



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:40 PM UTC

PDB ID : 5A2D / pdb_00005a2d
Title : CRYSTAL STRUCTURE OF BETAINES ALDEHYDE DEHYDROGENASE
FROM SPINACH SHOWING A THIOHEMIACETAL WITH BETAINES
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

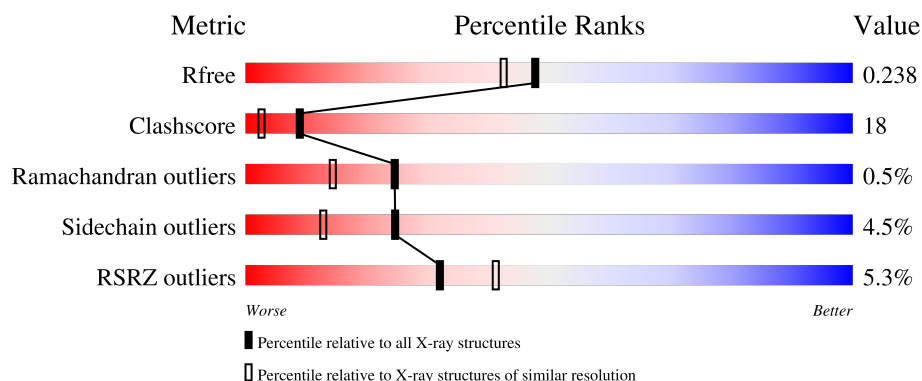
1 Overall quality at a glance

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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	82% 16%
1	B	497	78% 19%
2	C	497	55% 36% 6%
3	D	497	80% 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

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			

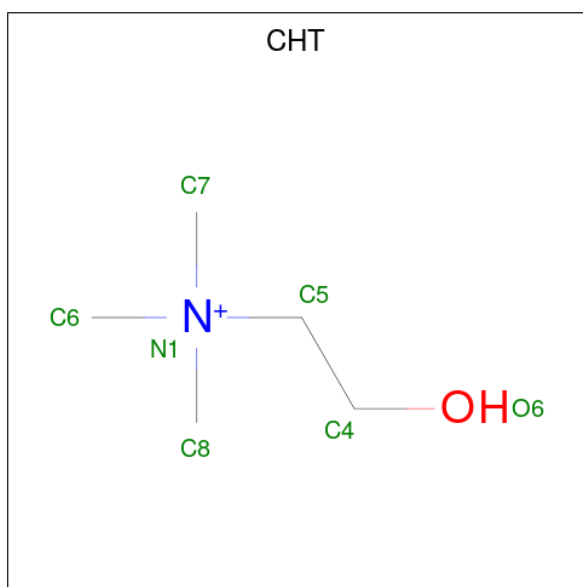
- Molecule 2 is a protein called BETAINE ALDEHYDE DEHYDROGENASE, CHLORO-PLASTIC.

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.

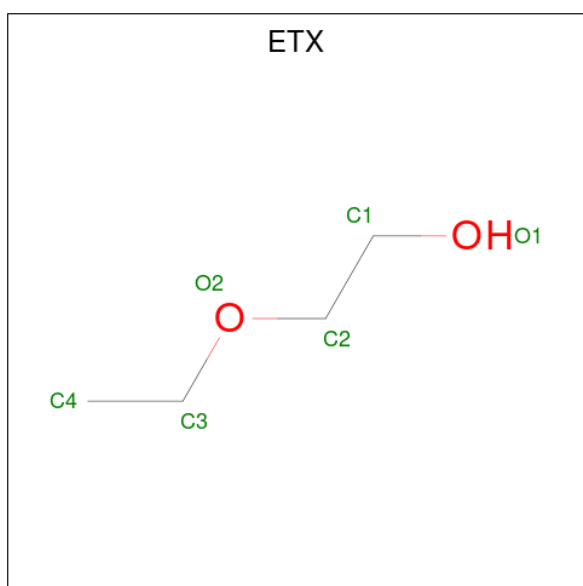
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	493	Total	C	N	O	S	0	3	0
			3817	2447	635	719	16			

- Molecule 4 is CHOLINE ION (CCD ID: 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 (CCD ID: ETX) (formula: $C_4H_{10}O_2$).

