



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:42 am GMT

PDB ID : 5A2D
Title : CRYSTAL STRUCTURE OF BETAIN ALDEHYDE DEHYDROGENASE
FROM SPINACH SHOWING A THIOHEMIACETAL WITH BETAIN
ALDEHYDE
Authors : Zarate-Romero, A.; Munoz-Clares, R.A.
Deposited on : 2015-05-17
Resolution : 1.98 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

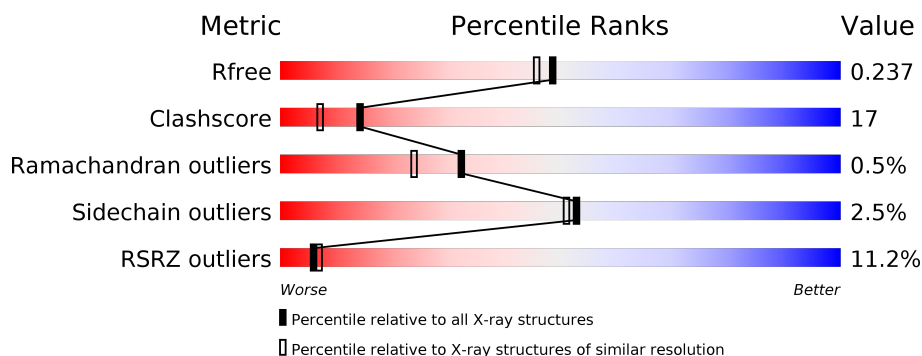
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	9293 (2.00-1.96)
Clashscore	112137	10621 (2.00-1.96)
Ramachandran outliers	110173	10502 (2.00-1.96)
Sidechain outliers	110143	10501 (2.00-1.96)
RSRZ outliers	101464	9395 (2.00-1.96)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	<div> <div>4%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	B	497	<div> <div>10%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
2	C	497	<div> <div>22%</div> <div>59%</div> <div>36%</div> <div>..</div> </div>
3	D	497	<div> <div>8%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CHT	A	1497	-	-	-	X
4	CHT	B	1497	-	-	-	X
5	ETX	D	1498	-	-	X	X
9	GOL	D	1500	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16066 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 BETAINE ALDEHYDE DEHYDROGENASE, CHLORO-PLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	7	0
			3841	2458	641	724	18			
1	B	493	Total	C	N	O	S	0	11	0
			3874	2479	647	731	17			

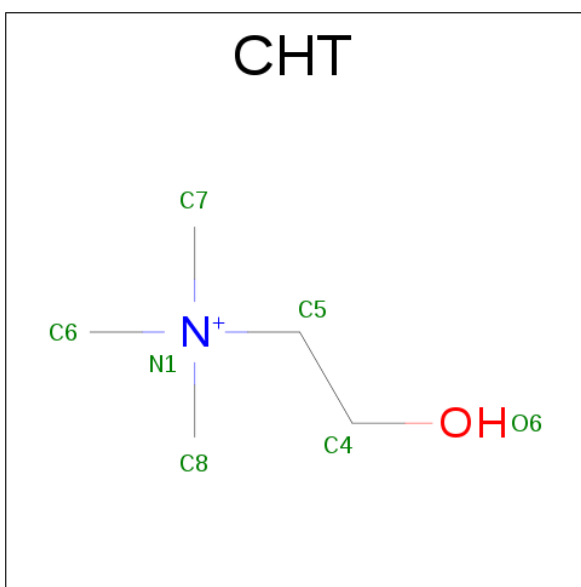
- Molecule 2 is a protein called BETAINE ALDEHYDE DEHYDROGENASE, CHLORO-PLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	492	Total	C	N	O	S	0	3	0
			3806	2437	636	717	16			

- Molecule 3 is a protein called BETAINE ALDEHYDE DEHYDROGENASE, CHLORO-PLASTIC.

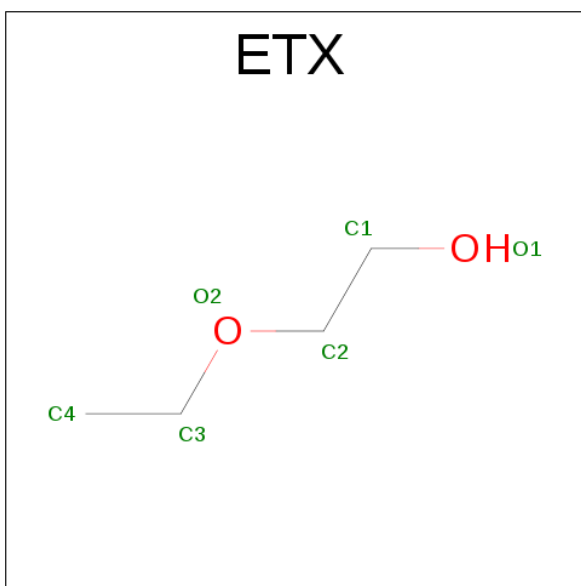
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	493	Total	C	N	O	S	0	3	0
			3817	2447	635	719	16			

- Molecule 4 is CHOLINE ION (three-letter code: CHT) (formula: C₅H₁₄NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			7	5	1	1		
4	B	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 5 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: $C_4H_{10}O_2$).

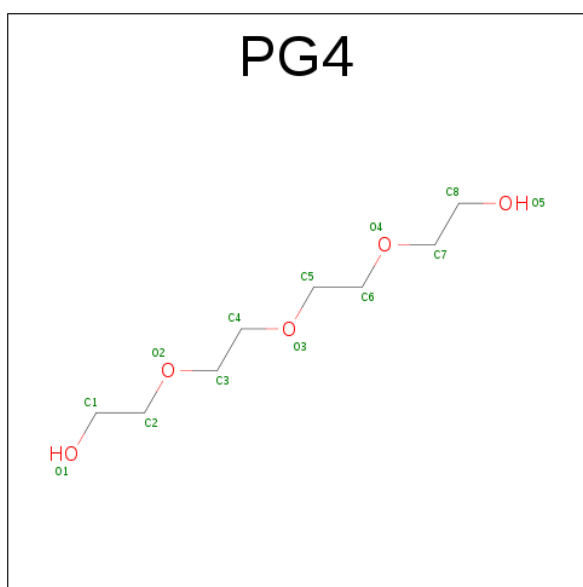


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		
5	D	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

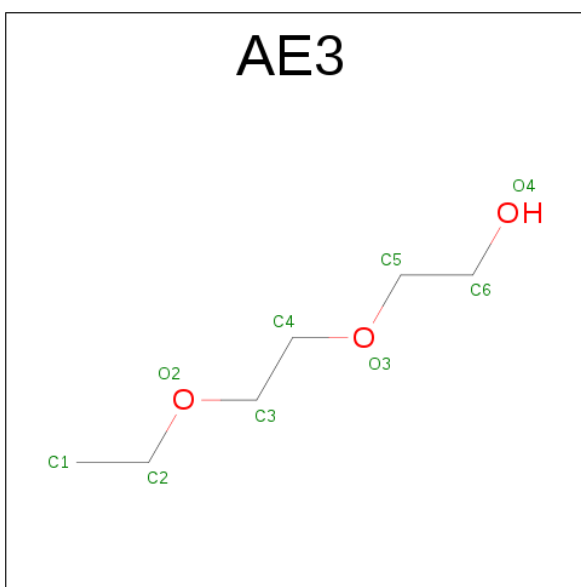
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total K 1 1	0	0
6	A	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0
6	C	1	Total K 1 1	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



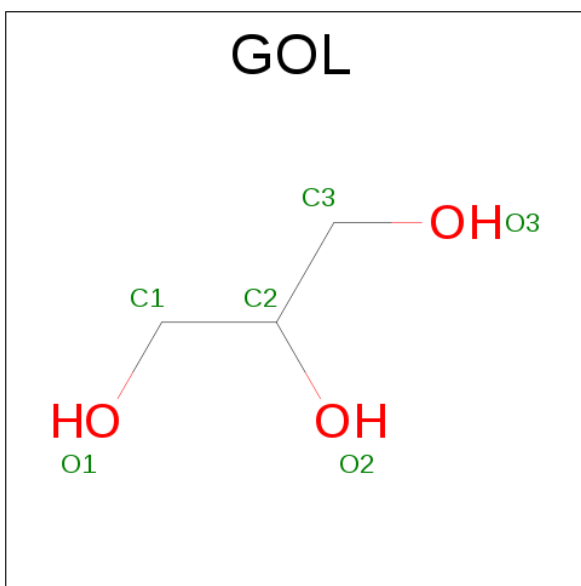
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 12 8 4	0	0

- Molecule 8 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula: C₆H₁₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			9	6	3		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			6	3	3		

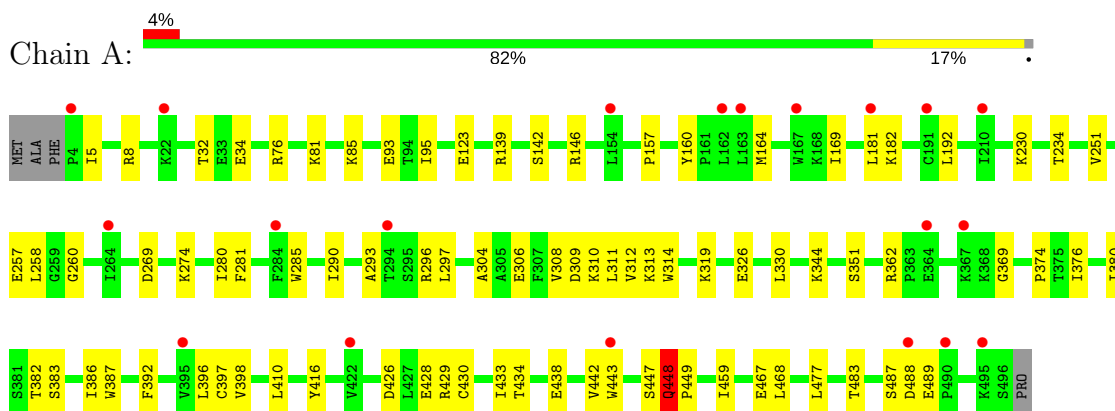
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	239	Total 239	O 239	0	0
10	B	150	Total 150	O 150	0	0
10	C	103	Total 103	O 103	0	0
10	D	179	Total 179	O 179	0	0

