Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:43 PM GMT

PDB ID	:	1QAL
Title	:	THE ACTIVE SITE BASE CONTROLS COFACTOR REACTIVITY IN ESCHERICHIA COLI AMINE OXIDASE : X-RAY CRYSTALLOGRAPHIC STUDIES WITH MUTATIONAL VARIANTS
Authors	:	Murray, J.M.; Wilmot, C.M.; Saysell, C.G.; Jaeger, J.; Knowles, P.F.; Phillips, S.E.; McPherson, M.J.
Deposited on	:	1999-03-19
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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:

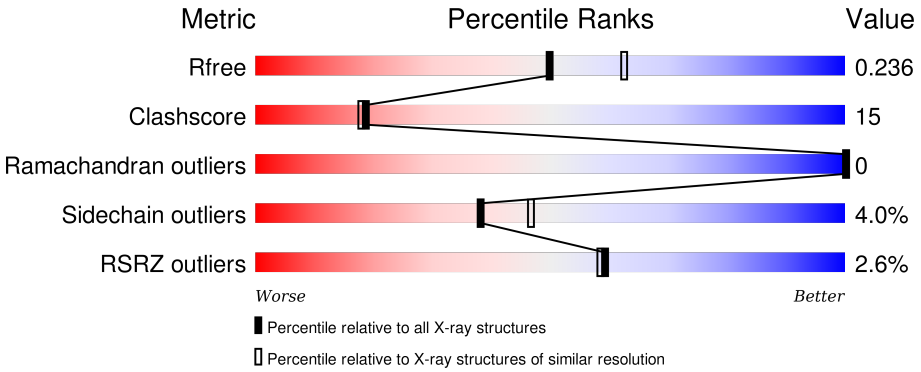
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	721	2% 66% 28% 5%
1	B	721	3% 68% 26% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12909 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 COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	0	1
			5665	3602	966	1075	22			
1	B	721	Total	C	N	O	S	0	0	0
			5692	3618	971	1081	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	ASN	ASP	ENGINEERED	UNP P46883
A	466	TPQ	TYR	MODIFIED RESIDUE	UNP P46883
B	383	ASN	ASP	ENGINEERED	UNP P46883
B	466	TPQ	TYR	MODIFIED RESIDUE	UNP P46883

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

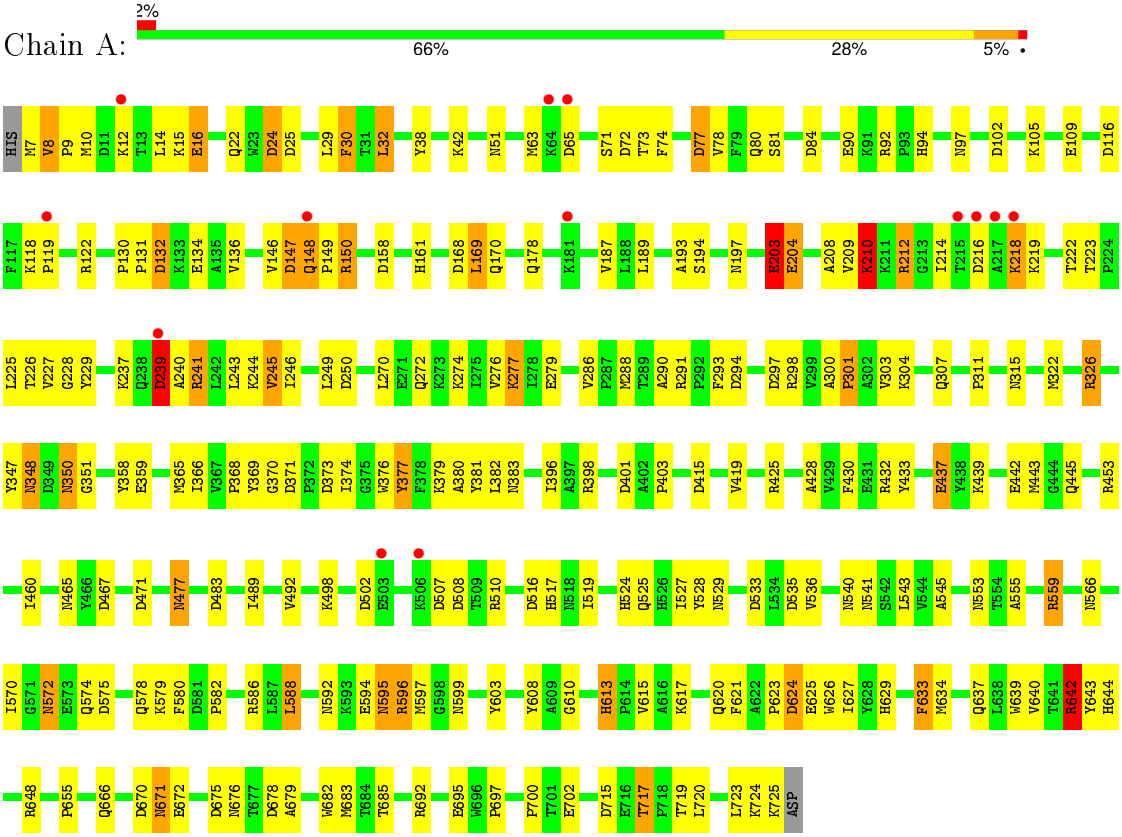
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	801	Total O 801 801	0	0
4	B	745	Total O 745 745	0	0

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.

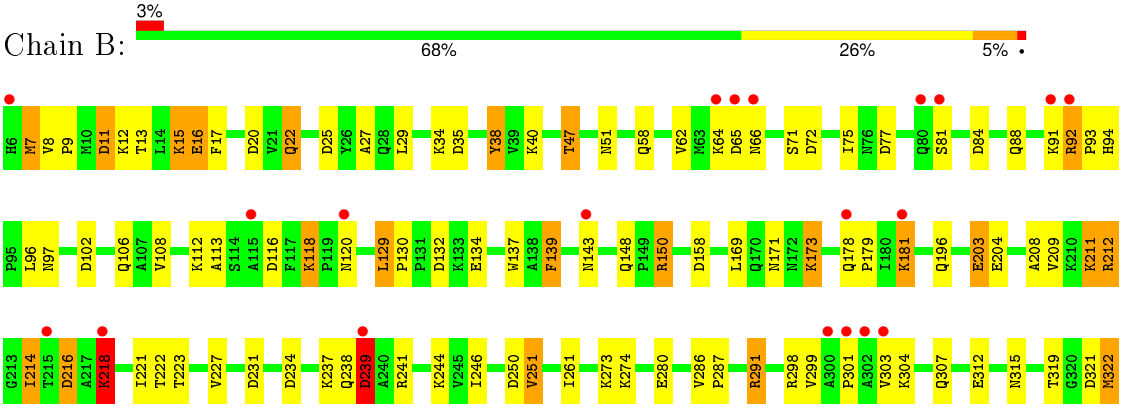
- Molecule 1: COPPER AMINE OXIDASE

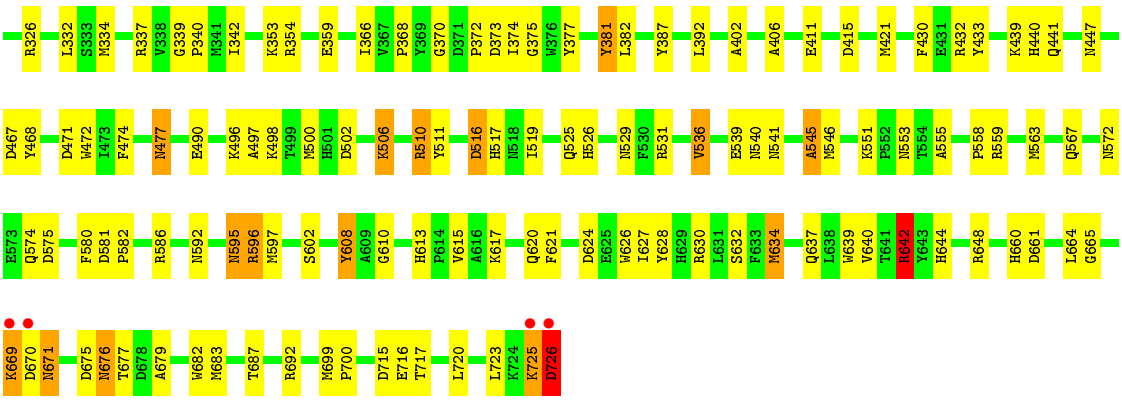
Chain A:



- Molecule 1: COPPER AMINE OXIDASE

Chain B:




R326 L332 S333 M334 R337 Y338 G339 P340 M341 I342 K353 R354 E359 I366 V367 P368 Y369 G370 D371 P372 D373 I374 G375 W376 Y377 Y381 L382 Y387 L392 A402 A406 E411 D415 M421 F430 E431 R432 Y433 K439 H440 Q441 N447
D467 Y468 D471 W472 I473 F474 N477 E490 K496 A497 K498 T499 M500 H501 D502 K506 R510 Y511 D516 H517 N518 I519 Q525 H526 N529 F530 R531 V536 E539 N540 N541 A545 M546 K551 P552 N553 T554 A555 P558 R559 M563 Q567 N572
E573 Q574 D575 F580 D581 P582 R586 N592 N595 R596 M597 S602 Y608 A609 G610 H613 P614 V615 A616 K617 Q620 F621 D624 E625 W626 I627 Y628 H629 R630 L631 S632 F633 M634 Q637 L638 W639 V640 T641 R642 Y643 H644 R648 H660 D661 L664 G665
K669 D670 M671 D675 M676 T677 D678 A679 W682 M683 T687 R692 M699 P700 D715 E716 T717 L720 L723 K724 K725 D726

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.05Å 166.52Å 79.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.91 – 2.19	Depositor EDS
% Data completeness (in resolution range)	93.7 (20.00-2.20) 92.9 (19.91-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.05 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.241 0.178 , 0.236	Depositor DCC
R_{free} test set	2902 reflections (3.52%)	DCC
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 65.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 86197 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12909	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, TPQ, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.59	0/5794	1.78	119/7888 (1.5%)
1	B	0.57	0/5822	1.70	104/7923 (1.3%)
All	All	0.58	0/11616	1.74	223/15811 (1.4%)

There are no bond length outliers.

