



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 02:18 PM EDT

PDB ID : 3PCM
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 6-HYDROXYNICOTINIC ACID N-OXIDE AND CYANIDE
Authors : Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-07-18
Resolution : 2.25 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)
Xtrriage (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) : 2.35.1

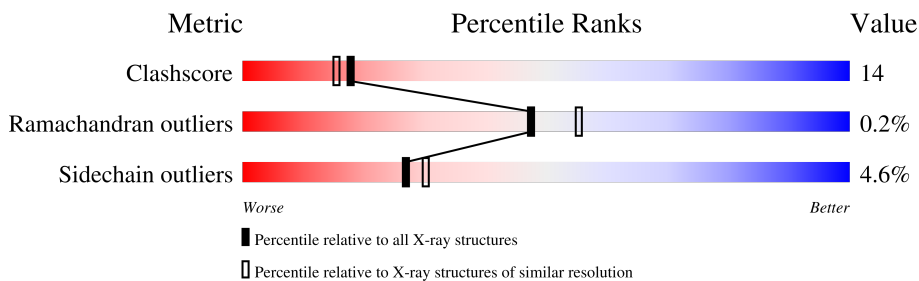
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)





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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	71% 24% .
1	B	200	74% 21% .
1	C	200	74% 22% .
1	D	200	70% 24% 6%
1	E	200	70% 24% .
1	F	200	64% 30% 5%
2	M	238	66% 29% . .
2	N	238	73% 21% . .

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Mol	Chain	Length	Quality of chain
2	O	238	 71% 23% . .
2	P	238	 68% 26% . . .
2	Q	238	 68% 23% 6% .
2	R	238	 69% 24% . . .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 21966 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.

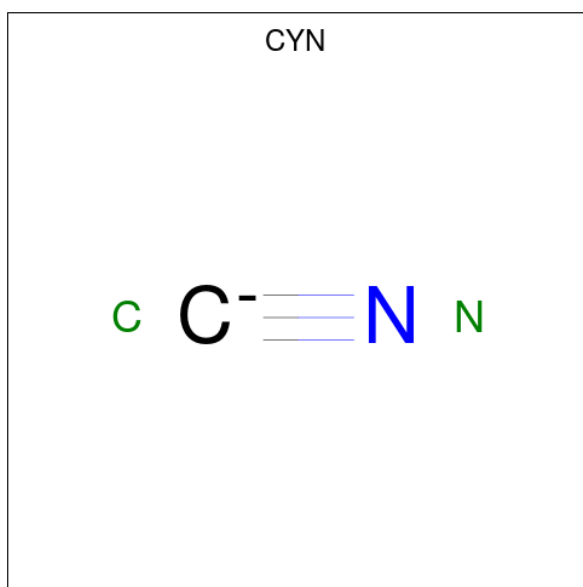
- Molecule 1 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1571	993	276	299	3	0	0	0
1	B	200	1571	993	276	299	3	0	0	0
1	C	200	1571	993	276	299	3	0	0	0
1	D	200	1571	993	276	299	3	0	0	0
1	E	200	1571	993	276	299	3	0	0	0
1	F	200	1571	993	276	299	3	0	0	0

- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	233	1840	1171	334	328	7	0	0	0
2	N	233	1840	1171	334	328	7	0	0	0
2	O	233	1840	1171	334	328	7	0	0	0
2	P	233	1840	1171	334	328	7	0	0	0
2	Q	233	1840	1171	334	328	7	0	0	0
2	R	233	1840	1171	334	328	7	0	0	0

- Molecule 3 is CYANIDE ION (three-letter code: CYN) (formula: CN).

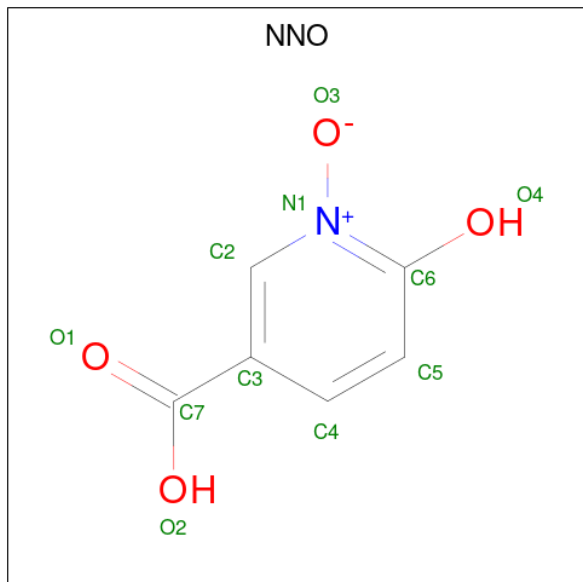


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	N	0	0
			2	1	1		
3	N	1	Total	C	N	0	0
			2	1	1		
3	O	1	Total	C	N	0	0
			2	1	1		
3	P	1	Total	C	N	0	0
			2	1	1		
3	Q	1	Total	C	N	0	0
			2	1	1		
3	R	1	Total	C	N	0	0
			2	1	1		

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		
4	N	1	Total	Fe	0	0
			1	1		
4	O	1	Total	Fe	0	0
			1	1		
4	P	1	Total	Fe	0	0
			1	1		
4	Q	1	Total	Fe	0	0
			1	1		
4	R	1	Total	Fe	0	0
			1	1		

- Molecule 5 is 6-HYDROXYISONICOTINIC ACID N-OXIDE (three-letter code: NNO) (formula: C₆H₅NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	M	1	11	6	1	4	0	0
5	N	1	11	6	1	4	0	0
5	O	1	11	6	1	4	0	0
5	P	1	11	6	1	4	0	0
5	Q	1	11	6	1	4	0	0
5	R	1	11	6	1	4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	77	77	77	0	0
6	M	154	154	154	0	0
6	B	86	86	86	0	0
6	N	156	156	156	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	78	Total 78	O 78	0	0
6	O	156	Total 156	O 156	0	0
6	D	80	Total 80	O 80	0	0
6	P	151	Total 151	O 151	0	0
6	E	79	Total 79	O 79	0	0
6	Q	161	Total 161	O 161	0	0
6	F	78	Total 78	O 78	0	0
6	R	160	Total 160	O 160	0	0

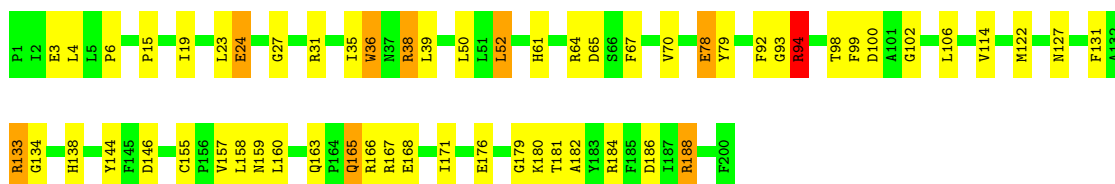
3 Residue-property plots [i](#)

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: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A: 



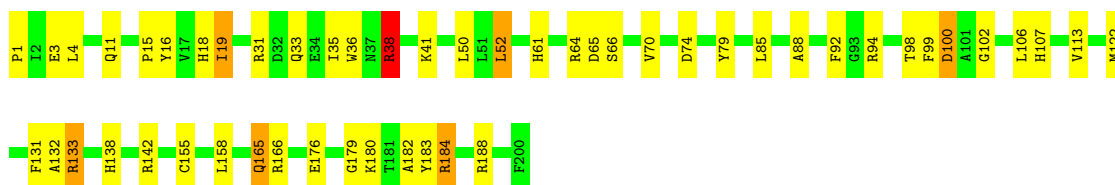
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B: 



- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

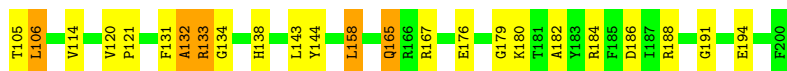
Chain C: 



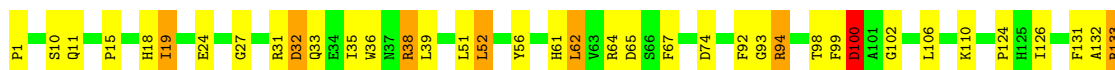
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D: 

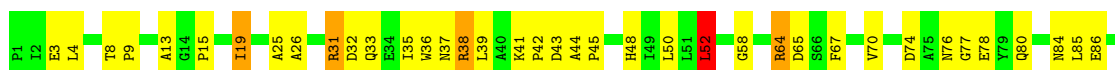




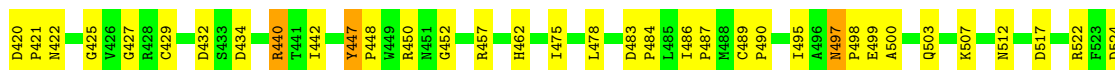
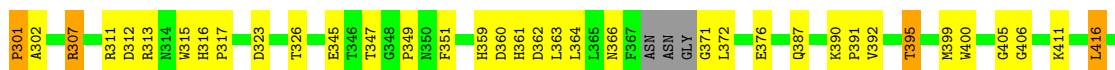
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



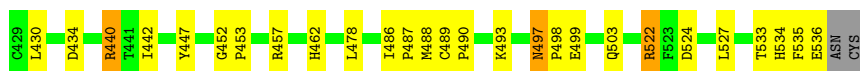
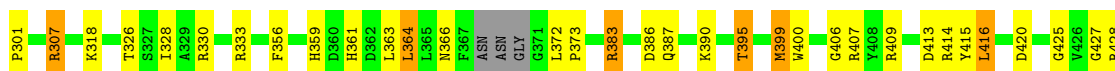
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

