Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 01:15 pm GMT

PDB ID	:	5A2D
Title	:	CRYSTAL STRUCTURE OF BETAINE ALDEHYDE DEHYDROGENASE FROM SPINACH SHOWING A THIOHEMIACETAL WITH BETAINE 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

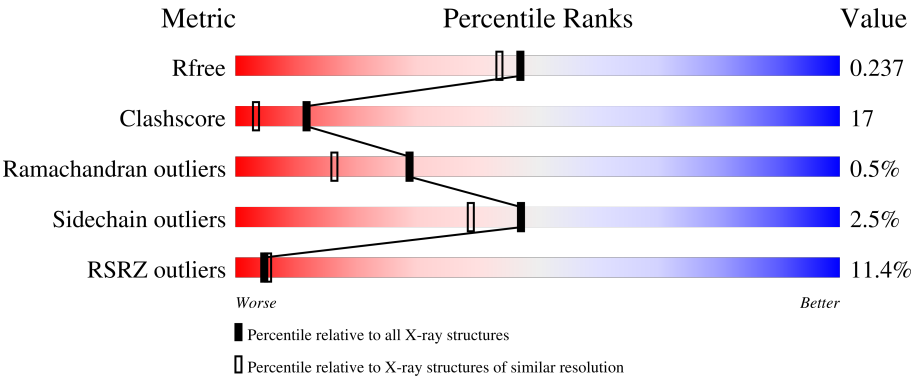
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	4% 82% 17%
1	B	497	10% 79% 19%
2	C	497	23% 59% 36%
3	D	497	8% 81% 16%

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	ETX	D	1498	-	-	X	-

2 Entry composition (i)

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, CHLOROPLASTIC.

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			

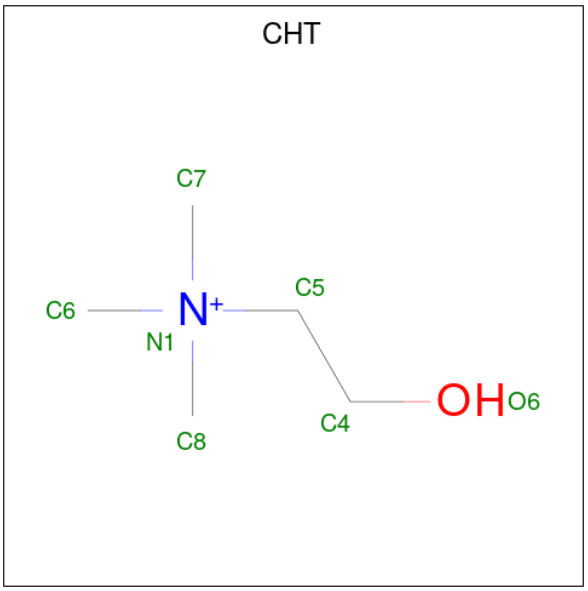
- Molecule 2 is a protein called BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC.

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, CHLOROPLASTIC.

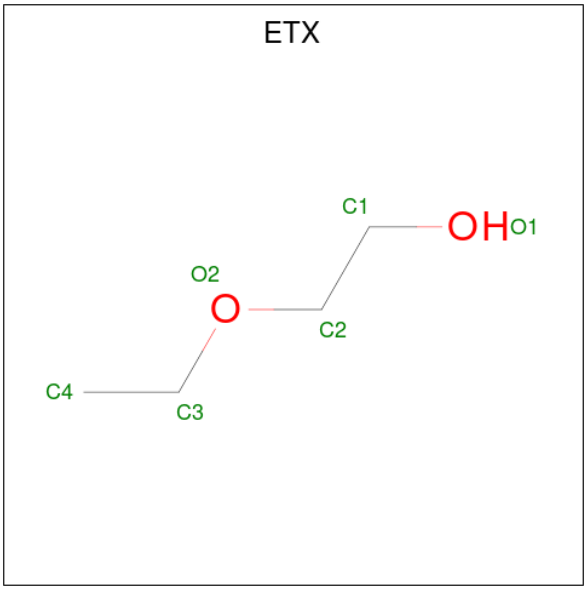
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	493	Total	C	N	O	S	0	3	0
			3817	2447	635	719	16			

- Molecule 4 is CHOLINE ION (three-letter code: CHT) (formula: $C_5H_{14}NO$).



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: $C_4H_{10}O_2$).