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	642	ARG	NE-CZ-NH2	-31.57	104.51	120.30
1	A	596	ARG	NE-CZ-NH2	-29.75	105.42	120.30
1	A	692	ARG	NE-CZ-NH2	-19.56	110.52	120.30
1	B	692	ARG	NE-CZ-NH2	-19.48	110.56	120.30
1	A	298	ARG	NE-CZ-NH2	-16.41	112.09	120.30
1	B	337	ARG	NE-CZ-NH1	15.85	128.22	120.30
1	A	642	ARG	NH1-CZ-NH2	15.75	136.72	119.40
1	B	291	ARG	NE-CZ-NH2	15.02	127.81	120.30
1	B	291	ARG	NE-CZ-NH1	-14.86	112.87	120.30
1	A	212	ARG	NE-CZ-NH1	13.88	127.24	120.30
1	A	596	ARG	NH1-CZ-NH2	13.86	134.65	119.40
1	A	241	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	B	241	ARG	NE-CZ-NH1	12.46	126.53	120.30
1	B	92	ARG	NE-CZ-NH1	-12.14	114.23	120.30
1	B	726	ASP	CB-CG-OD1	11.91	129.02	118.30
1	A	415	ASP	CB-CG-OD1	11.75	128.87	118.30
1	B	72	ASP	CB-CG-OD1	11.60	128.74	118.30
1	B	432	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	B	326	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	B	25	ASP	CB-CG-OD2	-11.32	108.11	118.30
1	A	147	ASP	CB-CG-OD1	11.29	128.46	118.30
1	B	608	TYR	CB-CG-CD2	-11.13	114.32	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	511	TYR	CB-CG-CD1	-10.98	114.41	121.00
1	A	16	GLU	OE1-CD-OE2	-10.78	110.36	123.30
1	B	132	ASP	CB-CG-OD1	-10.69	108.68	118.30
1	A	508	ASP	CB-CG-OD1	10.54	127.79	118.30
1	A	398	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	B	511	TYR	CB-CG-CD2	10.34	127.20	121.00
1	A	648	ARG	NE-CZ-NH2	-10.23	115.19	120.30
1	A	102	ASP	CB-CG-OD2	10.13	127.42	118.30
1	A	147	ASP	CB-CG-OD2	-9.95	109.34	118.30
1	B	586	ARG	NE-CZ-NH1	9.69	125.15	120.30
1	B	116	ASP	CB-CG-OD1	9.69	127.02	118.30
1	B	72	ASP	CB-CG-OD2	-9.61	109.65	118.30
1	B	648	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	A	432	ARG	NE-CZ-NH1	-9.29	115.66	120.30
1	B	608	TYR	CB-CG-CD1	9.28	126.57	121.00
1	B	11	ASP	CB-CG-OD2	-9.14	110.07	118.30
1	A	535	ASP	CB-CG-OD1	8.71	126.14	118.30
1	B	116	ASP	CB-CG-OD2	8.69	126.12	118.30
1	B	116	ASP	OD1-CG-OD2	-8.65	106.86	123.30
1	A	158	ASP	CB-CG-OD1	8.53	125.98	118.30
1	B	596	ARG	NE-CZ-NH1	-8.49	116.06	120.30
1	B	216	ASP	CB-CG-OD2	8.41	125.87	118.30
1	B	212	ARG	NE-CZ-NH2	8.41	124.50	120.30
1	B	234	ASP	CB-CG-OD1	8.40	125.86	118.30
1	A	30	PHE	CB-CG-CD1	-8.10	115.13	120.80
1	A	77	ASP	CB-CG-OD1	8.08	125.57	118.30
1	B	326	ARG	CD-NE-CZ	8.04	134.85	123.60
1	A	132	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	A	437	GLU	OE1-CD-OE2	-7.87	113.86	123.30
1	A	65	ASP	CB-CG-OD1	7.78	125.30	118.30
1	A	401	ASP	CB-CG-OD1	7.76	125.28	118.30
1	B	134	GLU	OE1-CD-OE2	-7.73	114.02	123.30
1	B	433	TYR	CB-CG-CD1	-7.70	116.38	121.00
1	A	401	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	B	648	ARG	NH1-CZ-NH2	-7.60	111.04	119.40
1	B	150	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	A	692	ARG	NH1-CZ-NH2	7.59	127.75	119.40
1	A	510	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	312	GLU	OE1-CD-OE2	-7.53	114.26	123.30
1	A	150	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	84	ASP	CB-CG-OD1	7.46	125.02	118.30
1	B	516	ASP	CB-CG-OD1	7.41	124.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	628	TYR	CB-CG-CD2	7.41	125.45	121.00
1	B	675	ASP	CB-CG-OD2	7.41	124.97	118.30
1	A	724	LYS	O-C-N	7.30	134.39	122.70
1	B	725	LYS	O-C-N	7.20	134.22	122.70
1	B	630	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	226	THR	CA-CB-CG2	-7.18	102.35	112.40
1	B	648	ARG	NE-CZ-NH2	7.15	123.88	120.30
1	A	122	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	B	204	GLU	OE1-CD-OE2	7.14	131.87	123.30
1	A	471	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	A	294	ASP	CB-CG-OD1	7.05	124.64	118.30
1	A	291	ARG	NE-CZ-NH1	-7.03	116.79	120.30
1	A	528	TYR	CB-CG-CD2	6.96	125.18	121.00
1	B	531	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	528	TYR	CB-CG-CD1	-6.91	116.85	121.00
1	A	717	THR	CA-CB-CG2	-6.86	102.80	112.40
1	B	510	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	92	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	307	GLN	CG-CD-OE1	6.82	135.23	121.60
1	B	16	GLU	OE1-CD-OE2	-6.77	115.18	123.30
1	A	373	ASP	CB-CG-OD2	6.75	124.38	118.30
1	B	7	MET	N-CA-CB	-6.75	98.44	110.60
1	B	113	ALA	CB-CA-C	-6.73	100.00	110.10
1	A	210	LYS	CD-CE-NZ	6.67	127.03	111.70
1	B	92	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	B	373	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	471	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	250	ASP	CB-CG-OD1	6.55	124.20	118.30
1	A	675	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	A	24	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	471	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	415	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	24	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	602	SER	N-CA-CB	-6.48	100.78	110.50
1	B	38	TYR	CB-CG-CD1	-6.45	117.13	121.00
1	B	25	ASP	OD1-CG-OD2	6.43	135.53	123.30
1	A	193	ALA	N-CA-CB	6.42	119.08	110.10
1	A	194	SER	N-CA-CB	6.40	120.10	110.50
1	A	678	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	347	TYR	CB-CG-CD1	6.36	124.82	121.00
1	A	168	ASP	CB-CG-OD1	6.34	124.00	118.30
1	A	239	ASP	CB-CG-OD1	6.32	123.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	726	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	695	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	B	624	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	A	586	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	603	TYR	CB-CG-CD1	6.28	124.77	121.00
1	A	442	GLU	OE1-CD-OE2	-6.27	115.78	123.30
1	B	497	ALA	CB-CA-C	-6.26	100.71	110.10
1	B	337	ARG	NH1-CZ-NH2	-6.26	112.52	119.40
1	B	725	LYS	CA-C-O	-6.24	107.00	120.10
1	B	692	ARG	NH1-CZ-NH2	6.22	126.24	119.40
1	A	102	ASP	OD1-CG-OD2	-6.17	111.57	123.30
1	B	15	LYS	O-C-N	6.13	132.51	122.70
1	A	507	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	566	ASN	CB-CG-OD1	6.07	133.74	121.60
1	A	301	PRO	N-CD-CG	-6.07	94.10	103.20
1	B	251	VAL	CA-CB-CG1	6.06	119.98	110.90
1	A	588	LEU	N-CA-C	-6.01	94.76	111.00
1	B	22	GLN	CG-CD-OE1	5.99	133.59	121.60
1	B	716	GLU	OE1-CD-OE2	-5.98	116.12	123.30
1	B	628	TYR	CG-CD1-CE1	5.98	126.08	121.30
1	A	507	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	326	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	502	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	326	ARG	CA-CB-CG	-5.95	100.32	113.40
1	B	239	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	A	65	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	321	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	B	84	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	20	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	245	VAL	CA-CB-CG1	5.83	119.64	110.90
1	A	168	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	B	359	GLU	CB-CA-C	5.82	122.03	110.40
1	A	502	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	212	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	116	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	B	692	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	586	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	A	467	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	B	158	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	30	PHE	CB-CG-CD2	5.77	124.84	120.80
1	B	628	TYR	CD1-CE1-CZ	-5.74	114.64	119.80
1	B	624	ASP	CB-CG-OD1	5.73	123.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	432	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	A	633	PHE	CB-CG-CD2	5.70	124.79	120.80
1	A	594	GLU	O-C-N	5.69	131.80	122.70
1	A	277	LYS	CD-CE-NZ	-5.68	98.63	111.70
1	B	218	LYS	CA-CB-CG	5.68	125.90	113.40
1	A	307	GLN	OE1-CD-NE2	-5.65	108.90	121.90
1	A	303	VAL	CA-CB-CG1	5.64	119.36	110.90
1	B	377	TYR	CG-CD2-CE2	5.64	125.81	121.30
1	A	77	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	297	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	373	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	B	58	GLN	N-CA-CB	5.58	120.65	110.60
1	B	354	ARG	NE-CZ-NH2	5.57	123.09	120.30
1	A	241	ARG	NH1-CZ-NH2	5.57	125.53	119.40
1	A	298	ARG	NH1-CZ-NH2	5.55	125.50	119.40
1	A	483	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	533	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	102	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	134	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	A	72	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	377	TYR	CZ-CE2-CD2	-5.49	114.86	119.80
1	A	90	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	A	586	ARG	NH1-CZ-NH2	-5.48	113.37	119.40
1	A	719	THR	CA-CB-CG2	-5.48	104.73	112.40
1	B	35	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	559	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	B	381	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	B	575	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	16	GLU	CG-CD-OE2	5.41	129.12	118.30
1	B	531	ARG	CD-NE-CZ	-5.41	116.03	123.60
1	A	169	LEU	CB-CG-CD2	-5.38	101.85	111.00
1	A	594	GLU	OE1-CD-OE2	5.38	129.76	123.30
1	B	129	LEU	N-CA-C	-5.32	96.64	111.00
1	A	178	GLN	CG-CD-OE1	-5.31	110.99	121.60
1	A	415	ASP	OD1-CG-OD2	-5.29	113.24	123.30
1	A	425	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	A	8	VAL	CA-CB-CG1	5.27	118.81	110.90
1	A	132	ASP	O-C-N	5.26	131.12	122.70
1	A	433	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	B	545	ALA	CB-CA-C	-5.25	102.23	110.10
1	B	468	TYR	CB-CG-CD1	-5.24	117.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	666	GLN	CG-CD-OE1	5.21	132.02	121.60
1	A	425	ARG	CD-NE-CZ	-5.20	116.32	123.60
1	B	261	ILE	N-CA-C	-5.20	96.95	111.00
1	B	536	VAL	CA-CB-CG2	-5.20	103.10	110.90
1	A	136	VAL	CA-CB-CG1	5.20	118.69	110.90
1	A	666	GLN	OE1-CD-NE2	-5.19	109.96	121.90
1	B	387	TYR	CB-CG-CD2	5.18	124.11	121.00
1	A	216	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	433	TYR	CB-CG-CD2	5.16	124.10	121.00
1	B	411	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	B	726	ASP	CA-C-O	-5.15	109.28	120.10
1	B	421	MET	N-CA-CB	-5.14	101.34	110.60
1	B	472	TRP	N-CA-C	-5.14	97.12	111.00
1	B	402	ALA	N-CA-CB	5.13	117.28	110.10
1	A	419	VAL	CA-CB-CG1	5.13	118.59	110.90
1	B	634	MET	CG-SD-CE	5.13	108.40	100.20
1	B	273	LYS	CA-CB-CG	-5.08	102.23	113.40
1	A	197	ASN	OD1-CG-ND2	-5.08	110.22	121.90
1	A	32	LEU	CB-CG-CD1	5.07	119.61	111.00
1	A	189	LEU	CB-CG-CD2	5.07	119.61	111.00
1	B	474	PHE	CB-CG-CD1	-5.05	117.27	120.80
1	B	642	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	624	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	A	203	GLU	OE1-CD-OE2	-5.04	117.26	123.30
1	A	439	LYS	O-C-N	5.03	130.75	122.70
1	A	290	ALA	O-C-N	5.03	130.74	122.70
1	B	15	LYS	CA-C-O	-5.03	109.54	120.10
1	B	139	PHE	CB-CG-CD1	-5.03	117.28	120.80
1	A	229	TYR	CB-CG-CD2	5.02	124.01	121.00
1	B	546	MET	N-CA-CB	5.02	119.63	110.60
1	A	685	THR	OG1-CB-CG2	-5.01	98.46	110.00
1	B	47	THR	CA-CB-OG1	5.01	119.53	109.00
1	B	640	VAL	CG1-CB-CG2	-5.01	102.89	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5665	0	5542	195	0
1	B	5692	0	5566	182	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	801	0	0	28	3
4	B	745	0	0	27	2
All	All	12909	0	11108	347	4

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 15.