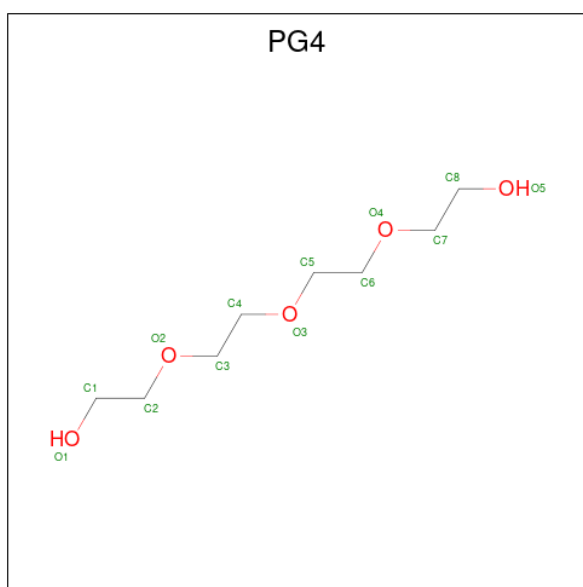


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		
5	D	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

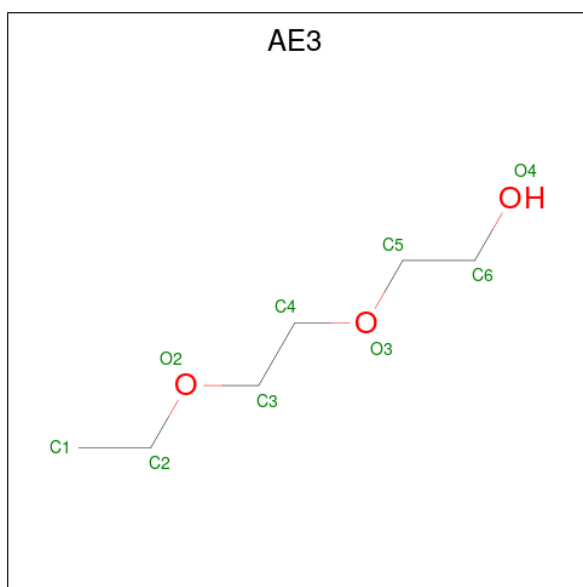
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0
6	B	1	Total K 1 1	0	0
6	C	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



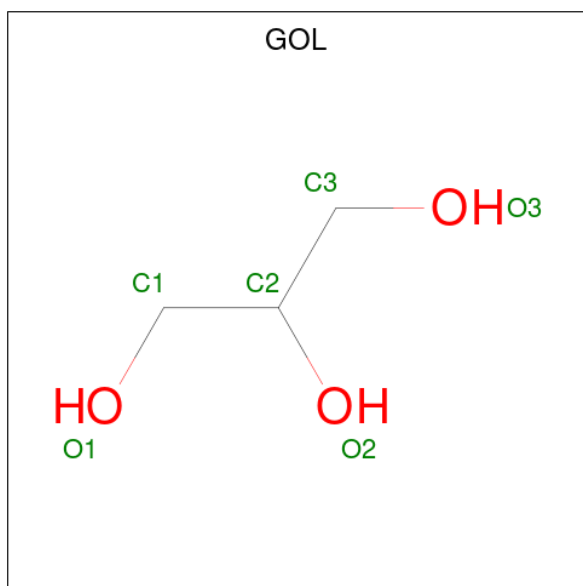
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 12 8 4	0	0

- Molecule 8 is 2-(2-ETHOXYETHOXY)ETHANOL (CCD ID: AE3) (formula: C₆H₁₄O₃).



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

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

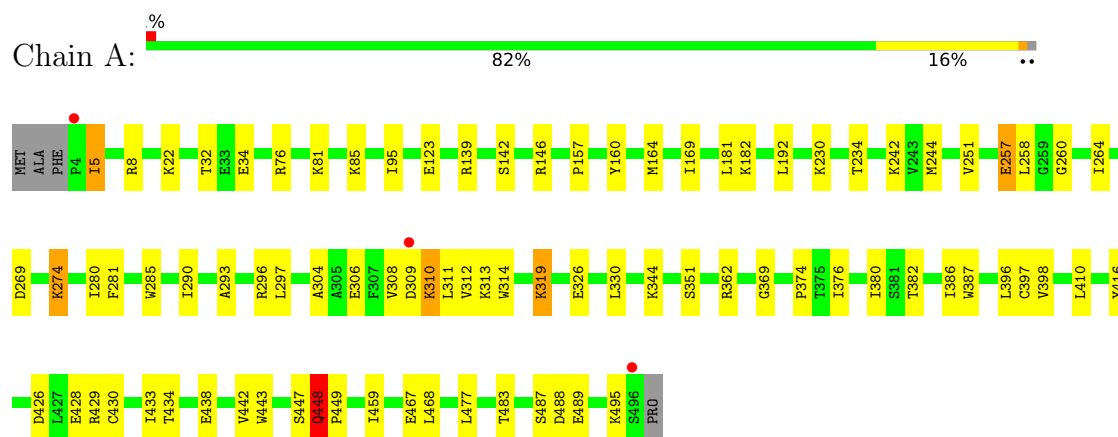
- Molecule 10 is water.

