Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:53 PM GMT

PDB ID	:	1MIO
Title	:	X-RAY CRYSTAL STRUCTURE OF THE NITROGENASE MOLYBDENUM-IRON PROTEIN FROM CLOSTRIDIUM PASTEURIANUM AT 3.0 ANGSTROMS RESOLUTION
Authors	:	Kim, J.; Woo, D.; Rees, D.C.
Deposited on	:	1993-03-24
Resolution	:	3.00 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 ⓘ symbol.

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

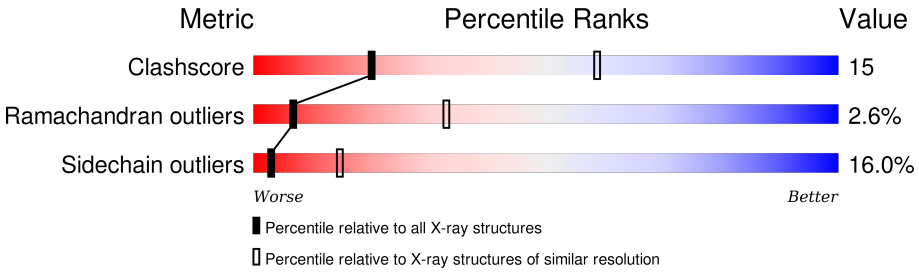
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	533	50% 35% 11%
1	C	533	49% 37% 10%
2	B	458	56% 35% 7%
2	D	458	57% 33% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CFM	B	496	-	-	X	-
5	CFM	D	496	-	-	X	-
6	CLP	B	498	-	-	X	-
6	CLP	D	498	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15269 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 NITROGENASE MOLYBDENUM IRON PROTEIN (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4074	2588	682	777	27			
1	C	525	Total	C	N	O	S	0	0	0
			4077	2589	683	778	27			

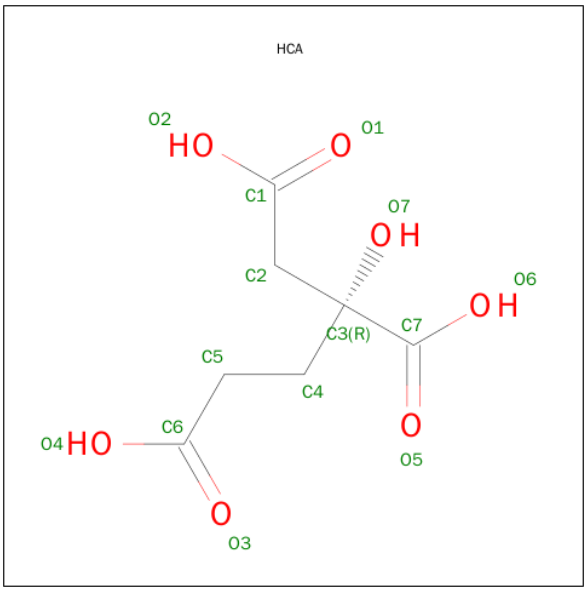
- Molecule 2 is a protein called NITROGENASE MOLYBDENUM IRON PROTEIN (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	457	Total	C	N	O	S	0	0	0
			3511	2231	579	681	20			
2	D	457	Total	C	N	O	S	0	0	0
			3511	2231	579	681	20			

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

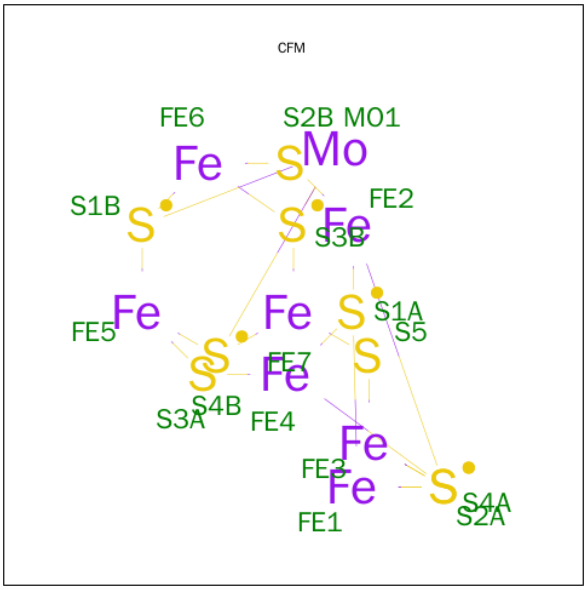
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).



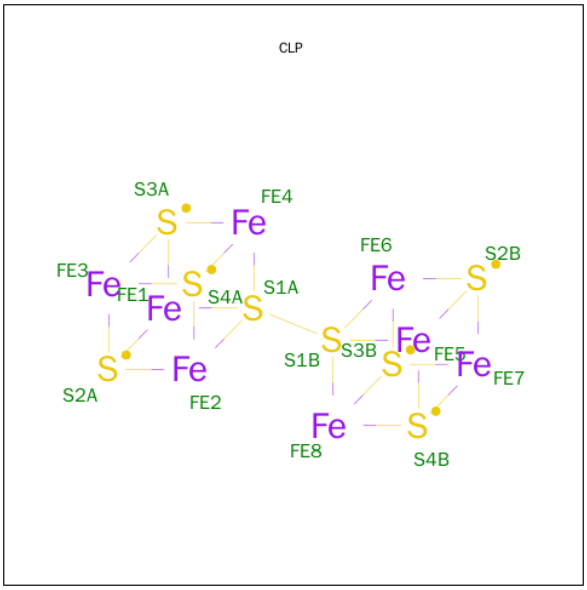
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 14 7 7	0	0
4	D	1	Total C O 14 7 7	0	0

- Molecule 5 is FE-MO-S CLUSTER (three-letter code: CFM) (formula: Fe_7MoS_9).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Fe Mo S 17 7 1 9	0	0
5	D	1	Total Fe Mo S 17 7 1 9	0	0

- Molecule 6 is FE-S CLUSTER (three-letter code: CLP) (formula: Fe_8S_8).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Fe S 16 8 8	0	0
6	D	1	Total Fe S 16 8 8	0	0

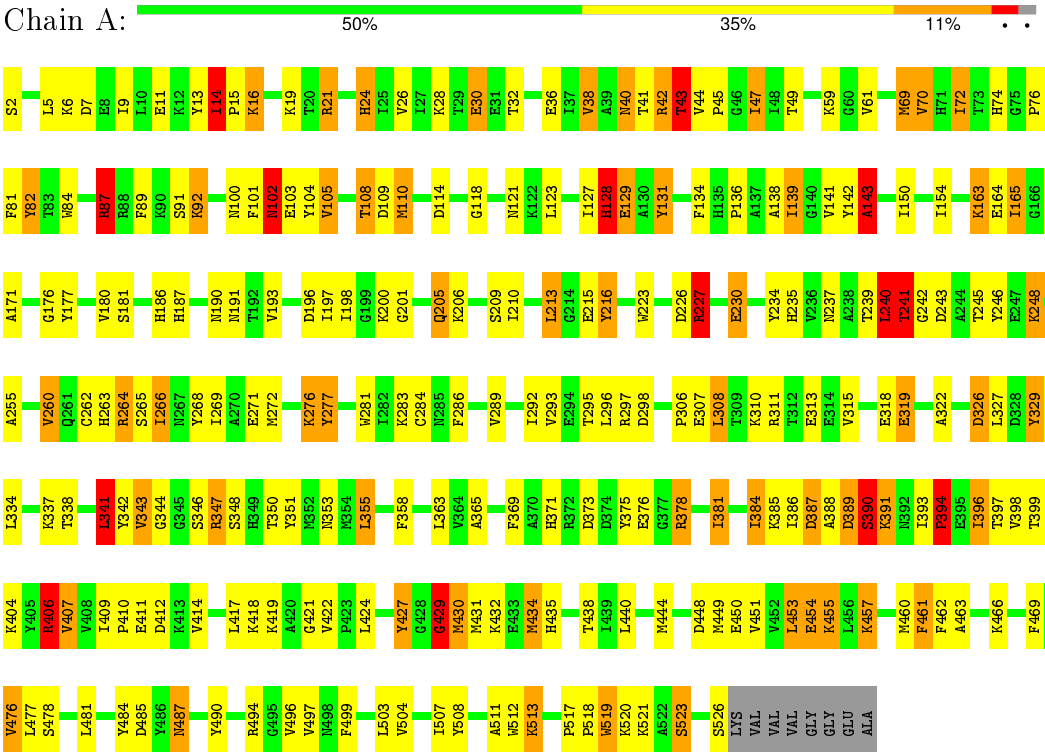
3 Residue-property plots (i)

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.

Note EDS was not executed.

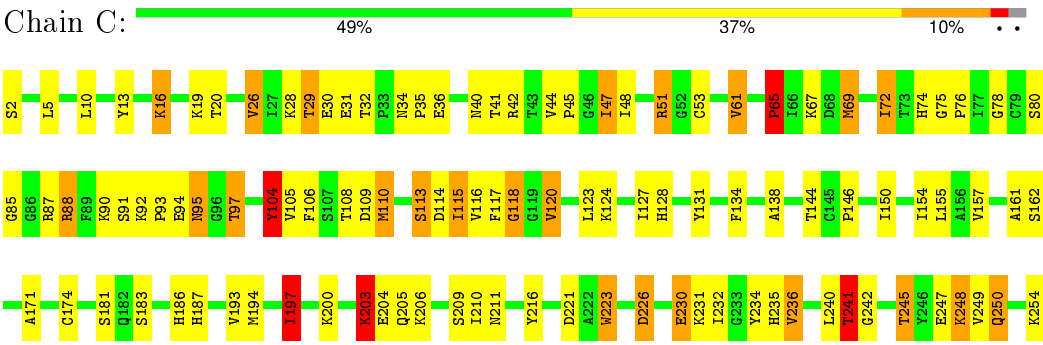
• Molecule 1: NITROGENASE MOLYBDENUM IRON PROTEIN (ALPHA CHAIN)

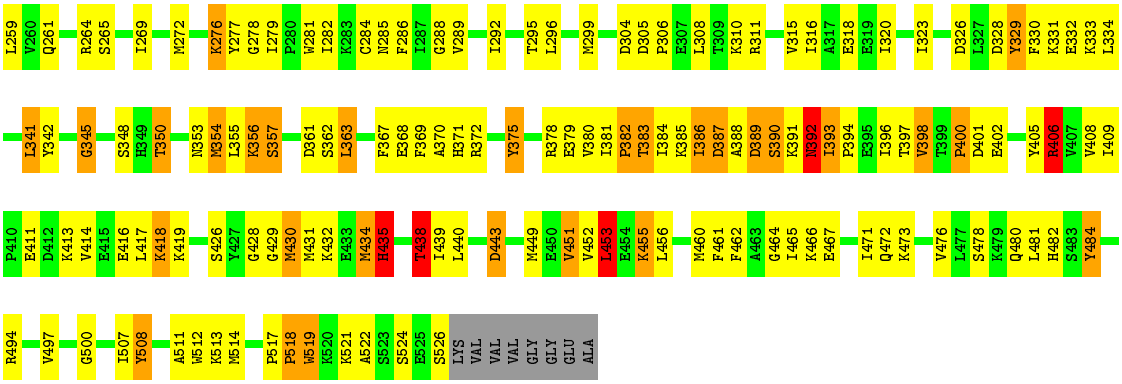
Chain A:



• Molecule 1: NITROGENASE MOLYBDENUM IRON PROTEIN (ALPHA CHAIN)

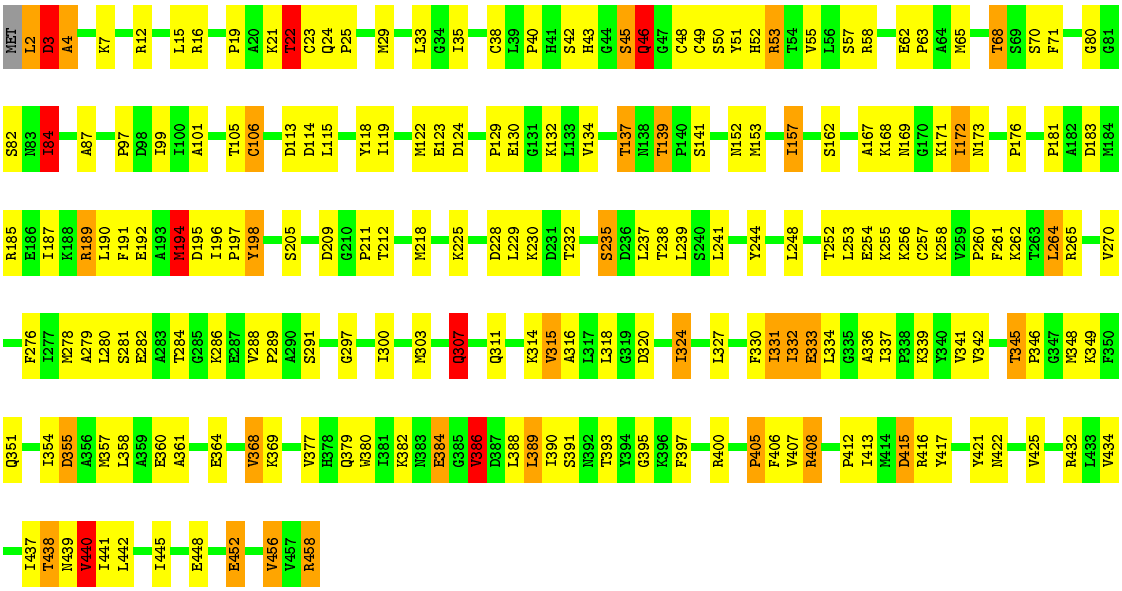
Chain C:





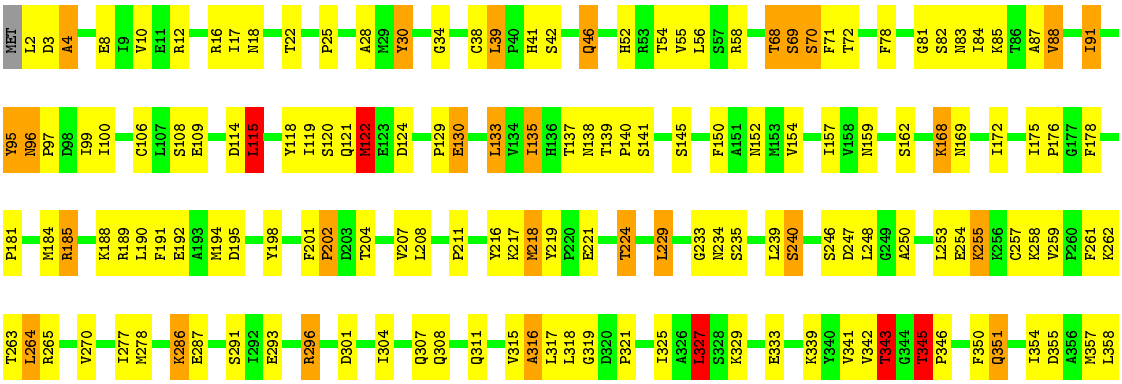
• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN (BETA CHAIN)

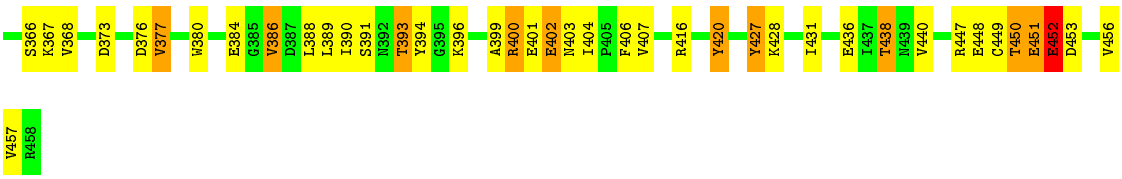
Chain B:



• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN (BETA CHAIN)

Chain D:




S366
K367
V368
D373
D376
V377
W380
E384
G385
V386
D387
L388
L389
I390
S391
N392
T393
Y394
G395
K396
A399
R400
E401
E402
N403
I404
P405
F406
V407
R416
Y420
Y427
K428
I431
E436
I437
T438
N439
V440
R447
E448
C449
T450
E451
E452
D453
V456
V457
R458

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.96Å 151.30Å 121.90Å 90.00° 110.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15269	wwPDB-VP
Average B, all atoms (Å^2)	8.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CFM, CLP, HCA

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	0.95	0/4163	1.90	105/5629 (1.9%)
1	C	0.98	3/4166 (0.1%)	1.84	95/5631 (1.7%)
2	B	0.91	0/3582	1.75	65/4845 (1.3%)
2	D	0.93	3/3582 (0.1%)	1.78	69/4845 (1.4%)
All	All	0.94	6/15493 (0.0%)	1.82	334/20950 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	5
2	B	0	2
2	D	0	4
All	All	0	13

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	141	SER	CA-CB	-6.37	1.43	1.52
1	C	390	SER	CA-CB	5.89	1.61	1.52
1	C	451	VAL	CA-CB	5.82	1.67	1.54
1	C	197	ILE	CA-CB	5.75	1.68	1.54
2	D	130	GLU	CB-CG	5.40	1.62	1.52
2	D	345	THR	CA-CB	5.17	1.66	1.53