All (347) 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:642:ARG:HD2	4:A:1498:HOH:O	1.34	1.27
1:A:625:GLU:O	1:A:629:HIS:CD2	2.11	1.02
1:A:130:PRO:HG2	4:A:1115:HOH:O	1.61	0.99
1:B:725:LYS:O	1:B:726:ASP:OD1	1.83	0.95
1:B:642:ARG:HH11	1:B:642:ARG:HB2	1.31	0.95
1:A:625:GLU:O	1:A:629:HIS:HD2	1.48	0.94
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.49	0.92
1:B:181:LYS:HE2	1:B:181:LYS:H	1.33	0.91
1:A:368:PRO:HG3	1:A:634:MET:HE1	1.53	0.90
1:A:304:LYS:H	1:B:315:ASN:HD21	1.17	0.90
1:B:572:ASN:HD22	1:B:671:ASN:HD21	1.21	0.86
1:A:368:PRO:HG3	1:A:634:MET:CE	2.04	0.86
1:A:130:PRO:O	4:A:1115:HOH:O	1.92	0.85
1:A:596:ARG:NH2	1:B:516:ASP:OD1	2.10	0.84
1:B:8:VAL:CG2	1:B:9:PRO:HD2	2.07	0.84
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.60	0.84
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.27	0.83
1:A:131:PRO:HB3	1:A:148:GLN:NE2	1.94	0.83
1:B:642:ARG:HH11	1:B:642:ARG:CB	1.94	0.81
1:A:279:GLU:OE1	1:A:374:ILE:HD11	1.80	0.81
1:B:525:GLN:HE22	1:B:620:GLN:H	1.27	0.81
1:B:181:LYS:CE	1:B:181:LYS:H	1.95	0.80
1:B:221:ILE:CD1	1:B:250:ASP:HB2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:NH2	1:B:303:VAL:HG13	1.98	0.79
1:B:540:ASN:HB3	1:B:676:ASN:ND2	1.97	0.78
1:B:617:LYS:HA	4:B:1051:HOH:O	1.84	0.77
1:B:580:PHE:H	1:B:637:GLN:HE21	1.33	0.76
1:B:181:LYS:HE2	1:B:181:LYS:N	2.00	0.76
1:A:624:ASP:HA	1:A:629:HIS:CE1	2.20	0.76
1:B:525:GLN:NE2	1:B:620:GLN:H	1.84	0.75
1:A:8:VAL:HG22	1:A:9:PRO:HD2	1.68	0.75
1:A:225:LEU:HD22	4:A:1575:HOH:O	1.86	0.75
1:B:94:HIS:HB3	1:B:97:ASN:ND2	2.00	0.75
1:B:94:HIS:HD2	1:B:96:LEU:H	1.34	0.75
1:A:580:PHE:H	1:A:637:GLN:HE21	1.33	0.75
1:B:94:HIS:HB3	1:B:97:ASN:HD21	1.51	0.74
1:A:527:ILE:HD12	1:A:634:MET:HE3	1.68	0.74
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.21	0.74
1:B:291:ARG:NH1	1:B:516:ASP:OD2	2.21	0.74
1:A:38:TYR:H	1:A:51:ASN:ND2	1.86	0.74
1:A:38:TYR:H	1:A:51:ASN:HD21	1.34	0.73
1:A:315:ASN:HD21	1:B:304:LYS:H	1.37	0.72
1:A:350:ASN:OD1	4:A:1074:HOH:O	2.08	0.71
1:A:624:ASP:C	1:A:629:HIS:NE2	2.44	0.71
1:B:27:ALA:HA	4:B:827:HOH:O	1.92	0.70
1:A:227:VAL:HG12	1:A:244:LYS:HG3	1.74	0.70
1:A:396:ILE:HD13	1:A:428:ALA:HB2	1.73	0.69
1:A:241:ARG:HG2	1:A:270:LEU:HD12	1.74	0.69
1:B:679:ALA:HB2	4:B:1177:HOH:O	1.93	0.69
1:B:227:VAL:HG12	1:B:244:LYS:HG3	1.74	0.69
1:B:574:GLN:H	1:B:671:ASN:ND2	1.90	0.69
1:B:700:PRO:HD2	4:B:1012:HOH:O	1.93	0.68
1:A:203:GLU:CD	1:A:203:GLU:H	1.97	0.68
1:A:525:GLN:HE22	1:A:620:GLN:H	1.41	0.68
1:B:38:TYR:H	1:B:51:ASN:HD21	1.41	0.68
1:B:717:THR:HB	1:B:720:LEU:HG	1.75	0.68
1:A:73:THR:HG23	1:A:77:ASP:OD2	1.94	0.67
1:B:580:PHE:H	1:B:637:GLN:NE2	1.93	0.66
1:B:12:LYS:O	1:B:16:GLU:HG2	1.94	0.66
1:A:639:TRP:HB2	1:A:682:TRP:HB2	1.77	0.66
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.60	0.66
1:A:210:LYS:HE2	1:A:214:ILE:O	1.96	0.66
1:A:368:PRO:HB2	1:A:621:PHE:CZ	2.31	0.66
1:B:203:GLU:H	1:B:203:GLU:CD	2.00	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ILE:HD11	1:A:627:ILE:HD11	1.78	0.65
1:B:670:ASP:HB2	4:B:1055:HOH:O	1.95	0.65
1:A:553:ASN:ND2	1:A:555:ALA:H	1.94	0.65
1:A:617:LYS:HE2	1:B:581:ASP:OD1	1.97	0.65
1:A:223:THR:HG22	1:A:246:ILE:O	1.97	0.65
1:B:173:LYS:HB3	1:B:173:LYS:NZ	2.12	0.64
1:A:498:LYS:O	1:A:517:HIS:HD2	1.81	0.64
1:B:38:TYR:H	1:B:51:ASN:ND2	1.97	0.63
1:A:572:ASN:ND2	1:A:575:ASP:H	1.96	0.63
1:A:527:ILE:HD12	1:A:634:MET:CE	2.28	0.63
1:B:441:GLN:OE1	1:B:447:ASN:HB2	1.98	0.63
1:A:570:ILE:HD13	1:A:578:GLN:HE22	1.62	0.63
1:A:368:PRO:HB2	1:A:621:PHE:HZ	1.64	0.62
1:A:559:ARG:HH22	1:B:370:GLY:HA2	1.63	0.62
1:A:149:PRO:HB3	1:A:170:GLN:HE21	1.65	0.62
1:B:506:LYS:CE	1:B:510:ARG:HH22	2.12	0.62
1:B:368:PRO:HG3	1:B:634:MET:HE3	1.82	0.62
1:A:382:LEU:HD13	1:A:655:PRO:HB2	1.82	0.62
1:A:536:VAL:H	1:A:541:ASN:HD21	1.46	0.62
1:B:221:ILE:N	1:B:221:ILE:HD12	2.15	0.61
1:A:379:LYS:HG3	4:A:1575:HOH:O	1.99	0.61
1:B:148:GLN:NE2	4:B:1287:HOH:O	2.34	0.61
1:A:381:TYR:CE2	4:A:1575:HOH:O	2.51	0.61
1:A:71:SER:OG	1:A:73:THR:HG22	2.00	0.61
1:A:365:MET:CE	1:A:383:ASN:HD22	2.14	0.60
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.50	0.59
1:B:366:ILE:HD11	1:B:627:ILE:HD11	1.83	0.59
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.17	0.59
1:A:326:ARG:HH22	1:B:303:VAL:HG13	1.64	0.59
1:A:572:ASN:HB2	1:A:671:ASN:ND2	2.18	0.59
1:A:237:LYS:HD3	1:A:240:ALA:HB2	1.83	0.59
1:A:326:ARG:NH1	1:B:303:VAL:HG22	2.17	0.59
1:A:572:ASN:CG	1:A:671:ASN:HD21	2.06	0.59
1:A:12:LYS:O	1:A:16:GLU:HG3	2.03	0.59
1:A:525:GLN:NE2	1:A:620:GLN:H	2.01	0.58
1:B:173:LYS:HB3	1:B:173:LYS:HZ3	1.68	0.58
1:B:216:ASP:OD1	1:B:218:LYS:HB2	2.03	0.58
1:B:334:MET:HB3	4:B:1464:HOH:O	2.02	0.58
1:B:572:ASN:ND2	1:B:671:ASN:HD21	1.95	0.58
1:B:120:ASN:CG	4:B:851:HOH:O	2.42	0.58
1:A:222:THR:HB	1:A:245:VAL:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASP:O	1:B:66:ASN:HB2	2.02	0.57
1:A:322:MET:HG2	4:A:1375:HOH:O	2.03	0.57
1:B:639:TRP:HB2	1:B:682:TRP:HB2	1.85	0.57
1:A:326:ARG:HH12	1:B:303:VAL:HG22	1.68	0.57
1:A:24:ASP:OD2	1:B:40:LYS:NZ	2.20	0.57
1:A:286:VAL:HG12	1:A:288:MET:HE3	1.87	0.57
1:B:130:PRO:HG3	4:B:1172:HOH:O	2.05	0.56
1:A:723:LEU:HD23	1:B:298:ARG:HD3	1.88	0.56
1:B:238:GLN:HA	1:B:238:GLN:HE21	1.71	0.55