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

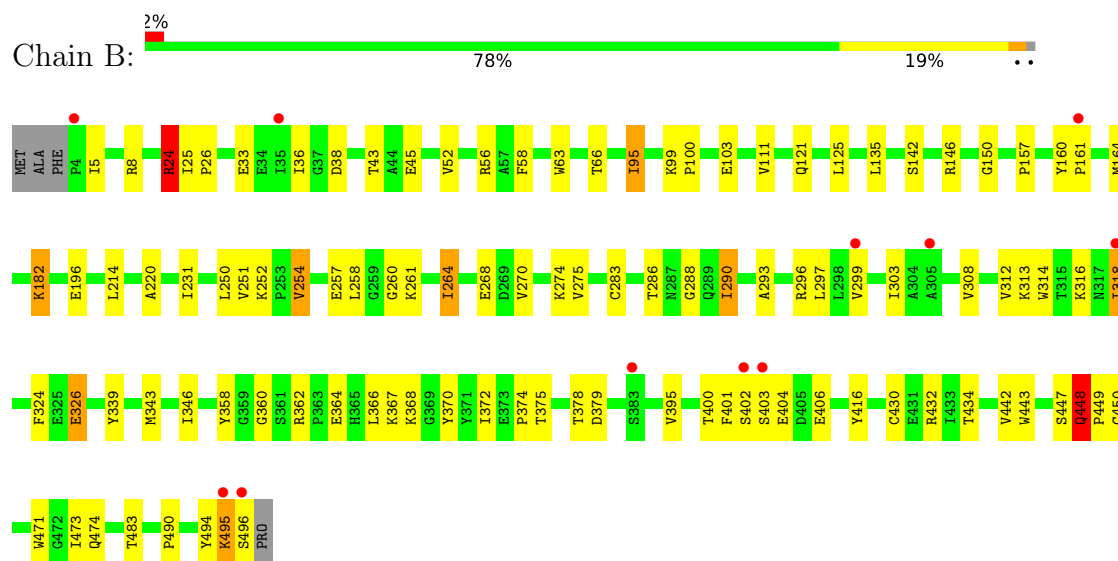
3 Residue-property plots

These plots are drawn for all protein, RNA, 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

