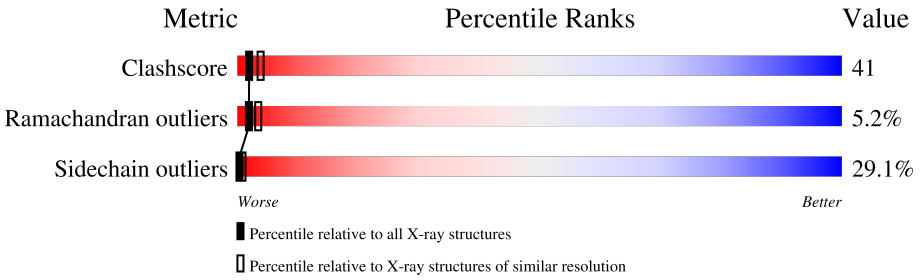
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	689	27% 43% 21% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5527 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
			Total	C	N	O	S			
1	A	689	5284	3318	934	994	38	15	0	0

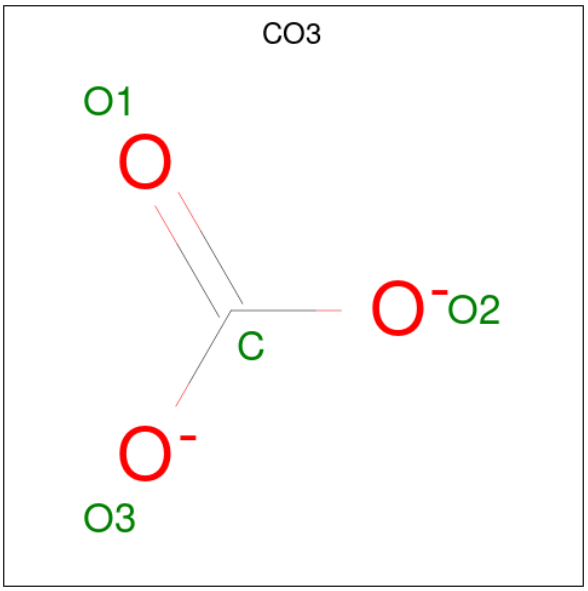
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	LYS	SER	SEE REMARK 999	UNP Q9TUM0
A	87	GLN	ASN	SEE REMARK 999	UNP Q9TUM0
A	242	PHE	SER	SEE REMARK 999	UNP Q9TUM0
A	312	LYS	SER	SEE REMARK 999	UNP Q9TUM0
A	477	ASP	ASN	SEE REMARK 999	UNP Q9TUM0
A	513	LEU	ASN	SEE REMARK 999	UNP Q9TUM0
A	523	LEU	TYR	SEE REMARK 999	UNP Q9TUM0
A	556	GLY	ASN	SEE REMARK 999	UNP Q9TUM0
A	608	ARG	GLU	SEE REMARK 999	UNP Q9TUM0
A	623	GLU	GLN	SEE REMARK 999	UNP Q9TUM0
A	658	ASP	GLU	SEE REMARK 999	UNP Q9TUM0

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

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

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	233	Total O 233 233	0	0

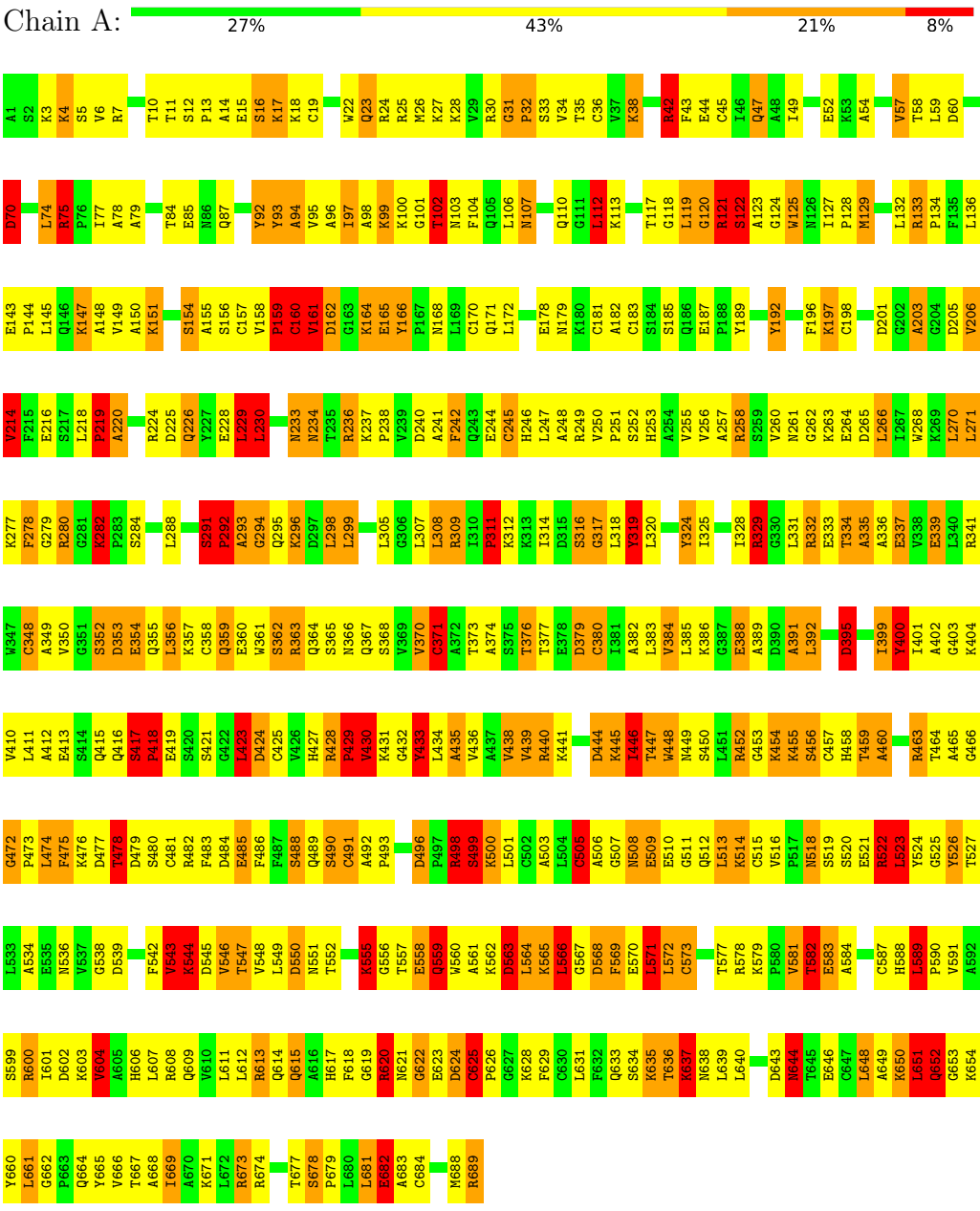
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

- Molecule 1: LACTOFERRIN

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.91Å 80.62Å 56.29Å 90.00° 92.37° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70	Depositor
% Data completeness (in resolution range)	94.1 (25.00-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.188 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5527	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, CO3

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	1.28	18/5392 (0.3%)	2.33	250/7293 (3.4%)

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	1	16

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	570	GLU	CB-CG	-43.78	0.69	1.52
1	A	430	VAL	C-N	-34.30	0.55	1.34
1	A	526	TYR	N-CA	23.48	1.93	1.46
1	A	526	TYR	CA-C	-19.58	1.02	1.52
1	A	572	LEU	C-N	-17.49	0.93	1.34
1	A	569	PHE	C-N	-17.30	0.94	1.34
1	A	571	LEU	CB-CG	-14.18	1.11	1.52
1	A	92	TYR	CA-CB	12.06	1.80	1.53
1	A	427	HIS	CB-CG	10.59	1.69	1.50
1	A	572	LEU	CB-CG	8.48	1.77	1.52
1	A	294	GLY	CA-C	6.78	1.62	1.51
1	A	293	ALA	C-N	-6.70	1.21	1.33
1	A	595	HIS	CB-CG	6.37	1.61	1.50
1	A	428	ARG	C-N	6.01	1.45	1.34
1	A	395	ASP	CA-CB	-5.94	1.40	1.53
1	A	432	GLY	CA-C	-5.93	1.42	1.51
1	A	120	GLY	N-CA	5.87	1.54	1.46
1	A	292	PRO	N-CA	5.15	1.56	1.47