1:A:7:MET:HE2	1:A:7:MET:HA	1.87	0.55
1:B:307:GLN:OE1	4:B:1189:HOH:O	2.18	0.55
1:A:670:ASP:OD2	1:A:672:GLU:HG3	2.06	0.55
1:B:723:LEU:HD23	1:B:726:ASP:OD1	2.07	0.55
1:A:29:LEU:HD13	1:A:30:PHE:N	2.21	0.55
1:A:77:ASP:O	1:A:81:SER:HB3	2.07	0.55
1:A:249:LEU:HD23	1:A:288:MET:HE1	1.89	0.55
1:A:326:ARG:NH2	1:B:303:VAL:HG22	2.22	0.54
1:A:624:ASP:HA	1:A:629:HIS:NE2	2.23	0.53
1:B:642:ARG:HH11	1:B:642:ARG:CG	2.21	0.53
1:B:596:ARG:HG2	1:B:596:ARG:NH1	2.24	0.53
1:A:225:LEU:HD21	1:A:381:TYR:OH	2.09	0.53
1:B:368:PRO:HB2	1:B:621:PHE:CZ	2.43	0.53
1:B:231:ASP:HB2	1:B:626:TRP:CZ2	2.44	0.53
1:B:596:ARG:HH11	1:B:596:ARG:HG2	1.74	0.53
1:B:216:ASP:OD1	1:B:218:LYS:N	2.41	0.53
1:B:291:ARG:HH11	1:B:291:ARG:CG	2.22	0.53
1:B:477:ASN:HD22	1:B:477:ASN:C	2.10	0.53
1:A:595:ASN:HB2	1:A:715:ASP:OD1	2.09	0.53
1:A:150:ARG:O	1:A:169:LEU:HB2	2.09	0.53
1:B:498:LYS:O	1:B:517:HIS:HD2	1.92	0.52
1:A:642:ARG:HH11	1:A:642:ARG:HB2	1.73	0.52
1:B:669:LYS:HA	1:B:669:LYS:HZ1	1.75	0.52
1:B:13:THR:HG22	1:B:75:ILE:CD1	2.38	0.52
1:A:326:ARG:HH22	1:B:303:VAL:HG22	1.74	0.52
1:B:94:HIS:CD2	1:B:96:LEU:H	2.22	0.52
1:A:274:LYS:NZ	1:A:276:VAL:HG12	2.24	0.52
1:B:553:ASN:ND2	1:B:555:ALA:H	2.06	0.52
1:A:10:MET:O	1:A:14:LEU:HD23	2.10	0.52
1:B:540:ASN:HB3	1:B:676:ASN:HD22	1.73	0.52
1:A:203:GLU:OE2	1:A:204:GLU:HG3	2.09	0.52
1:B:322:MET:CG	4:B:1160:HOH:O	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:LYS:HB3	1:A:498:LYS:NZ	2.24	0.52
1:B:572:ASN:HB2	1:B:671:ASN:ND2	2.24	0.52
1:A:29:LEU:HD13	1:A:30:PHE:O	2.09	0.52
1:A:130:PRO:HD2	4:A:1536:HOH:O	2.09	0.52
1:A:10:MET:CG	1:A:14:LEU:HD23	2.40	0.52
1:B:8:VAL:HG22	1:B:9:PRO:HD2	1.92	0.51
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.28	0.51
1:B:322:MET:HG3	4:B:1160:HOH:O	2.10	0.51
1:A:679:ALA:HB2	4:A:1524:HOH:O	2.10	0.51
1:A:210:LYS:HA	1:A:210:LYS:HE2	1.92	0.51
1:B:13:THR:HG22	1:B:75:ILE:HD11	1.91	0.51
1:A:326:ARG:CZ	1:B:303:VAL:HG22	2.41	0.51
1:A:377:TYR:CE1	1:B:558:PRO:HG2	2.46	0.51
1:A:700:PRO:HD2	4:A:975:HOH:O	2.11	0.51
1:A:579:LYS:HA	1:A:637:GLN:NE2	2.26	0.51
1:A:203:GLU:N	1:A:203:GLU:CD	2.64	0.51
1:A:94:HIS:HB3	1:A:97:ASN:ND2	2.26	0.50
1:A:643:TYR:O	1:A:644:HIS:CD2	2.64	0.50
1:B:223:THR:HG22	1:B:246:ILE:O	2.11	0.50
1:B:291:ARG:HH11	1:B:291:ARG:HG3	1.77	0.50
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.94	0.50
1:A:477:ASN:HD22	1:A:477:ASN:C	2.14	0.50
1:A:8:VAL:HG22	1:A:9:PRO:CD	2.41	0.50
1:B:669:LYS:HA	1:B:669:LYS:NZ	2.27	0.49
1:A:10:MET:HG3	1:A:14:LEU:CD2	2.43	0.49
1:A:371:ASP:HB3	1:A:376:TRP:HB3	1.94	0.49
1:A:572:ASN:HD21	1:A:575:ASP:CG	2.16	0.49
1:A:580:PHE:H	1:A:637:GLN:NE2	2.05	0.49
1:A:276:VAL:O	1:A:277:LYS:HB2	2.11	0.49
1:B:353:LYS:HE2	4:B:1031:HOH:O	2.12	0.49
1:A:223:THR:HG21	4:A:1302:HOH:O	2.11	0.49
1:B:299:VAL:O	1:B:301:PRO:HD3	2.13	0.49
1:A:274:LYS:HZ3	1:A:276:VAL:HG12	1.78	0.48
1:B:62:VAL:HG12	1:B:64:LYS:HG3	1.95	0.48
1:A:15:LYS:HE2	4:A:1264:HOH:O	2.12	0.48
1:A:725:LYS:N	4:A:1525:HOH:O	2.46	0.48
1:B:94:HIS:CD2	1:B:96:LEU:HB2	2.49	0.48
1:A:38:TYR:N	1:A:51:ASN:HD21	2.08	0.48
1:A:582:PRO:C	1:B:615:VAL:HG12	2.34	0.48
1:A:365:MET:CE	1:A:383:ASN:ND2	2.76	0.48
1:A:460:ILE:HG21	1:B:439:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ASP:OD1	1:B:239:ASP:C	2.51	0.48
1:B:17:PHE:O	1:B:34:LYS:HE2	2.13	0.48
1:A:10:MET:HG3	1:A:14:LEU:HD23	1.95	0.48
1:B:196:GLN:HE22	1:B:222:THR:H	1.62	0.48
1:A:437:GLU:OE2	1:B:700:PRO:HB3	2.14	0.48
1:A:572:ASN:HD22	1:A:575:ASP:H	1.61	0.48
1:A:592:ASN:HD21	1:A:676:ASN:ND2	2.04	0.47
1:B:529:ASN:HA	1:B:683:MET:O	2.14	0.47
1:B:92:ARG:HD2	4:B:1400:HOH:O	2.14	0.47
1:A:382:LEU:CD1	1:A:655:PRO:HB2	2.44	0.47
1:B:536:VAL:H	1:B:541:ASN:HD21	1.62	0.47
1:A:63:MET:HG3	4:A:1350:HOH:O	2.14	0.47
1:A:161:HIS:HB3	4:A:1256:HOH:O	2.15	0.47
1:A:219:LYS:HD2	4:A:1185:HOH:O	2.14	0.47
1:A:149:PRO:HB3	1:A:170:GLN:HB3	1.96	0.47
1:B:644:HIS:CD2	4:B:1003:HOH:O	2.68	0.47
1:B:644:HIS:HD2	4:B:1003:HOH:O	1.97	0.47
1:B:574:GLN:HB2	1:B:671:ASN:CG	2.35	0.47
1:B:27:ALA:C	4:B:827:HOH:O	2.53	0.47
1:A:272:GLN:NE2	1:A:274:LYS:NZ	2.63	0.47
1:B:209:VAL:CG1	1:B:214:ILE:HB	2.45	0.47
1:A:642:ARG:HH12	1:A:672:GLU:HB3	1.80	0.46
1:B:238:GLN:HA	1:B:238:GLN:NE2	2.30	0.46
1:B:22:GLN:HG3	4:B:838:HOH:O	2.14	0.46
1:B:642:ARG:NE	1:B:677:THR:OG1	2.48	0.46
1:B:108:VAL:CG1	1:B:112:LYS:HE3	2.46	0.46
1:B:725:LYS:O	1:B:726:ASP:CG	2.53	0.46
1:A:218:LYS:HE2	4:A:1571:HOH:O	2.15	0.46
1:B:118:LYS:HE2	1:B:118:LYS:HB3	1.41	0.46
1:B:660:HIS:HA	4:B:1242:HOH:O	2.16	0.46
1:A:105:LYS:O	1:A:109:GLU:HG3	2.15	0.46
1:A:642:ARG:NH2	4:A:1398:HOH:O	2.48	0.46
1:B:642:ARG:CG	1:B:642:ARG:NH1	2.77	0.46
1:A:615:VAL:CG2	1:B:582:PRO:HB2	2.46	0.46
1:B:595:ASN:HB2	1:B:715:ASP:OD1	2.16	0.46
1:A:626:TRP:HA	1:A:629:HIS:HD2	1.81	0.46
1:A:218:LYS:HZ3	1:A:218:LYS:HB2	1.81	0.46
1:B:574:GLN:HB2	1:B:671:ASN:ND2	2.30	0.45
1:A:209:VAL:HG12	1:A:214:ILE:HB	1.96	0.45
1:B:8:VAL:HG22	1:B:9:PRO:CD	2.47	0.45
1:A:74:PHE:CE1	1:A:78:VAL:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:VAL:CG2	1:B:9:PRO:CD	2.87	0.45
1:B:699:MET:HA	1:B:700:PRO:HD3	1.74	0.45
1:B:108:VAL:HG13	1:B:112:LYS:HE3	1.99	0.45
1:A:613:HIS:CE1	1:A:702:GLU:HG3	2.51	0.45