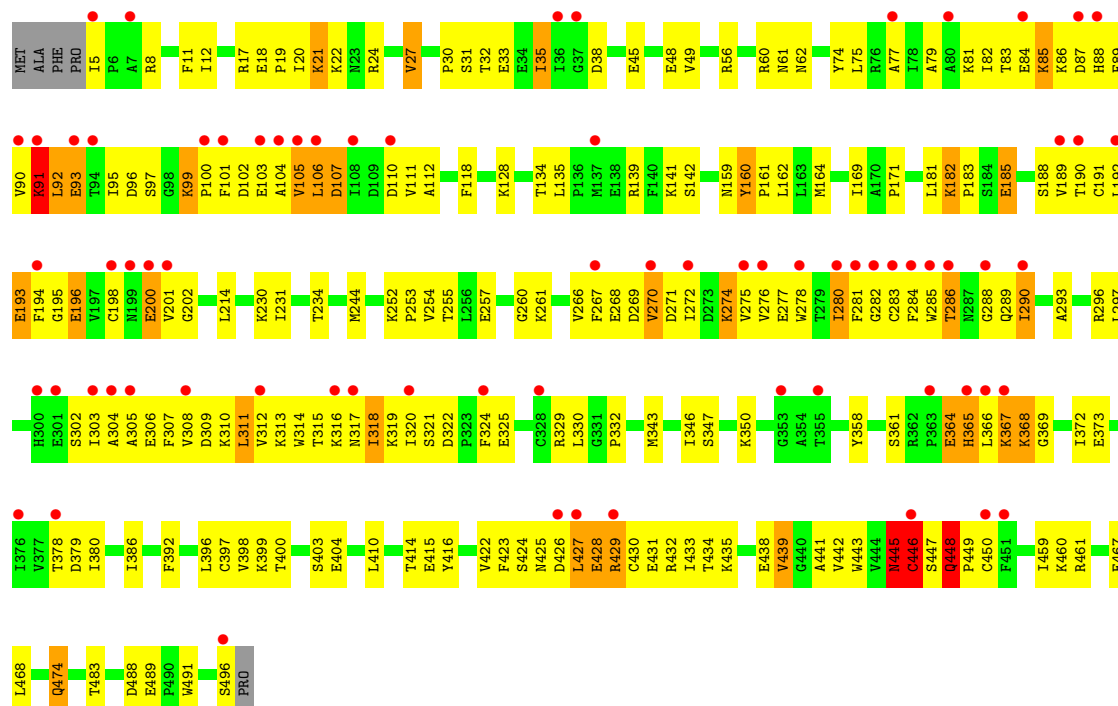


• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

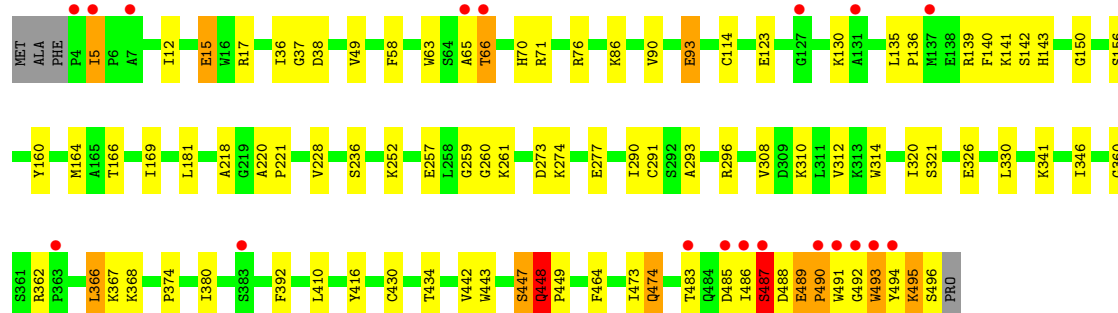
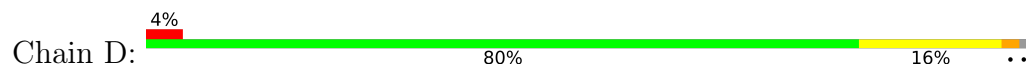


• Molecule 2: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC





● 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) 96.8 (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 0.196 , 0.238	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 , 57.3	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: PG4, CHT, CSO, AE3, ETX, GOL, 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	0.65	1/3934 (0.0%)	0.90	3/5350 (0.1%)
1	B	0.60	1/3964 (0.0%)	0.88	6/5390 (0.1%)
2	C	0.76	1/3890 (0.0%)	1.06	14/5289 (0.3%)
3	D	0.66	0/3891	0.93	9/5291 (0.2%)
All	All	0.67	3/15679 (0.0%)	0.94	32/21320 (0.2%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	LYS	C-O	-5.68	1.19	1.24
2	C	107	ASP	N-CA	-5.39	1.39	1.46
1	A	257	GLU	C-O	-5.08	1.18	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	446	CYS	CA-C-N	16.53	150.65	121.89
2	C	446	CYS	C-N-CA	16.53	150.65	121.89
3	D	487	SER	CB-CA-C	-16.01	75.85	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	GLN	N-CA-C	10.97	134.06	109.81
2	C	445	ASN	O-C-N	-9.98	109.31	122.59
2	C	91	LYS	N-CA-C	9.81	125.38	113.41
3	D	493	TRP	CA-C-N	-9.05	106.84	123.05
3	D	493	TRP	C-N-CA	-9.05	106.84	123.05
2	C	91	LYS	CB-CA-C	-9.00	93.48	109.24
2	C	105	VAL	N-CA-C	8.67	118.68	110.53
2	C	105	VAL	CB-CA-C	-8.23	101.24	112.02
1	B	24	ARG	O-C-N	-8.11	114.17	123.33
1	B	161	PRO	CB-CA-C	-7.50	100.53	113.20
1	B	220	ALA	CA-C-N	-7.36	112.21	119.64
1	B	220	ALA	C-N-CA	-7.36	112.21	119.64
1	B	161	PRO	N-CA-C	6.88	124.93	113.78
2	C	92	LEU	CB-CA-C	6.53	124.82	110.18
3	D	448	GLN	N-CA-C	6.23	123.58	109.81
3	D	220	ALA	CA-C-N	-5.88	113.62	119.56
3	D	220	ALA	C-N-CA	-5.88	113.62	119.56
2	C	448	GLN	CA-C-N	-5.78	112.62	119.84
2	C	448	GLN	C-N-CA	-5.78	112.62	119.84
2	C	270	VAL	N-CA-C	5.49	115.60	108.35
2	C	128	LYS	N-CA-C	-5.49	106.59	113.28
1	A	448	GLN	CB-CA-C	-5.40	99.54	110.17
3	D	447	SER	CB-CA-C	5.29	118.80	109.80
1	A	22	LYS	N-CA-C	5.20	118.89	112.24
2	C	87	ASP	N-CA-C	-5.20	106.20	112.54
3	D	156	SER	CA-C-N	5.10	125.31	120.31
3	D	156	SER	C-N-CA	5.10	125.31	120.31
2	C	274	LYS	N-CA-C	-5.10	105.18	111.40
1	B	314	TRP	N-CA-C	-5.07	105.65	111.07