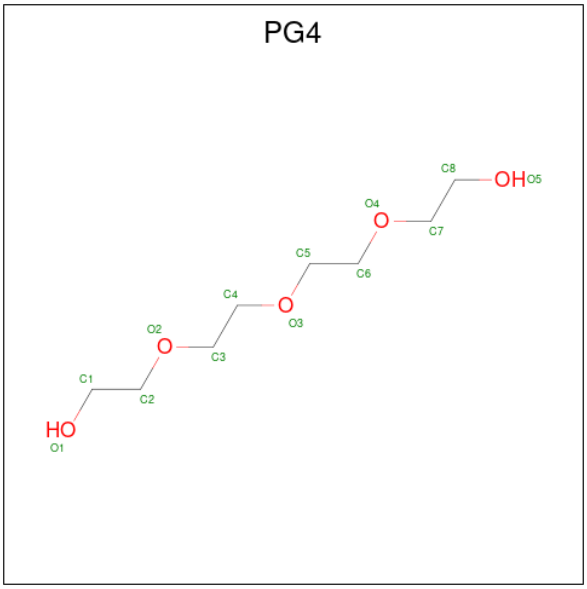


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			6	4	2			
5	D	1	Total	C	O		0	0
			6	4	2			

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

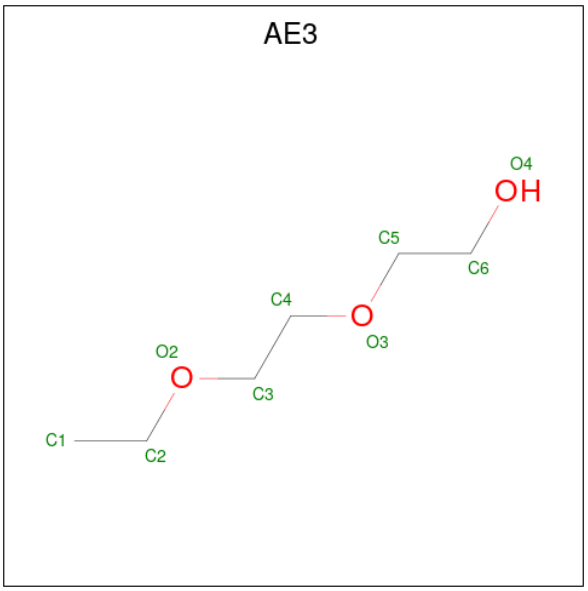
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0
6	B	1	Total K 1 1	0	0
6	C	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



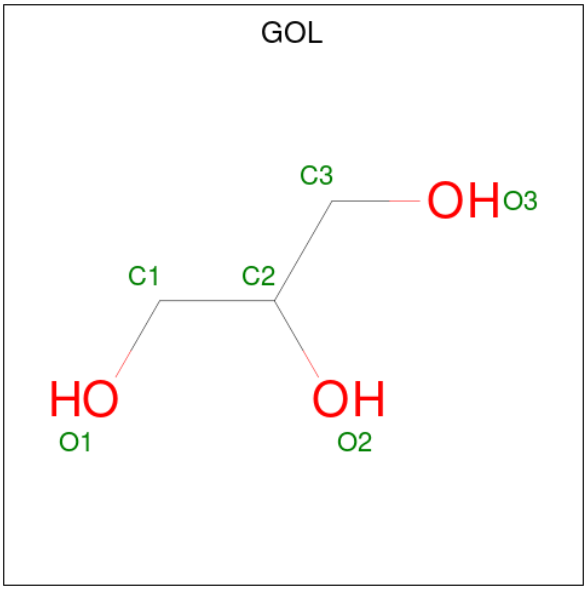
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 12 8 4	0	0

- Molecule 8 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula: $C_6H_{14}O_3$).



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

- 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 6 3 3	0	0

- Molecule 10 is water.

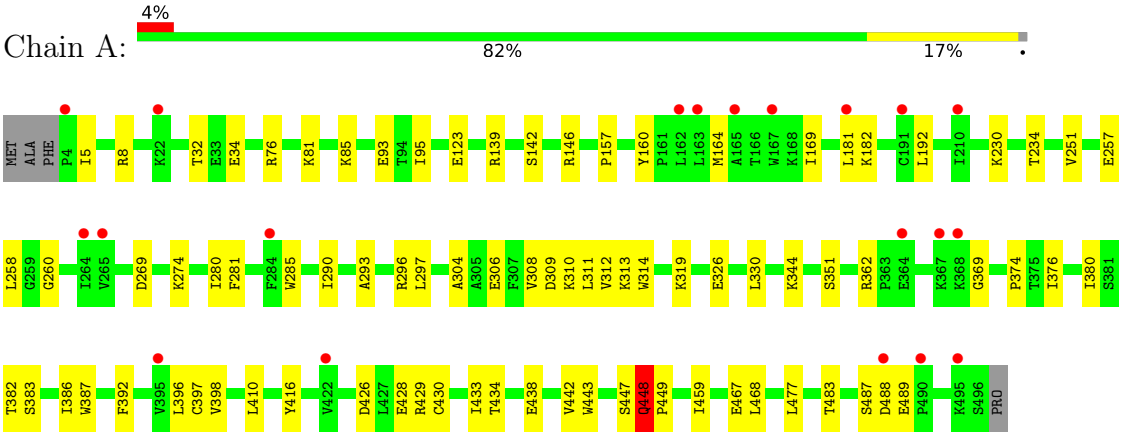
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	239	Total O 239 239	0	0
10	B	150	Total O 150 150	0	0
10	C	103	Total O 103 103	0	0
10	D	179	Total O 179 179	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