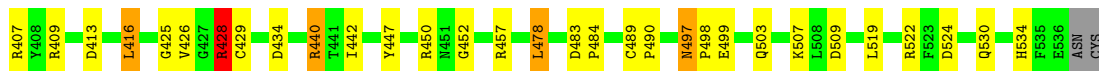


- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

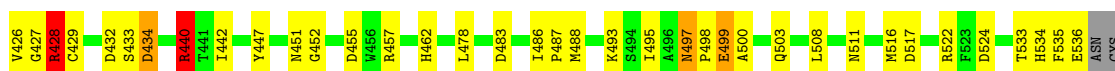
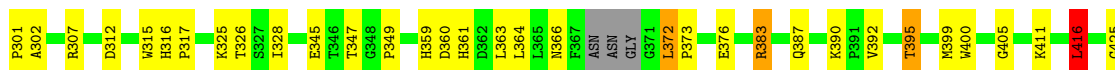


- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

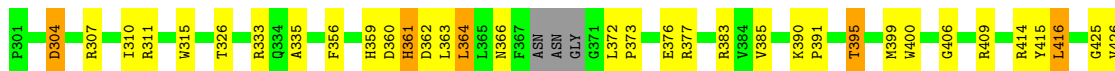




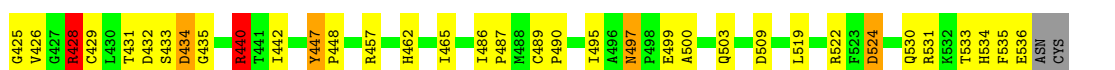
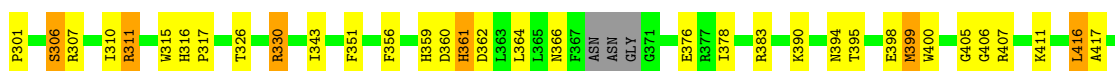
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.10Å 127.30Å 134.50Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.25	Depositor
% Data completeness (in resolution range)	91.0 (6.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	21966	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

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: CYN, NNO, 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	0.87	1/1611 (0.1%)	1.51	17/2195 (0.8%)
1	B	0.88	0/1611	1.51	20/2195 (0.9%)
1	C	0.88	0/1611	1.42	14/2195 (0.6%)
1	D	0.87	0/1611	1.47	19/2195 (0.9%)
1	E	0.88	0/1611	1.39	17/2195 (0.8%)
1	F	0.93	0/1611	1.54	14/2195 (0.6%)
2	M	0.93	1/1895 (0.1%)	1.46	21/2580 (0.8%)
2	N	0.92	0/1895	1.43	16/2580 (0.6%)
2	O	0.92	0/1895	1.51	26/2580 (1.0%)
2	P	0.94	1/1895 (0.1%)	1.46	22/2580 (0.9%)
2	Q	0.96	2/1895 (0.1%)	1.54	26/2580 (1.0%)
2	R	0.95	0/1895	1.45	17/2580 (0.7%)
All	All	0.91	5/21036 (0.0%)	1.48	229/28650 (0.8%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	345	GLU	CD-OE1	-6.08	1.19	1.25
1	A	94	ARG	CD-NE	-5.79	1.36	1.46
2	P	345	GLU	CD-OE1	-5.59	1.19	1.25
2	Q	433	SER	CB-OG	5.33	1.49	1.42
2	Q	428	ARG	CD-NE	-5.14	1.37	1.46