All (334) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	16	ARG	NE-CZ-NH1	12.84	126.72	120.30
1	A	240	LEU	CA-C-N	-12.72	89.21	117.20
1	A	390	SER	N-CA-C	11.99	143.38	111.00
1	A	240	LEU	O-C-N	11.33	140.83	122.70
1	C	406	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	C	375	TYR	CB-CG-CD1	-10.74	114.56	121.00
2	B	421	TYR	CB-CG-CD2	-10.67	114.60	121.00
2	D	400	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	A	390	SER	N-CA-CB	-9.96	95.56	110.50
1	A	240	LEU	C-N-CA	9.85	146.31	121.70
2	D	357	MET	CA-CB-CG	9.79	129.95	113.30
2	B	458	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	C	240	LEU	CA-C-N	-9.57	96.14	117.20
1	C	51	ARG	CA-CB-CG	9.39	134.06	113.40
1	C	281	TRP	CD1-CG-CD2	9.07	113.56	106.30
2	D	400	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	13	TYR	CB-CG-CD2	-8.93	115.64	121.00
1	C	240	LEU	O-C-N	8.85	136.86	122.70
1	A	21	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	241	THR	CA-C-N	8.82	133.85	116.20
1	C	519	TRP	CD1-CG-CD2	8.76	113.31	106.30
1	A	519	TRP	CD1-CG-CD2	8.75	113.30	106.30
1	C	443	ASP	CA-CB-CG	8.75	132.64	113.40
2	D	30	TYR	CB-CG-CD1	-8.70	115.78	121.00
1	A	490	TYR	CB-CG-CD2	-8.53	115.88	121.00
2	B	58	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	C	264	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	A	406	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	C	392	ASN	N-CA-C	-8.21	88.84	111.00
1	C	36	GLU	CA-CB-CG	8.16	131.35	113.40
1	A	281	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	A	264	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	C	512	TRP	CD1-CG-CD2	8.02	112.71	106.30
2	D	124	ASP	CA-CB-CG	7.98	130.97	113.40
2	B	244	TYR	CB-CG-CD1	7.98	125.79	121.00
1	A	79	CYS	CA-CB-SG	-7.94	99.72	114.00
1	C	131	TYR	CB-CG-CD1	-7.94	116.24	121.00
1	C	519	TRP	CE2-CD2-CG	-7.93	100.96	107.30
1	A	198	ILE	CA-C-N	7.88	131.97	116.20
2	B	53	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	C	372	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	227	ARG	CA-CB-CG	7.79	130.53	113.40
1	A	389	ASP	N-CA-C	-7.78	90.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	ASP	CB-CG-OD1	7.76	125.29	118.30
1	C	378	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	C	240	LEU	C-N-CA	7.67	140.89	121.70
2	D	58	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	A	519	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	C	512	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	C	104	TYR	CB-CG-CD2	-7.63	116.42	121.00
1	C	88	ARG	NE-CZ-NH1	7.61	124.11	120.30
2	D	416	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	512	TRP	CE2-CD2-CG	-7.50	101.30	107.30
2	B	416	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	434	MET	CA-CB-CG	7.47	126.00	113.30
1	C	411	GLU	CA-C-N	-7.45	100.80	117.20
2	B	3	ASP	N-CA-C	7.43	131.05	111.00
1	C	281	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	C	84	TRP	CD1-CG-CD2	7.38	112.20	106.30
1	A	213	LEU	CA-CB-CG	7.33	132.15	115.30
1	A	43	THR	CA-CB-CG2	-7.32	102.15	112.40
1	A	82	TYR	CB-CG-CD2	-7.32	116.61	121.00
1	A	494	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	C	342	TYR	CB-CG-CD2	-7.29	116.62	121.00
1	C	245	THR	CA-CB-CG2	7.27	122.58	112.40
2	B	377	VAL	CG1-CB-CG2	-7.26	99.28	110.90
2	B	29	MET	CG-SD-CE	-7.22	88.64	100.20
1	A	266	ILE	CB-CG1-CD1	-7.16	93.86	113.90
1	A	223	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	A	281	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	A	223	TRP	CD1-CG-CD2	7.07	111.96	106.30
1	A	512	TRP	CD1-CG-CD2	7.06	111.95	106.30
2	B	12	ARG	NE-CZ-NH2	-7.05	116.78	120.30
2	D	380	TRP	CD1-CG-CD2	7.04	111.93	106.30
1	A	108	THR	N-CA-C	-7.04	91.99	111.00
2	B	448	GLU	CA-CB-CG	7.02	128.85	113.40
2	D	3	ASP	N-CA-C	7.00	129.90	111.00
1	A	430	MET	CG-SD-CE	-6.97	89.04	100.20
1	C	378	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	341	LEU	CA-CB-CG	6.95	131.27	115.30
2	D	115	LEU	CA-CB-CG	6.94	131.26	115.30
2	D	380	TRP	CG-CD2-CE3	6.92	140.13	133.90
1	C	84	TRP	CE2-CD2-CG	-6.90	101.78	107.30
2	D	380	TRP	CE2-CD2-CG	-6.89	101.78	107.30
1	C	69	MET	CA-CB-CG	6.88	125.00	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	13	TYR	CB-CG-CD1	6.86	125.11	121.00
1	A	104	TYR	CB-CG-CD1	-6.84	116.90	121.00
2	D	185	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	B	440	VAL	CA-CB-CG2	-6.79	100.71	110.90
1	A	297	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	102	ASN	CA-CB-CG	6.75	128.25	113.40
2	D	447	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	C	281	TRP	CG-CD1-NE1	-6.70	103.40	110.10
1	C	411	GLU	N-CA-C	6.70	129.10	111.00
2	B	380	TRP	CD1-CG-CD2	6.69	111.65	106.30
1	C	354	MET	CG-SD-CE	-6.67	89.52	100.20
1	C	435	HIS	CA-CB-CG	6.65	124.91	113.60
2	B	2	LEU	CA-CB-CG	6.64	130.57	115.30
2	D	130	GLU	CA-CB-CG	6.64	128.00	113.40
1	C	51	ARG	N-CA-CB	-6.63	98.66	110.60
2	D	154	VAL	CA-CB-CG2	-6.62	100.97	110.90
2	D	16	ARG	NE-CZ-NH2	-6.61	117.00	120.30
2	B	380	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	A	397	THR	N-CA-CB	-6.50	97.94	110.30
1	A	129	GLU	N-CA-C	-6.50	93.45	111.00
1	A	38	VAL	CA-CB-CG2	6.50	120.65	110.90
1	A	128	HIS	CA-C-N	-6.48	102.94	117.20
1	A	390	SER	CA-CB-OG	6.48	128.71	111.20
2	D	69	SER	N-CA-C	-6.48	93.50	111.00
2	B	230	LYS	CA-CB-CG	6.48	127.66	113.40
2	D	343	THR	N-CA-CB	6.48	122.61	110.30
1	C	329	TYR	CB-CG-CD1	-6.48	117.11	121.00
2	B	22	THR	CA-CB-CG2	-6.46	103.35	112.40
2	B	440	VAL	N-CA-CB	-6.46	97.30	111.50
1	C	438	THR	N-CA-CB	-6.46	98.03	110.30
1	A	277	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	C	305	ASP	N-CA-C	6.45	128.42	111.00
2	D	88	VAL	CG1-CB-CG2	-6.43	100.60	110.90
2	D	118	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	A	108	THR	CA-CB-CG2	-6.41	103.43	112.40
1	C	40	ASN	N-CA-C	6.37	128.19	111.00
1	A	308	LEU	CA-CB-CG	6.36	129.93	115.30
2	D	327	LEU	CA-CB-CG	6.36	129.92	115.30
1	C	397	THR	CA-C-N	-6.31	103.33	117.20
1	A	386	ILE	N-CA-C	6.30	128.00	111.00
1	C	342	TYR	CB-CG-CD1	6.27	124.76	121.00
2	D	58	ARG	NE-CZ-NH1	6.27	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	165	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	A	347	ARG	CA-CB-CG	-6.27	99.61	113.40
2	B	2	LEU	CB-CA-C	6.27	122.11	110.20
1	C	434	MET	CG-SD-CE	-6.26	90.19	100.20
2	D	351	GLN	CA-CB-CG	6.25	127.15	113.40
2	B	324	ILE	CG1-CB-CG2	-6.25	97.66	111.40
1	A	343	VAL	CG1-CB-CG2	-6.24	100.91	110.90
2	B	400	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	B	257	CYS	CA-C-N	6.20	130.84	117.20
2	B	416	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	B	139	THR	N-CA-CB	-6.20	98.53	110.30
1	A	69	MET	CA-CB-CG	6.19	123.82	113.30
1	C	67	LYS	N-CA-CB	-6.18	99.47	110.60
1	A	143	ALA	N-CA-C	6.17	127.67	111.00
2	B	415	ASP	CB-CA-C	-6.17	98.05	110.40
1	A	105	VAL	CA-CB-CG2	-6.17	101.65	110.90
2	D	296	ARG	NE-CZ-NH1	6.15	123.37	120.30
2	B	244	TYR	CB-CG-CD2	-6.14	117.32	121.00
1	C	51	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	D	218	MET	CG-SD-CE	6.14	110.02	100.20
1	A	142	TYR	N-CA-C	6.13	127.54	111.00
1	A	24	HIS	CA-CB-CG	-6.11	103.21	113.60
1	C	223	TRP	CE2-CD2-CG	-6.09	102.42	107.30
2	B	218	MET	CG-SD-CE	6.09	109.95	100.20
1	C	519	TRP	CG-CD1-NE1	-6.09	104.01	110.10
2	D	394	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	A	281	TRP	CG-CD2-CE3	6.08	139.37	133.90
1	A	128	HIS	O-C-N	6.06	132.39	122.70
1	C	387	ASP	N-CA-C	-6.05	94.67	111.00
2	D	22	THR	CA-CB-CG2	6.05	120.87	112.40
2	B	384	GLU	CA-CB-CG	6.04	126.70	113.40
1	C	110	MET	CA-C-N	-6.04	103.91	117.20
2	B	408	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	142	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	A	168	PRO	CA-C-N	6.00	130.41	117.20
1	C	480	GLN	CA-CB-CG	5.99	126.58	113.40
1	A	21	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	D	70	SER	N-CA-CB	-5.96	101.56	110.50
2	D	296	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	B	380	TRP	CG-CD2-CE3	5.94	139.25	133.90
1	A	520	LYS	CA-C-N	-5.94	104.14	117.20
2	D	154	VAL	CA-CB-CG1	5.94	119.80	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	376	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	84	TRP	CD1-CG-CD2	5.93	111.04	106.30
1	A	84	TRP	CE2-CD2-CG	-5.92	102.56	107.30
1	A	406	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	490	TYR	CB-CG-CD1	5.91	124.54	121.00
1	A	87	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	C	385	LYS	CA-CB-CG	-5.89	100.44	113.40
1	C	245	THR	CA-CB-OG1	-5.89	96.63	109.00
1	C	174	CYS	CA-CB-SG	5.89	124.60	114.00
1	A	239	THR	N-CA-C	-5.87	95.14	111.00
2	B	386	VAL	N-CA-CB	-5.87	98.58	111.50
2	D	427	TYR	CB-CG-CD2	-5.86	117.48	121.00
2	B	2	LEU	N-CA-C	-5.86	95.19	111.00
1	A	198	ILE	N-CA-C	5.85	126.80	111.00
1	A	391	LYS	N-CA-C	5.85	126.79	111.00
1	A	424	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	521	LYS	N-CA-C	-5.83	95.26	111.00
1	A	526	SER	N-CA-C	-5.83	95.27	111.00
2	B	315	VAL	CG1-CB-CG2	-5.82	101.58	110.90
2	B	388	LEU	CA-CB-CG	5.82	128.69	115.30
2	D	393	THR	CA-C-N	5.82	130.00	117.20
2	D	296	ARG	CA-CB-CG	5.80	126.16	113.40
2	B	265	ARG	CB-CG-CD	-5.79	96.56	111.60
1	C	30	GLU	CA-C-N	-5.78	104.47	117.20
1	C	453	LEU	CA-CB-CG	5.78	128.58	115.30
1	C	226	ASP	N-CA-CB	-5.77	100.21	110.60
1	A	268	TYR	CB-CG-CD1	5.76	124.46	121.00
2	D	402	GLU	N-CA-C	-5.76	95.45	111.00
2	B	194	MET	CA-CB-CG	-5.75	103.52	113.30
1	C	134	PHE	CA-C-N	5.75	129.85	117.20
2	B	122	MET	CA-C-N	5.75	129.85	117.20
1	C	406	ARG	NE-CZ-NH2	-5.75	117.43	120.30
2	B	46	GLN	CA-CB-CG	5.74	126.02	113.40
2	B	333	GLU	CA-CB-CG	5.73	126.01	113.40
1	C	265	SER	CA-CB-OG	5.73	126.67	111.20
2	D	3	ASP	N-CA-CB	-5.72	100.31	110.60
2	B	386	VAL	CB-CA-C	5.70	122.23	111.40
1	A	234	TYR	CB-CG-CD2	-5.69	117.59	121.00
2	D	192	GLU	N-CA-CB	-5.68	100.38	110.60
1	A	92	LYS	CA-CB-CG	5.68	125.89	113.40
2	B	2	LEU	CA-C-N	-5.66	104.75	117.20
1	C	397	THR	O-C-N	5.65	131.75	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	135	ILE	CG1-CB-CG2	-5.65	98.96	111.40
1	A	376	GLU	N-CA-C	5.65	126.25	111.00
1	A	177	TYR	CB-CG-CD1	-5.64	117.62	121.00
1	A	38	VAL	CA-CB-CG1	-5.63	102.45	110.90
2	B	440	VAL	CA-CB-CG1	5.63	119.35	110.90
1	A	110	MET	CA-C-N	-5.61	104.86	117.20
1	A	476	VAL	CG1-CB-CG2	-5.61	101.93	110.90
2	D	141	SER	N-CA-C	5.58	126.06	111.00
1	A	2	SER	N-CA-CB	-5.57	102.14	110.50
1	A	108	THR	CA-C-N	5.57	129.45	117.20
1	A	163	LYS	CA-CB-CG	5.57	125.64	113.40
1	C	47	ILE	N-CA-C	-5.56	96.00	111.00
1	A	110	MET	O-C-N	5.56	131.59	122.70
2	B	212	THR	CA-C-N	-5.55	104.99	117.20
1	C	16	LYS	CA-CB-CG	5.55	125.60	113.40
2	B	84	ILE	CB-CA-C	-5.54	100.51	111.60
2	D	457	VAL	N-CA-C	-5.54	96.03	111.00
1	A	139	ILE	CA-C-N	5.53	127.25	116.20
1	A	508	TYR	CB-CG-CD2	5.52	124.31	121.00
1	A	427	TYR	CB-CG-CD2	-5.50	117.70	121.00
2	B	16	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	B	212	THR	CA-CB-CG2	5.48	120.08	112.40
1	A	519	TRP	CG-CD1-NE1	-5.48	104.62	110.10
1	A	281	TRP	CG-CD1-NE1	-5.47	104.63	110.10
2	B	205	SER	CA-C-N	5.47	127.15	116.20
1	C	221	ASP	CB-CA-C	-5.47	99.46	110.40
2	D	4	ALA	N-CA-C	5.46	125.75	111.00
2	B	12	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	B	51	TYR	CB-CG-CD1	5.46	124.27	121.00
1	C	10	LEU	CA-CB-CG	5.44	127.82	115.30
2	D	114	ASP	CB-CG-OD1	5.44	123.19	118.30
2	D	343	THR	CB-CA-C	-5.43	96.94	111.60
2	B	189	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	C	97	THR	N-CA-CB	-5.42	100.00	110.30
1	A	407	VAL	CG1-CB-CG2	-5.42	102.23	110.90
2	B	2	LEU	CD1-CG-CD2	-5.42	94.24	110.50
2	D	207	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	C	110	MET	O-C-N	5.41	131.35	122.70
1	C	231	LYS	CA-CB-CG	5.40	125.28	113.40
1	C	257	LEU	CA-CB-CG	5.39	127.70	115.30
2	B	2	LEU	CB-CG-CD1	5.39	120.16	111.00
1	C	241	THR	O-C-N	-5.39	114.04	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	428	GLY	N-CA-C	-5.39	99.63	113.10
1	C	84	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	C	94	GLU	CA-C-N	-5.36	105.41	117.20
2	B	58	ARG	CB-CG-CD	-5.34	97.71	111.60
1	C	281	TRP	CB-CG-CD1	-5.34	120.05	127.00
1	A	396	ILE	CG1-CB-CG2	-5.34	99.66	111.40
1	C	234	TYR	CB-CG-CD2	-5.33	117.80	121.00
2	D	333	GLU	CA-CB-CG	5.32	125.11	113.40
1	C	419	LYS	CA-CB-CG	5.32	125.11	113.40
2	D	191	PHE	CB-CG-CD2	-5.31	117.08	120.80
1	C	65	PRO	N-CA-C	5.31	125.90	112.10
1	C	356	LYS	CA-CB-CG	5.30	125.07	113.40
2	D	133	LEU	CA-CB-CG	5.30	127.49	115.30
2	D	449	CYS	CA-CB-SG	5.30	123.54	114.00
1	C	363	LEU	CA-CB-CG	5.30	127.48	115.30
1	C	13	TYR	CB-CG-CD2	-5.29	117.82	121.00
2	B	307	GLN	CA-CB-CG	5.29	125.03	113.40
1	C	372	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	D	12	ARG	CA-C-N	-5.27	105.60	117.20
1	C	167	ILE	N-CA-C	-5.26	96.79	111.00
1	C	386	ILE	CA-C-N	-5.26	105.63	117.20
1	C	519	TRP	CG-CD2-CE3	5.25	138.63	133.90
2	D	262	LYS	CB-CA-C	-5.25	99.90	110.40
2	D	221	GLU	N-CA-C	5.25	125.17	111.00
2	B	209	ASP	N-CA-C	-5.24	96.84	111.00
1	C	61	VAL	O-C-N	-5.24	114.31	122.70
1	C	211	ASN	CA-C-N	5.24	128.73	117.20
2	D	122	MET	CA-CB-CG	5.22	122.17	113.30
2	D	265	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	B	139	THR	CA-CB-CG2	5.19	119.67	112.40
1	C	223	TRP	CG-CD2-CE3	5.19	138.57	133.90
2	D	278	MET	CG-SD-CE	5.18	108.50	100.20
1	C	430	MET	CG-SD-CE	5.18	108.49	100.20
2	B	4	ALA	N-CA-C	5.18	124.98	111.00
1	A	342	TYR	N-CA-C	-5.17	97.03	111.00
1	C	276	LYS	CB-CG-CD	-5.17	98.15	111.60
1	A	271	GLU	CA-CB-CG	5.17	124.77	113.40
2	D	262	LYS	CA-CB-CG	5.17	124.76	113.40
1	A	198	ILE	O-C-N	-5.16	114.44	123.20
1	A	70	VAL	N-CA-C	-5.15	97.09	111.00
2	D	355	ASP	CB-CG-OD1	5.15	122.94	118.30
2	D	401	GLU	N-CA-CB	-5.15	101.33	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	316	ALA	N-CA-CB	5.14	117.30	110.10
2	B	211	PRO	CA-C-N	5.14	128.50	117.20
2	B	270	VAL	CG1-CB-CG2	-5.14	102.68	110.90
1	C	466	LYS	CA-C-N	-5.13	105.91	117.20
1	A	434	MET	N-CA-CB	-5.13	101.37	110.60
2	D	2	LEU	N-CA-C	-5.12	97.17	111.00
2	B	46	GLN	N-CA-CB	-5.12	101.39	110.60
2	D	122	MET	CB-CA-C	-5.11	100.18	110.40
1	C	357	SER	CA-CB-OG	5.10	124.98	111.20
1	A	131	TYR	CB-CG-CD2	-5.10	117.94	121.00
2	B	106	CYS	CB-CA-C	-5.10	100.20	110.40
2	D	219	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	C	134	PHE	O-C-N	-5.10	114.54	122.70
2	B	421	TYR	CA-CB-CG	5.09	123.08	113.40
2	D	452	GLU	N-CA-CB	-5.09	101.43	110.60
1	A	186	HIS	CB-CA-C	-5.09	100.22	110.40
1	C	95	ASN	CA-CB-CG	5.09	124.59	113.40
1	C	105	VAL	CA-CB-CG1	-5.09	103.27	110.90
2	D	191	PHE	CA-C-N	-5.08	106.03	117.20
1	A	30	GLU	N-CA-C	5.08	124.71	111.00
2	B	183	ASP	CB-CG-OD1	5.06	122.86	118.30
1	C	390	SER	CA-CB-OG	5.06	124.87	111.20
1	A	216	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	A	429	GLY	CA-C-N	-5.06	106.08	117.20
1	A	69	MET	CG-SD-CE	5.05	108.28	100.20
1	C	392	ASN	CA-CB-CG	5.05	124.51	113.40
1	A	384	ILE	CB-CA-C	-5.05	101.50	111.60
2	B	157	ILE	CA-C-N	5.04	128.30	117.20
1	A	386	ILE	CA-C-N	-5.04	106.11	117.20
1	C	512	TRP	CB-CG-CD1	-5.03	120.46	127.00
1	A	281	TRP	CA-CB-CG	5.02	123.24	113.70
2	B	320	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	C	248	LYS	CB-CG-CD	-5.02	98.54	111.60
1	A	47	ILE	N-CA-C	-5.02	97.44	111.00
2	D	122	MET	CB-CG-SD	-5.01	97.36	112.40
1	A	351	TYR	CB-CG-CD1	-5.01	117.99	121.00
2	D	124	ASP	CB-CG-OD1	5.01	122.81	118.30
2	D	355	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	C	318	GLU	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ILE	Peptide
1	A	240	LEU	Mainchain
2	B	198	TYR	Sidechain
2	B	337	ILE	Peptide
1	C	104	TYR	Sidechain
1	C	216	TYR	Sidechain
1	C	32	THR	Peptide
1	C	375	TYR	Sidechain
1	C	508	TYR	Sidechain
2	D	115	LEU	Peptide
2	D	216	TYR	Sidechain
2	D	30	TYR	Sidechain
2	D	420	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4074	0	3992	137	0
1	C	4077	0	3999	149	0
2	B	3511	0	3495	96	0
2	D	3511	0	3495	91	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	14	0	6	0	0
4	D	14	0	6	2	0
5	B	17	0	0	4	0
5	D	17	0	0	4	0
6	B	16	0	0	4	0
6	D	16	0	0	5	0
All	All	15269	0	14993	444	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 15.