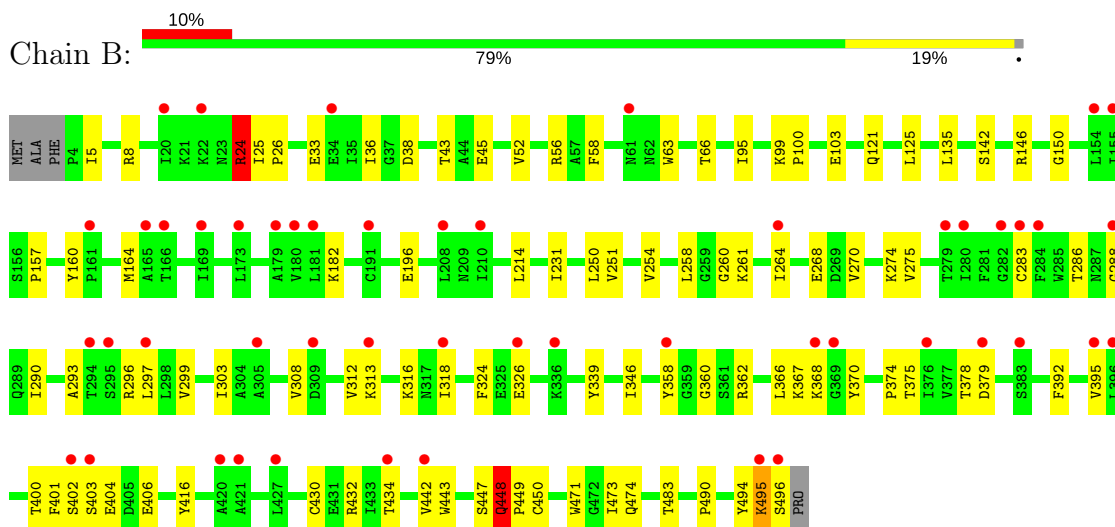
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

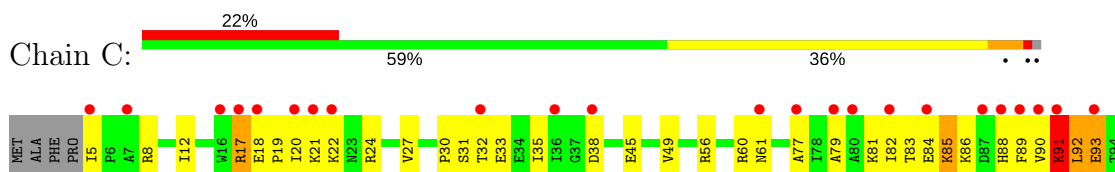
• Molecule 1: BETAINES ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

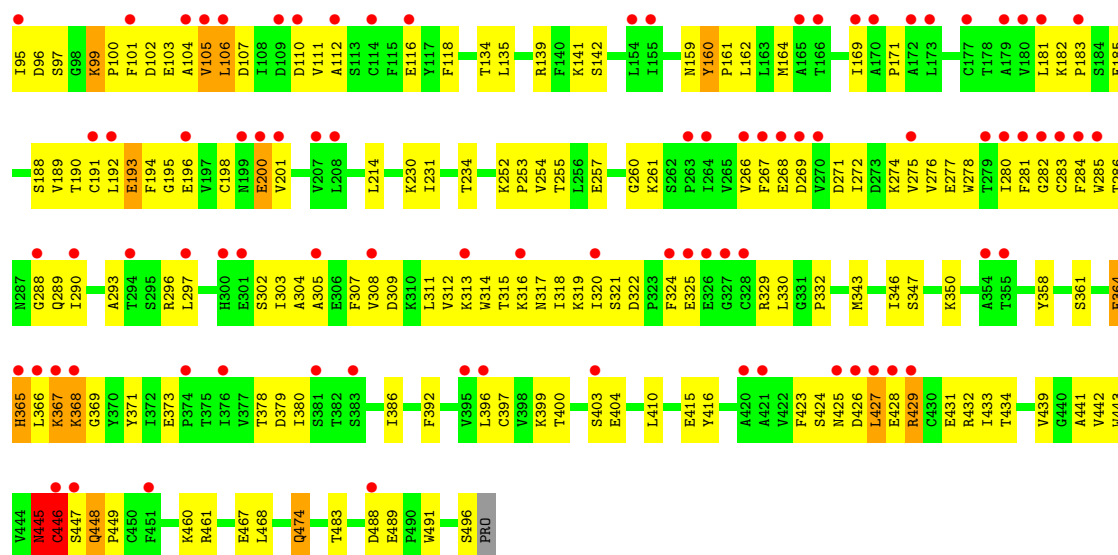


• Molecule 1: BETAINES ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

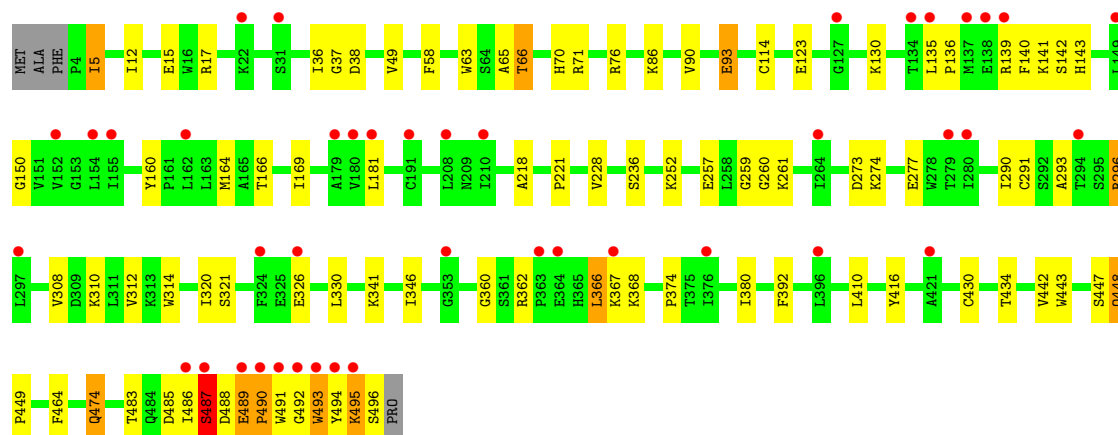
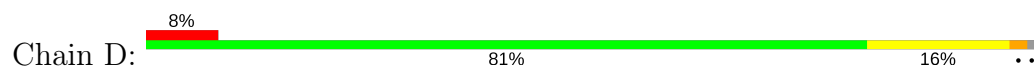


• Molecule 2: BETAINES ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC





● Molecule 3: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.72Å 82.29Å 87.72Å 79.41° 84.75° 77.40°	Depositor
Resolution (Å)	28.70 – 1.98 28.70 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.8 (28.70-1.98) 91.4 (28.70-1.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.194 , 0.237 0.194 , 0.237	Depositor DCC
R_{free} test set	6194 reflections (4.92%)	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16066	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CSO, ETX, AE3, PG4, CHT, K

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	0.51	0/3934	0.61	2/5350 (0.0%)
1	B	0.48	0/3964	0.59	1/5390 (0.0%)
2	C	0.57	0/3890	0.72	7/5289 (0.1%)
3	D	0.52	0/3891	0.66	3/5291 (0.1%)
All	All	0.52	0/15679	0.65	13/21320 (0.1%)

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	1
1	B	0	2
2	C	0	3
All	All	0	6

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	487	SER	CB-CA-C	-18.03	75.85	110.10
2	C	446	CYS	C-N-CA	11.58	150.65	121.70
1	A	448	GLN	N-CA-C	8.54	134.06	111.00
2	C	91	LYS	CB-CA-C	-8.46	93.48	110.40
2	C	445	ASN	O-C-N	-8.37	109.31	122.70
2	C	92	LEU	CB-CA-C	7.69	124.82	110.20
3	D	493	TRP	C-N-CA	-5.94	106.84	121.70
2	C	445	ASN	CA-C-N	5.57	129.46	117.20
1	B	24	ARG	O-C-N	-5.51	113.89	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	GLN	CB-CA-C	-5.43	99.54	110.40
3	D	296	ARG	NE-CZ-NH2	-5.39	117.60	120.30
2	C	105	VAL	CB-CA-C	-5.35	101.24	111.40
2	C	91	LYS	N-CA-C	5.33	125.38	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	396	LEU	Mainchain
1	B	24	ARG	Mainchain
2	C	21	LYS	Mainchain
2	C	445	ASN	Mainchain
2	C	446	CYS	Peptide

5.2 Too-close contacts

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	3841	0	3834	62	2
1	B	3874	0	3867	83	2
2	C	3806	0	3804	325	0
3	D	3817	0	3819	88	0
4	A	7	0	12	0	0
4	B	7	0	12	1	0
5	A	6	0	10	0	0
5	D	6	0	10	4	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	B	12	0	15	1	0
8	C	9	0	14	1	0
9	D	6	0	8	1	0
10	A	239	0	0	0	0
10	B	150	0	0	3	0
10	C	103	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	179	0	0	2	0
All	All	16066	0	15405	533	2

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 17.