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	571	LEU	CB-CG-CD2	-37.35	47.50	111.00
1	A	572	LEU	CB-CG-CD1	-22.51	72.73	111.00
1	A	569	PHE	O-C-N	-21.23	88.74	122.70
1	A	329	ARG	CD-NE-CZ	20.57	152.40	123.60
1	A	280	ARG	NE-CZ-NH1	18.16	129.38	120.30
1	A	682	GLU	CB-CG-CD	16.11	157.70	114.20
1	A	7	ARG	NE-CZ-NH1	16.04	128.32	120.30
1	A	482	ARG	NE-CZ-NH1	15.08	127.84	120.30
1	A	429	PRO	O-C-N	-14.18	100.02	122.70
1	A	571	LEU	CB-CG-CD1	14.08	134.93	111.00
1	A	280	ARG	CD-NE-CZ	13.86	143.01	123.60
1	A	42	ARG	NE-CZ-NH1	13.00	126.80	120.30
1	A	395	ASP	CA-CB-CG	12.99	141.98	113.40
1	A	689	ARG	NE-CZ-NH1	12.59	126.60	120.30
1	A	253	HIS	CA-CB-CG	12.25	134.43	113.60
1	A	625	CYS	N-CA-CB	12.13	132.43	110.60
1	A	189	TYR	CB-CG-CD1	12.06	128.23	121.00
1	A	673	ARG	NE-CZ-NH1	11.85	126.22	120.30
1	A	572	LEU	C-N-CA	-11.69	92.47	121.70
1	A	293	ALA	C-N-CA	-11.19	98.81	122.30
1	A	95	VAL	CG1-CB-CG2	-11.12	93.11	110.90
1	A	141	PRO	N-CA-C	11.05	140.83	112.10
1	A	482	ARG	CD-NE-CZ	10.82	138.75	123.60
1	A	42	ARG	CD-NE-CZ	10.69	138.56	123.60
1	A	192	TYR	CB-CG-CD1	-10.59	114.65	121.00
1	A	440	ARG	NE-CZ-NH2	10.53	125.56	120.30
1	A	293	ALA	CA-C-N	10.43	137.07	116.20
1	A	567	GLY	C-N-CA	10.34	147.56	121.70
1	A	673	ARG	CA-CB-CG	10.33	136.13	113.40
1	A	211	ASP	CB-CG-OD2	10.20	127.48	118.30
1	A	464	THR	N-CA-CB	-10.15	91.01	110.30
1	A	572	LEU	CA-C-N	-10.13	94.92	117.20
1	A	75	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	A	620	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	A	523	LEU	CA-CB-CG	9.99	138.28	115.30
1	A	673	ARG	CD-NE-CZ	9.78	137.29	123.60
1	A	431	LYS	C-N-CA	-9.63	102.07	122.30
1	A	572	LEU	CB-CG-CD2	9.57	127.26	111.00
1	A	224	ARG	NE-CZ-NH1	-9.55	115.52	120.30
1	A	682	GLU	CA-CB-CG	9.46	134.21	113.40
1	A	532	CYS	CA-CB-SG	9.43	130.96	114.00
1	A	617	HIS	CA-CB-CG	9.26	129.35	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	529	ALA	CB-CA-C	9.17	123.86	110.10
1	A	75	ARG	CA-CB-CG	9.16	133.54	113.40
1	A	229	LEU	CA-CB-CG	9.12	136.29	115.30
1	A	523	LEU	CB-CG-CD1	9.08	126.43	111.00
1	A	250	VAL	CA-CB-CG1	9.03	124.44	110.90
1	A	7	ARG	NH1-CZ-NH2	-9.02	109.48	119.40
1	A	363	ARG	CD-NE-CZ	9.00	136.20	123.60
1	A	624	ASP	CB-CG-OD1	9.00	126.40	118.30
1	A	637	LYS	CA-CB-CG	9.00	133.20	113.40
1	A	568	ASP	CB-CG-OD1	-8.92	110.27	118.30
1	A	309	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	A	567	GLY	CA-C-O	8.89	136.61	120.60
1	A	682	GLU	OE1-CD-OE2	-8.89	112.63	123.30
1	A	689	ARG	CD-NE-CZ	8.87	136.02	123.60
1	A	563	ASP	CA-CB-CG	8.67	132.47	113.40
1	A	613	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	A	531	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	A	280	ARG	NH1-CZ-NH2	-8.56	109.98	119.40
1	A	526	TYR	C-N-CA	8.52	142.99	121.70
1	A	253	HIS	CB-CA-C	8.51	127.42	110.40
1	A	563	ASP	CB-CG-OD2	8.51	125.96	118.30
1	A	482	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	A	508	ASN	CA-CB-CG	8.42	131.92	113.40
1	A	189	TYR	CB-CG-CD2	-8.39	115.97	121.00
1	A	350	VAL	CA-CB-CG2	8.38	123.47	110.90
1	A	569	PHE	CA-C-N	8.38	135.63	117.20
1	A	543	VAL	CA-CB-CG2	8.29	123.34	110.90
1	A	651	LEU	N-CA-CB	8.29	126.98	110.40
1	A	65	TYR	CB-CG-CD2	8.21	125.92	121.00
1	A	65	TYR	CB-CG-CD1	-8.19	116.09	121.00
1	A	652	GLN	CA-CB-CG	8.19	131.41	113.40
1	A	526	TYR	CB-CA-C	8.14	126.67	110.40
1	A	625	CYS	CA-CB-SG	8.10	128.58	114.00
1	A	66	ASP	CB-CG-OD1	8.08	125.57	118.30
1	A	433	TYR	CB-CA-C	8.07	126.55	110.40
1	A	572	LEU	CA-CB-CG	8.03	133.77	115.30
1	A	526	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	A	564	LEU	CA-CB-CG	7.86	133.38	115.30
1	A	604	VAL	CA-CB-CG1	7.76	122.54	110.90
1	A	309	ARG	NE-CZ-NH1	-7.75	116.43	120.30
1	A	620	ARG	CD-NE-CZ	7.70	134.38	123.60
1	A	224	ARG	NE-CZ-NH2	7.67	124.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	526	TYR	CB-CG-CD1	7.61	125.56	121.00
1	A	42	ARG	CA-CB-CG	7.58	130.08	113.40
1	A	309	ARG	NH1-CZ-NH2	7.55	127.70	119.40
1	A	432	GLY	C-N-CA	-7.48	103.00	121.70
1	A	192	TYR	CB-CG-CD2	7.43	125.46	121.00
1	A	664	GLN	CB-CG-CD	7.39	130.81	111.60
1	A	122	SER	C-N-CA	7.20	139.70	121.70
1	A	265	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	94	ALA	N-CA-CB	7.18	120.15	110.10
1	A	444	ASP	CA-CB-CG	7.16	129.16	113.40
1	A	219	PRO	CA-N-CD	-7.14	101.50	111.50
1	A	485	GLU	CA-CB-CG	7.12	129.06	113.40
1	A	250	VAL	CB-CA-C	7.08	124.86	111.40
1	A	509	GLU	OE1-CD-OE2	-7.05	114.84	123.30
1	A	354	GLU	OE1-CD-OE2	-7.03	114.86	123.30
1	A	544	LYS	N-CA-CB	7.03	123.25	110.60
1	A	582	THR	CA-CB-CG2	7.01	122.21	112.40
1	A	496	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	293	ALA	O-C-N	-6.96	111.37	123.20
1	A	564	LEU	N-CA-CB	6.95	124.30	110.40
1	A	348	CYS	N-CA-CB	6.89	123.00	110.60
1	A	460	ALA	N-CA-CB	6.88	119.73	110.10
1	A	570	GLU	CB-CG-CD	-6.86	95.68	114.20
1	A	107	ASN	CA-CB-CG	6.86	128.49	113.40
1	A	70	ASP	N-CA-CB	6.84	122.91	110.60
1	A	491	CYS	CA-CB-SG	6.80	126.24	114.00
1	A	492	ALA	N-CA-CB	6.78	119.59	110.10
1	A	240	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	558	GLU	OE1-CD-OE2	-6.74	115.21	123.30
1	A	230	LEU	CA-CB-CG	6.74	130.81	115.30
1	A	60	ASP	CA-CB-CG	6.64	128.01	113.40
1	A	417	SER	CB-CA-C	6.63	122.70	110.10
1	A	440	ARG	NH1-CZ-NH2	-6.63	112.11	119.40
1	A	624	ASP	CB-CG-OD2	-6.62	112.35	118.30
1	A	587	CYS	CA-CB-SG	6.60	125.87	114.00
1	A	532	CYS	CB-CA-C	6.59	123.59	110.40
1	A	430	VAL	C-N-CA	-6.59	105.23	121.70
1	A	291	SER	C-N-CD	-6.58	106.11	120.60
1	A	595	HIS	CA-CB-CG	6.58	124.79	113.60
1	A	106	LEU	CA-CB-CG	6.58	130.44	115.30
1	A	329	ARG	CA-CB-CG	6.56	127.84	113.40
1	A	423	LEU	N-CA-C	6.54	128.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	438	VAL	CA-CB-CG1	6.51	120.67	110.90
1	A	498	ARG	CD-NE-CZ	6.49	132.68	123.60
1	A	427	HIS	CB-CA-C	6.45	123.29	110.40
1	A	433	TYR	CA-CB-CG	6.43	125.62	113.40
1	A	354	GLU	CB-CG-CD	6.40	131.48	114.20
1	A	528	GLY	CA-C-O	6.40	132.12	120.60
1	A	418	PRO	N-CA-C	6.34	128.59	112.10
1	A	102	THR	CA-C-O	6.34	133.41	120.10
1	A	371	CYS	N-CA-CB	-6.33	99.21	110.60
1	A	201	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	683	ALA	N-CA-CB	6.28	118.89	110.10
1	A	567	GLY	O-C-N	-6.27	112.66	122.70
1	A	651	LEU	CB-CG-CD2	-6.26	100.35	111.00
1	A	170	CYS	N-CA-CB	6.26	121.87	110.60
1	A	363	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	276	GLU	CA-CB-CG	6.25	127.16	113.40
1	A	505	CYS	CB-CA-C	6.24	122.87	110.40
1	A	112	LEU	CA-CB-CG	6.23	129.62	115.30
1	A	624	ASP	CA-CB-CG	6.23	127.10	113.40
1	A	319	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	A	464	THR	CB-CA-C	6.20	128.33	111.60
1	A	584	ALA	N-CA-CB	6.18	118.76	110.10
1	A	252	SER	N-CA-CB	6.16	119.73	110.50
1	A	523	LEU	CB-CA-C	6.16	121.90	110.20
1	A	380	CYS	CA-CB-SG	-6.12	102.99	114.00
1	A	404	LYS	N-CA-CB	6.11	121.59	110.60
1	A	623	GLU	C-N-CA	6.11	136.96	121.70
1	A	526	TYR	N-CA-CB	-6.10	99.62	110.60
1	A	96	ALA	CA-C-O	-6.09	107.32	120.10
1	A	563	ASP	OD1-CG-OD2	-6.09	111.73	123.30
1	A	523	LEU	O-C-N	-6.08	112.97	122.70
1	A	65	TYR	O-C-N	6.08	132.43	122.70
1	A	79	ALA	N-CA-CB	-6.07	101.61	110.10
1	A	433	TYR	N-CA-CB	-6.06	99.70	110.60
1	A	589	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	684	CYS	CA-CB-SG	-6.05	103.11	114.00
1	A	572	LEU	O-C-N	-6.02	113.07	122.70
1	A	120	GLY	C-N-CA	6.01	136.74	121.70
1	A	309	ARG	CG-CD-NE	-5.98	99.25	111.80
1	A	559	GLN	N-CA-C	5.97	127.13	111.00
1	A	571	LEU	CA-CB-CG	-5.97	101.57	115.30
1	A	36	CYS	CA-CB-SG	-5.97	103.26	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	148	ALA	CA-C-O	-5.97	107.57	120.10
1	A	42	ARG	NH1-CZ-NH2	-5.96	112.84	119.40
1	A	657	TYR	CB-CG-CD2	5.95	124.57	121.00
1	A	433	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	A	92	TYR	CB-CG-CD1	5.91	124.55	121.00
1	A	555	LYS	CA-C-N	5.86	127.92	116.20
1	A	319	TYR	CB-CG-CD2	5.86	124.51	121.00
1	A	181	CYS	CA-CB-SG	5.84	124.51	114.00
1	A	280	ARG	CG-CD-NE	5.83	124.03	111.80
1	A	568	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	653	GLY	CA-C-O	5.80	131.05	120.60
1	A	93	TYR	CA-CB-CG	-5.77	102.44	113.40
1	A	19	CYS	CA-CB-SG	-5.71	103.72	114.00
1	A	491	CYS	N-CA-CB	5.71	120.88	110.60
1	A	337	GLU	CA-CB-CG	5.66	125.85	113.40
1	A	341	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	455	LYS	N-CA-CB	5.64	120.76	110.60
1	A	31	GLY	N-CA-C	-5.62	99.06	113.10
1	A	255	VAL	O-C-N	-5.61	113.73	122.70
1	A	555	LYS	N-CA-C	5.61	126.14	111.00
1	A	440	ARG	CD-NE-CZ	5.60	131.44	123.60
1	A	317	GLY	N-CA-C	5.60	127.09	113.10
1	A	341	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	245	CYS	CA-CB-SG	-5.55	104.01	114.00
1	A	224	ARG	N-CA-CB	5.54	120.56	110.60
1	A	427	HIS	CA-CB-CG	5.53	123.01	113.60
1	A	448	TRP	CA-C-N	5.51	129.33	117.20
1	A	159	PRO	CB-CA-C	5.50	125.76	112.00
1	A	455	LYS	CB-CA-C	-5.49	99.41	110.40
1	A	277	LYS	CB-CA-C	5.46	121.33	110.40
1	A	391	ALA	CA-C-O	5.46	131.56	120.10
1	A	651	LEU	CA-C-O	-5.46	108.64	120.10
1	A	42	ARG	O-C-N	-5.45	113.98	122.70
1	A	392	LEU	CB-CG-CD2	5.42	120.22	111.00
1	A	233	ASN	N-CA-CB	5.38	120.29	110.60
1	A	440	ARG	CG-CD-NE	5.38	123.10	111.80
1	A	339	GLU	CB-CA-C	5.38	121.15	110.40
1	A	649	ALA	CA-C-O	5.37	131.38	120.10
1	A	352	SER	N-CA-C	5.36	125.48	111.00
1	A	349	ALA	N-CA-CB	-5.35	102.61	110.10
1	A	681	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	456	SER	N-CA-CB	5.34	118.51	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	657	TYR	N-CA-CB	5.33	120.20	110.60
1	A	324	TYR	CB-CG-CD1	-5.33	117.81	121.00
1	A	644	ASN	N-CA-CB	5.32	120.17	110.60
1	A	93	TYR	CB-CG-CD2	5.30	124.18	121.00
1	A	278	PHE	CB-CA-C	-5.30	99.80	110.40
1	A	119	LEU	CB-CA-C	-5.29	100.14	110.20
1	A	57	VAL	CA-C-O	-5.29	108.99	120.10
1	A	106	LEU	CB-CG-CD2	5.29	119.98	111.00
1	A	203	ALA	CB-CA-C	5.27	118.00	110.10
1	A	481	CYS	CA-CB-SG	5.27	123.48	114.00
1	A	384	VAL	CA-CB-CG2	5.26	118.79	110.90
1	A	550	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	A	563	ASP	CB-CA-C	5.26	120.92	110.40
1	A	125	TRP	CA-CB-CG	5.25	123.67	113.70
1	A	478	THR	N-CA-CB	5.24	120.25	110.30
1	A	515	CYS	CA-C-O	5.24	131.09	120.10
1	A	566	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	242	PHE	CB-CA-C	-5.20	100.00	110.40
1	A	367	GLN	N-CA-C	5.17	124.96	111.00
1	A	400	TYR	CB-CG-CD1	5.17	124.10	121.00
1	A	652	GLN	N-CA-C	5.17	124.95	111.00
1	A	515	CYS	CB-CA-C	5.16	120.72	110.40
1	A	216	GLU	OE1-CD-OE2	-5.15	117.11	123.30
1	A	673	ARG	NH1-CZ-NH2	-5.15	113.73	119.40
1	A	337	GLU	CG-CD-OE1	5.14	128.59	118.30
1	A	4	LYS	CA-CB-CG	5.14	124.71	113.40
1	A	542	PHE	CB-CA-C	5.14	120.68	110.40
1	A	569	PHE	C-N-CA	5.14	134.54	121.70
1	A	250	VAL	CA-CB-CG2	5.11	118.56	110.90
1	A	522	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	319	TYR	N-CA-CB	5.10	119.79	110.60
1	A	465	ALA	O-C-N	5.10	131.87	123.20
1	A	565	LYS	CA-CB-CG	5.08	124.58	113.40
1	A	122	SER	CA-C-N	-5.06	106.06	117.20
1	A	324	TYR	CB-CG-CD2	5.06	124.03	121.00
1	A	509	GLU	CB-CG-CD	5.05	127.83	114.20
1	A	214	VAL	CB-CA-C	-5.03	101.84	111.40
1	A	689	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	657	TYR	CA-CB-CG	5.01	122.92	113.40
1	A	408	VAL	CA-CB-CG2	5.01	118.41	110.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	70	ASP	CA