All (444) 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)
6:B:498:CLP:S1A	6:B:498:CLP:S1B	2.30	1.28
6:D:498:CLP:S1B	6:D:498:CLP:S1A	2.33	1.26
1:C:345:GLY:HA3	5:D:496:CFM:S1A	2.01	0.99
1:C:197:ILE:HD11	1:C:249:VAL:HB	1.43	0.99
2:D:162:SER:HB3	2:D:257:CYS:SG	2.06	0.96
2:B:278:MET:HE3	1:C:519:TRP:HB3	1.53	0.90
1:A:43:THR:HG21	1:A:49:THR:HG21	1.58	0.86
2:D:325:ILE:HD11	2:D:350:PHE:HA	1.59	0.83
1:A:191:ASN:HD22	1:A:396:ILE:CG2	1.93	0.82
1:A:391:LYS:HE3	1:A:393:ILE:HB	1.66	0.77
1:C:76:PRO:HB2	6:D:498:CLP:S2B	2.24	0.77
2:B:452:GLU:HG2	1:C:92:LYS:HB3	1.66	0.77
1:A:76:PRO:HB2	6:B:498:CLP:S2B	2.25	0.76
1:C:72:ILE:HD11	1:C:108:THR:HG23	1.66	0.76
1:A:213:LEU:HB3	1:A:266:ILE:HD11	1.68	0.76
1:C:187:HIS:ND1	1:C:391:LYS:HB2	2.02	0.75
1:C:48:ILE:HD11	2:D:218:MET:HE1	1.68	0.74
1:C:2:SER:N	1:C:29:THR:HG1	1.84	0.73
1:C:369:PHE:HZ	5:D:496:CFM:S1A	2.10	0.73
1:C:48:ILE:CD1	2:D:218:MET:HE1	2.18	0.73
1:A:388:ALA:H	1:A:390:SER:HB3	1.53	0.73
1:C:48:ILE:HD11	2:D:218:MET:CE	2.18	0.73
2:B:300:ILE:HD13	2:B:303:MET:HE1	1.71	0.71
2:B:330:PHE:HA	2:B:333:GLU:HG2	1.72	0.71
2:B:332:ILE:HD11	2:B:358:LEU:HD12	1.73	0.71
2:D:318:LEU:HD11	2:D:377:VAL:HG11	1.72	0.71
1:C:323:ILE:HD12	1:C:497:VAL:HG11	1.72	0.71
1:C:193:VAL:HA	1:C:197:ILE:HG23	1.71	0.70
2:B:354:ILE:HD11	2:B:368:VAL:HB	1.72	0.70
2:D:145:SER:OG	2:D:345:THR:HB	1.91	0.70
1:A:450:GLU:O	1:A:454:GLU:HG2	1.92	0.69
1:C:232:ILE:HG12	1:C:315:VAL:HG11	1.75	0.69
2:B:297:GLY:HA3	2:D:211:PRO:HB3	1.75	0.68
1:A:191:ASN:ND2	1:A:396:ILE:CG2	2.55	0.68
2:B:129:PRO:HG2	2:B:132:LYS:HG3	1.75	0.68
2:D:69:SER:HB3	2:D:83:ASN:HB3	1.74	0.68
1:A:87:ARG:NH1	5:B:496:CFM:S5	2.67	0.67
2:D:325:ILE:HA	2:D:354:ILE:HD11	1.76	0.67
2:B:169:ASN:OD1	2:B:235:SER:HA	1.95	0.67
1:C:28:LYS:HB3	1:C:438:THR:HG22	1.75	0.67
1:C:74:HIS:O	1:C:144:THR:HB	1.95	0.66
2:B:176:PRO:HA	2:B:241:LEU:HD12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:GLY:O	2:D:85:LYS:HG2	1.96	0.66
1:A:431:MET:HG2	1:A:440:LEU:HD21	1.78	0.66
1:A:190:ASN:OD1	1:A:269:ILE:HG12	1.95	0.65
1:C:93:PRO:HB2	1:C:97:THR:O	1.95	0.65
1:C:65:PRO:HB2	1:C:241:THR:HB	1.78	0.65
2:B:137:THR:HG21	2:B:152:ASN:O	1.96	0.65
1:C:144:THR:HG22	1:C:146:PRO:HD2	1.78	0.65
1:A:343:VAL:HG21	1:A:481:LEU:HD23	1.76	0.65
1:C:154:ILE:HD12	1:C:171:ALA:HB1	1.79	0.65
1:C:389:ASP:HA	1:C:392:ASN:OD1	1.97	0.64
1:C:261:GLN:HE22	1:C:286:PHE:H	1.44	0.64
1:A:191:ASN:HD22	1:A:396:ILE:HG21	1.62	0.64
1:C:209:SER:HB3	1:C:255:ALA:HA	1.80	0.63
2:D:319:GLY:O	2:D:343:THR:HG22	1.98	0.63
1:C:471:ILE:HB	1:C:478:SER:HB2	1.80	0.63
1:C:209:SER:O	1:C:256:ASP:HB2	1.99	0.63
1:C:482:HIS:CE1	4:D:494:HCA:H51	2.34	0.63
1:A:180:VAL:HG13	1:A:390:SER:HB2	1.81	0.62
1:C:48:ILE:CD1	2:D:218:MET:CE	2.76	0.62
2:D:138:ASN:O	2:D:140:PRO:HD3	1.99	0.62
1:A:276:LYS:HA	1:A:400:PRO:HA	1.82	0.62
2:B:57:SER:HA	2:B:62:GLU:O	2.01	0.61
1:C:353:ASN:HA	1:C:356:LYS:HE3	1.83	0.61
2:B:254:GLU:O	2:B:258:LYS:HA	2.01	0.61
2:B:45:SER:HB2	6:B:498:CLP:S2A	2.41	0.61
1:C:259:LEU:HD21	1:C:299:MET:SD	2.41	0.60
2:B:241:LEU:HD23	2:B:264:LEU:HD13	1.82	0.60
1:A:378:ARG:HG3	1:A:427:TYR:HB3	1.83	0.60
1:C:369:PHE:CZ	5:D:496:CFM:S1A	2.94	0.60
2:B:84:ILE:HD11	2:B:118:TYR:CD2	2.37	0.60
1:C:123:LEU:HD23	1:C:157:VAL:HG21	1.83	0.59
2:D:254:GLU:O	2:D:258:LYS:HA	2.03	0.59
1:A:469:PHE:HB3	2:B:63:PRO:HD3	1.84	0.59
2:D:189:ARG:NH2	2:D:428:LYS:HG3	2.17	0.59
1:A:272:MET:SD	1:A:396:ILE:CG2	2.90	0.58
1:C:465:ILE:HG21	2:D:54:THR:HG23	1.84	0.58
1:C:65:PRO:HB3	1:C:242:GLY:H	1.69	0.58
1:C:114:ASP:O	1:C:118:GLY:HA2	2.03	0.58
1:C:381:ILE:HA	1:C:384:ILE:HD12	1.86	0.58
1:C:51:ARG:HG2	2:D:46:GLN:HE22	1.67	0.57
1:A:326:ASP:HA	1:A:329:TYR:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLY:HA2	1:C:110:MET:CE	2.34	0.57
1:A:42:ARG:N	1:A:388:ALA:HB1	2.19	0.57
1:C:434:MET:HB3	1:C:438:THR:HG21	1.86	0.57
2:B:24:GLN:HB3	2:B:139:THR:HG23	1.84	0.57
1:C:316:ILE:O	1:C:320:ILE:HG22	2.05	0.57
1:A:401:ASP:HB3	1:A:404:LYS:H	1.68	0.57
1:A:511:ALA:HB3	2:D:304:ILE:HG13	1.87	0.57
1:C:78:GLY:O	1:C:82:TYR:HD2	1.88	0.57
2:B:441:ILE:O	2:B:445:ILE:HG23	2.04	0.57
1:C:183:SER:HA	1:C:186:HIS:HD1	1.69	0.57
1:A:191:ASN:ND2	1:A:396:ILE:HG22	2.18	0.57
1:C:104:TYR:HA	2:D:18:ASN:HD21	1.70	0.57
1:C:118:GLY:HA2	1:C:150:ILE:HD12	1.87	0.57
1:A:347:ARG:HA	1:A:350:THR:OG1	2.05	0.57
2:D:39:LEU:HG	2:D:218:MET:HE2	1.87	0.56
1:A:378:ARG:HH12	1:A:381:ILE:HD12	1.69	0.56
2:B:351:GLN:O	2:B:355:ASP:HB2	2.05	0.56
1:A:190:ASN:HD21	1:A:266:ILE:HG22	1.70	0.56
2:B:456:VAL:HG11	1:C:85:GLY:HA3	1.88	0.56
2:D:253:LEU:HD22	2:D:259:VAL:HB	1.88	0.56
2:B:314:LYS:HB3	2:B:339:LYS:HG3	1.87	0.56
1:C:226:ASP:O	1:C:230:GLU:HB2	2.06	0.56
1:C:511:ALA:HA	1:C:514:MET:HG2	1.87	0.56
1:A:298:ASP:HB3	1:A:422:VAL:HG13	1.87	0.56
1:A:170:HIS:HE1	1:A:246:TYR:OH	1.89	0.56
2:B:405:PRO:HB3	2:B:440:VAL:HG13	1.87	0.56
2:B:171:LYS:HG2	2:B:197:PRO:HB2	1.87	0.55
1:A:284:CYS:HB2	1:A:295:THR:HG23	1.88	0.55
2:B:35:ILE:HD12	2:B:229:LEU:HD11	1.89	0.55
2:B:417:TYR:HB2	2:D:438:THR:HG21	1.87	0.55
2:D:389:LEU:HD23	2:D:399:ALA:HB2	1.89	0.55
1:A:327:LEU:HA	1:A:330:PHE:CD2	2.41	0.55
1:C:409:ILE:O	1:C:413:LYS:HE2	2.06	0.55
1:C:482:HIS:ND1	4:D:494:HCA:H51	2.21	0.55
2:D:390:ILE:HG12	2:D:407:VAL:HB	1.88	0.55
2:D:34:GLY:HA3	2:D:202:PRO:HB3	1.88	0.55
1:C:203:LYS:O	1:C:254:LYS:HG2	2.07	0.55
1:C:311:ARG:O	1:C:315:VAL:HG12	2.07	0.55
2:B:43:HIS:CE1	2:B:84:ILE:HG12	2.42	0.55
2:B:252:THR:HG22	2:B:256:LYS:NZ	2.22	0.55
1:C:183:SER:HB2	1:C:369:PHE:HD1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:PRO:HG2	2:B:65:MET:O	2.07	0.54
1:C:210:ILE:HG13	1:C:259:LEU:HD11	1.89	0.54
1:C:383:THR:O	1:C:384:ILE:HG13	2.07	0.54
2:B:194:MET:HB3	2:B:196:ILE:HD12	1.89	0.54
1:C:245:THR:HG22	1:C:247:GLU:HB2	1.89	0.54
1:C:432:LYS:NZ	1:C:432:LYS:HB3	2.23	0.54
2:D:393:THR:O	2:D:396:LYS:HG2	2.08	0.54
2:B:239:LEU:HD23	2:B:262:LYS:HB3	1.89	0.54
2:D:137:THR:HG23	2:D:139:THR:HG23	1.90	0.54
2:B:281:SER:HB3	1:C:526:SER:C	2.29	0.54
1:A:141:VAL:HB	1:A:171:ALA:HA	1.88	0.54
2:D:18:ASN:O	2:D:373:ASP:HB2	2.09	0.53
2:D:321:PRO:HG3	2:D:343:THR:HG21	1.90	0.53
1:A:276:LYS:HD3	1:A:399:THR:O	2.08	0.53
1:A:77:ILE:HG21	2:B:21:LYS:HE2	1.90	0.53
1:A:289:VAL:HG23	1:A:496:VAL:HG21	1.90	0.53
1:C:194:MET:HE2	1:C:269:ILE:HG12	1.91	0.53
1:A:365:ALA:O	1:A:440:LEU:HA	2.09	0.53
1:C:431:MET:HA	1:C:434:MET:HE3	1.91	0.53
1:A:260:VAL:HG12	1:A:283:LYS:HD2	1.91	0.52
1:A:499:PHE:CE1	1:A:503:LEU:HD22	2.45	0.52
1:C:75:GLY:HA2	1:C:110:MET:HE2	1.92	0.52
1:C:277:TYR:HB2	1:C:279:ILE:HG13	1.91	0.52
2:B:153:MET:O	2:B:157:ILE:HG13	2.10	0.52