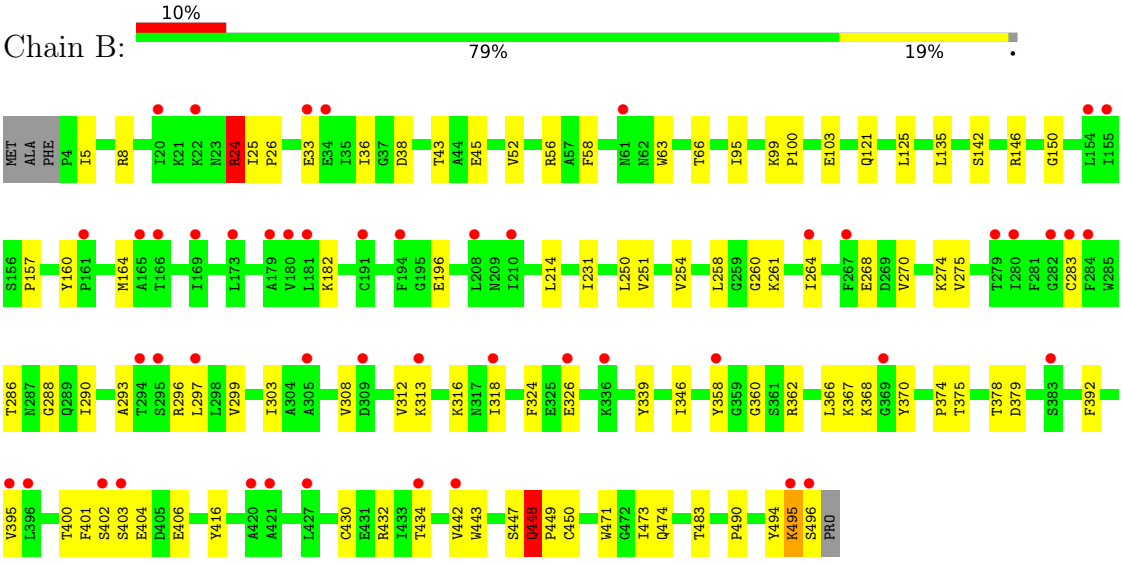
• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

Chain A:



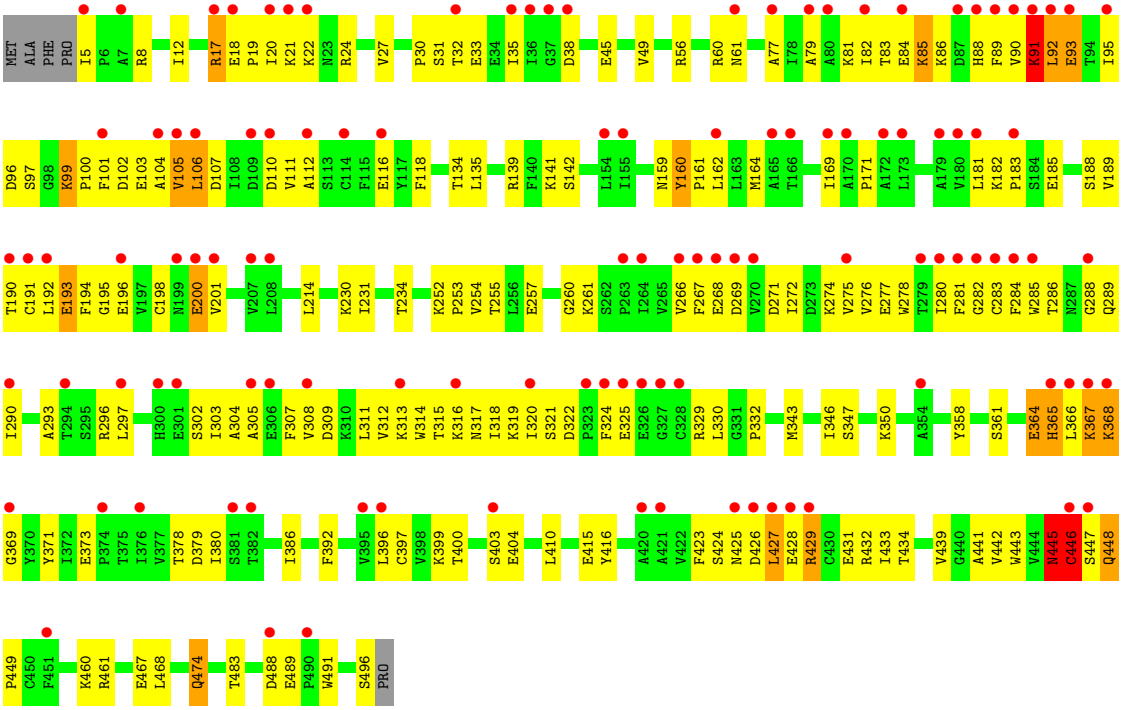
• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