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	LYS	Mainchain
1	A	319	TYR	Sidechain
1	A	379	ASP	Mainchain
1	A	400	TYR	Mainchain
1	A	429	PRO	Mainchain
1	A	430	VAL	Mainchain
1	A	435	ALA	Mainchain
1	A	499	SER	Mainchain
1	A	529	ALA	Mainchain
1	A	569	PHE	Mainchain
1	A	572	LEU	Peptide,Mainchain
1	A	622	GLY	Mainchain
1	A	636	THR	Mainchain
1	A	70	ASP	Sidechain
1	A	94	ALA	Mainchain

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	5284	0	5237	433	0
2	A	2	0	0	0	0
3	A	8	0	0	0	0
4	A	233	0	0	8	0
All	All	5527	0	5237	433	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 41.

All (433) 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:92:TYR:CB	1:A:92:TYR:CA	1.80	1.58
1:A:526:TYR:N	1:A:526:TYR:CA	1.93	1.31
1:A:343:ALA:O	1:A:606:HIS:NE2	1.66	1.29
1:A:423:LEU:HD12	1:A:423:LEU:O	1.25	1.27
1:A:233:ASN:O	1:A:234:ASN:HB2	1.50	1.11
1:A:423:LEU:O	1:A:423:LEU:CD1	1.98	1.11
1:A:23:GLN:HB2	1:A:34:VAL:O	1.51	1.07
1:A:18:LYS:NZ	1:A:288:LEU:O	1.90	1.03
1:A:463:ARG:HG2	1:A:463:ARG:HH11	1.22	1.03
1:A:168:ASN:HA	1:A:171:GLN:HB2	1.36	1.03
1:A:423:LEU:HD12	1:A:423:LEU:C	1.84	0.98
1:A:334:THR:O	1:A:336:ALA:N	1.98	0.96
1:A:440:ARG:HD2	1:A:536:ASN:HD21	1.29	0.96
1:A:364:GLN:HG3	1:A:629:PHE:HB2	1.47	0.95
1:A:679:PRO:HA	1:A:682:GLU:HG3	1.50	0.94
1:A:543:VAL:HG11	1:A:547:THR:HG21	1.50	0.94
1:A:352:SER:O	1:A:355:GLN:HB3	1.68	0.93
1:A:44:GLU:HA	1:A:47:GLN:HE21	1.31	0.93
1:A:518:ASN:HD22	1:A:519:SER:H	1.13	0.93
1:A:430:VAL:CG1	1:A:594:ASN:HD22	1.83	0.92
1:A:178:GLU:O	1:A:178:GLU:HG2	1.70	0.91
1:A:410:VAL:HG11	1:A:607:LEU:HD23	1.53	0.90
1:A:469:ILE:HD13	1:A:590:PRO:HG2	1.53	0.89
1:A:16:SER:HB3	1:A:38:LYS:HG2	1.56	0.87
1:A:548:VAL:HG11	1:A:581:VAL:HG21	1.56	0.87
1:A:638:ASN:HD22	1:A:643:ASP:H	1.21	0.87
1:A:219:PRO:O	1:A:220:ALA:O	1.93	0.85
1:A:334:THR:OG1	1:A:337:GLU:OE2	1.93	0.85
1:A:160:CYS:HG	1:A:183:CYS:HG	1.22	0.84
1:A:97:ILE:O	1:A:206:VAL:HG12	1.78	0.83
1:A:145:LEU:HD23	1:A:145:LEU:O	1.78	0.83
1:A:484:ASP:HB2	1:A:500:LYS:HD3	1.59	0.83
1:A:160:CYS:SG	4:A:724:HOH:O	2.36	0.82
1:A:14:ALA:HA	1:A:17:LYS:HD3	1.59	0.82
1:A:430:VAL:HG12	1:A:594:ASN:HD22	1.43	0.81
1:A:395:ASP:O	1:A:399:ILE:HG13	1.80	0.81
1:A:638:ASN:ND2	1:A:643:ASP:H	1.77	0.80
1:A:382:ALA:HA	1:A:385:LEU:HD12	1.63	0.80
1:A:589:LEU:HB3	1:A:590:PRO:HD2	1.64	0.79
1:A:44:GLU:HA	1:A:47:GLN:NE2	1.99	0.78
1:A:559:GLN:H	1:A:562:LYS:HG3	1.48	0.78
1:A:120:GLY:O	4:A:820:HOH:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LEU:HG	1:A:591:VAL:CG2	2.14	0.77
1:A:472:GLY:HA3	1:A:668:ALA:HA	1.65	0.77
1:A:364:GLN:HG3	1:A:629:PHE:CB	2.16	0.76
1:A:380:CYS:HB3	1:A:392:LEU:HD22	1.66	0.76
1:A:571:LEU:HD12	1:A:581:VAL:HA	1.67	0.76
1:A:507:GLY:HA3	1:A:514:LYS:HG2	1.67	0.76
1:A:615:GLN:HE22	1:A:648:LEU:H	1.35	0.74
1:A:593:PRO:HG2	1:A:661:LEU:HD12	1.68	0.74
1:A:660:TYR:HD2	1:A:661:LEU:HD13	1.53	0.74
1:A:469:ILE:O	1:A:473:PRO:HD2	1.87	0.74
1:A:143:GLU:HG3	1:A:147:LYS:HE2	1.69	0.73
1:A:342:ARG:HH11	1:A:342:ARG:HA	1.52	0.73
1:A:430:VAL:HG12	1:A:594:ASN:ND2	2.03	0.73
1:A:32:PRO:HB2	1:A:270:LEU:HB2	1.69	0.73
1:A:229:LEU:HB2	1:A:237:LYS:O	1.89	0.73
1:A:429:PRO:HA	1:A:652:GLN:HE22	1.53	0.73
1:A:429:PRO:HA	1:A:652:GLN:NE2	2.04	0.72
1:A:133:ARG:HB3	1:A:134:PRO:HD3	1.72	0.72
1:A:119:LEU:HD23	1:A:120:GLY:N	2.05	0.71
1:A:383:LEU:HD22	1:A:388:GLU:HB3	1.70	0.71
1:A:460:ALA:HA	1:A:493:PRO:HD2	1.73	0.71
1:A:129:MET:HE2	1:A:149:VAL:HG22	1.72	0.71
1:A:376:THR:OG1	1:A:377:THR:N	2.18	0.70
1:A:343:ALA:O	1:A:606:HIS:CE1	2.43	0.70
1:A:518:ASN:HD22	1:A:519:SER:N	1.88	0.70
1:A:133:ARG:HB3	1:A:134:PRO:CD	2.22	0.70
1:A:530:PHE:HB2	1:A:547:THR:HG22	1.74	0.70
1:A:447:THR:HG23	1:A:450:SER:HB3	1.73	0.70
1:A:352:SER:O	1:A:356:LEU:HG	1.92	0.70
1:A:582:THR:HG22	1:A:583:GLU:HG3	1.73	0.69
1:A:67:ALA:HB1	1:A:74:LEU:HD12	1.75	0.69
1:A:560:TRP:CZ3	1:A:561:ALA:HB2	2.27	0.69
1:A:16:SER:CB	1:A:38:LYS:HG2	2.21	0.69
1:A:530:PHE:HB2	1:A:547:THR:CG2	2.23	0.69
1:A:107:ASN:OD1	1:A:234:ASN:ND2	2.26	0.68
1:A:233:ASN:O	1:A:234:ASN:CB	2.31	0.68
1:A:242:PHE:O	1:A:246:HIS:HB3	1.92	0.68
1:A:160:CYS:HA	1:A:183:CYS:HB2	1.75	0.68
1:A:529:ALA:CB	1:A:543:VAL:HG13	2.23	0.68
1:A:476:LYS:HD2	1:A:667:THR:HG21	1.75	0.68
1:A:119:LEU:HD23	1:A:120:GLY:H	1.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ASN:ND2	1:A:519:SER:H	1.90	0.67
1:A:434:LEU:HG	1:A:591:VAL:HG22	1.76	0.67
1:A:445:LYS:O	1:A:446:ILE:HB	1.91	0.67
1:A:145:LEU:HD23	1:A:145:LEU:C	2.14	0.67
1:A:295:GLN:OE1	1:A:295:GLN:HA	1.94	0.67
1:A:23:GLN:OE1	1:A:35:THR:HG22	1.95	0.67
1:A:499:SER:HB2	1:A:500:LYS:HE2	1.77	0.67
1:A:136:LEU:O	1:A:137:ASP:HB2	1.94	0.66
1:A:346:VAL:HA	1:A:370:VAL:HG23	1.76	0.66
1:A:433:TYR:CD2	1:A:544:LYS:HB3	2.30	0.66
1:A:358:CYS:HB3	1:A:371:CYS:SG	2.36	0.66
1:A:469:ILE:HG21	1:A:590:PRO:HD2	1.76	0.66
1:A:159:PRO:O	1:A:161:VAL:N	2.29	0.66
1:A:334:THR:C	1:A:336:ALA:H	1.99	0.66