All (533) 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)
2:C:278:TRP:HE3	2:C:281:PHE:CZ	1.24	1.54
2:C:5:ILE:HD11	2:C:95:ILE:CD1	1.16	1.52
2:C:314:TRP:HA	2:C:317:ASN:ND2	1.29	1.41
2:C:278:TRP:HA	2:C:281:PHE:CE2	0.88	1.41
2:C:5:ILE:CD1	2:C:95:ILE:CD1	2.07	1.32
2:C:278:TRP:CE3	2:C:281:PHE:CZ	2.16	1.30
2:C:317:ASN:OD1	2:C:318:ILE:HD12	1.26	1.30
2:C:365:HIS:NE2	2:C:366:LEU:HD12	1.48	1.26
2:C:102:ASP:OD2	2:C:329:ARG:NH2	1.69	1.25
2:C:314:TRP:O	2:C:317:ASN:ND2	1.72	1.23
2:C:5:ILE:CD1	2:C:95:ILE:HD12	1.64	1.22
2:C:278:TRP:CA	2:C:281:PHE:HE2	1.24	1.21
1:B:316:LYS:HE3	1:B:358:TYR:CE1	1.78	1.18
2:C:281:PHE:HE1	2:C:447:SER:O	1.21	1.17
2:C:61:ASN:OD1	2:C:61:ASN:O	1.63	1.16
2:C:314:TRP:C	2:C:317:ASN:ND2	1.98	1.14
2:C:317:ASN:OD1	2:C:318:ILE:CD1	1.96	1.13
2:C:18:GLU:HG3	2:C:19:PRO:HD2	1.26	1.12
2:C:5:ILE:HD11	2:C:95:ILE:HD11	1.23	1.11
2:C:365:HIS:NE2	2:C:366:LEU:CD1	2.15	1.08
1:B:316:LYS:NZ	1:B:358:TYR:CD1	2.22	1.08
1:A:304:ALA:O	1:A:308:VAL:HG23	1.49	1.07
2:C:312:VAL:HG12	2:C:316:LYS:HE2	1.36	1.07
2:C:278:TRP:HA	2:C:281:PHE:CZ	1.90	1.06
2:C:5:ILE:CD1	2:C:95:ILE:HD11	1.77	1.05
2:C:111:VAL:HG21	2:C:162:LEU:CD2	1.89	1.03
1:B:316:LYS:CE	1:B:358:TYR:CE1	2.42	1.03
2:C:314:TRP:CA	2:C:317:ASN:HD22	1.56	1.02
1:B:495:LYS:HE3	1:B:495:LYS:HA	1.41	1.02
2:C:281:PHE:CE1	2:C:447:SER:O	2.13	1.01
2:C:272:ILE:HD11	2:C:303:ILE:CG2	1.92	1.00
2:C:316:LYS:HG3	2:C:358:TYR:CE1	1.98	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:185:GLU:OE1	2:C:214:LEU:HA	1.62	0.99
2:C:276:VAL:HG13	2:C:311:LEU:HD12	1.45	0.99
2:C:111:VAL:HG21	2:C:162:LEU:HD22	1.40	0.98
2:C:88:HIS:O	2:C:92:LEU:HD13	1.64	0.98
2:C:83:THR:HG23	2:C:86:LYS:HD3	1.44	0.98
1:B:63:TRP:O	1:B:66:THR:HG22	1.62	0.98
3:D:139:ARG:HG3	3:D:487:SER:HB2	1.46	0.96
3:D:63:TRP:O	3:D:66:THR:HB	1.66	0.96
2:C:91:LYS:NZ	2:C:101:PHE:CD2	2.34	0.95
2:C:32:THR:O	2:C:368:LYS:NZ	2.00	0.95
2:C:272:ILE:HD11	2:C:303:ILE:HG23	1.48	0.95
2:C:278:TRP:CE3	2:C:281:PHE:HZ	1.66	0.95
1:B:8:ARG:NH2	1:B:196:GLU:OE1	2.01	0.94
1:A:314:TRP:CH2	1:B:496:SER:HB3	2.01	0.94
2:C:77:ALA:HB1	2:C:201:VAL:HG23	1.49	0.93
2:C:93:GLU:O	2:C:97:SER:OG	1.86	0.93
2:C:272:ILE:CD1	2:C:303:ILE:HG23	1.98	0.92
2:C:278:TRP:HA	2:C:281:PHE:CD2	1.98	0.92
2:C:81:LYS:NZ	2:C:85:LYS:HD3	1.86	0.91
2:C:319:LYS:H	3:D:495:LYS:NZ	1.67	0.91
2:C:367:LYS:HE3	2:C:368:LYS:HG2	1.50	0.90
2:C:17:ARG:NH1	2:C:49:VAL:HG21	1.87	0.90
2:C:272:ILE:CD1	2:C:303:ILE:CG2	2.50	0.90
2:C:314:TRP:CA	2:C:317:ASN:HD21	1.80	0.90
2:C:314:TRP:HA	2:C:317:ASN:HD22	0.74	0.89
1:A:314:TRP:CZ2	1:B:496:SER:HB3	2.07	0.89
2:C:314:TRP:O	2:C:318:ILE:CD1	2.21	0.88
2:C:319:LYS:H	3:D:495:LYS:HZ1	1.22	0.88
3:D:5:ILE:HD11	3:D:37:GLY:HA3	1.53	0.87
2:C:91:LYS:NZ	2:C:101:PHE:HD2	1.70	0.87
2:C:77:ALA:HB1	2:C:201:VAL:CG2	2.05	0.86
1:B:378:THR:HG22	1:B:379:ASP:H	1.39	0.85
2:C:431:GLU:OE2	3:D:130:LYS:NZ	2.10	0.85
2:C:367:LYS:HD3	2:C:367:LYS:H	1.40	0.85
2:C:278:TRP:HE3	2:C:281:PHE:HZ	0.89	0.85
2:C:196:GLU:OE1	2:C:200:GLU:OE2	1.94	0.84
2:C:277:GLU:O	2:C:281:PHE:CD2	2.30	0.84
2:C:20:ILE:HD12	2:C:45:GLU:HB3	1.57	0.84
2:C:83:THR:CG2	2:C:86:LYS:HD3	2.07	0.83
2:C:271:ASP:HB3	2:C:274:LYS:HD3	1.61	0.83
2:C:277:GLU:O	2:C:281:PHE:HD2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:77:ALA:CB	2:C:201:VAL:CG2	2.57	0.82
2:C:312:VAL:HG12	2:C:316:LYS:CE	2.10	0.82
2:C:364:GLU:O	2:C:365:HIS:HB3	1.79	0.82
2:C:434:THR:HG22	2:C:442:VAL:HG11	1.62	0.81
2:C:8:ARG:HB2	2:C:192:LEU:HD13	1.59	0.81
2:C:188:SER:C	10:C:2038:HOH:O	2.18	0.81
3:D:367:LYS:HG3	3:D:368:LYS:HD2	1.61	0.81
2:C:81:LYS:HZ3	2:C:85:LYS:HD3	1.44	0.81
3:D:139:ARG:O	3:D:486:ILE:CG1	2.29	0.81
2:C:378:THR:HG22	2:C:379:ASP:H	1.45	0.81
2:C:18:GLU:HG3	2:C:19:PRO:CD	2.08	0.81
1:B:316:LYS:HE3	1:B:358:TYR:HE1	1.40	0.80
2:C:234:THR:HG23	2:C:257:GLU:OE1	1.81	0.80
2:C:278:TRP:C	2:C:281:PHE:CE2	2.55	0.80
2:C:33:GLU:HG3	2:C:369:GLY:HA2	1.62	0.80
2:C:104:ALA:O	2:C:107:ASP:HB2	1.80	0.80
2:C:318:ILE:HD12	2:C:318:ILE:N	1.96	0.80
3:D:139:ARG:O	3:D:486:ILE:HG12	1.83	0.79
2:C:364:GLU:O	2:C:365:HIS:CB	2.29	0.79
2:C:81:LYS:O	2:C:84:GLU:HB3	1.81	0.79
1:A:309:ASP:O	1:A:313:LYS:HD3	1.83	0.79
2:C:267:PHE:CE2	2:C:429:ARG:NH2	2.50	0.79
1:B:447:SER:O	1:B:448:GLN:HB2	1.80	0.78
2:C:365:HIS:CD2	2:C:366:LEU:HD12	2.17	0.78
2:C:111:VAL:CG2	2:C:162:LEU:CD2	2.62	0.78
1:B:316:LYS:NZ	1:B:358:TYR:CE1	2.52	0.77
2:C:89:PHE:CE1	2:C:193:GLU:OE2	2.38	0.77
1:B:318:ILE:HD11	1:B:374:PRO:HG3	1.65	0.77
2:C:278:TRP:CE3	2:C:281:PHE:CE2	2.73	0.77
2:C:429:ARG:O	2:C:432:ARG:N	2.16	0.77
3:D:93:GLU:OE2	10:D:2055:HOH:O	2.02	0.77
2:C:90:VAL:HG21	2:C:105:VAL:HG22	1.65	0.77
2:C:107:ASP:O	2:C:110:ASP:HB2	1.84	0.76
1:A:139:ARG:HG3	1:A:487:SER:HB3	1.67	0.76
2:C:271:ASP:O	2:C:274:LYS:HG2	1.85	0.76
2:C:272:ILE:HD11	2:C:303:ILE:HG21	1.68	0.76
2:C:18:GLU:CG	2:C:19:PRO:HD2	2.11	0.75
2:C:302:SER:HB2	2:C:303:ILE:HD12	1.68	0.75
10:C:2062:HOH:O	3:D:493:TRP:O	2.05	0.75
1:B:95:ILE:HG23	1:B:324:PHE:HE2	1.50	0.75
2:C:5:ILE:HD13	2:C:95:ILE:HD11	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LYS:O	1:B:496:SER:OG	2.05	0.74
1:B:261:LYS:O	1:B:296:ARG:NH1	2.20	0.74
1:B:434:THR:HG22	1:B:442:VAL:HG11	1.68	0.74
1:B:24:ARG:NE	1:B:38:ASP:OD2	2.20	0.74
2:C:5:ILE:HD11	2:C:95:ILE:HD12	0.74	0.74
2:C:365:HIS:CD2	2:C:366:LEU:CD1	2.71	0.73
2:C:111:VAL:HG11	2:C:162:LEU:HD21	1.70	0.73
1:B:160:TYR:HB2	1:B:164:MET:HG2	1.68	0.73
2:C:312:VAL:CG1	2:C:316:LYS:HE2	2.18	0.73
2:C:86:LYS:O	2:C:90:VAL:HG12	1.87	0.73
2:C:91:LYS:NZ	2:C:101:PHE:CE2	2.56	0.72
1:B:366[B]:LEU:O	1:B:368:LYS:N	2.22	0.72
3:D:139:ARG:HG3	3:D:487:SER:CB	2.19	0.72
1:B:495:LYS:CE	1:B:495:LYS:HA	2.18	0.72
2:C:60:ARG:HG3	2:C:60:ARG:HH11	1.55	0.72
3:D:434[A]:THR:HG22	3:D:442:VAL:HG11	1.72	0.71
2:C:347:SER:HA	2:C:350:LYS:HE2	1.72	0.71
1:A:362:ARG:NH2	1:A:369:GLY:O	2.19	0.71
2:C:89:PHE:CD1	2:C:193:GLU:OE2	2.44	0.71