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	94	ARG	NE-CZ-NH1	22.79	131.70	120.30
1	A	94	ARG	CD-NE-CZ	19.61	151.05	123.60
2	P	440	ARG	NE-CZ-NH2	-16.40	112.10	120.30
2	N	440	ARG	NE-CZ-NH2	-14.88	112.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	ARG	NE-CZ-NH2	-14.88	112.86	120.30
1	D	94	ARG	NE-CZ-NH2	-14.80	112.90	120.30
2	P	428	ARG	NE-CZ-NH1	14.74	127.67	120.30
1	B	94	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	A	94	ARG	NE-CZ-NH1	14.00	127.30	120.30
1	F	94	ARG	NE-CZ-NH2	-13.83	113.39	120.30
2	Q	428	ARG	CD-NE-CZ	12.99	141.79	123.60
2	Q	414	ARG	NE-CZ-NH1	12.22	126.41	120.30
2	R	428	ARG	NE-CZ-NH1	11.98	126.29	120.30
1	A	94	ARG	NE-CZ-NH2	-11.78	114.41	120.30
2	O	428	ARG	NE-CZ-NH1	11.76	126.18	120.30
2	M	450	ARG	NE-CZ-NH1	11.75	126.18	120.30
2	O	457	ARG	NE-CZ-NH1	11.62	126.11	120.30
2	R	440	ARG	NE-CZ-NH2	-11.58	114.51	120.30
2	Q	428	ARG	NE-CZ-NH1	11.50	126.05	120.30
2	O	428	ARG	CD-NE-CZ	11.39	139.55	123.60
1	C	142	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	D	94	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	A	133	ARG	NE-CZ-NH2	-10.36	115.12	120.30
2	M	440	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	D	184	ARG	NE-CZ-NH1	9.84	125.22	120.30
2	O	311	ARG	NE-CZ-NH2	-9.63	115.48	120.30
2	Q	377	ARG	NE-CZ-NH1	-9.60	115.50	120.30
2	N	409	ARG	NE-CZ-NH1	-9.43	115.58	120.30
2	O	330	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	D	186	ASP	CB-CG-OD1	9.42	126.78	118.30
2	Q	440	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	B	133	ARG	NE-CZ-NH2	-9.30	115.65	120.30
2	N	457	ARG	NE-CZ-NH2	-9.00	115.80	120.30
2	Q	311	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	A	184	ARG	NE-CZ-NH2	-8.81	115.89	120.30
2	N	409	ARG	NE-CZ-NH2	8.77	124.69	120.30
2	M	524	ASP	CB-CG-OD1	8.56	126.01	118.30
1	E	166	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	B	38	ARG	NE-CZ-NH2	-8.51	116.05	120.30
2	Q	428	ARG	NE-CZ-NH2	-8.48	116.06	120.30
2	O	333	ARG	NE-CZ-NH2	-8.44	116.08	120.30
2	Q	522	ARG	NE-CZ-NH1	-8.40	116.10	120.30
2	Q	457	ARG	NE-CZ-NH1	8.33	124.46	120.30
2	O	457	ARG	NE-CZ-NH2	-8.29	116.16	120.30
2	N	307	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	166	ARG	NE-CZ-NH1	8.25	124.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	428	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	D	167	ARG	NE-CZ-NH1	8.22	124.41	120.30
2	O	428	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	E	133	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	B	133	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	C	184	ARG	NE-CZ-NH1	7.93	124.26	120.30
2	O	440	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	C	188	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	A	31	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	D	38	ARG	CD-NE-CZ	-7.67	112.86	123.60
1	D	65	ASP	CB-CG-OD1	7.67	125.20	118.30
2	P	428	ARG	NE-CZ-NH2	-7.66	116.47	120.30
2	Q	409	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	D	184	ARG	NE-CZ-NH2	-7.60	116.50	120.30
2	M	313	ARG	NE-CZ-NH1	7.56	124.08	120.30
2	Q	457	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	146	ASP	CB-CG-OD1	7.38	124.94	118.30
2	N	428	ARG	CD-NE-CZ	7.34	133.88	123.60
1	F	31	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	B	74	ASP	CB-CG-OD1	7.24	124.82	118.30
2	O	440	ARG	CD-NE-CZ	-7.21	113.50	123.60
2	Q	377	ARG	CD-NE-CZ	-7.20	113.52	123.60
1	D	133	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	E	166	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	81	ASP	CB-CG-OD1	7.12	124.70	118.30
2	R	457	ARG	CD-NE-CZ	7.11	133.55	123.60
1	B	186	ASP	CB-CG-OD1	7.11	124.70	118.30
2	O	360	ASP	CB-CG-OD2	-7.08	111.92	118.30
2	Q	304	ASP	CB-CG-OD1	7.08	124.67	118.30
2	Q	428	ARG	CG-CD-NE	7.04	126.58	111.80
1	B	184	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	166	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	B	94	ARG	CG-CD-NE	7.01	126.51	111.80
2	R	524	ASP	CB-CG-OD2	-6.97	112.03	118.30
2	O	330	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	186	ASP	CB-CG-OD1	6.88	124.49	118.30
1	E	94	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	F	94	ARG	CD-NE-CZ	6.85	133.19	123.60
2	R	531	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	P	428	ARG	CG-CD-NE	6.79	126.07	111.80
1	D	188	ARG	NE-CZ-NH1	6.77	123.69	120.30
2	O	323	ASP	CB-CG-OD1	6.76	124.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	428	ARG	CG-CD-NE	6.76	126.00	111.80
1	D	133	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	F	166	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	M	528	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	E	38	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	166	ARG	NE-CZ-NH2	-6.65	116.97	120.30
2	N	383	ARG	NE-CZ-NH2	-6.65	116.97	120.30
2	R	407	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	M	312	ASP	CB-CG-OD2	-6.46	112.49	118.30
2	Q	333	ARG	NE-CZ-NH2	-6.45	117.07	120.30
2	M	457	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	Q	360	ASP	CB-CG-OD1	6.42	124.08	118.30
2	M	312	ASP	CB-CG-OD1	6.37	124.03	118.30
2	P	440	ARG	NH1-CZ-NH2	6.35	126.39	119.40
2	P	457	ARG	CD-NE-CZ	6.34	132.48	123.60
2	M	307	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	N	420	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	C	11	GLN	N-CA-CB	6.31	121.95	110.60
2	P	457	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	P	457	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	94	ARG	NE-CZ-NH1	-6.23	117.18	120.30
2	N	522	ARG	CD-NE-CZ	6.19	132.26	123.60
1	C	133	ARG	CA-CB-CG	6.18	127.00	113.40
2	M	311	ARG	CD-NE-CZ	6.17	132.24	123.60
1	F	36	TRP	CB-CA-C	6.12	122.65	110.40
1	F	64	ARG	NE-CZ-NH1	-6.12	117.24	120.30
2	N	307	ARG	NE-CZ-NH1	6.11	123.36	120.30
2	M	440	ARG	CD-NE-CZ	-6.03	115.15	123.60
2	Q	524	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	146	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	78	GLU	OE1-CD-OE2	5.94	130.43	123.30
1	E	142	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	P	524	ASP	CB-CG-OD1	5.91	123.62	118.30
1	E	31	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	65	ASP	CB-CG-OD1	5.88	123.59	118.30
2	R	407	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	R	432	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	F	133	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	E	133	ARG	CA-CB-CG	5.83	126.22	113.40
2	R	509	ASP	CB-CG-OD1	5.83	123.54	118.30
1	F	183	TYR	CA-CB-CG	5.82	124.45	113.40
1	E	100	ASP	CB-CG-OD2	5.82	123.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	323	ASP	CB-CG-OD1	5.81	123.53	118.30
2	P	383	ARG	CD-NE-CZ	-5.81	115.46	123.60
1	F	52	LEU	CA-CB-CG	5.81	128.66	115.30
1	F	186	ASP	CB-CG-OD1	5.80	123.52	118.30
2	R	434	ASP	CB-CG-OD2	-5.79	113.09	118.30
2	P	447	TYR	N-CA-CB	-5.78	100.19	110.60
2	P	432	ASP	CB-CG-OD1	5.73	123.46	118.30
2	O	313	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	52	LEU	CA-CB-CG	5.69	128.40	115.30
2	O	307	ARG	NE-CZ-NH1	5.69	123.15	120.30
2	O	407	ARG	NE-CZ-NH2	-5.69	117.46	120.30
2	M	323	ASP	CB-CG-OD2	-5.66	113.20	118.30
2	R	457	ARG	CA-CB-CG	5.66	125.85	113.40
2	N	440	ARG	NH1-CZ-NH2	5.66	125.62	119.40
2	M	524	ASP	CB-CG-OD2	-5.62	113.24	118.30
2	N	524	ASP	CB-CG-OD1	5.62	123.36	118.30
1	F	199	ASP	CB-CG-OD2	5.62	123.36	118.30
1	E	133	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	57	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	81	ASP	CB-CG-OD2	-5.59	113.27	118.30
2	Q	361	HIS	CA-CB-CG	-5.59	104.09	113.60
2	R	447	TYR	N-CA-CB	-5.58	100.55	110.60
1	A	38	ARG	CD-NE-CZ	-5.58	115.79	123.60
2	O	450	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	36	TRP	CB-CA-C	5.57	121.55	110.40
1	D	188	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	133	ARG	CA-CB-CG	5.56	125.63	113.40
1	C	133	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	E	74	ASP	CB-CG-OD1	5.55	123.30	118.30
2	P	452	GLY	N-CA-C	-5.55	99.22	113.10
2	M	457	ARG	CD-NE-CZ	5.54	131.36	123.60
2	N	452	GLY	N-CA-C	-5.54	99.25	113.10
1	E	38	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	O	524	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	43	ASP	CB-CG-OD1	5.52	123.27	118.30
1	F	38	ARG	CD-NE-CZ	-5.51	115.89	123.60
2	O	353	HIS	CA-CB-CG	-5.50	104.24	113.60
2	M	411	LYS	CA-CB-CG	5.50	125.51	113.40
1	E	36	TRP	CB-CA-C	5.49	121.38	110.40
1	B	186	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	C	188	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	64	ARG	CD-NE-CZ	-5.44	115.98	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	330	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	31	ARG	NE-CZ-NH2	-5.43	117.59	120.30
2	M	450	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	167	ARG	CD-NE-CZ	-5.42	116.01	123.60
1	D	78	GLU	CG-CD-OE2	-5.42	107.47	118.30
1	A	188	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	F	13	ALA	CB-CA-C	5.40	118.19	110.10
1	C	36	TRP	CB-CA-C	5.38	121.16	110.40
2	O	409	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	A	52	LEU	CB-CA-C	5.33	120.32	110.20
2	R	362	ASP	CB-CG-OD2	5.31	123.08	118.30
2	P	432	ASP	CB-CG-OD2	-5.30	113.53	118.30
2	Q	452	GLY	N-CA-C	-5.28	99.91	113.10
2	P	517	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	183	TYR	N-CA-CB	5.25	120.06	110.60
1	D	36	TRP	CB-CA-C	5.24	120.89	110.40
2	N	457	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	52	LEU	CA-CB-CG	5.23	127.33	115.30
2	P	312	ASP	CB-CG-OD1	5.23	123.01	118.30
2	N	420	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	62	LEU	CA-CB-CG	5.21	127.27	115.30
2	P	499	GLU	CA-CB-CG	5.20	124.84	113.40
2	M	517	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	94	ARG	CD-NE-CZ	5.16	130.82	123.60
1	E	186	ASP	CB-CG-OD1	5.15	122.94	118.30
2	R	361	HIS	CA-CB-CG	-5.15	104.84	113.60
2	M	432	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	A	23	LEU	CB-CA-C	5.13	119.95	110.20
2	Q	360	ASP	CB-CA-C	5.13	120.67	110.40
2	M	452	GLY	N-CA-C	-5.13	100.28	113.10
2	Q	430	LEU	N-CA-CB	-5.12	100.15	110.40
1	C	183	TYR	N-CA-CB	5.12	119.82	110.60
2	P	416	LEU	CB-CA-C	5.12	119.93	110.20
1	C	166	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	C	38	ARG	CD-NE-CZ	-5.11	116.45	123.60
2	P	372	LEU	CB-CA-C	5.10	119.89	110.20
2	O	409	ARG	NE-CZ-NH1	-5.09	117.75	120.30
2	O	452	GLY	N-CA-C	-5.09	100.37	113.10
2	Q	377	ARG	NE-CZ-NH2	5.09	122.85	120.30
2	N	414	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	Q	499	GLU	CA-CB-CG	5.09	124.59	113.40
1	C	183	TYR	CB-CG-CD2	5.08	124.05	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	174	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	M	447	TYR	N-CA-CB	-5.08	101.46	110.60
2	O	413	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	158	LEU	CB-CA-C	5.07	119.83	110.20
2	P	517	ASP	CB-CG-OD2	-5.06	113.75	118.30
2	Q	383	ARG	CD-NE-CZ	-5.05	116.53	123.60
2	Q	522	ARG	CD-NE-CZ	-5.04	116.54	123.60
2	R	311	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	O	457	ARG	CD-NE-CZ	5.04	130.66	123.60
2	P	428	ARG	CD-NE-CZ	5.02	130.63	123.60
2	Q	524	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	D	106	LEU	CA-CB-CG	5.01	126.83	115.30
2	P	428	ARG	CB-CG-CD	5.01	124.64	111.60
1	E	32	ASP	CB-CG-OD2	-5.01	113.79	118.30
2	O	509	ASP	CB-CG-OD1	5.00	122.80	118.30