1:A:559:GLN:N	1:A:562:LYS:HG3	2.11	0.66
1:A:311:PRO:HB2	1:A:314:ILE:HD12	1.78	0.65
1:A:122:SER:O	1:A:127:ILE:N	2.23	0.65
1:A:660:TYR:CD2	1:A:661:LEU:HD13	2.32	0.65
1:A:156:SER:HA	1:A:172:LEU:HD12	1.78	0.64
1:A:523:LEU:HG	1:A:532:CYS:HB3	1.80	0.64
1:A:436:VAL:HG11	1:A:545:ASP:HB3	1.78	0.64
1:A:522:ARG:HD3	1:A:531:ARG:NH1	2.13	0.64
1:A:637:LYS:NZ	1:A:639:LEU:HD21	2.12	0.64
1:A:168:ASN:CA	1:A:171:GLN:HB2	2.20	0.64
1:A:526:TYR:HD2	1:A:543:VAL:HG12	1.61	0.64
1:A:293:ALA:O	1:A:294:GLY:C	2.27	0.63
1:A:359:GLN:O	1:A:363:ARG:HG3	1.97	0.63
1:A:448:TRP:O	1:A:449:ASN:HB2	1.97	0.63
1:A:84:THR:HG23	1:A:87:GLN:H	1.64	0.63
1:A:219:PRO:C	1:A:220:ALA:O	2.34	0.63
1:A:484:ASP:HB2	1:A:500:LYS:CD	2.29	0.63
1:A:27:LYS:HD3	4:A:834:HOH:O	1.99	0.62
1:A:334:THR:C	1:A:336:ALA:N	2.50	0.62
1:A:275:GLN:NE2	1:A:307:LEU:HB2	2.15	0.62
1:A:119:LEU:HD12	1:A:161:VAL:HA	1.82	0.62
1:A:467:TRP:HD1	1:A:468:ASN:HD22	1.48	0.62
1:A:77:ILE:HD12	1:A:257:ALA:HB3	1.82	0.61
1:A:507:GLY:CA	1:A:514:LYS:HG2	2.29	0.61
1:A:529:ALA:HB3	1:A:543:VAL:HG13	1.83	0.61
1:A:317:GLY:HA2	1:A:325:ILE:HD11	1.81	0.61
1:A:473:PRO:HD3	1:A:668:ALA:CA	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:MET:O	1:A:475:PHE:HB2	2.01	0.61
1:A:334:THR:O	1:A:335:ALA:C	2.36	0.61
1:A:418:PRO:HD3	1:A:644:ASN:HB2	1.82	0.61
1:A:500:LYS:HE2	1:A:500:LYS:H	1.67	0.60
1:A:101:GLY:O	1:A:102:THR:C	2.39	0.60
1:A:157:CYS:SG	1:A:159:PRO:HD3	2.41	0.60
1:A:413:GLU:HB2	1:A:595:HIS:O	2.01	0.60
1:A:30:ARG:NH2	1:A:31:GLY:O	2.34	0.60
1:A:282:LYS:HE3	1:A:282:LYS:HA	1.83	0.60
1:A:339:GLU:HA	1:A:342:ARG:HB2	1.82	0.60
1:A:129:MET:CE	1:A:149:VAL:HG22	2.32	0.60
1:A:600:ARG:HB3	1:A:602:ASP:OD2	2.01	0.60
1:A:125:TRP:O	1:A:129:MET:HB2	2.02	0.59
1:A:573:CYS:HB3	1:A:577:THR:O	2.02	0.59
1:A:593:PRO:HG3	1:A:661:LEU:HA	1.84	0.59
1:A:358:CYS:CB	1:A:371:CYS:SG	2.90	0.59
1:A:144:PRO:HG2	1:A:147:LYS:HD2	1.84	0.59
1:A:332:ARG:CG	1:A:332:ARG:O	2.47	0.59
1:A:513:LEU:HD13	1:A:516:VAL:HG11	1.85	0.59
1:A:548:VAL:HG21	1:A:581:VAL:HG11	1.85	0.59
1:A:92:TYR:CB	1:A:92:TYR:N	2.64	0.58
1:A:145:LEU:C	1:A:145:LEU:CD2	2.71	0.58
1:A:657:TYR:O	1:A:661:LEU:HD22	2.03	0.58
1:A:113:LYS:HB3	1:A:172:LEU:HD11	1.86	0.58
1:A:119:LEU:CD2	1:A:120:GLY:N	2.66	0.58
1:A:344:GLN:NE2	4:A:726:HOH:O	2.35	0.58
1:A:529:ALA:HB3	1:A:543:VAL:CG1	2.34	0.58
1:A:588:HIS:ND1	1:A:589:LEU:O	2.37	0.58
1:A:99:LYS:HE3	1:A:226:GLN:O	2.04	0.57
1:A:384:VAL:HA	1:A:389:ALA:O	2.04	0.57
1:A:434:LEU:O	1:A:436:VAL:HG13	2.05	0.57
1:A:544:LYS:HD2	1:A:546:VAL:HG23	1.85	0.57
1:A:42:ARG:NH2	4:A:709:HOH:O	2.32	0.57
1:A:473:PRO:HD3	1:A:668:ALA:HA	1.86	0.57
1:A:385:LEU:HD21	1:A:405:CYS:HB3	1.86	0.57
1:A:513:LEU:HD22	1:A:516:VAL:HG21	1.86	0.57
1:A:230:LEU:HD12	1:A:236:ARG:HD2	1.87	0.56
1:A:15:GLU:HG3	1:A:299:LEU:HD23	1.86	0.56
1:A:162:ASP:C	1:A:164:LYS:H	2.08	0.56
1:A:400:TYR:O	1:A:401:ILE:C	2.44	0.56
1:A:408:VAL:O	1:A:598:VAL:HA	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:SER:CB	1:A:500:LYS:HE2	2.36	0.56
1:A:637:LYS:HG3	1:A:639:LEU:HG	1.86	0.56
1:A:433:TYR:CE2	1:A:544:LYS:HB3	2.40	0.56
1:A:526:TYR:N	1:A:526:TYR:CB	2.68	0.56
1:A:92:TYR:CB	1:A:92:TYR:C	2.71	0.56
1:A:529:ALA:HB1	1:A:543:VAL:HG13	1.88	0.56
1:A:45:CYS:O	1:A:49:ILE:HG13	2.06	0.56
1:A:619:GLY:O	1:A:622:GLY:N	2.35	0.56
1:A:144:PRO:HG2	1:A:147:LYS:CD	2.36	0.56
1:A:615:GLN:O	1:A:619:GLY:N	2.38	0.55
1:A:229:LEU:HD22	1:A:238:PRO:O	2.06	0.55
1:A:448:TRP:O	1:A:449:ASN:CB	2.52	0.55
1:A:665:TYR:CE2	1:A:669:ILE:HD11	2.41	0.55
1:A:113:LYS:HA	1:A:155:ALA:O	2.07	0.55
1:A:133:ARG:CB	1:A:134:PRO:CD	2.84	0.55
1:A:656:THR:HB	1:A:659:GLU:HB3	1.88	0.55
1:A:562:LYS:O	1:A:563:ASP:C	2.45	0.55
1:A:65:TYR:HB2	1:A:320:LEU:HD11	1.87	0.55
1:A:158:VAL:O	1:A:159:PRO:O	2.25	0.55
1:A:678:SER:O	1:A:681:LEU:HB3	2.07	0.54
1:A:452:ARG:HA	1:A:486:PHE:O	2.08	0.54
1:A:463:ARG:HG2	1:A:463:ARG:NH1	2.00	0.54
1:A:469:ILE:HG21	1:A:590:PRO:CD	2.36	0.54
1:A:133:ARG:HD2	1:A:133:ARG:O	2.08	0.54
1:A:556:GLY:HA3	1:A:561:ALA:HB3	1.90	0.54
1:A:17:LYS:HE3	1:A:292:PRO:HG2	1.90	0.53
1:A:147:LYS:O	1:A:151:LYS:HD3	2.08	0.53
1:A:410:VAL:HG11	1:A:607:LEU:CD2	2.33	0.53
1:A:665:TYR:O	1:A:669:ILE:HG12	2.09	0.53
1:A:395:ASP:O	1:A:399:ILE:CG1	2.55	0.53
1:A:456:SER:OG	1:A:490:SER:HB3	2.09	0.53
1:A:476:LYS:NZ	4:A:898:HOH:O	2.41	0.53
1:A:160:CYS:CB	1:A:183:CYS:HG	2.21	0.53
1:A:324:TYR:CE2	1:A:328:ILE:HD11	2.43	0.53
1:A:429:PRO:CA	1:A:652:GLN:HE22	2.19	0.53
1:A:456:SER:OG	1:A:458:HIS:NE2	2.42	0.53
1:A:460:ALA:HA	1:A:493:PRO:HG2	1.89	0.53
1:A:448:TRP:CH2	1:A:474:LEU:HD13	2.44	0.53
1:A:159:PRO:O	1:A:160:CYS:C	2.45	0.52
1:A:97:ILE:HG22	1:A:98:ALA:H	1.75	0.52
1:A:353:ASP:HB2	1:A:639:LEU:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LEU:HD23	1:A:588:HIS:CG	2.44	0.52
1:A:549:LEU:HB3	1:A:566:LEU:HD13	1.90	0.52
1:A:344:GLN:HG3	1:A:370:VAL:HG22	1.92	0.52