Chain B:



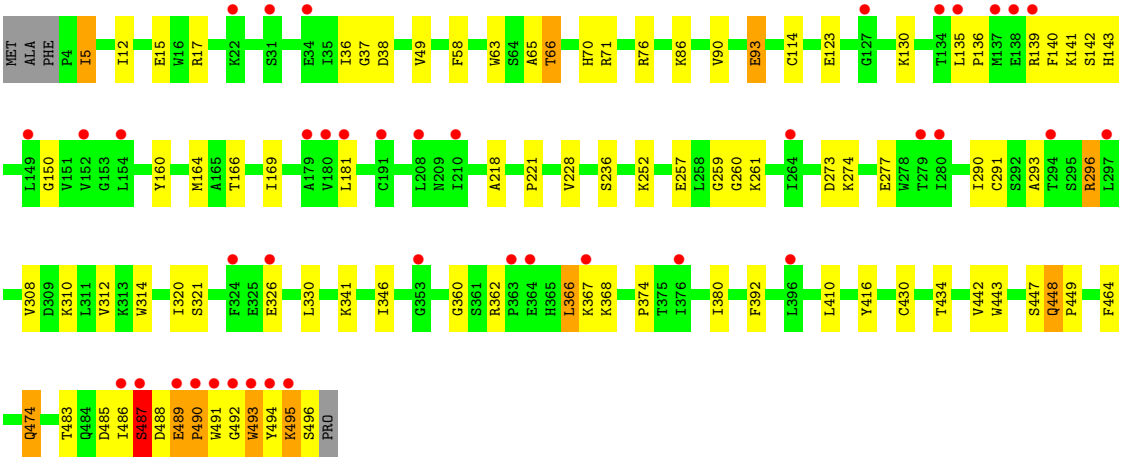
• Molecule 2: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

Chain C:



• Molecule 3: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

Chain D:



4 Data and refinement statistics (i)

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) 96.8 (28.70-1.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 1.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.194 , 0.237 0.195 , 0.237	Depositor DCC
R_{free} test set	6195 reflections (4.92%)	wwPDB-VP
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 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ETX, PG4, CHT, GOL, K, CSO, AE3