1:A:574:GLN:H	1:A:671:ASN:ND2	2.14	0.45
1:A:541:ASN:HD22	1:A:588:LEU:HD21	1.81	0.45
1:B:29:LEU:HD11	1:B:40:LYS:HB3	1.99	0.45
1:A:368:PRO:CG	1:A:634:MET:HE1	2.37	0.45
1:A:697:PRO:HD2	1:B:720:LEU:HD11	1.98	0.45
1:B:580:PHE:N	1:B:637:GLN:HE21	2.07	0.45
1:B:173:LYS:CB	1:B:173:LYS:NZ	2.78	0.45
1:B:51:ASN:N	1:B:51:ASN:HD22	2.14	0.45
1:A:187:VAL:HG22	1:A:243:LEU:HD21	1.97	0.45
1:A:369:TYR:CD2	1:A:524:HIS:HB3	2.52	0.45
1:B:203:GLU:N	1:B:203:GLU:CD	2.70	0.44
1:A:237:LYS:HZ2	1:A:239:ASP:CG	2.19	0.44
1:A:599:ASN:ND2	1:B:500:MET:HG3	2.33	0.44
1:A:366:ILE:CD1	1:A:627:ILE:HD11	2.46	0.44
1:A:150:ARG:N	4:A:1242:HOH:O	2.49	0.44
1:A:131:PRO:CB	1:A:148:GLN:NE2	2.73	0.44
1:A:225:LEU:HD21	1:A:381:TYR:CZ	2.52	0.44
1:A:595:ASN:HD22	1:A:595:ASN:C	2.21	0.44
1:A:599:ASN:ND2	4:A:950:HOH:O	2.49	0.44
1:A:300:ALA:HA	1:A:301:PRO:HD3	1.89	0.44
1:B:595:ASN:ND2	1:B:597:MET:H	2.15	0.44
1:A:608:TYR:HE2	1:B:608:TYR:HE2	1.66	0.43
1:A:597:MET:SD	1:B:516:ASP:HA	2.58	0.43
1:B:227:VAL:CG1	1:B:244:LYS:HG3	2.44	0.43
1:A:366:ILE:HD11	1:A:380:ALA:HB1	2.00	0.43
1:A:228:GLY:HA3	4:A:1599:HOH:O	2.18	0.43
1:A:7:MET:HE2	1:A:7:MET:CA	2.48	0.43
1:B:620:GLN:HG3	4:B:995:HOH:O	2.17	0.43
1:A:209:VAL:CG1	1:A:214:ILE:HB	2.48	0.43
1:B:209:VAL:HG13	1:B:214:ILE:HB	2.01	0.43
1:B:339:GLY:HA3	1:B:340:PRO:HD2	1.82	0.43
1:B:551:LYS:NZ	4:B:1478:HOH:O	2.40	0.43
1:A:624:ASP:CA	1:A:629:HIS:NE2	2.81	0.43
1:A:131:PRO:HG2	1:A:146:VAL:HG11	2.00	0.43
1:B:332:LEU:CD1	1:B:342:ILE:HD13	2.49	0.43
1:A:720:LEU:HA	1:A:720:LEU:HD23	1.87	0.43
1:A:453:ARG:NH2	4:A:1573:HOH:O	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:PHE:CZ	1:B:440:HIS:HD2	2.37	0.43
1:A:208:ALA:O	1:A:212:ARG:HG3	2.18	0.43
1:B:106:GLN:OE1	4:B:1166:HOH:O	2.21	0.43
1:A:623:PRO:O	1:A:629:HIS:CE1	2.72	0.43
1:B:77:ASP:O	1:B:81:SER:HB3	2.19	0.43
1:B:150:ARG:O	1:B:169:LEU:HB2	2.18	0.43
1:B:178:GLN:HA	1:B:179:PRO:HD3	1.86	0.42
1:B:129:LEU:HD12	1:B:130:PRO:HD2	2.01	0.42
1:B:545:ALA:O	1:B:567:GLN:HA	2.19	0.42
1:B:88:GLN:O	1:B:319:THR:HA	2.19	0.42
1:B:332:LEU:HD13	1:B:342:ILE:HD13	2.02	0.42
1:A:465:ASN:HB2	1:A:489:ILE:O	2.19	0.42
1:A:80:GLN:OE1	1:A:80:GLN:N	2.53	0.42
1:A:403:PRO:HG3	1:A:430:PHE:CD2	2.53	0.42
1:B:506:LYS:HE2	1:B:510:ARG:HH22	1.81	0.42
1:B:129:LEU:HA	1:B:130:PRO:HD2	1.81	0.42
1:A:516:ASP:HB3	1:A:519:ILE:HB	2.01	0.42
1:B:632:SER:OG	1:B:661:ASP:OD2	2.35	0.42
1:A:633:PHE:HA	1:A:639:TRP:CZ2	2.55	0.42
1:B:171:ASN:HB3	1:B:173:LYS:HE2	2.01	0.42
1:A:572:ASN:C	1:A:572:ASN:HD22	2.23	0.42
1:B:120:ASN:ND2	4:B:851:HOH:O	2.53	0.42
1:A:272:GLN:NE2	1:A:274:LYS:HZ2	2.17	0.42
1:A:516:ASP:HA	1:B:597:MET:SD	2.60	0.42
1:A:38:TYR:CG	1:A:311:PRO:HA	2.55	0.42
1:B:148:GLN:HB3	4:B:1144:HOH:O	2.19	0.42
1:B:665:GLY:O	1:B:669:LYS:NZ	2.49	0.42
1:A:492:VAL:HB	1:A:519:ILE:HG23	2.00	0.42
1:B:526:HIS:HB2	1:B:687:THR:OG1	2.19	0.42
1:A:580:PHE:CE2	1:A:582:PRO:HA	2.54	0.42
1:B:723:LEU:HA	1:B:723:LEU:HD12	1.90	0.42
1:B:366:ILE:HA	1:B:381:TYR:O	2.19	0.42
1:A:595:ASN:C	1:A:595:ASN:ND2	2.73	0.42
1:A:717:THR:HB	1:A:720:LEU:HG	2.02	0.42
1:B:496:LYS:HE3	4:B:1255:HOH:O	2.19	0.42
1:A:443:MET:CE	1:B:392:LEU:HD22	2.50	0.42
1:B:572:ASN:HD22	1:B:671:ASN:ND2	2.02	0.41
1:A:572:ASN:CB	1:A:671:ASN:HD21	2.32	0.41
1:B:353:LYS:CE	4:B:1031:HOH:O	2.67	0.41
1:A:608:TYR:HE2	1:B:608:TYR:CE2	2.39	0.41
1:B:7:MET:HG2	1:B:71:SER:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:PHE:HA	4:A:1287:HOH:O	2.20	0.41
1:A:237:LYS:NZ	1:A:239:ASP:OD1	2.45	0.41
1:A:288:MET:CE	1:A:288:MET:HA	2.50	0.41
1:B:92:ARG:HA	1:B:93:PRO:HD2	1.85	0.41
1:B:196:GLN:NE2	1:B:222:THR:H	2.18	0.41
1:B:374:ILE:HG13	1:B:375:GLY:N	2.35	0.41
1:A:22:GLN:HG3	4:A:1278:HOH:O	2.20	0.41
1:A:203:GLU:OE2	1:A:204:GLU:OE2	2.39	0.41
1:B:286:VAL:HA	1:B:287:PRO:HD3	1.88	0.41
1:A:118:LYS:HA	1:A:119:PRO:HD3	1.87	0.41
1:B:27:ALA:CA	4:B:827:HOH:O	2.60	0.41
1:A:543:LEU:HD22	1:A:640:VAL:HG21	2.03	0.41
1:A:629:HIS:CD2	1:A:629:HIS:H	2.39	0.41
1:B:368:PRO:HB2	1:B:621:PHE:CE2	2.56	0.41
4:A:959:HOH:O	1:B:563:MET:HB3	2.21	0.41
1:B:208:ALA:O	1:B:211:LYS:HG2	2.21	0.41
1:A:348:ASN:HD21	1:A:351:GLY:CA	2.34	0.41
1:B:406:ALA:HA	1:B:430:PHE:HB3	2.03	0.41
1:A:626:TRP:HA	1:A:629:HIS:CD2	2.55	0.41
1:A:529:ASN:HA	1:A:683:MET:O	2.20	0.41
1:A:529:ASN:HD21	1:A:682:TRP:HE3	1.68	0.41
1:A:149:PRO:HA	4:A:1242:HOH:O	2.21	0.41
1:B:639:TRP:CG	1:B:664:LEU:HD13	2.56	0.41
1:B:7:MET:HB3	1:B:7:MET:HE3	1.90	0.41
1:B:139:PHE:O	1:B:143:ASN:HA	2.21	0.41
1:A:223:THR:CG2	1:A:246:ILE:HB	2.51	0.41
1:A:29:LEU:HD13	1:A:30:PHE:C	2.41	0.41
1:A:608:TYR:CZ	1:A:615:VAL:HG21	2.56	0.41
1:A:132:ASP:HB3	4:A:1567:HOH:O	2.21	0.41
1:A:545:ALA:HB2	1:A:570:ILE:HD11	2.03	0.40
1:B:212:ARG:HH21	1:B:280:GLU:HB3	1.85	0.40
1:A:536:VAL:H	1:A:541:ASN:ND2	2.17	0.40
1:B:382:LEU:N	1:B:382:LEU:HD12	2.36	0.40
1:A:610:GLY:HA3	1:B:610:GLY:HA3	2.04	0.40
1:A:286:VAL:HG12	1:A:288:MET:CE	2.52	0.40
1:B:595:ASN:ND2	1:B:595:ASN:C	2.75	0.40
1:A:374:ILE:HD12	1:A:374:ILE:HA	1.83	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1283:HOH:O	4:B:1261:HOH:O[2_565]	1.53	0.67
4:B:827:HOH:O	4:B:1460:HOH:O[2_565]	1.88	0.32
4:A:1175:HOH:O	4:A:1434:HOH:O[2_565]	2.05	0.15
4:A:1153:HOH:O	4:A:1552:HOH:O[2_565]	2.14	0.06