1:A:358:CYS:O	1:A:362:SER:HB2	2.09	0.52
1:A:298:LEU:O	1:A:299:LEU:HB2	2.10	0.52
1:A:399:ILE:HG22	1:A:661:LEU:HD21	1.92	0.52
1:A:544:LYS:HD2	1:A:546:VAL:CG2	2.40	0.52
1:A:455:LYS:HB2	1:A:539:ASP:H	1.74	0.51
1:A:197:LYS:O	1:A:198:CYS:C	2.48	0.51
1:A:219:PRO:O	1:A:220:ALA:C	2.48	0.51
1:A:430:VAL:CG1	1:A:594:ASN:ND2	2.62	0.51
1:A:552:THR:HA	1:A:564:LEU:HD12	1.91	0.51
1:A:329:ARG:O	1:A:333:GLU:HG3	2.10	0.51
1:A:14:ALA:CA	1:A:17:LYS:HD3	2.38	0.51
1:A:241:ALA:O	1:A:245:CYS:HB3	2.11	0.51
1:A:556:GLY:HA3	1:A:561:ALA:CB	2.41	0.51
1:A:625:CYS:HB3	1:A:626:PRO:CD	2.40	0.51
1:A:457:CYS:SG	1:A:538:GLY:HA3	2.51	0.51
1:A:560:TRP:CE3	1:A:561:ALA:HB2	2.46	0.51
1:A:460:ALA:HA	1:A:493:PRO:CD	2.40	0.50
1:A:182:ALA:H	1:A:187:GLU:HB2	1.75	0.50
1:A:332:ARG:O	1:A:332:ARG:HG2	2.10	0.50
1:A:133:ARG:CB	1:A:134:PRO:HD3	2.41	0.50
1:A:473:PRO:HA	1:A:476:LYS:HD3	1.92	0.50
1:A:636:THR:O	1:A:637:LYS:CB	2.59	0.50
1:A:635:LYS:O	1:A:637:LYS:HG2	2.11	0.50
1:A:5:SER:HB3	1:A:33:SER:OG	2.12	0.50
1:A:68:GLY:HA3	1:A:316:SER:HB2	1.94	0.50
1:A:356:LEU:HA	1:A:359:GLN:HG3	1.94	0.50
1:A:59:LEU:HD11	1:A:256:VAL:HG21	1.94	0.50
1:A:489:GLN:HG2	1:A:503:ALA:HB3	1.94	0.49
1:A:506:ALA:HB3	1:A:521:GLU:OE1	2.12	0.49
1:A:509:GLU:OE2	1:A:522:ARG:NH2	2.45	0.49
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.94	0.49
1:A:440:ARG:NH1	1:A:534:ALA:O	2.43	0.49
1:A:5:SER:O	1:A:263:LYS:NZ	2.38	0.49
1:A:411:LEU:HD23	1:A:650:LYS:HA	1.92	0.49
1:A:688:MET:SD	1:A:688:MET:N	2.86	0.49
1:A:251:PRO:HB2	1:A:319:TYR:CE2	2.48	0.49
1:A:365:SER:O	1:A:366:ASN:HB2	2.12	0.49
1:A:475:PHE:HB3	1:A:671:LYS:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ASP:HB2	1:A:639:LEU:HD11	1.95	0.49
1:A:476:LYS:CD	1:A:667:THR:HG21	2.42	0.49
1:A:499:SER:OG	1:A:501:LEU:HB2	2.13	0.49
1:A:416:GLN:O	1:A:417:SER:HB2	2.12	0.48
1:A:352:SER:HA	1:A:355:GLN:HB2	1.95	0.48
1:A:469:ILE:HD13	1:A:590:PRO:CG	2.37	0.48
1:A:92:TYR:CA	1:A:92:TYR:CG	2.85	0.48
1:A:78:ALA:HA	1:A:308:LEU:O	2.13	0.48
1:A:402:ALA:O	1:A:407:LEU:HB2	2.14	0.48
1:A:429:PRO:CA	1:A:652:GLN:NE2	2.76	0.48
1:A:77:ILE:CD1	1:A:257:ALA:HB3	2.42	0.48
1:A:433:TYR:CE2	1:A:544:LYS:HG2	2.49	0.48
1:A:470:PRO:O	1:A:474:LEU:HB2	2.13	0.48
1:A:445:LYS:HE2	1:A:454:LYS:CE	2.44	0.48
1:A:423:LEU:CD1	1:A:423:LEU:C	2.58	0.48
1:A:138:TRP:HH2	1:A:331:LEU:O	1.96	0.48
1:A:611:LEU:O	1:A:615:GLN:HB3	2.14	0.48
1:A:374:ALA:HB3	1:A:380:CYS:SG	2.54	0.47
1:A:615:GLN:NE2	1:A:648:LEU:H	2.07	0.47
1:A:160:CYS:CB	1:A:183:CYS:SG	3.03	0.47
1:A:516:VAL:O	1:A:521:GLU:HB3	2.14	0.47
1:A:100:LYS:HE2	1:A:225:ASP:O	2.14	0.47
1:A:452:ARG:HG2	4:A:862:HOH:O	2.14	0.47
1:A:17:LYS:HG2	1:A:18:LYS:N	2.28	0.47
1:A:258:ARG:O	1:A:262:GLY:HA3	2.14	0.47
1:A:526:TYR:HB3	1:A:547:THR:OG1	2.13	0.47
1:A:93:TYR:HB3	1:A:246:HIS:HB2	1.97	0.47
1:A:144:PRO:O	1:A:145:LEU:C	2.53	0.47
1:A:455:LYS:HB2	1:A:538:GLY:HA2	1.97	0.47
1:A:459:THR:HB	1:A:466:GLY:HA3	1.96	0.47
1:A:608:ARG:HE	1:A:650:LYS:NZ	2.13	0.47
1:A:634:SER:CB	1:A:639:LEU:H	2.28	0.47
1:A:93:TYR:CD2	1:A:93:TYR:N	2.81	0.47
1:A:133:ARG:HG2	1:A:133:ARG:HH11	1.80	0.47
1:A:463:ARG:NH1	1:A:463:ARG:CG	2.75	0.47
1:A:552:THR:HG21	1:A:566:LEU:HA	1.97	0.47
1:A:54:ALA:O	1:A:258:ARG:NH2	2.47	0.47
1:A:473:PRO:HD3	1:A:668:ALA:HB2	1.97	0.47
1:A:526:TYR:O	1:A:543:VAL:HG11	2.15	0.47
1:A:129:MET:HG3	1:A:149:VAL:HG21	1.97	0.46
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:SER:O	1:A:127:ILE:HG12	2.15	0.46
1:A:634:SER:HB2	1:A:639:LEU:H	1.79	0.46
1:A:496:ASP:OD2	1:A:498:ARG:HG3	2.15	0.46
1:A:258:ARG:HG3	1:A:260:VAL:O	2.16	0.46
1:A:271:LEU:O	1:A:275:GLN:HB2	2.14	0.46
1:A:434:LEU:HD23	1:A:588:HIS:ND1	2.30	0.46
1:A:10:THR:HA	1:A:15:GLU:HG2	1.98	0.46
1:A:49:ILE:HD11	1:A:57:VAL:HG12	1.97	0.46
1:A:268:TRP:O	1:A:272:VAL:HG23	2.16	0.46
1:A:505:CYS:HB3	1:A:521:GLU:OE2	2.15	0.46
1:A:162:ASP:OD1	1:A:164:LYS:HB2	2.15	0.46
1:A:417:SER:O	1:A:419:GLU:N	2.48	0.46
1:A:526:TYR:N	1:A:526:TYR:CG	2.84	0.46
1:A:433:TYR:HD2	1:A:544:LYS:HB3	1.77	0.46
1:A:293:ALA:O	1:A:295:GLN:N	2.48	0.46
1:A:296:LYS:HA	1:A:296:LYS:HD3	1.53	0.46
1:A:412:ALA:HB2	1:A:651:LEU:CD1	2.46	0.46
1:A:424:ASP:O	1:A:428:ARG:NE	2.48	0.46
1:A:127:ILE:HG21	1:A:248:ALA:HB3	1.97	0.45
1:A:147:LYS:HA	1:A:150:ALA:HB3	1.97	0.45
1:A:17:LYS:CE	1:A:292:PRO:HG2	2.45	0.45
1:A:348:CYS:N	1:A:391:ALA:O	2.46	0.45
1:A:279:GLY:O	1:A:282:LYS:HB2	2.16	0.45
1:A:75:ARG:O	1:A:256:VAL:HA	2.16	0.45
1:A:603:LYS:HE3	1:A:606:HIS:HD2	1.80	0.45
1:A:418:PRO:HD3	1:A:644:ASN:CB	2.45	0.45
1:A:43:PHE:O	1:A:47:GLN:HG3	2.17	0.45
1:A:358:CYS:CB	1:A:371:CYS:HG	2.29	0.45
1:A:424:ASP:O	1:A:428:ARG:NH2	2.46	0.45
1:A:228:GLU:HB3	1:A:236:ARG:HB3	1.99	0.45
1:A:489:GLN:NE2	1:A:503:ALA:CB	2.80	0.45
1:A:75:ARG:NH1	1:A:314:ILE:O	2.49	0.45
1:A:356:LEU:HG	1:A:356:LEU:H	1.53	0.45
1:A:478:THR:OG1	1:A:479:ASP:N	2.50	0.45
1:A:548:VAL:CG2	1:A:581:VAL:HG11	2.46	0.45