1:A:488:ASP:OD1	1:B:274:LYS:NZ	2.22	0.71
2:C:81:LYS:O	2:C:84:GLU:N	2.23	0.71
1:A:434[B]:THR:HB	1:A:442:VAL:HG11	1.72	0.71
2:C:314:TRP:O	2:C:317:ASN:OD1	2.09	0.70
2:C:111:VAL:CG2	2:C:162:LEU:HD23	2.22	0.70
2:C:277:GLU:OE2	3:D:494:TYR:N	2.19	0.70
2:C:267:PHE:CZ	2:C:429:ARG:NH1	2.59	0.70
2:C:314:TRP:O	2:C:318:ILE:HD11	1.92	0.69
2:C:267:PHE:CE2	2:C:429:ARG:NH1	2.59	0.69
2:C:364:GLU:O	2:C:365:HIS:ND1	2.26	0.69
2:C:365:HIS:CD2	2:C:366:LEU:HG	2.27	0.69
2:C:267:PHE:CE1	2:C:429:ARG:NH1	2.61	0.69
2:C:317:ASN:CG	2:C:318:ILE:HD12	2.10	0.69
2:C:83:THR:HA	2:C:86:LYS:HG3	1.75	0.69
1:B:316:LYS:CE	1:B:358:TYR:CD1	2.73	0.69
2:C:316:LYS:CG	2:C:358:TYR:CE1	2.75	0.69
2:C:267:PHE:CD2	2:C:429:ARG:NH1	2.61	0.69
2:C:33:GLU:HB2	2:C:368:LYS:NZ	2.08	0.68
1:A:483[B]:THR:CG2	1:B:443:TRP:CD1	2.76	0.68
2:C:399:LYS:HD2	2:C:410:LEU:HD21	1.76	0.68
2:C:488:ASP:OD1	3:D:274:LYS:NZ	2.25	0.68
1:A:139:ARG:NH2	1:A:489:GLU:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:315:THR:O	2:C:318:ILE:HD13	1.92	0.68
2:C:274:LYS:HG3	2:C:275:VAL:N	2.08	0.68
2:C:269:ASP:HB2	2:C:425:ASN:HB2	1.75	0.68
2:C:30:PRO:HB2	2:C:332:PRO:HG2	1.75	0.68
2:C:364:GLU:O	2:C:365:HIS:CG	2.47	0.68
3:D:485:ASP:OD1	3:D:487:SER:HB2	1.94	0.67
1:A:483[B]:THR:CG2	1:B:443:TRP:HD1	2.07	0.67
2:C:316:LYS:HG3	2:C:358:TYR:CZ	2.28	0.67
1:A:351:SER:OG	2:C:141:LYS:NZ	2.28	0.67
2:C:107:ASP:O	2:C:110:ASP:CB	2.43	0.67
3:D:139:ARG:O	3:D:486:ILE:HG13	1.94	0.67
1:A:296:ARG:NH2	1:A:410:LEU:O	2.27	0.67
2:C:267:PHE:CD1	2:C:429:ARG:NH1	2.63	0.66
2:C:278:TRP:CA	2:C:281:PHE:CD2	2.67	0.66
2:C:280:ILE:HG12	2:C:284:PHE:HD2	1.60	0.66
2:C:267:PHE:CD2	2:C:429:ARG:NH2	2.63	0.66
2:C:427:LEU:HG	2:C:428:GLU:N	2.10	0.66
2:C:281:PHE:O	2:C:285:TRP:HB2	1.96	0.66
2:C:303:ILE:O	2:C:303:ILE:HG22	1.96	0.66
1:B:346:ILE:HD13	1:B:360:GLY:HA2	1.78	0.65
2:C:230:LYS:HZ1	2:C:255:THR:HG23	1.61	0.65
2:C:319:LYS:N	3:D:495:LYS:NZ	2.44	0.65
1:A:309:ASP:O	1:A:313:LYS:CD	2.44	0.65
1:B:316:LYS:HE3	1:B:358:TYR:CD1	2.32	0.65
1:B:450[B]:CYS:HB2	4:B:1497:CHT:C4	2.26	0.65
2:C:17:ARG:HH12	2:C:49:VAL:HG21	1.58	0.65
2:C:169:ILE:HD11	2:C:181:LEU:HD22	1.78	0.65
2:C:272:ILE:HD13	2:C:303:ILE:HG23	1.78	0.65
2:C:314:TRP:C	2:C:317:ASN:HD21	1.92	0.65
2:C:365:HIS:HD2	2:C:366:LEU:HG	1.61	0.65
3:D:291:CSO:HB2	5:D:1498:ETX:H43	1.78	0.65
2:C:426:ASP:O	2:C:429:ARG:HB3	1.97	0.65
1:A:434[A]:THR:HG22	1:A:442:VAL:HG11	1.79	0.64
2:C:107:ASP:HA	2:C:110:ASP:OD2	1.98	0.64
2:C:190:THR:HG22	10:C:2018:HOH:O	1.97	0.64
2:C:100:PRO:O	2:C:103:GLU:N	2.29	0.64
3:D:491:TRP:CE3	3:D:491:TRP:HA	2.32	0.64
2:C:77:ALA:HB3	2:C:201:VAL:CG2	2.28	0.64
3:D:273:ASP:OD1	3:D:310:LYS:NZ	2.23	0.64
1:B:318:ILE:CD1	1:B:374:PRO:HG3	2.28	0.64
2:C:261:LYS:O	2:C:296:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:141:LYS:O	3:D:141:LYS:HG3	1.97	0.64
1:A:380:ILE:HG13	1:A:397[B]:CYS:HB2	1.80	0.63
2:C:320:ILE:HG12	2:C:330:LEU:HD23	1.80	0.63
3:D:5:ILE:CD1	3:D:37:GLY:HA3	2.25	0.63
2:C:308:VAL:HG23	2:C:309:ASP:N	2.13	0.63
2:C:267:PHE:CG	2:C:429:ARG:NH1	2.64	0.63
2:C:367:LYS:CD	2:C:368:LYS:H	2.12	0.63
3:D:368:LYS:HA	3:D:368:LYS:HE3	1.81	0.63
1:B:43:THR:OG1	1:B:45:GLU:OE1	2.16	0.63
1:B:313:LYS:O	1:B:313:LYS:HG2	1.98	0.62
2:C:347:SER:HA	2:C:350:LYS:CE	2.29	0.62
2:C:429:ARG:O	2:C:432:ARG:HB2	1.99	0.62
2:C:424:SER:OG	2:C:425:ASN:N	2.30	0.62
2:C:61:ASN:C	2:C:61:ASN:OD1	2.36	0.62
3:D:261:LYS:HG3	3:D:296:ARG:HD2	1.81	0.62
3:D:38:ASP:OD1	3:D:38:ASP:N	2.30	0.62
2:C:111:VAL:HG21	2:C:162:LEU:HD23	1.76	0.62
2:C:88:HIS:O	2:C:92:LEU:CD1	2.44	0.62
2:C:60:ARG:NH1	2:C:60:ARG:HG3	2.14	0.62
2:C:404:GLU:HG3	2:C:433:ILE:HD11	1.80	0.62
2:C:82:ILE:CG2	2:C:112:ALA:HB2	2.29	0.61
1:A:430:CYS:O	1:A:434[B]:THR:HG22	1.99	0.61
2:C:318:ILE:CD1	2:C:318:ILE:N	2.62	0.61
2:C:423:PHE:CZ	2:C:446:CYS:O	2.53	0.61
1:A:426:ASP:OD1	1:A:428:GLU:HG2	2.00	0.61
3:D:447:SER:O	3:D:449:PRO:HD3	2.00	0.61
2:C:367:LYS:HE2	2:C:368:LYS:HB2	1.82	0.61
2:C:91:LYS:HE3	2:C:324:PHE:CE2	2.35	0.61
2:C:268:GLU:HA	2:C:303:ILE:HD13	1.83	0.60
2:C:272:ILE:CD1	2:C:303:ILE:HG21	2.25	0.60
2:C:188:SER:CA	10:C:2038:HOH:O	2.49	0.60
2:C:268:GLU:HA	2:C:303:ILE:CD1	2.31	0.60
2:C:365:HIS:CD2	2:C:366:LEU:CG	2.84	0.60
3:D:58:PHE:CE1	3:D:150:GLY:HA2	2.36	0.60
2:C:314:TRP:O	2:C:318:ILE:HD12	2.00	0.60
2:C:427:LEU:HG	2:C:428:GLU:H	1.65	0.60
2:C:81:LYS:HZ1	2:C:85:LYS:HD3	1.66	0.60
1:B:378:THR:HG22	1:B:379:ASP:N	2.15	0.59
2:C:195:GLY:O	2:C:198:CYS:N	2.36	0.59
2:C:343:MET:HE1	2:C:346:ILE:HD12	1.84	0.59
2:C:297:LEU:HB2	2:C:396:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:404:GLU:HG2	2:C:404:GLU:O	2.02	0.59
2:C:83:THR:HG23	2:C:86:LYS:CD	2.25	0.59
3:D:66:THR:HG23	3:D:70:HIS:HB3	1.84	0.59
2:C:308:VAL:O	2:C:312:VAL:HG23	2.03	0.59
2:C:367:LYS:HE3	2:C:368:LYS:CG	2.28	0.59
1:B:25[B]:ILE:HG12	1:B:26:PRO:HD2	1.84	0.58
3:D:490:PRO:C	3:D:492:GLY:N	2.55	0.58
2:C:272:ILE:HD13	2:C:303:ILE:CG2	2.31	0.58
1:A:290:ILE:HB	1:A:293:ALA:HB2	1.86	0.58
2:C:367:LYS:N	2:C:367:LYS:HD3	2.12	0.58
1:A:169:ILE:HD11	1:A:181:LEU:HD22	1.84	0.58
1:A:430:CYS:O	1:A:434[A]:THR:HG23	2.04	0.58
2:C:18:GLU:CG	2:C:19:PRO:CD	2.77	0.58
2:C:230:LYS:NZ	2:C:255:THR:HG23	2.18	0.58
2:C:196:GLU:O	2:C:200:GLU:HG3	2.03	0.57
2:C:278:TRP:O	2:C:281:PHE:CE2	2.58	0.57
3:D:261:LYS:HG3	3:D:296:ARG:CD	2.34	0.57
2:C:278:TRP:CB	2:C:281:PHE:CE2	2.82	0.57
3:D:321:SER:HA	3:D:366:LEU:HD21	1.85	0.57
2:C:159:ASN:C	2:C:160:TYR:CD1	2.78	0.57
2:C:361:SER:O	2:C:373:GLU:HG3	2.04	0.57
2:C:89:PHE:CE1	2:C:193:GLU:CD	2.78	0.57
3:D:485:ASP:OD1	3:D:487:SER:N	2.38	0.57
3:D:491:TRP:HE3	3:D:491:TRP:HA	1.70	0.56
1:A:306:GLU:OE2	1:A:310:LYS:NZ	2.38	0.56
3:D:490:PRO:O	3:D:492:GLY:N	2.38	0.56
2:C:278:TRP:CD1	2:C:423:PHE:HE2	2.22	0.56
2:C:269:ASP:CB	2:C:425:ASN:HB2	2.36	0.56
3:D:139:ARG:NH2	3:D:489:GLU:O	2.38	0.56
3:D:490:PRO:O	3:D:491:TRP:C	2.42	0.56
2:C:367:LYS:CE	2:C:368:LYS:H	2.18	0.56