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (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	3841	0	3834	62	2
1	B	3874	0	3867	83	2
2	C	3806	0	3804	328	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	536	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 (536) 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:CA	2:C:281:PHE:CE2	1.82	1.60
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:314:TRP:CA	2:C:317:ASN:ND2	1.84	1.40
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:314:TRP:O	2:C:317:ASN:CG	1.72	1.27
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:HA	1:B:495:LYS:HE3	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H	2:C:367:LYS:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:33:GLU:HG3	2:C:369:GLY:HA2	1.62	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: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:81:LYS:O	2:C:84:GLU:HB3	1.81	0.79
2:C:364:GLU:O	2:C:365:HIS:CB	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HA	1:B:495:LYS:CE	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:83:THR:HA	2:C:86:LYS:HG3	1.75	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
1:B:316:LYS:CE	1:B:358:TYR:CD1	2.73	0.69
2:C:267:PHE:CD2	2:C:429:ARG:NH1	2.61	0.69
2:C:316:LYS:CG	2:C:358:TYR:CE1	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HA	3:D:491:TRP:CE3	2.32	0.64
2:C:77:ALA:HB3	2:C:201:VAL:CG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:141:LYS:HG3	3:D:141:LYS:O	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:267:PHE:CG	2:C:429:ARG:NH1	2.64	0.63
2:C:308:VAL:HG23	2:C:309:ASP:N	2.13	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:HG2	1:B:313:LYS:O	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:61:ASN:OD1	2:C:61:ASN:C	2.36	0.62
2:C:424:SER:OG	2:C:425:ASN:N	2.30	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:88:HIS:O	2:C:92:LEU:CD1	2.44	0.62
2:C:111:VAL:HG21	2:C:162:LEU:HD23	1.76	0.62
2:C:60:ARG:HG3	2:C:60:ARG:NH1	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:91:LYS:HE3	2:C:324:PHE:CE2	2.35	0.61
2:C:367:LYS:HE2	2:C:368:LYS:HB2	1.82	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:81:LYS:HZ1	2:C:85:LYS:HD3	1.66	0.60
2:C:427:LEU:HG	2:C:428:GLU:H	1.65	0.60
1:B:378:THR:HG22	1:B:379:ASP:N	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:83:THR:HG23	2:C:86:LYS:CD	2.25	0.59
2:C:404:GLU:O	2:C:404:GLU:HG2	2.02	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:HD3	2:C:367:LYS:N	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:HA	3:D:491:TRP:HE3	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:81:LYS:O	2:C:84:GLU:CB	2.54	0.56
2:C:274:LYS:CG	2:C:275:VAL:N	2.68	0.56
2:C:314:TRP:CH2	3:D:496:SER:HA	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:315:THR:HA	2:C:318:ILE:HD13	1.89	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
2:C:423:PHE:CE2	2:C:445:ASN:O	2.60	0.55
2:C:404:GLU:O	2:C:404:GLU:CG	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:280:ILE:HG22	1:B:494:TYR:CE2	2.44	0.53
1:A:447:SER:O	1:A:449:PRO:HD3	2.08	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:31:SER:HG	2:C:371:TYR:HH	1.56	0.52
2:C:107:ASP:O	2:C:110:ASP:N	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:140:PHE:HD1	3:D:485:ASP:HA	1.78	0.49
3:D:430:CYS:O	3:D:434[A]:THR:HG23	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:HD22	1:B:473:ILE:HD11	1.94	0.48
1:B:268:GLU:HA	1:B:303:ILE:HD13	1.95	0.48
1:B:495:LYS:HE3	1:B:495:LYS:CA	2.29	0.48
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:97:SER:OG	2:C:99:LYS:HG2	2.14	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:182:LYS:NZ	2:C:183:PRO:O	2.44	0.48
2:C:303:ILE:CG2	2:C:303:ILE:O	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:32:THR:O	2:C:33:GLU:HB2	2.13	0.47
2:C:285:TRP:HD1	2:C:286:THR:H	1.61	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
1:B:260:GLY:HA2	1:B:416:TYR:CD1	2.50	0.47
2:C:33:GLU:HB2	2:C:368:LYS:HZ1	1.79	0.47
2:C:367:LYS:CE	2:C:368:LYS:HB2	2.45	0.47
2:C:443:TRP:CD1	2:C:449:PRO:HD2	2.50	0.47
1:B:447:SER:O	1:B:448:GLN:CB	2.57	0.47
2:C:56:ARG:NH2	10:C:2006:HOH:O	2.45	0.47
2:C:260:GLY:HA2	2:C:416:TYR:CD1	2.50	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:146[A]:ARG:HB3	1:A:477:LEU:HD13	1.96	0.46
1:A:260:GLY:HA2	1:A:416:TYR:CD1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H	2:C:364:GLU:HG2	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:258:LEU:CD1	1:B:251:VAL:HG21	2.46	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
2:C:96:ASP:OD2	10:C:2018:HOH:O	2.21	0.45
2:C:296:ARG:NH2	2:C:410:LEU:O	2.50	0.44
2:C:368:LYS:HD2	2:C:368:LYS:HA	1.61	0.44
1:A:488:ASP:OD1	1:A:488:ASP:O	2.35	0.44
2:C:252:LYS:HB2	2:C:252:LYS:HE3	1.71	0.44
2:C:86:LYS:HB2	2:C:86:LYS:HE2	1.57	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:185:GLU:H	2:C:185:GLU:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:316:LYS:CG	2:C:358:TYR:HE1	2.30	0.44
3:D:86:LYS:O	3:D:90:VAL:HG23	2.18	0.44
3:D:443:TRP:CZ2	3:D:448:GLN:HA	2.53	0.44
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: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:102:ASP:CB	2:C:329:ARG:HH12	2.32	0.43
2:C:86:LYS:O	2:C:90:VAL:N	2.45	0.43
2:C:365:HIS:CE1	2:C:366:LEU:HD12	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:140:PHE:CD1	3:D:485:ASP:HA	2.55	0.42
3:D:330:LEU:CD2	3:D:374:PRO:HD3	2.49	0.42
1:A:274:LYS:HG2	1:B:490:PRO:HA	2.02	0.42
1:A:483[B]:THR:HG23	1:A:483[B]:THR:O	2.18	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:CD2	2:C:365:HIS:C	2.93	0.41
2:C:95:ILE:HG23	2:C:324:PHE:HZ	1.85	0.41
2:C:468:LEU:N	2:C:468:LEU:HD12	2.35	0.41
3:D:474:GLN:HE21	3:D:474:GLN:HB2	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
1:B:326:GLU:H	1:B:326:GLU:HG2	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
2:C:429:ARG:O	2:C:432:ARG:CB	2.67	0.41
3:D:135:LEU:HA	3:D:136:PRO:HD3	1.95	0.41
3:D:380:ILE:HD13	3:D:380:ILE:HA	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:27:VAL:HG12	2:C:38:ASP:N	2.36	0.40
2:C:111:VAL:CG1	2:C:162:LEU:CD2	2.99	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%)	47	38
1	B	502/497 (101%)	474 (94%)	26 (5%)	2 (0%)	34	22
2	C	492/497 (99%)	447 (91%)	40 (8%)	5 (1%)	15	6
3	D	492/497 (99%)	474 (96%)	16 (3%)	2 (0%)	34	22
All	All	1984/1988 (100%)	1877 (95%)	97 (5%)	10 (0%)	29	16