2:D:317:LEU:HD23	2:D:327:LEU:HD13	1.92	0.52
2:D:25:PRO:HG3	6:D:498:CLP:S3B	2.49	0.52
1:A:289:VAL:O	1:A:293:VAL:HG13	2.10	0.52
2:D:41:HIS:HE1	2:D:87:ALA:HB1	1.74	0.52
1:A:74:HIS:HD2	1:A:108:THR:OG1	1.92	0.52
1:C:209:SER:HA	1:C:235:HIS:O	2.10	0.52
1:C:431:MET:HE3	1:C:440:LEU:HD22	1.91	0.51
1:C:278:GLY:HA3	1:C:406:ARG:O	2.09	0.51
1:C:210:ILE:HG22	1:C:236:VAL:HB	1.93	0.51
2:B:238:THR:O	2:B:261:PHE:HA	2.10	0.51
1:A:209:SER:HB3	1:A:255:ALA:HA	1.91	0.51
2:B:452:GLU:HB3	1:C:91:SER:O	2.10	0.51
1:A:272:MET:SD	1:A:396:ILE:HG21	2.51	0.51
2:B:348:MET:O	2:B:351:GLN:HB3	2.11	0.51
2:B:35:ILE:HD11	2:B:157:ILE:HD13	1.93	0.51
2:B:173:ASN:HB2	2:B:238:THR:HG23	1.93	0.51
2:D:38:CYS:HA	2:D:99:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TYR:HB2	1:A:139:ILE:HD11	1.93	0.51
1:C:461:PHE:O	1:C:478:SER:HA	2.11	0.51
1:A:14:ILE:HG23	1:A:16:LYS:HD3	1.91	0.51
1:A:451:VAL:O	1:A:455:LYS:HB2	2.11	0.51
1:A:216:TYR:CE2	5:B:496:CFM:S2A	3.04	0.51
2:B:71:PHE:CZ	2:B:80:GLY:HA3	2.46	0.51
1:A:108:THR:HG21	1:A:123:LEU:HA	1.92	0.51
1:A:61:VAL:HG13	1:A:87:ARG:HH12	1.76	0.50
1:C:276:LYS:O	1:C:405:TYR:HD1	1.93	0.50
2:D:317:LEU:HD23	2:D:327:LEU:CD1	2.41	0.50
1:C:90:LYS:HB3	1:C:223:TRP:CH2	2.46	0.50
1:C:464:GLY:H	1:C:467:GLU:HG3	1.76	0.50
2:B:48:CYS:SG	2:B:105:THR:HG21	2.50	0.50
1:A:209:SER:HA	1:A:235:HIS:O	2.11	0.50
2:B:187:ILE:O	2:B:191:PHE:HD2	1.94	0.50
1:A:16:LYS:HD2	1:A:16:LYS:H	1.76	0.50
1:A:180:VAL:HG11	1:A:388:ALA:HB3	1.93	0.50
2:D:97:PRO:HG2	2:D:100:ILE:HD13	1.94	0.50
2:B:276:PHE:O	2:B:280:LEU:HD12	2.11	0.50
1:A:248:LYS:HB3	1:A:248:LYS:NZ	2.26	0.50
1:C:462:PHE:HB3	1:C:481:LEU:HG	1.94	0.50
1:C:106:PHE:HD1	2:D:17:ILE:HG12	1.76	0.50
2:B:300:ILE:HD13	2:B:303:MET:CE	2.40	0.50
2:B:49:CYS:O	2:B:53:ARG:HG3	2.11	0.50
2:B:68:THR:HB	2:B:70:SER:H	1.76	0.50
1:C:53:CYS:HB3	6:D:498:CLP:S2A	2.52	0.50
1:A:201:GLY:HA3	1:A:251:ASN:ND2	2.27	0.50
1:C:113:SER:HA	1:C:116:VAL:HG22	1.93	0.50
2:D:119:ILE:HA	2:D:122:MET:SD	2.52	0.49
2:D:169:ASN:OD1	2:D:235:SER:HA	2.12	0.49
1:A:205:GLN:HG3	1:A:254:LYS:O	2.12	0.49
1:A:334:LEU:HG	1:A:504:VAL:HG12	1.93	0.49
2:B:141:SER:HB3	6:B:498:CLP:S3B	2.52	0.49
2:D:436:GLU:O	2:D:440:VAL:HG13	2.12	0.49
2:B:194:MET:O	2:B:195:ASP:HB3	2.12	0.49
1:A:519:TRP:HZ2	2:D:293:GLU:HG2	1.77	0.49
1:A:409:ILE:HG22	1:A:410:PRO:O	2.12	0.49
1:A:15:PRO:O	1:A:19:LYS:HD2	2.13	0.49
1:C:272:MET:HB3	1:C:398:VAL:HG11	1.94	0.49
1:C:306:PRO:O	1:C:310:LYS:HB2	2.13	0.48
1:C:210:ILE:HG22	1:C:236:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:MET:O	1:C:453:LEU:HB2	2.13	0.48
1:A:378:ARG:NH1	1:A:381:ILE:HD12	2.28	0.48
1:A:143:ALA:HB2	1:A:154:ILE:HD13	1.94	0.48
2:D:85:LYS:NZ	2:D:121:GLN:HE21	2.11	0.48
2:D:135:ILE:HG21	2:D:157:ILE:HG22	1.95	0.48
1:A:444:MET:HG3	1:A:448:ASP:HB2	1.95	0.48
1:C:187:HIS:CE1	1:C:391:LYS:HB2	2.49	0.48
2:B:172:ILE:O	2:B:198:TYR:HA	2.13	0.48
1:A:292:ILE:O	1:A:296:LEU:HD13	2.14	0.48
2:B:23:CYS:HB2	2:B:141:SER:HB2	1.95	0.48
2:B:330:PHE:O	2:B:334:LEU:HG	2.13	0.48
1:C:435:HIS:O	1:C:438:THR:HB	2.14	0.48
1:A:14:ILE:HA	1:A:14:ILE:HD12	1.75	0.48
2:D:296:ARG:HH11	2:D:296:ARG:HG3	1.78	0.48
2:B:97:PRO:HB2	2:B:99:ILE:O	2.13	0.48
1:C:414:VAL:O	1:C:418:LYS:HD2	2.13	0.48
2:D:358:LEU:HD13	2:D:366:SER:HB2	1.96	0.48
1:C:277:TYR:HA	1:C:405:TYR:HA	1.96	0.48
2:B:408:ARG:HB3	2:B:413:ILE:HG12	1.96	0.48
2:B:237:LEU:HA	2:B:260:PRO:HG2	1.96	0.47
1:C:379:GLU:O	1:C:382:PRO:HD2	2.14	0.47
1:A:5:LEU:O	1:A:9:ILE:HG13	2.14	0.47
1:C:341:LEU:HD12	1:C:348:SER:O	2.14	0.47
1:C:494:ARG:O	1:C:497:VAL:HG22	2.14	0.47
2:B:169:ASN:HD21	2:B:235:SER:HB3	1.78	0.47
1:A:100:ASN:OD1	1:A:102:ASN:HB3	2.14	0.47
1:A:226:ASP:O	1:A:230:GLU:HB2	2.14	0.47
2:B:239:LEU:HB3	2:B:264:LEU:HD11	1.96	0.47
2:D:109:GLU:HG3	2:D:140:PRO:HA	1.96	0.47
2:B:393:THR:OG1	2:B:413:ILE:HA	2.14	0.47
1:C:451:VAL:O	1:C:455:LYS:HB2	2.15	0.47
1:C:90:LYS:HB3	1:C:223:TRP:CZ3	2.49	0.47
1:C:128:HIS:ND1	1:C:165:ILE:HD13	2.29	0.47
2:D:69:SER:O	2:D:71:PHE:N	2.48	0.47
1:A:315:VAL:HA	1:A:318:GLU:HG2	1.97	0.47
1:C:401:ASP:O	1:C:405:TYR:HB2	2.14	0.47
1:C:197:ILE:HD12	1:C:250:GLN:HG3	1.97	0.47
1:A:378:ARG:O	1:A:381:ILE:HB	2.14	0.47
1:C:181:SER:OG	1:C:369:PHE:HB2	2.15	0.47
2:D:38:CYS:HA	2:D:99:ILE:O	2.15	0.47
2:B:354:ILE:HD11	2:B:368:VAL:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:PHE:CE1	1:A:295:THR:HG21	2.51	0.46
2:B:434:VAL:O	2:B:438:THR:HB	2.14	0.46
2:D:427:TYR:O	2:D:431:ILE:HG13	2.15	0.46
1:C:116:VAL:HG23	1:C:117:PHE:CD2	2.50	0.46
2:D:175:ILE:HB	2:D:246:SER:HB3	1.97	0.46
1:A:213:LEU:HB3	1:A:266:ILE:CD1	2.41	0.46
1:C:51:ARG:HD2	1:C:368:GLU:O	2.16	0.46
1:A:24:HIS:CE1	1:A:38:VAL:HG23	2.50	0.46
2:B:307:GLN:O	2:B:311:GLN:HG2	2.16	0.46
1:A:187:HIS:CE1	1:A:394:PRO:O	2.68	0.46
2:D:255:LYS:HA	2:D:258:LYS:NZ	2.31	0.46
1:A:519:TRP:HA	1:A:523:SER:O	2.15	0.46
1:C:363:LEU:HD13	1:C:456:LEU:HD23	1.98	0.46
2:D:240:SER:HB2	2:D:263:THR:HG23	1.98	0.46
2:B:84:ILE:HD11	2:B:118:TYR:HD2	1.79	0.46
2:D:41:HIS:CE1	2:D:87:ALA:HB1	2.51	0.46
2:B:49:CYS:HB2	2:B:68:THR:HG23	1.98	0.46
1:A:307:GLU:O	1:A:311:ARG:HG3	2.15	0.46
2:B:397:PHE:HZ	2:D:456:VAL:HG12	1.80	0.46
2:D:345:THR:HA	2:D:346:PRO:HD3	1.72	0.45
1:C:276:LYS:HG2	1:C:401:ASP:HB2	1.98	0.45
2:D:391:SER:HB3	2:D:406:PHE:HE1	1.80	0.45
1:A:434:MET:SD	1:A:438:THR:HG21	2.57	0.45
1:A:263:HIS:HB2	1:A:283:LYS:HE2	1.98	0.45
1:A:369:PHE:HZ	5:B:496:CFM:S1A	2.39	0.45
1:C:284:CYS:HB2	1:C:295:THR:HG23	1.99	0.45
1:A:375:TYR:O	1:A:431:MET:HG3	2.17	0.45
1:C:452:VAL:O	1:C:456:LEU:HB2	2.15	0.45
2:D:402:GLU:O	2:D:404:ILE:HG13	2.17	0.45
1:C:48:ILE:HD12	2:D:218:MET:HE1	1.99	0.45
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.73	0.45
1:C:120:VAL:HG12	1:C:157:VAL:HG11	1.96	0.45
2:D:224:THR:HB	2:D:229:LEU:HD11	1.97	0.45
2:B:316:ALA:HB2	2:B:386:VAL:HG11	1.98	0.45
1:C:308:LEU:HA	1:C:311:ARG:HG2	1.98	0.45
1:A:344:GLY:HA3	5:B:496:CFM:S1B	2.57	0.45
1:C:278:GLY:O	1:C:408:VAL:HG13	2.17	0.45
1:C:106:PHE:CD1	2:D:17:ILE:HG12	2.52	0.45
1:C:88:ARG:NH1	1:C:484:TYR:HB2	2.32	0.45
1:A:341:LEU:O	1:A:365:ALA:HA	2.17	0.45
1:A:457:LYS:HB2	1:A:457:LYS:HE3	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:TYR:CD1	1:A:241:THR:OG1	2.70	0.45
2:B:389:LEU:O	2:B:406:PHE:HA	2.17	0.45
2:B:278:MET:HA	2:B:278:MET:CE	2.47	0.45
1:C:414:VAL:O	1:C:418:LYS:HB2	2.16	0.45
1:A:472:GLN:HG2	1:A:476:VAL:O	2.16	0.45
1:C:48:ILE:HD11	2:D:218:MET:HE3	1.99	0.44
2:B:43:HIS:HE1	2:B:80:GLY:O	2.01	0.44
1:A:453:LEU:HD11	1:A:471:ILE:HG23	1.99	0.44
1:A:101:PHE:CZ	1:A:134:PHE:HB3	2.52	0.44
1:A:517:PRO:HA	1:A:518:PRO:HD3	1.84	0.44
2:B:237:LEU:HG	2:B:238:THR:N	2.32	0.44