3:D:447:SER:O	3:D:448:GLN:HB2	2.05	0.56
2:C:100:PRO:O	2:C:103:GLU:HB2	2.06	0.56
2:C:278:TRP:CA	2:C:281:PHE:CZ	2.68	0.56
1:B:316:LYS:NZ	1:B:358:TYR:CG	2.72	0.56
2:C:274:LYS:CG	2:C:275:VAL:N	2.68	0.56
2:C:81:LYS:O	2:C:84:GLU:CB	2.54	0.56
2:C:315:THR:HA	2:C:318:ILE:HD13	1.89	0.55
2:C:314:TRP:CH2	3:D:496:SER:HA	2.41	0.55
1:B:474:GLN:NE2	10:B:2059:HOH:O	2.38	0.55
2:C:160:TYR:CD1	2:C:160:TYR:N	2.73	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:423:PHE:CE2	2:C:445:ASN:O	2.60	0.55
2:C:404:GLU:CG	2:C:404:GLU:O	2.55	0.55
3:D:447:SER:C	3:D:449:PRO:HD3	2.28	0.55
1:B:430:CYS:O	1:B:434:THR:HG23	2.07	0.55
3:D:259:GLY:HA3	5:D:1498:ETX:H22	1.89	0.54
1:B:5:ILE:HG13	1:B:36:ILE:HD12	1.90	0.54
2:C:278:TRP:N	2:C:281:PHE:HE2	1.98	0.54
1:A:304:ALA:O	1:A:308:VAL:CG2	2.41	0.54
1:A:251:VAL:HG21	1:B:258:LEU:HD11	1.90	0.54
2:C:142:SER:OG	2:C:483:THR:HG22	2.08	0.54
1:A:330:LEU:HD22	1:A:374:PRO:HG3	1.90	0.54
2:C:111:VAL:HG11	2:C:162:LEU:CD2	2.37	0.54
2:C:12:ILE:HG21	2:C:49:VAL:HG12	1.89	0.54
3:D:362:ARG:NH2	3:D:367:LYS:O	2.41	0.53
3:D:260:GLY:HA2	3:D:416:TYR:CD1	2.42	0.53
2:C:403:SER:OG	2:C:404:GLU:N	2.41	0.53
1:A:447:SER:O	1:A:449:PRO:HD3	2.08	0.53
1:A:280:ILE:HG22	1:B:494:TYR:CE2	2.44	0.53
2:C:118:PHE:CZ	2:C:171:PRO:HG3	2.44	0.53
2:C:315:THR:C	2:C:318:ILE:HD13	2.29	0.53
3:D:5:ILE:HG12	3:D:36:ILE:O	2.08	0.53
3:D:142:SER:HB2	3:D:483:THR:HG22	1.91	0.53
2:C:267:PHE:CE2	2:C:429:ARG:CZ	2.91	0.53
2:C:35:ILE:HD13	2:C:35:ILE:N	2.23	0.53
2:C:268:GLU:HG3	2:C:269:ASP:OD1	2.07	0.52
1:A:5:ILE:HD11	1:A:95:ILE:HG21	1.92	0.52
1:B:290:ILE:HB	1:B:293:ALA:HB2	1.91	0.52
1:B:494:TYR:O	1:B:495:LYS:HE3	2.09	0.52
2:C:365:HIS:NE2	2:C:366:LEU:HD11	2.15	0.52
2:C:447:SER:C	2:C:449:PRO:HD3	2.30	0.52
2:C:107:ASP:O	2:C:110:ASP:N	2.33	0.52
2:C:31:SER:HG	2:C:371:TYR:HH	1.56	0.52
1:A:447:SER:C	1:A:449:PRO:HD3	2.30	0.52
1:B:33:GLU:HG3	1:B:370:TYR:CE1	2.45	0.52
1:B:58:PHE:CE1	1:B:150:GLY:HA2	2.45	0.52
2:C:139:ARG:NH2	2:C:489:GLU:O	2.43	0.52
2:C:460:LYS:HE3	9:D:1500:GOL:H32	1.92	0.52
2:C:260:GLY:HA2	2:C:416:TYR:CG	2.45	0.52
3:D:139:ARG:NE	3:D:487:SER:CB	2.74	0.51
2:C:286:THR:O	2:C:289:GLN:HG3	2.11	0.51
1:A:8:ARG:HB2	1:A:192:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483[B]:THR:HG23	1:B:443:TRP:HD1	1.75	0.51
2:C:274:LYS:O	2:C:277:GLU:N	2.43	0.51
1:B:448:GLN:N	1:B:449:PRO:HD3	2.25	0.51
2:C:105:VAL:C	2:C:107:ASP:H	2.13	0.51
3:D:236:SER:HA	5:D:1498:ETX:H12	1.92	0.51
1:A:32:THR:OG1	1:A:34:GLU:HB3	2.10	0.51
2:C:8:ARG:HG3	2:C:192:LEU:CD1	2.41	0.51
1:A:269:ASP:OD1	1:A:429:ARG:NH1	2.43	0.51
2:C:77:ALA:CB	2:C:201:VAL:HG22	2.40	0.50
2:C:79:ALA:O	2:C:82:ILE:HG22	2.11	0.50
2:C:308:VAL:HG23	2:C:309:ASP:H	1.75	0.50
1:A:443:TRP:CZ2	1:A:448:GLN:HA	2.46	0.50
2:C:318:ILE:HA	3:D:495:LYS:NZ	2.25	0.50
1:B:100:PRO:HD2	1:B:103:GLU:CD	2.32	0.50
1:B:270:VAL:HB	1:B:275:VAL:HG21	1.92	0.50
2:C:319:LYS:HZ1	2:C:325:GLU:CD	2.14	0.50
2:C:282:GLY:HA2	2:C:448:GLN:HG2	1.94	0.50
3:D:66:THR:CG2	3:D:71:ARG:HG3	2.41	0.50
1:B:25[B]:ILE:HD12	1:B:214:LEU:HD21	1.94	0.50
2:C:367:LYS:HG2	2:C:368:LYS:N	2.26	0.49
2:C:367:LYS:CG	2:C:368:LYS:N	2.74	0.49
2:C:192:LEU:HD12	2:C:192:LEU:C	2.32	0.49
3:D:430:CYS:O	3:D:434[A]:THR:HG23	2.13	0.49
3:D:140:PHE:HD1	3:D:485:ASP:HA	1.78	0.49
1:A:142:SER:OG	1:A:483[A]:THR:HG22	2.12	0.49
1:B:402:SER:OG	1:B:403:SER:N	2.45	0.49
2:C:111:VAL:HG22	2:C:162:LEU:HD23	1.94	0.49
2:C:315:THR:HA	2:C:318:ILE:CD1	2.43	0.49
3:D:139:ARG:CG	3:D:487:SER:HB2	2.32	0.49
3:D:296:ARG:NH2	3:D:410:LEU:O	2.45	0.49
1:B:261:LYS:NZ	10:B:2109:HOH:O	2.46	0.49
2:C:305:ALA:HA	2:C:308:VAL:HG22	1.95	0.48
2:C:82:ILE:HG21	2:C:112:ALA:HB2	1.96	0.48
2:C:275:VAL:HG23	2:C:423:PHE:CD2	2.48	0.48
3:D:130:LYS:HE2	3:D:143:HIS:CE1	2.47	0.48
1:A:260:GLY:HA2	1:A:416:TYR:CG	2.49	0.48
2:C:321:SER:HB2	2:C:325:GLU:OE1	2.13	0.48
1:A:251:VAL:HG21	1:B:258:LEU:CD1	2.44	0.48
1:B:268:GLU:HA	1:B:303:ILE:HD13	1.95	0.48
1:B:125:LEU:HD22	1:B:473:ILE:HD11	1.94	0.48
1:B:495:LYS:CA	1:B:495:LYS:HE3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:ILE:HB	2:C:293:ALA:HB2	1.94	0.48
3:D:260:GLY:HA2	3:D:416:TYR:CG	2.48	0.48
1:A:76:ARG:NH1	1:A:123:GLU:OE2	2.28	0.48
2:C:111:VAL:CG1	2:C:162:LEU:HD21	2.43	0.48
2:C:314:TRP:CB	2:C:317:ASN:HD21	2.25	0.48
2:C:97:SER:OG	2:C:99:LYS:HG2	2.14	0.48
2:C:182:LYS:NZ	2:C:183:PRO:O	2.44	0.48
2:C:303:ILE:O	2:C:303:ILE:CG2	2.60	0.48
1:A:297:LEU:HD23	1:A:398:VAL:HG13	1.95	0.48
3:D:5:ILE:HG13	3:D:5:ILE:O	2.14	0.48
2:C:102:ASP:OD2	2:C:329:ARG:CZ	2.54	0.48
2:C:285:TRP:HD1	2:C:286:THR:H	1.61	0.47
2:C:32:THR:O	2:C:33:GLU:HB2	2.13	0.47
1:A:319:LYS:NZ	1:A:326:GLU:O	2.47	0.47
1:B:308:VAL:O	1:B:312:VAL:HG23	2.14	0.47
2:C:159:ASN:ND2	2:C:160:TYR:HE1	2.12	0.47
2:C:33:GLU:HB2	2:C:368:LYS:HZ1	1.79	0.47
2:C:443:TRP:CD1	2:C:449:PRO:HD2	2.50	0.47
1:B:260:GLY:HA2	1:B:416:TYR:CD1	2.50	0.47
2:C:367:LYS:CE	2:C:368:LYS:HB2	2.45	0.47
1:B:447:SER:O	1:B:448:GLN:CB	2.57	0.47
2:C:260:GLY:HA2	2:C:416:TYR:CD1	2.50	0.47
2:C:56:ARG:NH2	10:C:2006:HOH:O	2.45	0.47
3:D:139:ARG:HD3	3:D:140:PHE:CZ	2.49	0.47
1:B:99:LYS:HE3	1:B:286:THR:HG23	1.97	0.47
1:B:448:GLN:N	1:B:449:PRO:CD	2.78	0.47
3:D:169:ILE:HD11	3:D:181:LEU:HD22	1.98	0.47
3:D:491:TRP:CD1	3:D:493:TRP:HB2	2.49	0.47
2:C:272:ILE:O	2:C:276:VAL:HG23	2.14	0.46
2:C:380:ILE:O	2:C:399:LYS:NZ	2.48	0.46
1:A:260:GLY:HA2	1:A:416:TYR:CD1	2.50	0.46
1:A:146[A]:ARG:HB3	1:A:477:LEU:HD13	1.96	0.46
2:C:378:THR:HG22	2:C:379:ASP:N	2.24	0.46
1:B:135:LEU:HD11	1:B:142:SER:HB2	1.98	0.46
2:C:160:TYR:HB2	2:C:164:MET:HG2	1.98	0.46
2:C:367:LYS:CE	2:C:368:LYS:HG2	2.36	0.46
2:C:386:ILE:HG13	2:C:397:CYS:SG	2.55	0.46
3:D:489:GLU:O	3:D:490:PRO:C	2.54	0.46
2:C:191:CYS:C	2:C:193:GLU:N	2.67	0.46
1:B:378:THR:CG2	1:B:379:ASP:H	2.20	0.46
3:D:76:ARG:NH1	3:D:123:GLU:OE2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:283:CYS:O	2:C:288:GLY:HA2	2.16	0.46