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	716/721 (99%)	689 (96%)	27 (4%)	0	100	100
1	B	718/721 (100%)	695 (97%)	23 (3%)	0	100	100
All	All	1434/1442 (99%)	1384 (96%)	50 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	609/612 (100%)	590 (97%)	19 (3%)	47	59
1	B	612/612 (100%)	582 (95%)	30 (5%)	31	36
All	All	1221/1224 (100%)	1172 (96%)	49 (4%)	38	47

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	42	LYS
1	A	147	ASP
1	A	148	GLN
1	A	203	GLU
1	A	204	GLU
1	A	210	LYS
1	A	218	LYS
1	A	239	ASP
1	A	348	ASN
1	A	350	ASN
1	A	377	TYR
1	A	445	GLN
1	A	477	ASN
1	A	572	ASN
1	A	595	ASN
1	A	613	HIS
1	A	642	ARG
1	A	671	ASN
1	B	11	ASP
1	B	15	LYS
1	B	47	THR
1	B	91	LYS
1	B	118	LYS
1	B	137	TRP
1	B	173	LYS
1	B	181	LYS
1	B	203	GLU
1	B	211	LYS
1	B	214	ILE
1	B	218	LYS
1	B	237	LYS
1	B	239	ASP
1	B	251	VAL
1	B	274	LYS
1	B	322	MET
1	B	372	PRO
1	B	467	ASP
1	B	477	ASN
1	B	490	GLU
1	B	506	LYS
1	B	539	GLU
1	B	595	ASN