1:A:472:GLN:HE21	1:A:477:LEU:HA	1.83	0.44
1:C:517:PRO:HA	1:C:518:PRO:HD2	1.66	0.44
1:A:277:TYR:O	1:A:406:ARG:HD2	2.17	0.44
1:C:53:CYS:CB	6:D:498:CLP:S2A	3.06	0.44
2:B:38:CYS:SG	2:B:101:ALA:HB2	2.58	0.44
1:C:354:MET:O	1:C:357:SER:HB2	2.17	0.44
1:C:393:ILE:HG23	1:C:394:PRO:HD2	1.98	0.44
1:C:256:ASP:O	1:C:408:VAL:HG21	2.18	0.44
2:B:339:LYS:HA	2:B:339:LYS:HD2	1.73	0.44
2:D:88:VAL:HA	2:D:91:ILE:HD12	1.98	0.44
2:B:315:VAL:HG21	2:B:331:ILE:HG21	2.00	0.44
2:D:315:VAL:HG13	2:D:388:LEU:HB3	1.98	0.44
2:B:341:VAL:O	2:B:368:VAL:HA	2.18	0.44
1:A:78:GLY:HA3	2:B:23:CYS:SG	2.58	0.44
1:A:343:VAL:HG12	1:A:344:GLY:H	1.83	0.44
1:A:401:ASP:O	1:A:402:GLU:HB2	2.18	0.44
2:B:331:ILE:HG22	2:B:336:ALA:HB3	2.00	0.44
1:A:81:PHE:CD2	2:B:22:THR:HG23	2.53	0.44
1:A:81:PHE:CG	2:B:22:THR:HG23	2.52	0.44
1:A:330:PHE:CZ	1:A:497:VAL:HA	2.52	0.43
1:C:289:VAL:HA	1:C:292:ILE:HD12	2.00	0.43
1:A:82:TYR:CZ	2:B:22:THR:HG21	2.53	0.43
2:D:176:PRO:HG3	2:D:184:MET:HG2	2.01	0.43
2:D:42:SER:HB2	2:D:68:THR:HG23	2.01	0.43
1:A:191:ASN:ND2	1:A:396:ILE:CB	2.81	0.43
2:B:332:ILE:CD1	2:B:357:MET:HG2	2.49	0.43
2:D:96:ASN:HA	2:D:97:PRO:HD3	1.72	0.43
1:C:326:ASP:O	1:C:329:TYR:HB3	2.18	0.43
2:B:255:LYS:HA	2:B:255:LYS:HD3	1.81	0.43
2:D:52:HIS:O	2:D:55:VAL:HG12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:ILE:HD12	2:B:134:VAL:HG23	2.00	0.43
1:A:213:LEU:HA	1:A:240:LEU:HB2	2.01	0.43
1:A:181:SER:HB2	1:A:369:PHE:HB3	1.99	0.43
1:A:410:PRO:O	1:A:412:ASP:N	2.51	0.43
1:C:334:LEU:HD11	1:C:507:ILE:HD12	1.99	0.43
2:B:379:GLN:O	2:B:382:LYS:HB2	2.18	0.43
2:B:284:THR:OG1	2:B:286:LYS:HG2	2.19	0.43
1:A:338:THR:HG23	1:A:363:LEU:HG	2.00	0.43
2:B:25:PRO:HB2	2:B:52:HIS:CE1	2.53	0.43
1:A:163:LYS:HB2	1:A:163:LYS:HE3	1.75	0.43
1:C:472:GLN:HA	1:C:476:VAL:O	2.19	0.43
1:A:69:MET:HG2	1:A:138:ALA:HB3	2.01	0.43
1:C:146:PRO:O	1:C:150:ILE:HG12	2.18	0.43
1:A:193:VAL:HA	1:A:197:ILE:HD12	1.99	0.43
1:A:513:LYS:N	1:A:513:LYS:HD2	2.33	0.43
1:C:65:PRO:CB	1:C:241:THR:HB	2.47	0.43
1:C:69:MET:HG2	1:C:138:ALA:HB3	1.99	0.43
2:D:316:ALA:HB2	2:D:386:VAL:HG11	1.99	0.43
1:A:205:GLN:HG2	1:A:206:LYS:N	2.33	0.43
1:C:292:ILE:HG22	1:C:296:LEU:HD23	2.00	0.43
1:A:262:CYS:SG	1:A:265:SER:OG	2.69	0.43
1:A:103:GLU:H	1:A:103:GLU:HG2	1.67	0.43
2:D:88:VAL:HG21	2:D:122:MET:CE	2.48	0.43
1:A:26:VAL:HG11	1:A:36:GLU:O	2.19	0.43
2:B:390:ILE:HA	2:B:407:VAL:O	2.18	0.43
1:A:227:ARG:HH11	1:A:227:ARG:HG3	1.83	0.43
1:C:205:GLN:HG2	1:C:206:LYS:N	2.33	0.43
1:A:355:LEU:O	1:A:358:PHE:HB2	2.19	0.42
1:C:333:LYS:HB2	1:C:334:LEU:HD13	2.01	0.42
2:B:342:VAL:HG22	2:B:369:LYS:HB3	2.01	0.42
1:C:330:PHE:HE2	1:C:497:VAL:HA	1.84	0.42
1:A:131:TYR:CD1	1:A:167:ILE:HD12	2.54	0.42
1:C:88:ARG:HH12	1:C:484:TYR:HB2	1.84	0.42
1:A:449:MET:O	1:A:453:LEU:HB2	2.19	0.42
1:A:461:PHE:O	1:A:478:SER:HA	2.19	0.42
1:A:91:SER:O	2:D:452:GLU:HB2	2.19	0.42
1:C:391:LYS:HA	1:C:393:ILE:HB	2.01	0.42
1:C:26:VAL:HG11	1:C:431:MET:HE2	2.00	0.42
2:B:115:LEU:O	2:B:119:ILE:HG12	2.19	0.42
1:A:430:MET:HG2	1:A:434:MET:HE2	2.01	0.42
1:A:337:LYS:HE2	1:A:507:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ILE:HG13	1:C:259:LEU:CD1	2.50	0.42
2:B:276:PHE:O	2:B:279:ALA:HB3	2.20	0.42
2:D:367:LYS:HD3	2:D:368:VAL:N	2.35	0.42
1:C:434:MET:HE3	1:C:440:LEU:HD21	2.02	0.42
1:C:511:ALA:HA	1:C:514:MET:CG	2.49	0.42
1:A:131:TYR:HA	1:A:136:PRO:HD3	2.02	0.42
1:A:14:ILE:HG23	1:A:16:LYS:CD	2.49	0.42
2:D:176:PRO:HD2	2:D:201:PHE:O	2.20	0.42
2:D:115:LEU:HD23	2:D:115:LEU:H	1.84	0.42
1:C:330:PHE:CE2	1:C:500:GLY:HA3	2.54	0.42
2:B:288:VAL:HA	2:B:289:PRO:HD3	1.80	0.42
1:C:245:THR:HB	1:C:248:LYS:HB2	2.02	0.42
1:A:358:PHE:HE2	1:A:499:PHE:CE1	2.38	0.42
2:D:195:ASP:O	2:D:286:LYS:NZ	2.53	0.42
1:A:44:VAL:HA	1:A:45:PRO:HD3	1.79	0.42
2:D:87:ALA:O	2:D:91:ILE:HG13	2.20	0.41
1:C:331:LYS:HG2	1:C:357:SER:O	2.20	0.41
1:C:288:GLY:O	1:C:292:ILE:HG13	2.20	0.41
2:B:345:THR:HA	2:B:346:PRO:HD2	1.66	0.41
1:C:127:ILE:HG21	1:C:161:ALA:HB1	2.02	0.41
1:A:484:TYR:O	1:A:487:ASN:ND2	2.53	0.41
2:B:391:SER:OG	2:B:395:GLY:HA3	2.19	0.41
2:B:46:GLN:HA	2:B:68:THR:HG21	2.01	0.41
2:D:194:MET:O	2:D:286:LYS:HG2	2.20	0.41
1:A:319:GLU:O	1:A:322:ALA:HB3	2.20	0.41
1:C:76:PRO:HG2	2:D:106:CYS:SG	2.60	0.41
1:A:131:TYR:CD2	1:A:165:ILE:HG12	2.55	0.41
1:A:216:TYR:HA	1:A:242:GLY:H	1.85	0.41
1:C:115:ILE:HG22	1:C:116:VAL:HG13	2.02	0.41
1:C:333:LYS:HB3	1:C:508:TYR:HE2	1.84	0.41
2:D:233:GLY:HA2	2:D:257:CYS:SG	2.60	0.41
1:C:75:GLY:HA2	1:C:110:MET:HE3	2.00	0.41
2:D:95:TYR:HB3	2:D:218:MET:SD	2.61	0.41
2:D:137:THR:OG1	2:D:152:ASN:HB3	2.20	0.41
2:D:204:THR:CG2	2:D:208:LEU:HB2	2.51	0.41
2:B:162:SER:OG	2:B:253:LEU:HD13	2.20	0.41
1:C:87:ARG:NH1	5:D:496:CFM:S5	2.94	0.41
1:C:75:GLY:HA3	1:C:144:THR:HG21	2.02	0.41
1:A:343:VAL:CG2	1:A:481:LEU:HD23	2.47	0.41
2:D:28:ALA:HB2	2:D:139:THR:HG21	2.02	0.41
1:A:70:VAL:HG12	1:A:72:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ILE:HA	1:A:394:PRO:HD2	1.94	0.41
1:A:193:VAL:HG13	1:A:269:ILE:HD11	2.03	0.41
1:C:48:ILE:CD1	2:D:218:MET:HE3	2.51	0.41
1:C:330:PHE:CE2	1:C:497:VAL:HA	2.55	0.41
1:A:462:PHE:HB3	1:A:481:LEU:HD22	2.02	0.41
1:A:61:VAL:HG13	1:A:87:ARG:NH1	2.36	0.41
1:C:461:PHE:HB3	1:C:471:ILE:HG21	2.02	0.41
2:D:250:ALA:HB1	2:D:261:PHE:CD2	2.55	0.41
1:A:114:ASP:O	1:A:118:GLY:N	2.51	0.41
2:D:450:THR:HB	2:D:453:ASP:HB3	2.03	0.41
2:D:239:LEU:HD22	2:D:264:LEU:HD21	2.03	0.41
1:C:431:MET:CE	1:C:440:LEU:HD22	2.50	0.41
1:A:128:HIS:CG	1:A:165:ILE:HD11	2.56	0.41
2:B:232:THR:HG22	2:B:253:LEU:HD21	2.03	0.41
2:B:181:PRO:O	2:B:185:ARG:HG3	2.21	0.41
1:C:5:LEU:HD23	1:C:439:ILE:HG12	2.02	0.41
2:D:172:ILE:O	2:D:198:TYR:HA	2.21	0.41
1:C:74:HIS:HA	1:C:108:THR:OG1	2.21	0.41
1:C:154:ILE:O	1:C:157:VAL:HG22	2.21	0.41
2:B:438:THR:HG22	2:B:439:ASN:ND2	2.36	0.41
2:D:150:PHE:CD2	2:D:178:PHE:HD1	2.39	0.41
2:D:181:PRO:O	2:D:185:ARG:HG3	2.20	0.41
1:C:261:GLN:HE22	1:C:286:PHE:N	2.13	0.40
2:D:168:LYS:HA	2:D:234:ASN:O	2.21	0.40
1:A:427:TYR:CZ	1:A:429:GLY:HA2	2.56	0.40
1:A:45:PRO:O	2:B:87:ALA:HA	2.20	0.40
1:A:40:ASN:O	1:A:388:ALA:HB2	2.20	0.40
1:A:216:TYR:HD1	1:A:241:THR:OG1	2.04	0.40
1:C:259:LEU:HB3	1:C:284:CYS:SG	2.62	0.40
1:A:308:LEU:HD23	1:A:311:ARG:NH1	2.36	0.40
2:D:188:LYS:HD2	2:D:198:TYR:HE2	1.85	0.40
1:C:285:ASN:OD1	1:C:350:THR:HG22	2.22	0.40
1:C:367:PHE:CD2	1:C:370:ALA:HB3	2.56	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	523/533 (98%)	447 (86%)	58 (11%)	18 (3%)	5 25
1	C	523/533 (98%)	452 (86%)	51 (10%)	20 (4%)	4 22
2	B	455/458 (99%)	414 (91%)	35 (8%)	6 (1%)	15 53
2	D	455/458 (99%)	411 (90%)	37 (8%)	7 (2%)	13 50
All	All	1956/1982 (99%)	1724 (88%)	181 (9%)	51 (3%)	7 33