2:C:319:LYS:NZ	2:C:325:GLU:CD	2.69	0.45
2:C:364:GLU:HG2	2:C:364:GLU:H	1.50	0.45
1:A:281:PHE:O	1:A:285:TRP:HB3	2.17	0.45
1:B:339:TYR:OH	1:B:362:ARG:NH1	2.50	0.45
2:C:266:VAL:HG11	2:C:307:PHE:HE2	1.81	0.45
2:C:320:ILE:HG23	2:C:330:LEU:HG	1.98	0.45
3:D:228:VAL:O	3:D:252:LYS:HE2	2.16	0.45
2:C:278:TRP:O	2:C:281:PHE:CD2	2.70	0.45
1:A:160:TYR:HB2	1:A:164:MET:HG2	1.98	0.45
1:A:447:SER:O	1:A:448:GLN:HB2	2.16	0.45
1:B:283:CYS:O	1:B:288:GLY:HA2	2.16	0.45
2:C:278:TRP:N	2:C:281:PHE:CE2	2.72	0.45
3:D:66:THR:HG22	3:D:71:ARG:HG3	1.97	0.45
1:B:471:TRP:CE2	7:B:1498:PG4:H31	2.50	0.45
2:C:266:VAL:HG11	2:C:307:PHE:CE2	2.51	0.45
1:B:443:TRP:CD1	1:B:449:PRO:HD2	2.51	0.45
1:A:81:LYS:HD2	1:A:85:LYS:HD2	1.99	0.45
2:C:102:ASP:HB2	2:C:329:ARG:HH12	1.82	0.45
1:B:33:GLU:HG3	1:B:370:TYR:CZ	2.51	0.45
3:D:65:ALA:HB3	10:D:2039:HOH:O	2.16	0.45
1:A:344:LYS:HG3	2:C:134:THR:HG21	1.98	0.45
1:A:429:ARG:O	1:A:433:ILE:HG12	2.17	0.45
1:A:258:LEU:CD1	1:B:251:VAL:HG21	2.46	0.45
2:C:96:ASP:OD2	10:C:2018:HOH:O	2.21	0.45
2:C:368:LYS:HD2	2:C:368:LYS:HA	1.61	0.44
2:C:296:ARG:NH2	2:C:410:LEU:O	2.50	0.44
1:A:488:ASP:O	1:A:488:ASP:OD1	2.35	0.44
2:C:252:LYS:HB2	2:C:252:LYS:HE3	1.71	0.44
2:C:231:ILE:HB	2:C:254:VAL:HG12	1.98	0.44
2:C:272:ILE:HA	2:C:275:VAL:HG12	1.98	0.44
2:C:439:VAL:HG13	2:C:441:ALA:H	1.81	0.44
2:C:86:LYS:HE2	2:C:86:LYS:HB2	1.57	0.44
2:C:185:GLU:HG2	2:C:185:GLU:H	1.43	0.44
2:C:278:TRP:CD1	2:C:423:PHE:CE2	3.04	0.44
2:C:317:ASN:OD1	2:C:317:ASN:C	2.56	0.44
1:A:157:PRO:HG2	1:A:164:MET:HG3	1.99	0.44
1:A:157:PRO:HD3	1:A:234:THR:HB	1.98	0.44
2:C:316:LYS:CG	2:C:358:TYR:HE1	2.30	0.44
3:D:443:TRP:CZ2	3:D:448:GLN:HA	2.53	0.44
3:D:86:LYS:O	3:D:90:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:GLU:C	1:A:459:ILE:HD11	2.38	0.44
1:B:146[A]:ARG:HH11	1:B:474:GLN:HE22	1.66	0.44
3:D:160:TYR:HB2	3:D:164:MET:HG2	2.00	0.44
3:D:290:ILE:HB	3:D:293:ALA:HB2	1.99	0.44
1:B:264:ILE:HG23	1:B:297:LEU:HA	2.00	0.44
2:C:191:CYS:O	2:C:194:PHE:N	2.50	0.44
2:C:267:PHE:CD2	2:C:429:ARG:CZ	3.01	0.43
2:C:280:ILE:CG1	2:C:284:PHE:HD2	2.31	0.43
2:C:315:THR:CA	2:C:318:ILE:HD13	2.47	0.43
2:C:105:VAL:C	2:C:107:ASP:N	2.71	0.43
2:C:160:TYR:O	2:C:161:PRO:C	2.57	0.43
1:B:121:GLN:NE2	10:B:2053:HOH:O	2.51	0.43
1:B:299:VAL:O	1:B:400:THR:HA	2.18	0.43
2:C:102:ASP:CB	2:C:329:ARG:HH12	2.32	0.43
2:C:33:GLU:HB2	2:C:368:LYS:HZ3	1.80	0.43
2:C:92:LEU:HD12	2:C:92:LEU:H	1.82	0.43
2:C:365:HIS:CE1	2:C:366:LEU:HD12	2.38	0.43
2:C:86:LYS:O	2:C:90:VAL:N	2.45	0.43
1:A:382:THR:HG22	1:A:387:TRP:CE2	2.53	0.43
1:B:375:THR:HB	1:B:395:VAL:HG22	2.01	0.43
2:C:81:LYS:O	2:C:82:ILE:C	2.56	0.43
3:D:218:ALA:O	3:D:221:PRO:HD2	2.18	0.43
2:C:427:LEU:C	2:C:429:ARG:H	2.22	0.43
2:C:467:GLU:HB3	2:C:468:LEU:HD13	2.01	0.43
2:C:99:LYS:O	2:C:100:PRO:C	2.57	0.43
3:D:12:ILE:HG21	3:D:49:VAL:HG12	2.00	0.43
1:B:404:GLU:OE2	1:B:432:ARG:NH2	2.51	0.43
2:C:18:GLU:CG	2:C:19:PRO:N	2.82	0.43
2:C:103:GLU:HG2	2:C:285:TRP:HE1	1.84	0.42
2:C:308:VAL:CG2	2:C:309:ASP:N	2.82	0.42
2:C:474:GLN:NE2	8:C:1497:AE3:H3C1	2.34	0.42
3:D:320:ILE:HG12	3:D:330:LEU:HD23	2.01	0.42
2:C:135:LEU:HD11	2:C:142:SER:HB2	2.02	0.42
3:D:341:LYS:HB2	3:D:341:LYS:HE3	1.76	0.42
1:A:467:GLU:O	1:A:468:LEU:HB2	2.20	0.42
1:B:250:LEU:O	1:B:251:VAL:HG12	2.19	0.42
2:C:8:ARG:CB	2:C:192:LEU:HD13	2.41	0.42
2:C:361:SER:O	2:C:373:GLU:OE1	2.37	0.42
2:C:415:GLU:OE2	2:C:461:ARG:HD2	2.20	0.42
1:B:260:GLY:HA2	1:B:416:TYR:CG	2.54	0.42
2:C:24:ARG:HE	2:C:38:ASP:CG	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:15:GLU:HG3	3:D:17:ARG:HE	1.84	0.42
2:C:106:LEU:O	2:C:110:ASP:OD2	2.37	0.42
3:D:330:LEU:CD2	3:D:374:PRO:HD3	2.49	0.42
3:D:140:PHE:CD1	3:D:485:ASP:HA	2.55	0.42
1:A:483[B]:THR:O	1:A:483[B]:THR:HG23	2.18	0.42
1:A:274:LYS:HG2	1:B:490:PRO:HA	2.02	0.42
2:C:269:ASP:O	2:C:425:ASN:CG	2.58	0.42
3:D:493:TRP:CD1	3:D:494:TYR:CZ	3.08	0.42
2:C:31:SER:HA	2:C:332:PRO:HG3	2.02	0.42
2:C:96:ASP:OD2	2:C:189:VAL:HG12	2.19	0.42
3:D:308:VAL:O	3:D:312:VAL:HG12	2.19	0.42
1:B:52:VAL:O	1:B:56:ARG:HG3	2.20	0.41
2:C:496:SER:HB3	3:D:314:TRP:CZ2	2.55	0.41
2:C:313:LYS:HD2	2:C:313:LYS:HA	1.83	0.41
2:C:365:HIS:C	2:C:365:HIS:CD2	2.93	0.41
2:C:468:LEU:N	2:C:468:LEU:HD12	2.35	0.41
2:C:95:ILE:HG23	2:C:324:PHE:HZ	1.85	0.41
3:D:474:GLN:HB2	3:D:474:GLN:HE21	1.70	0.41
1:B:157:PRO:HD2	1:B:164:MET:HB3	2.01	0.41
2:C:95:ILE:HG23	2:C:324:PHE:CZ	2.55	0.41
2:C:305:ALA:O	2:C:308:VAL:HG22	2.20	0.41
1:A:308:VAL:O	1:A:311:LEU:HB3	2.20	0.41
1:B:312:VAL:O	1:B:316:LYS:HG2	2.21	0.41
1:A:312:VAL:HG12	1:A:376:ILE:HD12	2.02	0.41
2:C:81:LYS:HZ1	2:C:85:LYS:CD	2.33	0.41
2:C:92:LEU:HD12	2:C:92:LEU:N	2.35	0.41
3:D:114:CYS:SG	3:D:166:THR:HG22	2.60	0.41
3:D:346:ILE:HD13	3:D:360:GLY:HA2	2.03	0.41
1:A:182:LYS:O	1:A:182:LYS:HG3	2.20	0.41
2:C:429:ARG:O	2:C:432:ARG:CB	2.67	0.41
3:D:380:ILE:HA	3:D:380:ILE:HD13	1.85	0.41
1:B:326:GLU:HG2	1:B:326:GLU:H	1.58	0.41
1:B:401:PHE:HB2	1:B:406:GLU:HG2	2.02	0.41
2:C:201:VAL:HG22	2:C:201:VAL:O	2.20	0.41
3:D:135:LEU:HA	3:D:136:PRO:HD3	1.95	0.41
1:B:231:ILE:HB	1:B:254:VAL:HG22	2.03	0.41
2:C:305:ALA:HA	2:C:308:VAL:CG2	2.51	0.40
2:C:322:ASP:OD1	2:C:324:PHE:HB2	2.20	0.40
1:A:386:ILE:HG23	1:A:397[A]:CYS:SG	2.62	0.40
2:C:277:GLU:OE1	3:D:492:GLY:N	2.55	0.40
2:C:491:TRP:HB3	3:D:277:GLU:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:253:PRO:HB3	3:D:464:PHE:CG	2.57	0.40
2:C:315:THR:C	2:C:317:ASN:H	2.24	0.40
3:D:259:GLY:CA	5:D:1498:ETX:H22	2.52	0.40
1:A:310:LYS:HA	1:A:313:LYS:HD3	2.03	0.40
1:B:58:PHE:CZ	1:B:150:GLY:HA2	2.57	0.40
2:C:111:VAL:CG1	2:C:162:LEU:CD2	2.99	0.40
2:C:27:VAL:HG12	2:C:38:ASP:N	2.36	0.40
2:C:304:ALA:O	2:C:308:VAL:HG13	2.22	0.40
3:D:493:TRP:HD1	3:D:494:TYR:CZ	2.39	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLU:OE2	1:B:313:LYS:NZ[1_465]	1.81	0.39
1:A:326:GLU:OE2	1:B:313:LYS:CE[1_465]	1.87	0.33