1:A:128:PRO:O	1:A:132:LEU:HD12	2.17	0.44
1:A:528:GLY:HA2	1:A:531:ARG:HB3	1.99	0.44
1:A:637:LYS:HG3	1:A:639:LEU:CG	2.46	0.44
1:A:473:PRO:HD3	1:A:668:ALA:CB	2.48	0.44
1:A:607:LEU:O	1:A:608:ARG:C	2.54	0.44
1:A:196:PHE:CZ	1:A:214:VAL:HG13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HD21	1:A:405:CYS:CB	2.46	0.44
1:A:625:CYS:CB	1:A:626:PRO:CD	2.95	0.44
1:A:658:ASP:HB3	1:A:666:VAL:HG21	1.98	0.44
1:A:15:GLU:HG3	1:A:299:LEU:CD2	2.47	0.44
1:A:160:CYS:HB3	1:A:183:CYS:SG	2.58	0.44
1:A:31:GLY:HA2	1:A:273:LYS:HD2	2.00	0.44
1:A:67:ALA:HB1	1:A:74:LEU:CD1	2.44	0.44
1:A:589:LEU:HB3	1:A:590:PRO:CD	2.42	0.44
1:A:637:LYS:HB2	1:A:637:LYS:HE2	1.81	0.44
1:A:374:ALA:HB1	1:A:379:ASP:HB2	1.99	0.44
1:A:471:MET:HB3	1:A:483:PHE:CE2	2.52	0.44
1:A:325:ILE:O	1:A:329:ARG:HG3	2.18	0.43
1:A:438:VAL:CG2	1:A:439:VAL:N	2.81	0.43
1:A:15:GLU:OE1	1:A:299:LEU:N	2.38	0.43
1:A:103:ASN:OD1	1:A:103:ASN:N	2.52	0.43
1:A:344:GLN:O	1:A:344:GLN:HG2	2.16	0.43
1:A:364:GLN:CG	1:A:629:PHE:HB2	2.34	0.43
1:A:448:TRP:CZ2	1:A:474:LEU:HD13	2.54	0.43
1:A:380:CYS:CB	1:A:392:LEU:HD22	2.42	0.43
1:A:125:TRP:CZ3	1:A:149:VAL:HG11	2.53	0.43
1:A:357:LYS:NZ	1:A:639:LEU:O	2.37	0.43
1:A:361:TRP:HZ2	1:A:614:GLN:HG3	1.83	0.43
1:A:555:LYS:HE3	1:A:555:LYS:HB2	1.78	0.43
1:A:353:ASP:HA	1:A:356:LEU:HG	2.00	0.43
1:A:435:ALA:O	1:A:588:HIS:HB2	2.19	0.43
1:A:599:SER:OG	1:A:600:ARG:N	2.48	0.43
1:A:556:GLY:CA	1:A:561:ALA:HB3	2.48	0.43
1:A:157:CYS:O	1:A:159:PRO:HD3	2.18	0.43
1:A:453:GLY:O	1:A:488:SER:HB2	2.18	0.43
1:A:101:GLY:O	1:A:102:THR:O	2.37	0.43
1:A:278:PHE:HA	1:A:282:LYS:HG2	2.01	0.43
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.74	0.43
1:A:400:TYR:HD1	1:A:657:TYR:HE2	1.66	0.43
1:A:22:TRP:O	1:A:26:MET:HB2	2.19	0.43
1:A:179:ASN:HA	1:A:182:ALA:HB2	2.00	0.43
1:A:441:LYS:O	1:A:441:LYS:HG2	2.18	0.43
1:A:469:ILE:HA	1:A:668:ALA:HB1	2.00	0.43
1:A:543:VAL:HG21	1:A:547:THR:CG2	2.49	0.43
1:A:601:ILE:HD12	1:A:604:VAL:HG11	2.01	0.43
1:A:618:PHE:O	1:A:631:LEU:HB2	2.18	0.43
1:A:117:THR:OG1	1:A:124:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLN:NE2	1:A:503:ALA:HB1	2.34	0.42
1:A:32:PRO:HG2	1:A:270:LEU:HA	2.01	0.42
1:A:113:LYS:HD2	1:A:203:ALA:O	2.18	0.42
1:A:473:PRO:HA	1:A:476:LYS:HB3	2.01	0.42
1:A:662:GLY:O	1:A:665:TYR:HB3	2.19	0.42
1:A:24:ARG:HD3	1:A:24:ARG:HA	1.80	0.42
1:A:118:GLY:HA2	1:A:159:PRO:HB2	2.01	0.42
1:A:143:GLU:HA	1:A:144:PRO:HD2	1.80	0.42
1:A:614:GLN:NE2	1:A:614:GLN:HA	2.34	0.42
1:A:182:ALA:N	1:A:187:GLU:HB2	2.34	0.42
1:A:229:LEU:O	1:A:236:ARG:HA	2.19	0.42
1:A:508:ASN:HD22	1:A:512:GLN:HB2	1.83	0.42
1:A:562:LYS:H	1:A:562:LYS:HG2	1.57	0.42
1:A:402:ALA:HB1	1:A:598:VAL:HG11	2.00	0.42
1:A:472:GLY:CA	1:A:668:ALA:HA	2.43	0.42
1:A:582:THR:HG22	1:A:583:GLU:H	1.84	0.42
1:A:84:THR:OG1	1:A:85:GLU:N	2.53	0.42
1:A:97:ILE:O	1:A:206:VAL:CG1	2.58	0.42
1:A:506:ALA:HB2	1:A:523:LEU:HD13	2.01	0.42
1:A:26:MET:HG3	1:A:32:PRO:O	2.19	0.42
1:A:107:ASN:CG	1:A:234:ASN:HD21	2.22	0.42
1:A:526:TYR:HA	1:A:543:VAL:HG12	2.01	0.42
1:A:23:GLN:OE1	1:A:35:THR:HA	2.20	0.42
1:A:352:SER:O	1:A:355:GLN:CB	2.52	0.42
1:A:260:VAL:O	1:A:261:ASN:C	2.57	0.42
1:A:291:SER:HB3	1:A:295:GLN:O	2.20	0.42
1:A:399:ILE:O	1:A:403:GLY:N	2.46	0.42
1:A:455:LYS:HG2	1:A:539:ASP:OD2	2.19	0.42
1:A:651:LEU:O	1:A:654:LYS:HB2	2.19	0.42
1:A:13:PRO:O	1:A:17:LYS:N	2.49	0.42
1:A:121:ARG:HD3	1:A:121:ARG:HA	1.72	0.42
1:A:416:GLN:OE1	1:A:620:ARG:NH2	2.52	0.42
1:A:469:ILE:HG21	1:A:590:PRO:CG	2.50	0.42
1:A:165:GLU:HB2	1:A:166:TYR:CD1	2.54	0.41
1:A:453:GLY:O	1:A:488:SER:CB	2.68	0.41
1:A:49:ILE:CD1	1:A:57:VAL:HG12	2.50	0.41
1:A:123:ALA:HB3	1:A:192:TYR:OH	2.20	0.41
1:A:447:THR:CG2	1:A:450:SER:HB3	2.47	0.41
1:A:260:VAL:HG12	1:A:261:ASN:HB2	2.03	0.41
1:A:460:ALA:HA	1:A:493:PRO:CG	2.50	0.41
1:A:522:ARG:HD3	1:A:531:ARG:HH12	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PHE:HZ	1:A:205:ASP:O	2.04	0.41
1:A:157:CYS:C	1:A:159:PRO:HD3	2.41	0.41
1:A:214:VAL:CG1	1:A:218:LEU:HD12	2.51	0.41
1:A:412:ALA:O	1:A:648:LEU:HA	2.21	0.41
1:A:418:PRO:HG3	1:A:644:ASN:ND2	2.35	0.41
1:A:99:LYS:O	1:A:236:ARG:NH2	2.55	0.41
1:A:543:VAL:HG21	1:A:547:THR:HG21	2.03	0.41
1:A:104:PHE:CD1	1:A:112:LEU:HD11	2.56	0.40
1:A:11:THR:H	1:A:15:GLU:HG2	1.86	0.40
1:A:360:GLU:O	1:A:364:GLN:HB2	2.20	0.40
1:A:6:VAL:HG23	1:A:266:LEU:HG	2.03	0.40
1:A:358:CYS:HB2	1:A:640:LEU:HD11	2.02	0.40
1:A:110:GLN:HB3	4:A:838:HOH:O	2.22	0.40
1:A:143:GLU:CG	1:A:147:LYS:HE2	2.44	0.40
1:A:353:ASP:HA	1:A:356:LEU:CD1	2.51	0.40
1:A:364:GLN:NE2	1:A:364:GLN:HA	2.37	0.40
1:A:467:TRP:HD1	1:A:468:ASN:ND2	2.18	0.40
1:A:525:GLY:C	1:A:526:TYR:CA	2.80	0.40
1:A:636:THR:O	1:A:637:LYS:HB3	2.21	0.40
1:A:102:THR:HB	1:A:104:PHE:CE1	2.56	0.40
1:A:113:LYS:HD3	1:A:172:LEU:HD21	2.03	0.40
1:A:608:ARG:HE	1:A:650:LYS:HZ2	1.69	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	687/689 (100%)	562 (82%)	89 (13%)	36 (5%)	2 3