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	143	ALA
1	A	241	THR
1	A	387	ASP
1	A	411	GLU
1	A	523	SER
2	B	3	ASP
2	B	361	ALA
1	C	34	ASN
1	C	241	THR
1	C	345	GLY
1	C	429	GLY
2	D	4	ALA
2	D	70	SER
1	A	176	GLY
1	A	205	GLN
1	A	390	SER
1	C	388	ALA
1	C	524	SER
1	A	129	GLU
1	A	168	PRO
1	A	346	SER

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Mol	Chain	Res	Type
1	A	394	PRO
1	A	463	ALA
2	B	4	ALA
2	B	114	ASP
1	C	203	LYS
1	C	402	GLU
1	C	484	TYR
2	D	129	PRO
1	A	429	GLY
1	C	35	PRO
1	C	109	ASP
1	C	389	ASP
1	C	521	LYS
1	C	522	ALA
2	D	115	LEU
2	D	451	GLU
1	C	390	SER
1	C	400	PRO
1	A	419	LYS
2	B	167	ALA
1	C	118	GLY
1	A	306	PRO
1	C	65	PRO
1	A	421	GLY
2	D	91	ILE
2	D	270	VAL
1	C	166	GLY
1	C	518	PRO
2	B	412	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	434/446 (97%)	355 (82%)	79 (18%)	2 11
1	C	435/446 (98%)	369 (85%)	66 (15%)	3 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	383/384 (100%)	322 (84%)	61 (16%)	3 15
2	D	383/384 (100%)	327 (85%)	56 (15%)	4 18
All	All	1635/1660 (98%)	1373 (84%)	262 (16%)	3 15