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	1571	0	1499	46	0
1	B	1571	0	1499	37	0
1	C	1571	0	1499	40	0
1	D	1571	0	1499	51	0
1	E	1571	0	1499	52	0
1	F	1571	0	1499	60	0
2	M	1840	0	1794	55	0
2	N	1840	0	1794	48	0
2	O	1840	0	1794	48	0
2	P	1840	0	1794	54	0
2	Q	1840	0	1794	59	0
2	R	1840	0	1794	55	0
3	M	2	0	0	1	0
3	N	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	2	0	0	1	0
3	P	2	0	0	1	0
3	Q	2	0	0	1	0
3	R	2	0	0	1	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
5	M	11	0	3	0	0
5	N	11	0	3	0	0
5	O	11	0	3	0	0
5	P	11	0	3	0	0
5	Q	11	0	3	0	0
5	R	11	0	3	0	0
6	A	77	0	0	1	0
6	B	86	0	0	0	0
6	C	78	0	0	0	0
6	D	80	0	0	1	0
6	E	79	0	0	3	0
6	F	78	0	0	0	0
6	M	154	0	0	7	0
6	N	156	0	0	4	0
6	O	156	0	0	4	0
6	P	151	0	0	7	0
6	Q	161	0	0	5	0
6	R	160	0	0	5	0
All	All	21966	0	19776	548	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (548) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLN:H	1:B:165:GLN:NE2	1.49	1.09
1:C:64:ARG:NH1	1:C:100:ASP:O	1.92	1.02
1:F:64:ARG:NH1	1:F:100:ASP:O	1.92	1.00
1:B:165:GLN:HE21	1:B:165:GLN:N	1.59	1.00
1:D:64:ARG:NH1	1:D:100:ASP:O	1.93	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:GLN:H	1:F:165:GLN:NE2	1.68	0.91
2:N:390:LYS:HE2	6:N:723:HOH:O	1.69	0.91
2:N:390:LYS:HD3	6:N:647:HOH:O	1.73	0.88
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.56	0.88
2:R:497:ASN:HD22	2:R:499:GLU:H	1.22	0.88
1:A:64:ARG:NH1	1:A:100:ASP:O	2.06	0.88
1:E:165:GLN:H	1:E:165:GLN:HE21	1.21	0.88
1:D:165:GLN:H	1:D:165:GLN:HE21	1.16	0.88
1:F:165:GLN:H	1:F:165:GLN:HE21	1.18	0.88
1:B:64:ARG:NH1	1:B:100:ASP:O	2.07	0.86
2:M:390:LYS:HD2	6:M:641:HOH:O	1.74	0.86
2:Q:361:HIS:CD2	2:Q:361:HIS:H	1.91	0.86
1:E:64:ARG:NH1	1:E:100:ASP:O	2.08	0.85
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.57	0.85
1:D:78:GLU:HG2	2:P:301:PRO:HG2	1.58	0.84
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.60	0.83
2:Q:390:LYS:HD3	6:Q:1020:HOH:O	1.77	0.83
1:F:176:GLU:HG3	1:F:180:LYS:O	1.79	0.83
2:R:497:ASN:ND2	2:R:499:GLU:H	1.75	0.83
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.62	0.81
1:D:134:GLY:HA3	2:P:326:THR:HG22	1.60	0.81
1:A:165:GLN:H	1:A:165:GLN:NE2	1.79	0.81
2:N:488:MET:CE	1:C:1:PRO:HG3	2.10	0.80
2:R:361:HIS:H	2:R:361:HIS:CD2	1.98	0.78
1:C:165:GLN:H	1:C:165:GLN:NE2	1.81	0.78
1:F:33:GLN:HG2	1:F:85:LEU:HD12	1.66	0.77
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.32	0.77
2:M:361:HIS:H	2:M:361:HIS:CD2	2.02	0.77
1:C:165:GLN:H	1:C:165:GLN:HE21	1.29	0.77
1:E:165:GLN:H	1:E:165:GLN:NE2	1.83	0.77
2:P:361:HIS:H	2:P:361:HIS:CD2	1.99	0.76
2:N:497:ASN:ND2	2:N:499:GLU:H	1.83	0.76
1:B:176:GLU:HG3	1:B:180:LYS:O	1.85	0.76
1:D:165:GLN:H	1:D:165:GLN:NE2	1.82	0.76
2:R:306:SER:CB	2:R:530:GLN:HE21	1.98	0.76
2:O:497:ASN:HD22	2:O:499:GLU:H	1.34	0.75
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.68	0.75
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.68	0.75
2:N:497:ASN:HD22	2:N:499:GLU:H	1.32	0.75
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.67	0.75
2:N:453:PRO:HB2	2:O:310:ILE:HD12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.32	0.74
2:M:497:ASN:HD22	2:M:499:GLU:H	1.32	0.73
2:Q:497:ASN:ND2	2:Q:499:GLU:OE1	2.20	0.73
1:A:70:VAL:HG11	1:A:106:LEU:HD21	1.71	0.73
2:R:361:HIS:H	2:R:361:HIS:HD2	1.37	0.73
2:P:361:HIS:H	2:P:361:HIS:HD2	1.37	0.72
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.04	0.72
2:O:497:ASN:ND2	2:O:499:GLU:H	1.86	0.72
1:B:165:GLN:H	1:B:165:GLN:HE21	0.76	0.72
1:D:78:GLU:CG	2:P:301:PRO:HG2	2.21	0.71
1:D:176:GLU:HG3	1:D:180:LYS:O	1.90	0.71
2:M:361:HIS:H	2:M:361:HIS:HD2	1.39	0.70
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.57	0.70
1:F:3:GLU:OE1	1:F:3:GLU:HA	1.92	0.69
1:A:176:GLU:HG3	1:A:180:LYS:O	1.93	0.69
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.57	0.69
1:B:103:GLU:OE2	1:B:184:ARG:NH2	2.23	0.69
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.42	0.68
2:R:536:GLU:HB2	6:R:1336:HOH:O	1.93	0.68
2:N:361:HIS:CD2	2:N:361:HIS:H	2.11	0.68
1:E:100:ASP:OD1	1:E:100:ASP:N	2.26	0.68
2:Q:522:ARG:NH1	6:Q:1057:HOH:O	2.26	0.67
2:M:536:GLU:HB2	6:M:698:HOH:O	1.95	0.67
2:P:497:ASN:HD22	2:P:499:GLU:H	1.41	0.67
2:Q:399:MET:HA	2:Q:462:HIS:O	1.96	0.66
2:M:497:ASN:ND2	2:M:499:GLU:H	1.93	0.66
2:Q:356:PHE:CZ	2:Q:430:LEU:HD13	2.30	0.66
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.28	0.66
1:D:65:ASP:OD2	1:D:133:ARG:HD3	1.96	0.66
2:O:361:HIS:H	2:O:361:HIS:CD2	2.14	0.65
1:D:100:ASP:OD1	1:D:100:ASP:N	2.28	0.65
2:O:390:LYS:HE2	6:O:727:HOH:O	1.96	0.65
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.60	0.65
1:D:79:TYR:O	2:P:301:PRO:HB3	1.96	0.65
2:N:488:MET:HE2	1:C:1:PRO:HG3	1.77	0.65
1:C:19:ILE:O	2:O:426:VAL:HG21	1.98	0.64
2:Q:390:LYS:HE2	6:Q:1137:HOH:O	1.97	0.64
2:R:416:LEU:C	2:R:416:LEU:HD23	2.18	0.64
2:M:416:LEU:C	2:M:416:LEU:HD23	2.17	0.64
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.33	0.64
1:A:79:TYR:O	2:M:301:PRO:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:522:ARG:NH1	6:M:665:HOH:O	2.28	0.63
2:R:364:LEU:HD22	2:R:440:ARG:HD3	1.81	0.63
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.79	0.63
2:R:497:ASN:HD22	2:R:499:GLU:N	1.93	0.63
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.27	0.63
2:P:497:ASN:ND2	2:P:499:GLU:H	1.96	0.62
2:O:356:PHE:HD1	2:O:428:ARG:HD2	1.65	0.62
1:F:48:HIS:HA	1:F:109:VAL:HG12	1.82	0.62
1:F:176:GLU:OE2	1:F:179:GLY:HA2	2.00	0.62
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.34	0.62
2:M:359:HIS:O	2:M:366:ASN:HB3	2.00	0.62
2:O:356:PHE:CE1	2:O:428:ARG:HD3	2.35	0.62
1:F:70:VAL:HG21	1:F:106:LEU:HD21	1.81	0.61
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.65	0.61
1:D:35:ILE:HG22	1:D:94:ARG:HG3	1.82	0.61
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.34	0.61
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.83	0.61
1:F:78:GLU:CD	2:R:301:PRO:HG3	2.21	0.61
2:N:400:TRP:HA	2:N:425:GLY:O	2.00	0.61
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.98	0.61
2:Q:364:LEU:HD11	2:Q:442:ILE:HG23	1.81	0.61
1:A:134:GLY:HA3	2:M:326:THR:HG22	1.83	0.60
2:N:359:HIS:O	2:N:366:ASN:HB3	2.01	0.60
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.81	0.60
2:P:416:LEU:C	2:P:416:LEU:HD23	2.22	0.60
1:F:25:ALA:O	2:R:411:LYS:NZ	2.34	0.60
2:O:478:LEU:HD23	2:O:478:LEU:C	2.21	0.60
1:F:19:ILE:O	2:R:426:VAL:HG21	2.01	0.60
1:F:131:PHE:O	1:F:132:ALA:HB2	2.02	0.60
2:P:405:GLY:HA3	6:P:651:HOH:O	2.02	0.59
1:B:176:GLU:OE2	1:B:179:GLY:O	2.20	0.59
1:F:50:LEU:O	1:F:182:ALA:HA	2.01	0.59
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.65	0.59
1:E:24:GLU:O	1:E:27:GLY:N	2.35	0.59
2:N:399:MET:HA	2:N:462:HIS:O	2.01	0.59
1:A:78:GLU:HG2	2:M:301:PRO:HG3	1.84	0.59
1:E:35:ILE:HG21	1:E:92:PHE:HE2	1.68	0.58
2:Q:364:LEU:HD22	2:Q:440:ARG:HD3	1.85	0.58
1:C:79:TYR:O	2:O:301:PRO:HB3	2.03	0.58
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.03	0.58
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:PRO:HD2	3:O:575:CYN:N	2.17	0.58
2:O:359:HIS:O	2:O:366:ASN:HB3	2.03	0.58
1:D:131:PHE:O	1:D:132:ALA:HB2	2.03	0.58
2:R:406:GLY:O	2:R:447:TYR:HD1	1.87	0.58
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.03	0.58
2:R:497:ASN:HD22	2:R:497:ASN:C	2.08	0.57
2:P:390:LYS:HD2	6:P:648:HOH:O	2.05	0.57
2:N:364:LEU:HD12	2:N:373:PRO:HG2	1.86	0.57
1:E:176:GLU:HG3	1:E:180:LYS:O	2.04	0.57
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.40	0.57
2:P:400:TRP:HA	2:P:425:GLY:O	2.04	0.57
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.04	0.57
1:B:70:VAL:HG21	1:B:106:LEU:HD21	1.85	0.56
1:B:147:ASP:OD2	1:B:174:ARG:NH1	2.38	0.56
1:F:115:ASN:HA	1:F:121:PRO:HA	1.86	0.56
1:B:168:GLU:HA	1:B:171:ILE:HD12	1.87	0.56
2:R:536:GLU:HG3	6:R:1229:HOH:O	2.04	0.56
1:D:77:GLY:O	1:D:114:VAL:HG12	2.05	0.56
2:R:416:LEU:HD23	2:R:417:ALA:N	2.19	0.56
2:O:326:THR:HG22	2:O:326:THR:O	2.06	0.56
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.35	0.56
2:N:361:HIS:H	2:N:361:HIS:HD2	1.54	0.56
1:C:176:GLU:HG3	1:C:180:LYS:O	2.06	0.56
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.26	0.56
1:A:176:GLU:HA	1:A:180:LYS:O	2.05	0.56
3:M:575:CYN:N	6:M:602:HOH:O	2.33	0.56
2:P:376:GLU:O	2:P:442:ILE:HA	2.05	0.56
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.39	0.56
2:N:415:TYR:CE1	2:N:416:LEU:HD22	2.42	0.55
1:F:176:GLU:HG3	1:F:180:LYS:C	2.26	0.55
2:Q:364:LEU:CD2	2:Q:440:ARG:HD3	2.36	0.55
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.54	0.55
1:B:165:GLN:NE2	1:B:165:GLN:N	2.34	0.55
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	2.02	0.55
1:D:176:GLU:HG2	1:D:179:GLY:HA2	1.88	0.55
1:F:35:ILE:HD13	2:R:351:PHE:CE1	2.41	0.55
1:F:37:ASN:HB2	1:F:106:LEU:HD12	1.87	0.55
1:D:98:THR:O	1:D:102:GLY:HA2	2.07	0.55
1:F:143:LEU:C	1:F:143:LEU:HD23	2.26	0.55
1:C:100:ASP:OD1	1:C:100:ASP:N	2.39	0.54
1:A:176:GLU:OE2	1:A:179:GLY:HA2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:GLU:OE1	1:C:3:GLU:HA	2.05	0.54
2:Q:356:PHE:HD1	2:Q:428:ARG:HD2	1.72	0.54
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	2.05	0.54
1:E:98:THR:O	1:E:102:GLY:HA2	2.08	0.54
1:F:3:GLU:OE1	1:F:3:GLU:CA	2.55	0.54
2:M:406:GLY:O	2:M:447:TYR:HD1	1.91	0.54
2:N:383:ARG:NE	2:N:434:ASP:O	2.40	0.54