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Mol	Chain	Res	Type
1	B	613	HIS
1	B	642	ARG
1	B	669	LYS
1	B	671	ASN
1	B	676	ASN
1	B	726	ASP

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

Mol	Chain	Res	Type
1	A	22	GLN
1	A	51	ASN
1	A	97	ASN
1	A	148	GLN
1	A	161	HIS
1	A	170	GLN
1	A	178	GLN
1	A	196	GLN
1	A	200	ASN
1	A	272	GLN
1	A	307	GLN
1	A	315	ASN
1	A	324	HIS
1	A	327	ASN
1	A	348	ASN
1	A	383	ASN
1	A	445	GLN
1	A	447	ASN
1	A	477	ASN
1	A	517	HIS
1	A	525	GLN
1	A	529	ASN
1	A	541	ASN
1	A	553	ASN
1	A	567	GLN
1	A	572	ASN
1	A	595	ASN
1	A	599	ASN
1	A	604	GLN
1	A	629	HIS
1	A	637	GLN
1	A	660	HIS

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Mol	Chain	Res	Type
1	A	671	ASN
1	A	676	ASN
1	B	51	ASN
1	B	94	HIS
1	B	97	ASN
1	B	143	ASN
1	B	148	GLN
1	B	196	GLN
1	B	200	ASN
1	B	201	ASN
1	B	238	GLN
1	B	263	ASN
1	B	272	GLN
1	B	315	ASN
1	B	327	ASN
1	B	350	ASN
1	B	383	ASN
1	B	447	ASN
1	B	477	ASN
1	B	501	HIS
1	B	517	HIS
1	B	525	GLN
1	B	529	ASN
1	B	541	ASN
1	B	553	ASN
1	B	567	GLN
1	B	572	ASN
1	B	595	ASN
1	B	599	ASN
1	B	604	GLN
1	B	613	HIS
1	B	637	GLN
1	B	644	HIS
1	B	671	ASN
1	B	676	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPQ	A	466	1	13,14,15	2.67	6 (46%)	15,19,21	1.98	4 (26%)
1	TPQ	B	466	1	13,14,15	2.01	4 (30%)	15,19,21	2.01	3 (20%)

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
1	TPQ	A	466	1	-	0/4/22/24	0/1/1/1
1	TPQ	B	466	1	-	0/4/22/24	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	TPQ	C1-C2	-5.71	1.41	1.49
1	B	466	TPQ	C1-C2	-5.35	1.42	1.49
1	A	466	TPQ	O5-C5	-4.04	1.13	1.24
1	A	466	TPQ	O2-C2	-3.93	1.14	1.24
1	A	466	TPQ	C4-C5	-2.76	1.38	1.47
1	B	466	TPQ	C4-C5	-2.59	1.39	1.47
1	A	466	TPQ	CB-C1	2.02	1.55	1.50
1	B	466	TPQ	C3-C4	2.32	1.39	1.35
1	A	466	TPQ	C6-C1	2.57	1.41	1.34
1	B	466	TPQ	CB-C1	2.57	1.56	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	466	TPQ	O-C-CA	-3.86	115.45	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	466	TPQ	C4-C3-C2	-3.03	116.90	120.77
1	A	466	TPQ	C6-C1-C2	-2.12	116.94	118.44
1	A	466	TPQ	CB-C1-C2	2.32	121.94	118.33
1	B	466	TPQ	CB-C1-C2	3.65	124.02	118.33
1	A	466	TPQ	C3-C2-C1	4.26	121.49	118.30
1	B	466	TPQ	C3-C2-C1	4.71	121.83	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	718/721 (99%)	-0.46	13 (1%)	71	70	14, 25, 44, 65	0
1	B	720/721 (99%)	-0.36	24 (3%)	50	49	16, 26, 46, 66	0
All	All	1438/1442 (99%)	-0.41	37 (2%)	59	58	14, 26, 45, 66	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	PRO	6.9
1	B	302	ALA	5.5
1	B	726	ASP	5.1
1	B	6	HIS	4.6
1	A	64	LYS	4.2
1	A	218	LYS	4.1
1	A	215	THR	3.7
1	B	65	ASP	3.7
1	B	215	THR	3.3
1	B	239	ASP	3.2
1	A	148	GLN	3.2
1	B	92	ARG	3.0
1	B	91	LYS	2.9
1	B	303	VAL	2.9
1	A	65	ASP	2.9
1	A	217	ALA	2.7
1	B	115	ALA	2.6
1	A	12	LYS	2.5
1	A	216	ASP	2.4
1	B	178	GLN	2.4
1	A	503	GLU	2.4
1	A	239	ASP	2.4
1	B	143	ASN	2.3
1	B	300	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	119	PRO	2.3
1	B	64	LYS	2.3
1	B	725	LYS	2.2
1	B	218	LYS	2.2
1	A	506	LYS	2.2
1	B	66	ASN	2.2
1	B	181	LYS	2.1
1	B	670	ASP	2.1
1	B	80	GLN	2.1
1	B	669	LYS	2.1
1	B	120	ASN	2.0
1	A	181	LYS	2.0
1	B	81	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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
1	TPQ	A	466	14/15	0.91	0.20	-	24,50,58,59	0
1	TPQ	B	466	14/15	0.84	0.18	-	24,45,55,57	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	CA	A	802	1/1	1.00	0.13	0.54	25,25,25,25	0
3	CA	B	802	1/1	0.99	0.10	-0.70	25,25,25,25	0
3	CA	A	803	1/1	0.97	0.06	-1.41	47,47,47,47	0
3	CA	B	803	1/1	0.98	0.05	-1.60	45,45,45,45	0
2	CU	B	801	1/1	0.99	0.05	-	26,26,26,26	0
2	CU	A	801	1/1	0.99	0.05	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.