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	7	ASP
1	A	11	GLU
1	A	14	ILE
1	A	16	LYS
1	A	21	ARG
1	A	28	LYS
1	A	32	THR
1	A	40	ASN
1	A	41	THR
1	A	42	ARG
1	A	43	THR
1	A	47	ILE
1	A	59	LYS
1	A	72	ILE
1	A	87	ARG
1	A	89	PHE
1	A	92	LYS
1	A	102	ASN
1	A	105	VAL
1	A	109	ASP
1	A	110	MET
1	A	121	ASN
1	A	127	ILE
1	A	128	HIS
1	A	150	ILE
1	A	164	GLU
1	A	196	ASP
1	A	200	LYS
1	A	210	ILE
1	A	215	GLU
1	A	227	ARG
1	A	230	GLU
1	A	237	ASN

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Mol	Chain	Res	Type
1	A	240	LEU
1	A	243	ASP
1	A	245	THR
1	A	248	LYS
1	A	260	VAL
1	A	264	ARG
1	A	276	LYS
1	A	310	LYS
1	A	313	GLU
1	A	319	GLU
1	A	326	ASP
1	A	329	TYR
1	A	332	GLU
1	A	341	LEU
1	A	348	SER
1	A	353	ASN
1	A	355	LEU
1	A	371	HIS
1	A	373	ASP
1	A	378	ARG
1	A	381	ILE
1	A	384	ILE
1	A	385	LYS
1	A	387	ASP
1	A	389	ASP
1	A	394	PRO
1	A	398	VAL
1	A	401	ASP
1	A	406	ARG
1	A	407	VAL
1	A	414	VAL
1	A	417	LEU
1	A	418	LYS
1	A	432	LYS
1	A	435	HIS
1	A	453	LEU
1	A	454	GLU
1	A	455	LYS
1	A	457	LYS
1	A	460	MET
1	A	461	PHE
1	A	466	LYS

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Mol	Chain	Res	Type
1	A	485	ASP
1	A	487	ASN
1	A	513	LYS
2	B	2	LEU
2	B	3	ASP
2	B	7	LYS
2	B	15	LEU
2	B	19	PRO
2	B	22	THR
2	B	33	LEU
2	B	42	SER
2	B	45	SER
2	B	46	GLN
2	B	50	SER
2	B	55	VAL
2	B	68	THR
2	B	82	SER
2	B	84	ILE
2	B	106	CYS
2	B	113	ASP
2	B	123	GLU
2	B	124	ASP
2	B	130	GLU
2	B	137	THR
2	B	168	LYS
2	B	172	ILE
2	B	189	ARG
2	B	190	LEU
2	B	192	GLU
2	B	194	MET
2	B	225	LYS
2	B	228	ASP
2	B	235	SER
2	B	248	LEU
2	B	264	LEU
2	B	282	GLU
2	B	291	SER
2	B	307	GLN
2	B	318	LEU
2	B	324	ILE
2	B	327	LEU
2	B	331	ILE

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Mol	Chain	Res	Type
2	B	332	ILE
2	B	345	THR
2	B	349	LYS
2	B	355	ASP
2	B	360	GLU
2	B	364	GLU
2	B	368	VAL
2	B	384	GLU
2	B	386	VAL
2	B	389	LEU
2	B	405	PRO
2	B	415	ASP
2	B	422	ASN
2	B	425	VAL
2	B	432	ARG
2	B	437	ILE
2	B	438	THR
2	B	440	VAL
2	B	442	LEU
2	B	452	GLU
2	B	456	VAL
2	B	458	ARG
1	C	16	LYS
1	C	19	LYS
1	C	20	THR
1	C	26	VAL
1	C	29	THR
1	C	31	GLU
1	C	41	THR
1	C	42	ARG
1	C	44	VAL
1	C	45	PRO
1	C	47	ILE
1	C	61	VAL
1	C	65	PRO
1	C	72	ILE
1	C	80	SER
1	C	83	THR
1	C	95	ASN
1	C	113	SER
1	C	115	ILE
1	C	120	VAL

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Mol	Chain	Res	Type
1	C	124	LYS
1	C	155	LEU
1	C	162	SER
1	C	165	ILE
1	C	197	ILE
1	C	200	LYS
1	C	203	LYS
1	C	204	GLU
1	C	230	GLU
1	C	236	VAL
1	C	250	GLN
1	C	256	ASP
1	C	282	ILE
1	C	304	ASP
1	C	328	ASP
1	C	332	GLU
1	C	341	LEU
1	C	350	THR
1	C	355	LEU
1	C	361	ASP
1	C	362	SER
1	C	371	HIS
1	C	380	VAL
1	C	382	PRO
1	C	383	THR
1	C	386	ILE
1	C	387	ASP
1	C	392	ASN
1	C	393	ILE
1	C	396	ILE
1	C	398	VAL
1	C	400	PRO
1	C	406	ARG
1	C	416	GLU
1	C	417	LEU
1	C	418	LYS
1	C	426	SER
1	C	430	MET
1	C	435	HIS
1	C	438	THR
1	C	443	ASP
1	C	453	LEU

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Mol	Chain	Res	Type
1	C	455	LYS
1	C	460	MET
1	C	473	LYS
1	C	513	LYS
2	D	8	GLU
2	D	10	VAL
2	D	39	LEU
2	D	46	GLN
2	D	56	LEU
2	D	68	THR
2	D	72	THR
2	D	78	PHE
2	D	82	SER
2	D	84	ILE
2	D	95	TYR
2	D	96	ASN
2	D	108	SER
2	D	115	LEU
2	D	120	SER
2	D	122	MET
2	D	130	GLU
2	D	133	LEU
2	D	159	ASN
2	D	168	LYS
2	D	190	LEU
2	D	202	PRO
2	D	217	LYS
2	D	224	THR
2	D	229	LEU
2	D	240	SER
2	D	247	ASP
2	D	248	LEU
2	D	255	LYS
2	D	264	LEU
2	D	277	ILE
2	D	286	LYS
2	D	287	GLU
2	D	291	SER
2	D	307	GLN
2	D	308	GLN
2	D	311	GLN
2	D	327	LEU

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Mol	Chain	Res	Type
2	D	329	LYS
2	D	339	LYS
2	D	341	VAL
2	D	342	VAL
2	D	343	THR
2	D	345	THR
2	D	351	GLN
2	D	377	VAL
2	D	384	GLU
2	D	386	VAL
2	D	400	ARG
2	D	403	ASN
2	D	420	TYR
2	D	438	THR
2	D	448	GLU
2	D	450	THR
2	D	451	GLU
2	D	452	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	74	HIS
1	A	170	HIS
1	A	191	ASN
1	A	285	ASN
1	A	403	GLN
1	A	445	ASN
1	A	472	GLN
1	A	487	ASN
1	A	498	ASN
2	B	41	HIS
2	B	121	GLN
2	B	439	ASN
1	C	237	ASN
1	C	261	GLN
1	C	324	GLN
1	C	371	HIS
1	C	447	HIS
1	C	498	ASN
2	D	18	ASN

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Mol	Chain	Res	Type
2	D	90	ASN
2	D	121	GLN
2	D	159	ASN
2	D	308	GLN
2	D	439	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	HCA	B	494	-	4,13,13	0.82	0	3,18,18	1.73	1 (33%)
5	CFM	B	496	1	0,24,24	0.00	-	0,45,45	0.00	-
6	CLP	B	498	1,2	0,25,25	0.00	-	0,54,54	0.00	-
4	HCA	D	494	-	4,13,13	0.76	0	3,18,18	1.66	1 (33%)
5	CFM	D	496	1	0,24,24	0.00	-	0,45,45	0.00	-
6	CLP	D	498	1,2	0,25,25	0.00	-	0,54,54	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HCA	B	494	-	-	0/7/17/17	0/0/0/0
5	CFM	B	496	1	-	0/0/84/84	0/0/8/8
6	CLP	B	498	1,2	-	0/0/117/117	0/12/10/10
4	HCA	D	494	-	-	0/7/17/17	0/0/0/0
5	CFM	D	496	1	-	0/0/84/84	0/0/8/8
6	CLP	D	498	1,2	-	0/0/117/117	0/12/10/10

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	494	HCA	C3-C2-C1	2.12	118.35	114.96
4	D	494	HCA	C3-C2-C1	2.47	118.90	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	496	CFM	4	0
6	B	498	CLP	4	0
4	D	494	HCA	2	0
5	D	496	CFM	4	0
6	D	498	CLP	5	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.