2:Q:356:PHE:HZ	2:Q:430:LEU:HD13	1.73	0.54
1:E:143:LEU:HD23	1:E:143:LEU:C	2.28	0.54
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.89	0.54
2:O:522:ARG:NH1	6:O:673:HOH:O	2.36	0.54
1:F:15:PRO:HD2	3:R:575:CYN:N	2.22	0.54
2:N:497:ASN:HD22	2:N:497:ASN:C	2.10	0.54
2:O:406:GLY:O	2:O:447:TYR:HD1	1.90	0.54
2:O:416:LEU:C	2:O:416:LEU:HD23	2.27	0.54
1:D:78:GLU:CD	2:P:301:PRO:HG2	2.28	0.54
1:D:143:LEU:C	1:D:143:LEU:HD23	2.28	0.54
1:D:165:GLN:HE21	1:D:165:GLN:N	1.97	0.54
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.43	0.54
2:Q:487:PRO:O	2:Q:493:LYS:HD3	2.08	0.53
1:F:165:GLN:HE21	1:F:165:GLN:N	1.97	0.53
1:F:174:ARG:HB2	1:F:183:TYR:CE1	2.43	0.53
1:B:15:PRO:HB3	1:B:133:ARG:HD2	1.90	0.53
2:O:376:GLU:O	2:O:442:ILE:HA	2.08	0.53
1:F:19:ILE:HG22	1:F:26:ALA:HB1	1.90	0.53
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.43	0.53
2:O:356:PHE:HE1	2:O:428:ARG:HD3	1.74	0.53
1:D:134:GLY:CA	2:P:326:THR:HG22	2.37	0.53
2:M:416:LEU:C	2:M:416:LEU:CD2	2.77	0.53
2:M:405:GLY:HA3	6:M:644:HOH:O	2.07	0.53
1:B:98:THR:O	1:B:102:GLY:HA2	2.08	0.53
1:F:15:PRO:HB3	1:F:133:ARG:HD2	1.90	0.53
2:R:405:GLY:HA3	6:R:1260:HOH:O	2.09	0.53
2:R:306:SER:HB3	2:R:530:GLN:HE21	1.73	0.53
2:R:359:HIS:O	2:R:366:ASN:HB3	2.08	0.53
1:C:65:ASP:OD2	1:C:133:ARG:HD3	2.08	0.53
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.45	0.53
1:E:19:ILE:O	2:Q:426:VAL:HG21	2.09	0.53
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.24	0.52
2:N:363:LEU:HD11	2:N:427:GLY:HA3	1.91	0.52
1:F:74:ASP:OD1	1:F:74:ASP:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:PRO:HB3	1:C:133:ARG:HD2	1.92	0.52
1:E:15:PRO:HD2	3:Q:575:CYN:N	2.25	0.52
1:A:165:GLN:H	1:A:165:GLN:CD	2.13	0.52
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.44	0.52
1:B:176:GLU:HG3	1:B:180:LYS:C	2.30	0.52
2:O:306:SER:CB	2:O:530:GLN:HE21	2.23	0.52
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.73	0.52
2:M:399:MET:HA	2:M:462:HIS:O	2.10	0.51
2:O:385:VAL:HA	2:O:390:LYS:O	2.10	0.51
2:Q:483:ASP:HB3	2:Q:486:ILE:HG13	1.91	0.51
1:D:33:GLN:HB3	1:D:85:LEU:CD1	2.41	0.51
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.92	0.51
2:O:306:SER:OG	2:O:530:GLN:NE2	2.37	0.51
2:O:364:LEU:HD11	2:O:442:ILE:HG23	1.93	0.51
1:D:15:PRO:HD2	3:P:575:CYN:N	2.26	0.51
2:M:400:TRP:HA	2:M:425:GLY:O	2.11	0.51
1:C:38:ARG:HG3	1:C:107:HIS:HB2	1.92	0.51
1:D:61:HIS:ND1	1:E:163:GLN:HG3	2.24	0.51
1:A:168:GLU:HA	1:A:171:ILE:HD12	1.92	0.51
2:P:536:GLU:HB2	6:P:702:HOH:O	2.11	0.51
1:E:98:THR:HB	1:E:100:ASP:OD1	2.11	0.51
1:D:33:GLN:HB3	1:D:85:LEU:HD11	1.92	0.51
2:N:497:ASN:HD22	2:N:498:PRO:N	2.10	0.50
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.38	0.50
1:E:33:GLN:O	2:Q:428:ARG:NH2	2.41	0.50
1:A:188:ARG:NH1	6:A:259:HOH:O	2.43	0.50
2:M:486:ILE:HB	2:M:487:PRO:HD3	1.92	0.50
1:D:32:ASP:HB2	6:P:730:HOH:O	2.10	0.50
1:E:32:ASP:HB2	6:E:267:HOH:O	2.10	0.50
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.93	0.50
2:Q:361:HIS:CD2	2:Q:361:HIS:N	2.66	0.50
1:D:19:ILE:O	2:P:426:VAL:HG21	2.10	0.50
1:C:176:GLU:HA	1:C:180:LYS:O	2.11	0.50
2:O:326:THR:HG22	2:O:330:ARG:HD2	1.92	0.50
1:A:157:VAL:O	1:A:160:LEU:HB2	2.11	0.50
2:P:316:HIS:HB3	2:P:317:PRO:HD2	1.93	0.50
2:R:399:MET:HA	2:R:462:HIS:O	2.12	0.50
1:A:78:GLU:CG	2:M:301:PRO:HG3	2.42	0.50
1:B:64:ARG:HD3	1:B:99:PHE:O	2.12	0.50
2:O:356:PHE:CD1	2:O:428:ARG:HD2	2.46	0.50
1:F:31:ARG:HH11	2:R:428:ARG:HG2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:302:ALA:HB1	2:P:347:THR:HG22	1.93	0.50
2:M:497:ASN:HD22	2:M:499:GLU:N	2.07	0.49
2:R:356:PHE:CD1	2:R:428:ARG:HD3	2.47	0.49
2:R:360:ASP:OD2	2:R:428:ARG:HD2	2.12	0.49
2:N:536:GLU:HB2	6:N:701:HOH:O	2.12	0.49
1:F:33:GLN:CG	1:F:85:LEU:HD12	2.39	0.49
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	1.95	0.49
1:A:92:PHE:CG	2:M:349:PRO:HG3	2.47	0.49
1:B:134:GLY:HA3	2:N:326:THR:HG22	1.94	0.49
2:O:497:ASN:HD22	2:O:498:PRO:N	2.09	0.49
2:N:406:GLY:O	2:N:447:TYR:HD1	1.94	0.49
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.76	0.49
2:O:497:ASN:HD22	2:O:497:ASN:C	2.16	0.49
2:P:522:ARG:NH1	6:P:670:HOH:O	2.37	0.49
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.43	0.49
1:C:70:VAL:HG11	1:C:106:LEU:HD21	1.95	0.49
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.28	0.49
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.28	0.49
2:Q:356:PHE:CD1	2:Q:428:ARG:HD2	2.48	0.49
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.76	0.49
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.48	0.49
1:E:165:GLN:HE21	1:E:165:GLN:N	2.01	0.49
2:Q:451:ASN:HB3	2:Q:455:ASP:OD2	2.13	0.48
2:Q:497:ASN:ND2	2:Q:499:GLU:HB2	2.28	0.48
1:E:10:SER:O	1:E:11:GLN:HG2	2.13	0.48
2:R:390:LYS:HE2	6:R:1373:HOH:O	2.13	0.48
1:A:98:THR:O	1:A:102:GLY:HA2	2.14	0.48
2:M:361:HIS:CD2	2:M:361:HIS:N	2.73	0.48
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.47	0.48
1:E:52:LEU:HD23	1:E:184:ARG:NH1	2.28	0.48
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.49	0.48
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.13	0.48
2:O:356:PHE:CD1	2:O:428:ARG:CD	2.96	0.48
1:F:35:ILE:CD1	2:R:351:PHE:CE1	2.96	0.48
1:D:98:THR:OG1	1:D:102:GLY:N	2.38	0.48
1:B:3:GLU:CA	1:B:3:GLU:OE1	2.61	0.48
1:B:132:ALA:HB3	1:B:135:ILE:HD12	1.96	0.48
2:P:497:ASN:HD22	2:P:497:ASN:C	2.17	0.48
1:E:176:GLU:HG2	1:E:179:GLY:HA2	1.94	0.48
1:F:77:GLY:O	1:F:114:VAL:HG12	2.13	0.48
2:R:486:ILE:HB	2:R:487:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:356:PHE:CZ	2:N:430:LEU:HD13	2.49	0.48
1:F:64:ARG:HD3	1:F:99:PHE:O	2.14	0.48
1:D:39:LEU:HD12	1:D:39:LEU:N	2.29	0.48
1:D:191:GLY:O	1:D:194:GLU:HB2	2.14	0.48
2:R:497:ASN:ND2	2:R:499:GLU:N	2.54	0.48
1:A:3:GLU:OE1	1:A:3:GLU:HA	2.14	0.48
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.48	0.48
1:C:131:PHE:O	1:C:132:ALA:HB2	2.14	0.47
1:E:188:ARG:HG3	1:E:188:ARG:HH11	1.79	0.47
1:A:100:ASP:OD1	1:A:100:ASP:N	2.44	0.47
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.96	0.47
2:O:302:ALA:HB1	2:O:347:THR:CG2	2.44	0.47
2:N:326:THR:HG22	2:N:330:ARG:HD2	1.96	0.47
2:N:328:ILE:HD12	2:O:335:ALA:HB2	1.96	0.47
1:D:26:ALA:O	2:P:411:LYS:HG3	2.14	0.47
2:P:359:HIS:O	2:P:366:ASN:HB3	2.13	0.47
2:P:399:MET:HA	2:P:462:HIS:O	2.14	0.47
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.14	0.47
1:D:15:PRO:HB3	1:D:133:ARG:HD2	1.96	0.47
1:E:35:ILE:HG21	1:E:92:PHE:CE2	2.49	0.47
1:D:50:LEU:O	1:D:182:ALA:HA	2.14	0.47
1:D:51:LEU:O	1:D:105:THR:HA	2.14	0.47
1:E:51:LEU:HD11	1:E:126:ILE:HD12	1.96	0.47
2:Q:415:TYR:CE1	2:Q:416:LEU:HD23	2.49	0.47
1:F:98:THR:O	1:F:102:GLY:HA2	2.15	0.47
2:R:306:SER:OG	2:R:530:GLN:NE2	2.48	0.47
2:R:394:ASN:HA	2:R:431:THR:O	2.15	0.47
1:A:180:LYS:HG2	1:A:181:THR:N	2.29	0.47
1:E:176:GLU:OE2	1:E:179:GLY:HA2	2.15	0.47
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.30	0.47
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.96	0.47
2:Q:372:LEU:HA	2:Q:373:PRO:HD3	1.84	0.47
2:Q:497:ASN:HD21	2:Q:499:GLU:HB2	1.80	0.47
2:R:400:TRP:HA	2:R:425:GLY:O	2.15	0.47
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.97	0.47
1:A:6:PRO:HG2	2:M:503:GLN:NE2	2.31	0.47
2:M:363:LEU:N	2:M:363:LEU:HD12	2.30	0.47
2:M:392:VAL:HG12	2:M:395:THR:HB	1.97	0.47
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.74	0.47
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.97	0.47
2:Q:385:VAL:HA	2:Q:390:LYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:VAL:HG11	1:D:106:LEU:HD21	1.96	0.46
1:D:144:TYR:CE1	1:D:158:LEU:HD13	2.50	0.46
1:E:131:PHE:O	1:E:132:ALA:HB2	2.16	0.46
2:Q:304:ASP:OD1	2:Q:307:ARG:NH1	2.37	0.46
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.83	0.46
2:N:486:ILE:N	2:N:487:PRO:HD2	2.30	0.46
2:Q:536:GLU:HB2	6:Q:1100:HOH:O	2.15	0.46
1:F:143:LEU:HD23	1:F:144:TYR:N	2.30	0.46
1:E:19:ILE:O	2:Q:426:VAL:CG2	2.64	0.46
1:A:65:ASP:OD2	1:A:133:ARG:HD3	2.15	0.46
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.50	0.46
2:P:315:TRP:HZ2	2:P:503:GLN:HE21	1.62	0.46
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.31	0.46
1:D:92:PHE:CG	2:P:349:PRO:HG3	2.51	0.46
1:F:165:GLN:NE2	1:F:165:GLN:N	2.49	0.46
1:C:113:VAL:HG13	1:C:122:MET:O	2.15	0.46
2:O:313:ARG:O	2:O:318:LYS:HE2	2.16	0.46
2:P:416:LEU:C	2:P:416:LEU:CD2	2.84	0.46
1:E:147:ASP:OD2	1:E:174:ARG:NH1	2.48	0.46
2:Q:473:LYS:NZ	6:Q:1036:HOH:O	2.31	0.46
2:R:356:PHE:CE1	2:R:428:ARG:HD3	2.51	0.46
1:A:155:CYS:O	1:A:159:ASN:ND2	2.49	0.46
1:B:1:PRO:HA	2:P:508:LEU:O	2.16	0.46
2:O:390:LYS:HA	2:O:391:PRO:HD3	1.75	0.46
2:P:390:LYS:NZ	6:P:666:HOH:O	2.43	0.46
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.84	0.46
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.67	0.46
1:A:163:GLN:HB3	1:A:165:GLN:NE2	2.30	0.46
2:M:512:ASN:O	2:Q:534:HIS:HE1	1.99	0.46
1:B:50:LEU:O	1:B:182:ALA:HA	2.16	0.46
1:E:51:LEU:HB2	1:E:106:LEU:HB3	1.98	0.46
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.64	0.46
1:B:65:ASP:OD2	1:B:133:ARG:HD3	2.16	0.46
2:N:486:ILE:HB	2:N:487:PRO:HD3	1.97	0.46
1:C:158:LEU:HD12	1:C:158:LEU:HA	1.85	0.46
2:Q:362:ASP:OD2	2:Q:440:ARG:NH1	2.48	0.46
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.98	0.45
2:N:372:LEU:HA	2:N:373:PRO:HD3	1.85	0.45
1:C:98:THR:OG1	1:C:102:GLY:N	2.50	0.45
2:O:318:LYS:HA	2:O:318:LYS:HD3	1.64	0.45