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ARG
1	A	159	PRO
1	A	160	CYS
1	A	220	ALA
1	A	335	ALA
1	A	418	PRO
1	A	429	PRO
1	A	446	ILE
1	A	513	LEU
1	A	604	VAL
1	A	154	SER
1	A	234	ASN
1	A	454	LYS
1	A	547	THR
1	A	571	LEU
1	A	624	ASP
1	A	637	LYS
1	A	650	LYS
1	A	102	THR
1	A	137	ASP
1	A	292	PRO
1	A	311	PRO
1	A	472	GLY
1	A	563	ASP
1	A	133	ARG
1	A	417	SER
1	A	511	GLY
1	A	620	ARG
1	A	625	CYS
1	A	122	SER
1	A	551	ASN
1	A	559	GLN
1	A	589	LEU
1	A	209	VAL
1	A	161	VAL
1	A	32	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	570/570 (100%)	404 (71%)	166 (29%)	0 1

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	LYS
1	A	12	SER
1	A	16	SER
1	A	17	LYS
1	A	23	GLN
1	A	25	ARG
1	A	28	LYS
1	A	38	LYS
1	A	42	ARG
1	A	47	GLN
1	A	52	GLU
1	A	58	THR
1	A	69	LEU
1	A	70	ASP
1	A	74	LEU
1	A	75	ARG
1	A	97	ILE
1	A	99	LYS
1	A	112	LEU
1	A	121	ARG
1	A	122	SER
1	A	129	MET
1	A	141	PRO
1	A	147	LYS
1	A	151	LYS
1	A	154	SER
1	A	160	CYS
1	A	161	VAL
1	A	162	ASP
1	A	164	LYS
1	A	165	GLU
1	A	166	TYR
1	A	185	SER
1	A	197	LYS
1	A	206	VAL