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 (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	414/410 (101%)	407 (98%)	7 (2%)	60	53
1	B	417/410 (102%)	411 (99%)	6 (1%)	67	62
2	C	408/409 (100%)	389 (95%)	19 (5%)	26	13
3	D	408/408 (100%)	396 (97%)	12 (3%)	42	31
All	All	1647/1637 (101%)	1603 (97%)	44 (3%)	47	35

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
3	CSO	D	450	3	3,6,7	0.78	0	0,6,8	-	-
2	CSO	C	291	2	3,6,7	0.55	0	0,6,8	-	-
3	CSO	D	291	3	3,6,7	0.98	0	0,6,8	-	-

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 monosaccharides 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	B	1497	1	6,6,6	1.98	1 (16%)	8,8,8	1.10	1 (12%)
8	AE3	C	1497	-	8,8,8	0.71	0	7,7,7	0.38	0
4	CHT	A	1497	1	6,6,6	1.97	1 (16%)	8,8,8	1.20	1 (12%)
5	ETX	A	1498	-	5,5,5	0.44	0	4,4,4	0.29	0
5	ETX	D	1498	-	5,5,5	0.39	0	4,4,4	0.51	0
7	PG4	B	1498	-	11,11,12	0.75	0	10,10,11	0.45	0
9	GOL	D	1500	-	5,5,5	0.35	0	5,5,5	0.30	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	B	1497	1	-	1/4/4/4	-
8	AE3	C	1497	-	-	3/6/6/6	-
4	CHT	A	1497	1	-	0/4/4/4	-
5	ETX	A	1498	-	-	2/3/3/3	-
5	ETX	D	1498	-	-	1/3/3/3	-
7	PG4	B	1498	-	-	7/9/9/10	-
9	GOL	D	1500	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1497	CHT	O6-C4	-3.82	1.22	1.42
4	A	1497	CHT	O6-C4	-3.70	1.23	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1497	CHT	C8-N1-C5	2.29	119.29	109.92
4	B	1497	CHT	C8-N1-C5	2.00	118.10	109.92

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1497	AE3	C4-C3-O2-C2
5	A	1498	ETX	O1-C1-C2-O2
8	C	1497	AE3	O3-C5-C6-O4
7	B	1498	PG4	O2-C3-C4-O3
7	B	1498	PG4	O1-C1-C2-O2
5	D	1498	ETX	C4-C3-O2-C2
7	B	1498	PG4	C8-C7-O4-C6
7	B	1498	PG4	C1-C2-O2-C3
7	B	1498	PG4	C4-C3-O2-C2
5	A	1498	ETX	C1-C2-O2-C3
7	B	1498	PG4	C6-C5-O3-C4
4	B	1497	CHT	C4-C5-N1-C7
7	B	1498	PG4	O3-C5-C6-O4
8	C	1497	AE3	O2-C3-C4-O3