2:O:364:LEU:CD2	2:O:440:ARG:HD3	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:376:GLU:OE1	6:P:642:HOH:O	2.21	0.45
2:Q:356:PHE:HE2	2:Q:430:LEU:HD22	1.81	0.45
1:F:94:ARG:NH2	2:R:398:GLU:OE2	2.38	0.45
1:F:131:PHE:CE2	1:F:138:HIS:HB3	2.52	0.45
1:B:176:GLU:HG2	1:B:179:GLY:HA2	1.98	0.45
2:N:478:LEU:C	2:N:478:LEU:HD23	2.36	0.45
2:Q:364:LEU:HB2	2:Q:440:ARG:HD3	1.97	0.45
1:C:74:ASP:C	1:C:74:ASP:OD1	2.55	0.45
1:F:41:LYS:O	1:F:44:ALA:N	2.49	0.45
2:M:390:LYS:HD3	6:M:717:HOH:O	2.16	0.45
1:C:98:THR:O	1:C:102:GLY:HA2	2.17	0.45
1:E:56:TYR:CE2	1:E:62:LEU:HD23	2.52	0.45
2:Q:484:PRO:O	2:Q:487:PRO:HD2	2.17	0.45
2:M:478:LEU:HD23	2:M:478:LEU:C	2.37	0.45
2:P:364:LEU:HD22	2:P:440:ARG:CD	2.44	0.45
1:E:52:LEU:CD2	1:E:184:ARG:NH1	2.80	0.45
2:O:400:TRP:HA	2:O:425:GLY:O	2.15	0.45
2:P:478:LEU:C	2:P:478:LEU:HD23	2.37	0.45
1:F:32:ASP:HB2	6:R:1383:HOH:O	2.17	0.45
2:P:483:ASP:HB3	2:P:486:ILE:HG13	1.99	0.45
1:F:74:ASP:OD1	1:F:76:ASN:N	2.50	0.45
2:M:512:ASN:O	2:Q:534:HIS:CE1	2.69	0.45
1:B:143:LEU:C	1:B:143:LEU:HD23	2.37	0.45
1:D:176:GLU:HG3	1:D:180:LYS:C	2.37	0.45
1:F:58:GLY:HA3	1:F:190:GLN:OE1	2.16	0.45
1:A:176:GLU:HG2	1:A:179:GLY:CA	2.47	0.45
2:M:326:THR:HG22	2:M:326:THR:O	2.17	0.45
1:C:35:ILE:HG21	1:C:92:PHE:CE2	2.52	0.45
1:C:50:LEU:O	1:C:182:ALA:HA	2.16	0.45
1:D:28:ASN:HB3	1:D:29:PRO:HD2	1.99	0.45
2:P:360:ASP:O	2:P:427:GLY:HA2	2.17	0.45
1:B:98:THR:HB	1:B:100:ASP:OD1	2.17	0.44
2:R:378:ILE:HA	2:R:519:LEU:O	2.17	0.44
1:E:176:GLU:HA	1:E:180:LYS:O	2.17	0.44
2:N:386:ASP:HA	2:N:527:LEU:O	2.18	0.44
1:F:98:THR:OG1	1:F:101:ALA:HB3	2.17	0.44
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.52	0.44
1:C:16:TYR:O	1:C:19:ILE:HG23	2.18	0.44
2:P:325:LYS:HD3	2:Q:335:ALA:HB1	1.98	0.44
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.99	0.44
2:Q:428:ARG:O	2:Q:429:CYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.20	0.44
1:F:39:LEU:N	1:F:39:LEU:HD12	2.33	0.44
2:N:488:MET:HE1	1:C:1:PRO:HG3	1.96	0.44
2:O:315:TRP:HZ2	2:O:503:GLN:HE21	1.65	0.44
2:P:486:ILE:HB	2:P:487:PRO:HD3	1.99	0.44
2:Q:395:THR:O	2:Q:430:LEU:HA	2.18	0.44
2:N:364:LEU:HD11	2:N:442:ILE:HG23	2.00	0.44
2:Q:453:PRO:HG2	2:R:310:ILE:HG23	1.99	0.44
2:M:497:ASN:HA	2:M:498:PRO:HD2	1.89	0.44
2:R:307:ARG:CG	2:R:533:THR:HG22	2.48	0.44
2:R:326:THR:HG22	2:R:330:ARG:HD2	2.00	0.44
1:A:50:LEU:O	1:A:182:ALA:HA	2.17	0.44
2:M:316:HIS:HB3	2:M:317:PRO:HD2	1.98	0.44
1:E:134:GLY:HA3	2:Q:326:THR:HG22	2.00	0.44
1:F:65:ASP:OD2	1:F:133:ARG:HD3	2.17	0.44
1:A:70:VAL:HG11	1:A:106:LEU:CD2	2.46	0.44
1:F:131:PHE:CD2	1:F:138:HIS:HB3	2.52	0.44
1:A:131:PHE:CE2	1:A:138:HIS:HB3	2.53	0.43
1:C:176:GLU:HG3	1:C:180:LYS:C	2.38	0.43
2:P:372:LEU:HA	2:P:373:PRO:HD3	1.89	0.43
2:P:488:MET:C	2:P:493:LYS:HE2	2.38	0.43
1:E:176:GLU:HG3	1:E:180:LYS:C	2.38	0.43
1:E:176:GLU:HG2	1:E:179:GLY:CA	2.48	0.43
1:A:24:GLU:O	1:A:27:GLY:N	2.47	0.43
2:N:395:THR:O	2:N:430:LEU:HA	2.18	0.43
1:D:5:LEU:O	2:P:387:GLN:HG2	2.19	0.43
2:Q:363:LEU:HD11	2:Q:427:GLY:HA3	1.99	0.43
2:O:361:HIS:H	2:O:361:HIS:HD2	1.61	0.43
1:E:1:PRO:HB2	6:E:201:HOH:O	2.17	0.43
1:A:15:PRO:HB3	1:A:133:ARG:HD2	2.00	0.43
2:R:383:ARG:HA	2:R:435:GLY:O	2.19	0.43
1:B:66:SER:HB2	1:B:130:LEU:HD11	2.01	0.43
1:D:33:GLN:CD	1:D:85:LEU:HD12	2.39	0.43
2:P:495:ILE:CG2	2:P:500:ALA:HB3	2.49	0.43
1:E:94:ARG:HH11	1:E:94:ARG:HD3	1.71	0.43
1:A:64:ARG:HD3	1:A:99:PHE:O	2.19	0.43
1:E:18:HIS:CE1	1:E:99:PHE:CE1	3.06	0.43
2:R:311:ARG:HH11	2:R:311:ARG:HD2	1.67	0.43
2:M:362:ASP:OD2	2:M:440:ARG:NH1	2.52	0.43
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.73	0.43
1:C:18:HIS:CE1	1:C:99:PHE:CE1	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:360:ASP:HB3	2:O:428:ARG:HG3	2.01	0.43
1:B:5:LEU:O	2:N:387:GLN:HG2	2.19	0.43
1:D:39:LEU:HB3	1:D:90:ASN:O	2.19	0.43
1:F:48:HIS:CD2	1:F:109:VAL:HG12	2.53	0.43
1:A:165:GLN:NE2	1:A:165:GLN:N	2.59	0.42
2:N:497:ASN:ND2	2:N:499:GLU:OE1	2.43	0.42
2:O:356:PHE:HD1	2:O:428:ARG:CD	2.31	0.42
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.39	0.42
1:F:168:GLU:HA	1:F:171:ILE:CD1	2.38	0.42
1:D:120:VAL:HA	1:D:121:PRO:HD3	1.83	0.42
1:A:61:HIS:ND1	1:B:163:GLN:HG3	2.34	0.42
2:N:307:ARG:HA	2:N:307:ARG:HD3	1.79	0.42
2:N:486:ILE:N	2:N:487:PRO:CD	2.82	0.42
2:O:483:ASP:HA	2:O:484:PRO:HD2	1.94	0.42
1:D:176:GLU:HG2	1:D:179:GLY:CA	2.49	0.42
2:M:483:ASP:HB3	2:M:486:ILE:HG13	2.02	0.42
1:B:190:GLN:HG3	2:N:333:ARG:HG2	2.01	0.42
2:N:356:PHE:HZ	2:N:430:LEU:HD13	1.85	0.42
1:E:110:LYS:CE	1:E:148:GLU:OE2	2.67	0.42
1:F:8:THR:HA	1:F:9:PRO:HD3	1.87	0.42
2:R:447:TYR:HA	2:R:448:PRO:HD3	1.89	0.42
2:R:497:ASN:ND2	2:R:499:GLU:OE1	2.41	0.42
1:A:36:TRP:CE3	1:A:36:TRP:HA	2.54	0.42
2:N:522:ARG:HD3	6:N:669:HOH:O	2.19	0.42
2:Q:362:ASP:OD1	2:Q:364:LEU:HB2	2.20	0.42
2:R:442:ILE:O	2:R:442:ILE:HG13	2.19	0.42
2:M:448:PRO:HB2	2:P:516:MET:HA	2.01	0.42
2:P:302:ALA:HB1	2:P:347:THR:CG2	2.50	0.42
1:C:38:ARG:HH11	1:C:38:ARG:HD2	1.68	0.42
1:C:155:CYS:HB3	1:C:158:LEU:HB2	2.02	0.42
1:F:84:ASN:OD1	1:F:86:GLU:HB2	2.20	0.42
2:M:307:ARG:HD2	6:M:653:HOH:O	2.18	0.41
2:N:407:ARG:HD2	2:N:413:ASP:OD2	2.19	0.41
2:P:363:LEU:HD11	2:P:427:GLY:HA3	2.00	0.41
1:D:131:PHE:O	1:D:132:ALA:CB	2.68	0.41
2:P:451:ASN:HB3	2:P:455:ASP:OD2	2.20	0.41
1:E:161:ILE:O	1:E:167:ARG:NH2	2.48	0.41
2:Q:390:LYS:HA	2:Q:391:PRO:HD3	1.78	0.41
2:M:420:ASP:HA	2:M:421:PRO:HD2	1.89	0.41
1:C:176:GLU:OE2	1:C:179:GLY:HA2	2.20	0.41
1:E:124:PRO:HA	6:E:221:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.85	0.41
2:M:371:GLY:HA3	2:M:422:ASN:ND2	2.36	0.41
2:M:390:LYS:HA	2:M:391:PRO:HD3	1.92	0.41
1:D:18:HIS:NE2	6:D:944:HOH:O	2.27	0.41
2:M:376:GLU:O	2:M:442:ILE:HA	2.21	0.41
2:P:497:ASN:HD22	2:P:498:PRO:N	2.18	0.41
1:F:44:ALA:O	1:F:48:HIS:NE2	2.36	0.41
2:R:376:GLU:O	2:R:442:ILE:HA	2.21	0.41
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.55	0.41
2:M:302:ALA:HB1	2:M:347:THR:CG2	2.50	0.41
2:M:484:PRO:O	2:M:487:PRO:HD2	2.21	0.41
2:N:453:PRO:CB	2:O:310:ILE:HD12	2.46	0.41
1:C:19:ILE:HG13	2:O:426:VAL:HG22	2.02	0.41
1:B:6:PRO:HG2	2:N:503:GLN:NE2	2.35	0.41
2:O:390:LYS:HD3	6:O:651:HOH:O	2.20	0.41
2:Q:415:TYR:CE1	2:Q:416:LEU:CD2	3.04	0.41
1:F:78:GLU:HB2	1:F:80:GLN:NE2	2.36	0.41
2:P:392:VAL:HG12	2:P:395:THR:HB	2.01	0.41
1:E:35:ILE:HG22	1:E:94:ARG:HG3	2.02	0.41
1:F:19:ILE:O	2:R:426:VAL:CG2	2.68	0.41
1:A:35:ILE:CD1	2:M:351:PHE:CE1	3.04	0.41
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.36	0.41
1:E:110:LYS:HE2	1:E:148:GLU:OE2	2.21	0.41
2:Q:406:GLY:O	2:Q:447:TYR:HD1	2.04	0.41
2:N:318:LYS:HA	2:N:318:LYS:HD3	1.80	0.41
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.21	0.41
2:P:383:ARG:NE	2:P:434:ASP:O	2.41	0.41
2:O:405:GLY:HA3	6:O:654:HOH:O	2.20	0.40
1:E:158:LEU:HD12	1:E:158:LEU:HA	1.97	0.40
2:R:495:ILE:HG21	2:R:500:ALA:HB3	2.04	0.40
2:M:495:ILE:CG2	2:M:500:ALA:HB3	2.51	0.40
1:B:3:GLU:OE1	1:B:3:GLU:HA	2.22	0.40
1:B:79:TYR:O	2:N:301:PRO:CB	2.70	0.40
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.63	0.40
2:P:315:TRP:HZ2	2:P:503:GLN:NE2	2.18	0.40
2:Q:513:ALA:O	2:Q:515:PRO:HD3	2.21	0.40
1:F:44:ALA:HA	1:F:45:PRO:HD2	1.82	0.40
2:R:316:HIS:HB3	2:R:317:PRO:HD2	2.04	0.40
2:N:493:LYS:HB2	2:N:493:LYS:HE3	1.69	0.40
1:A:114:VAL:HG23	1:A:122:MET:HE2	2.04	0.40
2:M:360:ASP:O	2:M:427:GLY:HA2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ILE:HD13	1:C:19:ILE:HG21	1.74	0.40
2:O:356:PHE:CD1	2:O:428:ARG:HD3	2.57	0.40
1:D:64:ARG:HD3	1:D:99:PHE:O	2.21	0.40
1:E:39:LEU:HD11	1:E:93:GLY:HA3	2.02	0.40
2:Q:310:ILE:HD13	2:Q:310:ILE:HA	1.82	0.40
1:A:70:VAL:HA	1:A:127:ASN:O	2.21	0.40
2:O:378:ILE:HA	2:O:519:LEU:O	2.21	0.40
1:D:52:LEU:HA	1:D:104:TRP:O	2.21	0.40
2:P:328:ILE:HD12	2:Q:335:ALA:HB2	2.02	0.40
2:R:465:ILE:HD12	2:R:465:ILE:N	2.36	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	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
1	B	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
1	C	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
1	D	198/200 (99%)	187 (94%)	10 (5%)	1 (0%)	29	29
1	E	198/200 (99%)	186 (94%)	12 (6%)	0	100	100
1	F	198/200 (99%)	187 (94%)	9 (4%)	2 (1%)	15	13
2	M	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	N	229/238 (96%)	219 (96%)	9 (4%)	1 (0%)	34	37
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	220 (96%)	8 (4%)	1 (0%)	34	37
2	Q	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	R	229/238 (96%)	220 (96%)	8 (4%)	1 (0%)	34	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2562/2628 (98%)	2450 (96%)	106 (4%)	6 (0%)	47 55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	535	PHE
2	R	535	PHE
2	N	535	PHE
1	D	132	ALA
1	F	132	ALA
1	F	42	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	162/163 (99%)	155 (96%)	7 (4%)	29 33
1	B	162/163 (99%)	155 (96%)	7 (4%)	29 33
1	C	162/163 (99%)	155 (96%)	7 (4%)	29 33
1	D	162/163 (99%)	155 (96%)	7 (4%)	29 33
1	E	162/163 (99%)	157 (97%)	5 (3%)	40 49
1	F	162/163 (99%)	155 (96%)	7 (4%)	29 33
2	M	196/202 (97%)	187 (95%)	9 (5%)	27 30
2	N	196/202 (97%)	190 (97%)	6 (3%)	40 49
2	O	196/202 (97%)	186 (95%)	10 (5%)	24 25
2	P	196/202 (97%)	186 (95%)	10 (5%)	24 25
2	Q	196/202 (97%)	184 (94%)	12 (6%)	18 18
2	R	196/202 (97%)	184 (94%)	12 (6%)	18 18
All	All	2148/2190 (98%)	2049 (95%)	99 (5%)	27 30