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Mol	Chain	Res	Type
1	A	214	VAL
1	A	219	PRO
1	A	226	GLN
1	A	229	LEU
1	A	230	LEU
1	A	236	ARG
1	A	244	GLU
1	A	247	LEU
1	A	249	ARG
1	A	258	ARG
1	A	264	GLU
1	A	266	LEU
1	A	270	LEU
1	A	271	LEU
1	A	275	GLN
1	A	280	ARG
1	A	282	LYS
1	A	284	SER
1	A	291	SER
1	A	296	LYS
1	A	298	LEU
1	A	299	LEU
1	A	305	LEU
1	A	308	LEU
1	A	309	ARG
1	A	311	PRO
1	A	312	LYS
1	A	316	SER
1	A	318	LEU
1	A	329	ARG
1	A	332	ARG
1	A	334	THR
1	A	342	ARG
1	A	344	GLN
1	A	353	ASP
1	A	354	GLU
1	A	356	LEU
1	A	359	GLN
1	A	362	SER
1	A	368	SER
1	A	370	VAL
1	A	371	CYS

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Mol	Chain	Res	Type
1	A	373	THR
1	A	376	THR
1	A	386	LYS
1	A	388	GLU
1	A	395	ASP
1	A	399	ILE
1	A	407	LEU
1	A	408	VAL
1	A	415	GLN
1	A	421	SER
1	A	423	LEU
1	A	424	ASP
1	A	425	CYS
1	A	433	TYR
1	A	439	VAL
1	A	444	ASP
1	A	445	LYS
1	A	446	ILE
1	A	447	THR
1	A	452	ARG
1	A	459	THR
1	A	463	ARG
1	A	474	LEU
1	A	475	PHE
1	A	477	ASP
1	A	478	THR
1	A	480	SER
1	A	485	GLU
1	A	488	SER
1	A	490	SER
1	A	491	CYS
1	A	498	ARG
1	A	499	SER
1	A	500	LYS
1	A	505	CYS
1	A	510	GLU
1	A	514	LYS
1	A	518	ASN
1	A	520	SER
1	A	522	ARG
1	A	523	LEU
1	A	524	TYR

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Mol	Chain	Res	Type
1	A	527	THR
1	A	532	CYS
1	A	543	VAL
1	A	544	LYS
1	A	546	VAL
1	A	550	ASP
1	A	555	LYS
1	A	557	THR
1	A	558	GLU
1	A	559	GLN
1	A	563	ASP
1	A	565	LYS
1	A	566	LEU
1	A	568	ASP
1	A	573	CYS
1	A	578	ARG
1	A	579	LYS
1	A	581	VAL
1	A	582	THR
1	A	583	GLU
1	A	589	LEU
1	A	600	ARG
1	A	609	GLN
1	A	612	LEU
1	A	613	ARG
1	A	615	GLN
1	A	621	ASN
1	A	628	LYS
1	A	633	GLN
1	A	635	LYS
1	A	637	LYS
1	A	644	ASN
1	A	646	GLU
1	A	648	LEU
1	A	651	LEU
1	A	652	GLN
1	A	655	THR
1	A	658	ASP
1	A	661	LEU
1	A	669	ILE
1	A	673	ARG
1	A	674	ARG

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Mol	Chain	Res	Type
1	A	677	THR
1	A	678	SER
1	A	682	GLU
1	A	689	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	126	ASN
1	A	226	GLN
1	A	234	ASN
1	A	253	HIS
1	A	275	GLN
1	A	468	ASN
1	A	508	ASN
1	A	518	ASN
1	A	536	ASN
1	A	594	ASN
1	A	615	GLN
1	A	638	ASN
1	A	644	ASN
1	A	652	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 monosaccharides 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	CO3	A	692	-	2,3,3	0.96	0	2,3,3	1.73	0
3	CO3	A	693	2	2,3,3	0.96	0	2,3,3	2.90	2 (100%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	693	CO3	O3-C-O1	-3.43	110.64	119.55
3	A	693	CO3	O2-C-O1	2.25	125.39	119.55

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	569:PHE	C	570:GLU	N	0.94
1	A	572:LEU	C	573:CYS	N	0.93

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	430:VAL	C	431:LYS	N	0.55

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.