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	498/497 (100%)	482 (97%)	15 (3%)	1 (0%)	51	46
1	B	502/497 (101%)	474 (94%)	26 (5%)	2 (0%)	38	30
2	C	492/497 (99%)	447 (91%)	40 (8%)	5 (1%)	18	10
3	D	492/497 (99%)	474 (96%)	16 (3%)	2 (0%)	38	30
All	All	1984/1988 (100%)	1877 (95%)	97 (5%)	10 (0%)	32	24

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	GLN
1	B	367	LYS
1	B	448	GLN
2	C	365	HIS
2	C	448	GLN
3	D	448	GLN
2	C	446	CYS
2	C	445	ASN
2	C	106	LEU
3	D	490	PRO

5.3.2 Protein sidechains ⓘ

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	414/410 (101%)	407 (98%)	7 (2%)	66	67
1	B	417/410 (102%)	411 (99%)	6 (1%)	71	73
2	C	408/409 (100%)	389 (95%)	19 (5%)	30	23
3	D	408/408 (100%)	396 (97%)	12 (3%)	48	44
All	All	1647/1637 (101%)	1603 (97%)	44 (3%)	53	48

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93[A]	GLU
1	A	93[B]	GLU
1	A	230	LYS
1	A	257	GLU
1	A	383[A]	SER
1	A	383[B]	SER
1	A	392	PHE
1	B	182	LYS
1	B	392	PHE
1	B	448	GLN
1	B	483[A]	THR
1	B	483[B]	THR

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Mol	Chain	Res	Type
1	B	495	LYS
2	C	17	ARG
2	C	22	LYS
2	C	85	LYS
2	C	91	LYS
2	C	93	GLU
2	C	99	LYS
2	C	116	GLU
2	C	160	TYR
2	C	193	GLU
2	C	200	GLU
2	C	364	GLU
2	C	367	LYS
2	C	368	LYS
2	C	392	PHE
2	C	400	THR
2	C	427	LEU
2	C	429	ARG
2	C	446	CYS
2	C	474	GLN
3	D	5	ILE
3	D	66	THR
3	D	93	GLU
3	D	257	GLU
3	D	326	GLU
3	D	366	LEU
3	D	392	PHE
3	D	474	GLN
3	D	487	SER
3	D	488	ASP
3	D	489	GLU
3	D	495	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	61	ASN
2	C	88	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSO	C	291	2	4,6,7	1.28	1 (25%)	1,6,8	1.31	0
3	CSO	D	291	3	4,6,7	0.76	0	1,6,8	2.90	1 (100%)
3	CSO	D	450	3	4,6,7	0.70	0	1,6,8	1.89	0

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
2	CSO	C	291	2	-	0/1/5/7	0/0/0/0
3	CSO	D	291	3	-	0/1/5/7	0/0/0/0
3	CSO	D	450	3	-	0/1/5/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	291	CSO	CA-C	2.41	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	291	CSO	O-C-CA	-2.90	117.02	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	291	CSO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	CHT	A	1497	1	6,6,6	1.95	1 (16%)	8,8,8	1.28	1 (12%)
5	ETX	A	1498	-	5,5,5	0.45	0	4,4,4	0.30	0
4	CHT	B	1497	1	6,6,6	1.95	1 (16%)	8,8,8	1.19	1 (12%)
7	PG4	B	1498	-	11,11,12	0.76	0	10,10,11	0.45	0
8	AE3	C	1497	-	8,8,8	0.72	0	7,7,7	0.38	0
5	ETX	D	1498	-	5,5,5	0.40	0	4,4,4	0.49	0
9	GOL	D	1500	-	5,5,5	0.33	0	5,5,5	0.29	0