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
8	C	1497	AE3	1	0
5	D	1498	ETX	4	0
7	B	1498	PG4	1	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	493/497 (99%)	0.24	20 (4%) 37 39	20, 38, 67, 97	0
1	B	493/497 (99%)	0.58	49 (9%) 7 8	24, 48, 79, 118	0
2	C	491/497 (98%)	1.29	115 (23%) 0 0	30, 68, 109, 194	0
3	D	491/497 (98%)	0.35	40 (8%) 12 13	23, 41, 78, 183	0
All	All	1968/1988 (98%)	0.61	224 (11%) 5 5	20, 46, 92, 194	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	281	PHE	11.5
2	C	313	LYS	6.7
2	C	427	LEU	6.7
2	C	106	LEU	6.1
2	C	324	PHE	6.1
2	C	169	ILE	5.9
3	D	494	TYR	5.9
2	C	105	VAL	5.8
2	C	87	ASP	5.6
2	C	91	LYS	5.4
2	C	285	TRP	5.4
2	C	17	ARG	5.3
2	C	428	GLU	5.3
2	C	173	LEU	5.3
2	C	280	ILE	5.3
2	C	301	GLU	5.1
2	C	451	PHE	5.1
2	C	192	LEU	5.1
2	C	181	LEU	4.9
2	C	101	PHE	4.9
2	C	109	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
2	C	201	VAL	4.8
2	C	21	LYS	4.8
3	D	490	PRO	4.7
2	C	282	GLY	4.7
2	C	396	LEU	4.7
2	C	154	LEU	4.6
3	D	367	LYS	4.6
1	B	264	ILE	4.4
3	D	491	TRP	4.3
2	C	80	ALA	4.2
2	C	367	LYS	4.2
2	C	20	ILE	4.2
2	C	90	VAL	4.2
1	B	181	LEU	4.1
3	D	487	SER	4.0
2	C	18	GLU	4.0
1	B	169	ILE	4.0
1	B	402	SER	4.0
2	C	267	PHE	4.0
2	C	84	GLU	4.0
2	C	268	GLU	3.9
3	D	489	GLU	3.9
2	C	208	LEU	3.9
2	C	283	CYS	3.9
1	B	154	LEU	3.8
2	C	180	VAL	3.8
2	C	446	CYS	3.8
1	B	326	GLU	3.8
1	A	495	LYS	3.8
3	D	137	MET	3.7
2	C	368	LYS	3.7
1	A	264	ILE	3.7
2	C	61	ASN	3.7
1	B	208	LEU	3.7
2	C	288	GLY	3.7
2	C	305	ALA	3.6
1	B	191	CYS	3.6
2	C	264	ILE	3.6
2	C	300	HIS	3.6
2	C	22	LYS	3.6
2	C	170	ALA	3.6
2	C	95	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
3	D	495	LYS	3.5
1	B	20	ILE	3.5
1	B	283	CYS	3.5
3	D	486	ILE	3.4
1	B	421	ALA	3.4
2	C	179	ALA	3.4
1	B	336	LYS	3.3
2	C	155	ILE	3.3
1	B	396	LEU	3.3
2	C	328	CYS	3.3
1	A	367	LYS	3.3
2	C	326	GLU	3.3
3	D	181	LEU	3.3
1	B	403	SER	3.2
2	C	110	ASP	3.2
1	B	294	THR	3.2
1	B	305	ALA	3.2
2	C	290	ILE	3.2
2	C	36	ILE	3.2
2	C	376	ILE	3.2
1	B	427	LEU	3.1
3	D	134	THR	3.1
2	C	366	LEU	3.1
3	D	154	LEU	3.1
1	B	420	ALA	3.1
1	A	181	LEU	3.0
3	D	396	LEU	3.0
1	B	165	ALA	3.0
1	A	4	PRO	3.0
1	B	442	VAL	3.0
3	D	135	LEU	3.0
1	B	280	ILE	3.0
1	B	34	GLU	3.0
2	C	447	SER	3.0
1	B	297	LEU	3.0
3	D	493	TRP	2.9
3	D	279	THR	2.9
2	C	381	SER	2.9
3	D	139	ARG	2.9
1	B	279	THR	2.9
1	B	313	LYS	2.9
2	C	294	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	403	SER	2.9
2	C	327	GLY	2.8
3	D	138	GLU	2.8
2	C	426	ASP	2.8
1	B	395	VAL	2.8
3	D	22	LYS	2.8
3	D	180	VAL	2.8
2	C	77	ALA	2.8
3	D	210	ILE	2.8
2	C	196	GLU	2.8
3	D	326	GLU	2.8
1	B	383	SER	2.8