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	24	GLU
1	A	38	ARG
1	A	52	LEU
1	A	78	GLU
1	A	94	ARG
1	A	165	GLN
2	M	301	PRO
2	M	372	LEU
2	M	395	THR
2	M	416	LEU
2	M	429	CYS
2	M	434	ASP
2	M	497	ASN
2	M	507	LYS
2	M	534	HIS
1	B	24	GLU
1	B	32	ASP
1	B	38	ARG
1	B	52	LEU
1	B	165	GLN
1	B	176	GLU
1	B	184	ARG
2	N	364	LEU
2	N	395	THR
2	N	399	MET
2	N	416	LEU
2	N	497	ASN
2	N	534	HIS
1	C	4	LEU
1	C	19	ILE
1	C	38	ARG
1	C	52	LEU
1	C	66	SER
1	C	100	ASP
1	C	165	GLN
2	O	395	THR
2	O	399	MET
2	O	416	LEU
2	O	428	ARG
2	O	429	CYS
2	O	434	ASP
2	O	478	LEU

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Mol	Chain	Res	Type
2	O	497	ASN
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	38	ARG
1	D	43	ASP
1	D	52	LEU
1	D	100	ASP
1	D	165	GLN
2	P	395	THR
2	P	416	LEU
2	P	428	ARG
2	P	429	CYS
2	P	433	SER
2	P	434	ASP
2	P	440	ARG
2	P	497	ASN
2	P	511	ASN
2	P	534	HIS
1	E	19	ILE
1	E	38	ARG
1	E	52	LEU
1	E	100	ASP
1	E	165	GLN
2	Q	364	LEU
2	Q	395	THR
2	Q	416	LEU
2	Q	428	ARG
2	Q	429	CYS
2	Q	434	ASP
2	Q	438	SER
2	Q	478	LEU
2	Q	487	PRO
2	Q	497	ASN
2	Q	507	LYS
2	Q	515	PRO
1	F	4	LEU
1	F	19	ILE
1	F	38	ARG
1	F	43	ASP
1	F	52	LEU