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	CHT	A	1497	1	-	0/4/4/4	0/0/0/0
5	ETX	A	1498	-	-	0/3/3/3	0/0/0/0
4	CHT	B	1497	1	-	0/4/4/4	0/0/0/0
7	PG4	B	1498	-	-	0/9/9/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	AE3	C	1497	-	-	0/6/6/6	0/0/0/0
5	ETX	D	1498	-	-	0/3/3/3	0/0/0/0
9	GOL	D	1500	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1497	CHT	O6-C4	-3.74	1.22	1.42
4	A	1497	CHT	O6-C4	-3.62	1.23	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1497	CHT	C8-N1-C5	2.13	118.10	109.93
4	A	1497	CHT	C8-N1-C5	2.44	119.29	109.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1497	CHT	1	0
7	B	1498	PG4	1	0
8	C	1497	AE3	1	0
5	D	1498	ETX	4	0
9	D	1500	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	493/497 (99%)	0.24	20 (4%) 38 41	20, 38, 67, 97	0
1	B	493/497 (99%)	0.57	50 (10%) 8 9	24, 48, 79, 118	0
2	C	491/497 (98%)	1.27	109 (22%) 1 1	30, 68, 109, 194	0
3	D	491/497 (98%)	0.34	42 (8%) 11 13	23, 41, 78, 183	0
All	All	1968/1988 (98%)	0.60	221 (11%) 6 7	20, 46, 92, 194	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	281	PHE	11.1
2	C	427	LEU	6.5
2	C	313	LYS	6.4
2	C	106	LEU	6.0
3	D	494	TYR	6.0
2	C	169	ILE	5.9
2	C	105	VAL	5.8
2	C	91	LYS	5.6
2	C	87	ASP	5.5
2	C	101	PHE	5.5
2	C	324	PHE	5.5
2	C	109	ASP	5.3
2	C	17	ARG	5.3
2	C	428	GLU	5.3
2	C	285	TRP	5.3
2	C	301	GLU	5.2
2	C	280	ILE	5.1
2	C	173	LEU	5.1
2	C	192	LEU	5.1
2	C	181	LEU	5.0
2	C	80	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
2	C	154	LEU	4.8
2	C	21	LYS	4.7
3	D	490	PRO	4.6
1	B	181	LEU	4.5
2	C	451	PHE	4.5
2	C	396	LEU	4.5
3	D	487	SER	4.5
1	B	264	ILE	4.4
3	D	491	TRP	4.4
3	D	489	GLU	4.3
2	C	282	GLY	4.3
2	C	208	LEU	4.2
3	D	367	LYS	4.2
2	C	90	VAL	4.1
2	C	367	LYS	4.1
1	B	169	ILE	4.0
2	C	201	VAL	4.0
2	C	84	GLU	4.0
2	C	267	PHE	4.0
2	C	300	HIS	3.9
1	B	191	CYS	3.9
1	B	402	SER	3.8
1	A	264	ILE	3.8
2	C	95	ILE	3.8
1	B	154	LEU	3.8
2	C	305	ALA	3.8
2	C	446	CYS	3.8
2	C	180	VAL	3.7
2	C	283	CYS	3.7
1	B	396	LEU	3.6
1	B	283	CYS	3.6
2	C	20	ILE	3.6
2	C	22	LYS	3.6
2	C	264	ILE	3.6
3	D	134	THR	3.6
2	C	170	ALA	3.5
2	C	179	ALA	3.5
2	C	18	GLU	3.5
1	A	181	LEU	3.5
1	B	326	GLU	3.5
1	B	208	LEU	3.5
1	A	495	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	268	GLU	3.5
3	D	137	MET	3.5
2	C	368	LYS	3.4
3	D	181	LEU	3.4
2	C	155	ILE	3.4
2	C	61	ASN	3.3
2	C	36	ILE	3.3
3	D	495	LYS	3.3
2	C	288	GLY	3.2
1	B	294	THR	3.2
1	B	336	LYS	3.2
2	C	326	GLU	3.2
1	B	297	LEU	3.1
3	D	486	ILE	3.2
2	C	328	CYS	3.1
3	D	135	LEU	3.1
1	B	403	SER	3.1
1	B	421	ALA	3.1
2	C	290	ILE	3.1
2	C	110	ASP	3.1
1	B	427	LEU	3.1
2	C	366	LEU	3.1
3	D	154	LEU	3.1
1	B	313	LYS	3.1
2	C	376	ILE	3.0
2	C	294	THR	3.0
1	B	20	ILE	2.9
3	D	264	ILE	2.9
2	C	172	ALA	2.9
3	D	279	THR	2.9
2	C	426	ASP	2.9
1	A	367	LYS	2.9
3	D	139	ARG	2.9
1	B	442	VAL	2.9
3	D	210	ILE	2.9
1	B	165	ALA	2.9
2	C	327	GLY	2.8
2	C	403	SER	2.8
3	D	180	VAL	2.8
3	D	396	LEU	2.8
2	C	196	GLU	2.8
1	B	395	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	163	LEU	2.8
1	B	34	GLU	2.8
3	D	22	LYS	2.8
3	D	149	LEU	2.8
1	A	488	ASP	2.8
2	C	447	SER	2.8
1	B	420	ALA	2.7
2	C	320	ILE	2.7
3	D	324	PHE	2.7
2	C	88	HIS	2.7
1	A	4	PRO	2.7
2	C	279	THR	2.7
2	C	93	GLU	2.7
3	D	297	LEU	2.7
2	C	5	ILE	2.7
3	D	493	TRP	2.7
2	C	425	ASN	2.7
2	C	270	VAL	2.6
2	C	199	ASN	2.6
3	D	138	GLU	2.6
1	B	383	SER	2.6
1	B	305	ALA	2.6
3	D	280	ILE	2.6
1	A	422	VAL	2.6
3	D	152	VAL	2.6
2	C	104	ALA	2.6
3	D	492	GLY	2.6
1	A	210	ILE	2.6
2	C	191	CYS	2.6
3	D	363	PRO	2.6
1	B	279	THR	2.6
1	A	162	LEU	2.5
2	C	77	ALA	2.5
1	B	369	GLY	2.5
2	C	165	ALA	2.5
2	C	395	VAL	2.5
1	B	284	PHE	2.5
1	B	318	ILE	2.5
1	A	284	PHE	2.5
2	C	116	GLU	2.5
1	A	490	PRO	2.4
2	C	166	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	381	SER	2.4
3	D	326	GLU	2.4
3	D	364	GLU	2.4
1	B	280	ILE	2.4
3	D	353	GLY	2.4
1	B	495	LYS	2.4
1	B	179	ALA	2.4
3	D	294	THR	2.4
2	C	263	PRO	2.4
1	A	364	GLU	2.4
2	C	7	ALA	2.4
2	C	79	ALA	2.4
2	C	488	ASP	2.4
2	C	114	CYS	2.4
2	C	308	VAL	2.4
3	D	31	SER	2.3
2	C	32	THR	2.3
1	B	496	SER	2.3
2	C	297	LEU	2.3
1	B	210	ILE	2.3
2	C	429	ARG	2.3
2	C	284	PHE	2.3
1	A	191	CYS	2.3
2	C	89	PHE	2.3
2	C	365	HIS	2.3
2	C	207	VAL	2.3
2	C	275	VAL	2.3
1	B	161	PRO	2.3
3	D	179	ALA	2.3
1	B	61	ASN	2.2
1	B	166	THR	2.2
1	B	155	ILE	2.2
2	C	16	TRP	2.2
3	D	191	CYS	2.2
1	A	167	TRP	2.2
1	B	173	LEU	2.2
2	C	421	ALA	2.2
1	B	22	LYS	2.2
2	C	183	PRO	2.2
2	C	355	THR	2.2
2	C	316	LYS	2.2
1	B	376	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	154	LEU	2.1
2	C	269	ASP	2.1
2	C	177	CYS	2.1
1	A	294	THR	2.1
1	B	434	THR	2.1
3	D	208	LEU	2.1
3	D	127	GLY	2.1
3	D	162	LEU	2.1
1	B	358	TYR	2.1
1	A	443	TRP	2.1
1	A	395	VAL	2.1
2	C	266	VAL	2.1
2	C	82	ILE	2.1
2	C	38	ASP	2.1
2	C	200	GLU	2.1
1	B	282	GLY	2.1
1	B	295	SER	2.1
2	C	112	ALA	2.1
2	C	420	ALA	2.1
2	C	374	PRO	2.1
1	B	180	VAL	2.0
3	D	421	ALA	2.0
1	B	309	ASP	2.0
2	C	383[A]	SER	2.0
1	B	288	GLY	2.0
2	C	354	ALA	2.0
1	B	379	ASP	2.0
3	D	155	ILE	2.0
3	D	376	ILE	2.0
1	A	22	LYS	2.0
1	B	368	LYS	2.0
2	C	325	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CSO	D	291	7/8	0.96	0.12	-	29,30,62,92	0
2	CSO	C	291	7/8	0.92	0.14	-	54,59,75,80	0
3	CSO	D	450	7/8	0.89	0.15	-	38,43,61,89	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CHT	A	1497	7/7	0.91	0.40	12.56	53,55,61,61	7
5	ETX	D	1498	6/6	0.65	0.35	8.88	55,63,66,68	0
4	CHT	B	1497	7/7	0.94	0.26	4.59	59,60,65,66	7
9	GOL	D	1500	6/6	0.73	0.18	2.59	54,60,62,63	0
5	ETX	A	1498	6/6	0.85	0.16	0.78	57,58,60,62	0
6	K	D	1499	1/1	0.97	0.13	0.55	43,43,43,43	1
8	AE3	C	1497	9/9	0.82	0.14	0.26	50,53,56,59	0
7	PG4	B	1498	12/13	0.93	0.10	-0.37	35,40,48,51	0
6	K	C	1498	1/1	0.94	0.10	-1.19	48,48,48,48	1
6	K	B	1499	1/1	0.92	0.09	-1.35	45,45,45,45	1
6	K	A	1499	1/1	0.98	0.06	-3.77	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.