3	D	149	LEU	2.8
1	B	495	LYS	2.7
3	D	363	PRO	2.7
3	D	264	ILE	2.7
3	D	280	ILE	2.7
2	C	270	VAL	2.7
2	C	279	THR	2.7
2	C	88	HIS	2.7
2	C	425	ASN	2.7
3	D	364	GLU	2.7
1	A	210	ILE	2.6
1	A	488	ASP	2.6
1	B	318	ILE	2.6
1	B	284	PHE	2.6
2	C	269	ASP	2.6
2	C	114	CYS	2.6
1	A	163	LEU	2.6
1	A	422	VAL	2.6
2	C	395	VAL	2.6
2	C	112	ALA	2.6
3	D	297	LEU	2.5
2	C	199	ASN	2.5
3	D	152	VAL	2.5
2	C	172	ALA	2.5
2	C	284	PHE	2.5
1	A	162	LEU	2.5
2	C	191	CYS	2.5
2	C	382	THR	2.5
2	C	89	PHE	2.5
3	D	324	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	308	VAL	2.4
2	C	116	GLU	2.4
2	C	93	GLU	2.4
3	D	492	GLY	2.4
2	C	165	ALA	2.4
2	C	421	ALA	2.4
1	B	22	LYS	2.4
2	C	5	ILE	2.4
2	C	369	GLY	2.4
1	B	179	ALA	2.4
2	C	297	LEU	2.4
3	D	179	ALA	2.4
2	C	365	HIS	2.4
2	C	104	ALA	2.3
1	A	364	GLU	2.3
1	B	166	THR	2.3
2	C	207	VAL	2.3
2	C	316	LYS	2.3
3	D	31	SER	2.3
3	D	127	GLY	2.3
2	C	32	THR	2.3
1	A	395	VAL	2.3
2	C	320	ILE	2.3
1	A	191	CYS	2.3
1	A	490	PRO	2.3
2	C	162	LEU	2.3
1	A	167	TRP	2.3
1	B	282	GLY	2.2
2	C	263	PRO	2.2
1	B	369	GLY	2.2
1	A	284	PHE	2.2
2	C	275	VAL	2.2
1	B	61	ASN	2.2
3	D	191	CYS	2.2
1	B	194	PHE	2.2
1	B	434	THR	2.2
1	B	210	ILE	2.2
2	C	166	THR	2.2
2	C	190	THR	2.2
3	D	353	GLY	2.2
2	C	306	GLU	2.2
2	C	35	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	22	LYS	2.2
2	C	323	PRO	2.2
2	C	37	GLY	2.2
2	C	325	GLU	2.2
2	C	488	ASP	2.2
1	B	180	VAL	2.2
1	B	295	SER	2.1
2	C	200	GLU	2.1
1	B	309	ASP	2.1
1	A	368	LYS	2.1
1	B	155	ILE	2.1
1	B	173	LEU	2.1
2	C	7	ALA	2.1
1	B	358	TYR	2.1
3	D	294	THR	2.1
2	C	420	ALA	2.1
2	C	429	ARG	2.1
1	A	265	VAL	2.1
1	B	496	SER	2.1
3	D	376	ILE	2.1
2	C	92	LEU	2.1
3	D	208	LEU	2.1
2	C	374	PRO	2.1
2	C	266	VAL	2.1
2	C	79	ALA	2.1
1	B	161	PRO	2.1
1	B	33	GLU	2.0
1	B	267	PHE	2.0
2	C	354	ALA	2.0
2	C	183	PRO	2.0
2	C	490	PRO	2.0
2	C	38	ASP	2.0
1	A	165	ALA	2.0
3	D	34	GLU	2.0
2	C	82	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CSO	D	450	7/8	0.88	0.15	38,43,61,89	0
2	CSO	C	291	7/8	0.90	0.15	54,59,75,80	0
3	CSO	D	291	7/8	0.96	0.12	29,30,62,92	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ETX	D	1498	6/6	0.64	0.35	55,63,66,68	0
9	GOL	D	1500	6/6	0.72	0.21	54,60,62,63	0
8	AE3	C	1497	9/9	0.82	0.14	50,53,56,59	0
5	ETX	A	1498	6/6	0.84	0.18	57,58,60,62	0
4	CHT	A	1497	7/7	0.90	0.40	53,55,61,61	7
6	K	B	1499	1/1	0.92	0.10	45,45,45,45	1
7	PG4	B	1498	12/13	0.93	0.11	35,40,48,51	0
4	CHT	B	1497	7/7	0.94	0.26	59,60,65,66	7
6	K	C	1498	1/1	0.95	0.11	48,48,48,48	1
6	K	D	1499	1/1	0.96	0.13	43,43,43,43	1
6	K	A	1499	1/1	0.97	0.07	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.