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Mol	Chain	Res	Type
1	F	100	ASP
1	F	165	GLN
2	R	306	SER
2	R	343	ILE
2	R	395	THR
2	R	399	MET
2	R	416	LEU
2	R	428	ARG
2	R	429	CYS
2	R	433	SER
2	R	434	ASP
2	R	440	ARG
2	R	497	ASN
2	R	534	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
2	M	361	HIS
2	M	422	ASN
2	M	497	ASN
2	M	503	GLN
1	B	165	GLN
2	N	361	HIS
2	N	412	ASN
2	N	497	ASN
2	N	503	GLN
1	C	163	GLN
1	C	165	GLN
2	O	361	HIS
2	O	497	ASN
2	O	503	GLN
2	O	530	GLN
1	D	59	ASN
1	D	165	GLN
2	P	361	HIS
2	P	497	ASN
2	P	503	GLN
1	E	165	GLN
2	Q	334	GLN
2	Q	361	HIS

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Mol	Chain	Res	Type
2	Q	412	ASN
2	Q	422	ASN
2	Q	497	ASN
2	Q	503	GLN
2	Q	534	HIS
1	F	18	HIS
1	F	165	GLN
2	R	361	HIS
2	R	422	ASN
2	R	497	ASN
2	R	503	GLN
2	R	530	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	CYN	O	575	4	0,1,1	-	-	-		
5	NNO	Q	550	4	9,11,11	1.30	1 (11%)	9,15,15	1.20	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NNO	R	550	4	9,11,11	1.41	1 (11%)	9,15,15	1.48	2 (22%)
3	CYN	Q	575	4	0,1,1	-	-	-	-	-
5	NNO	N	550	4	9,11,11	1.52	3 (33%)	9,15,15	1.46	2 (22%)
5	NNO	P	550	4	9,11,11	1.46	3 (33%)	9,15,15	1.64	2 (22%)
3	CYN	N	575	4	0,1,1	-	-	-	-	-
3	CYN	P	575	4	0,1,1	-	-	-	-	-
3	CYN	M	575	4	0,1,1	-	-	-	-	-
3	CYN	R	575	4	0,1,1	-	-	-	-	-
5	NNO	O	550	4	9,11,11	1.70	3 (33%)	9,15,15	1.69	2 (22%)
5	NNO	M	550	4	9,11,11	1.42	0	9,15,15	1.27	1 (11%)

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
5	NNO	Q	550	4	-	0/4/4/4	0/1/1/1
5	NNO	R	550	4	-	0/4/4/4	0/1/1/1
5	NNO	N	550	4	-	0/4/4/4	0/1/1/1
5	NNO	P	550	4	-	0/4/4/4	0/1/1/1
5	NNO	O	550	4	-	0/4/4/4	0/1/1/1
5	NNO	M	550	4	-	0/4/4/4	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	550	NNO	O2-C7	-2.93	1.21	1.30
5	N	550	NNO	O2-C7	-2.49	1.22	1.30
5	O	550	NNO	C2-C3	2.45	1.42	1.39
5	P	550	NNO	C3-C7	2.36	1.54	1.49
5	N	550	NNO	C2-C3	2.29	1.42	1.39
5	N	550	NNO	C3-C7	2.22	1.54	1.49
5	R	550	NNO	C3-C7	2.14	1.54	1.49
5	P	550	NNO	C2-N1	-2.06	1.31	1.35
5	Q	550	NNO	C3-C7	2.05	1.53	1.49
5	P	550	NNO	O2-C7	-2.05	1.24	1.30
5	O	550	NNO	C3-C7	2.01	1.53	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	550	NNO	O2-C7-C3	3.42	123.71	114.85
5	O	550	NNO	O2-C7-O1	-3.11	116.44	123.35
5	N	550	NNO	O2-C7-O1	-2.90	116.91	123.35
5	P	550	NNO	O2-C7-C3	2.89	122.34	114.85
5	P	550	NNO	O2-C7-O1	-2.79	117.17	123.35
5	R	550	NNO	O2-C7-O1	-2.74	117.26	123.35
5	R	550	NNO	O2-C7-C3	2.56	121.49	114.85
5	N	550	NNO	O2-C7-C3	2.44	121.18	114.85
5	M	550	NNO	O2-C7-C3	2.32	120.88	114.85
5	Q	550	NNO	O2-C7-O1	-2.23	118.41	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	575	CYN	1	0
3	Q	575	CYN	1	0
3	P	575	CYN	1	0
3	M	575	CYN	1	0
3	R	575	CYN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.