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	64	2
1	B	3874	0	3867	86	2
2	C	3806	0	3805	352	0
3	D	3817	0	3819	94	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	1	0
10	B	150	0	0	3	0
10	C	103	0	0	6	0
10	D	179	0	0	3	0
All	All	16066	0	15406	569	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 18.

All (569) 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:314:TRP:O	2:C:317:ASN:CG	1.72	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:314:TRP:C	2:C:317:ASN:ND2	1.98	1.19
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:188:SER:C	10:C:2038:HOH:O	2.18	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:278:TRP:C	2:C:281:PHE:CE2	2.55	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
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
3:D:367:LYS:HG3	3:D:368:LYS:HD2	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:317:ASN:CG	2:C:318:ILE:HD12	2.10	0.73
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:81:LYS:HZ3	2:C:85:LYS:HD3	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:495:LYS:O	1:B:496:SER:OG	2.05	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:81:LYS:HZ1	2:C:85:LYS:HD3	1.57	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
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
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
2:C:343:MET:HE3	2:C:372:ILE:HD13	1.76	0.67
3:D:485:ASP:OD1	3:D:487:SER:HB2	1.94	0.67
2:C:61:ASN:OD1	2:C:61:ASN:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:314:TRP:C	2:C:317:ASN:HD21	1.92	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: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
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
3:D:490:PRO:C	3:D:492:GLY:N	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:261:LYS:HG3	3:D:296:ARG:HD2	1.81	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
3:D:38:ASP:OD1	3:D:38:ASP:N	2.30	0.62
2:C:159:ASN:C	2:C:160:TYR:CD1	2.78	0.62
2:C:404:GLU:HG3	2:C:433:ILE:HD11	1.80	0.62
3:D:273:ASP:OD1	3:D:310:LYS:NZ	2.23	0.62
2:C:82:ILE:CG2	2:C:112:ALA:HB2	2.29	0.61
2:C:89:PHE:CE1	2:C:193:GLU:CD	2.78	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
3:D:490:PRO:O	3:D:491:TRP:C	2.42	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: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
2:C:195:GLY:O	2:C:198:CYS:N	2.36	0.59
3:D:447:SER:C	3:D:449:PRO:HD3	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:315:THR:C	2:C:318:ILE:HD13	2.29	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
2:C:343:MET:HE2	2:C:343:MET:HA	1.87	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:361:SER:O	2:C:373:GLU:HG3	2.04	0.57
1:B:343:MET:HE2	1:B:372:ILE:HG12	1.86	0.57
2:C:447:SER:C	2:C:449:PRO:HD3	2.30	0.57
3:D:485:ASP:OD1	3:D:487:SER:N	2.38	0.57
1:A:447:SER:C	1:A:449:PRO:HD3	2.30	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
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
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
2:C:105:VAL:C	2:C:107:ASP:H	2.13	0.55
1:B:100:PRO:HD2	1:B:103:GLU:CD	2.32	0.55
1:B:430:CYS:O	1:B:434:THR:HG23	2.07	0.55
2:C:319:LYS:HZ1	2:C:325:GLU:CD	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:192:LEU:HD12	2:C:192:LEU:C	2.32	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
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
1:A:242:LYS:NZ	10:A:2146:HOH:O	2.41	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:107:ASP:O	2:C:110:ASP:N	2.33	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
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
3:D:236:SER:HA	5:D:1498:ETX:H12	1.92	0.51
3:D:489:GLU:O	3:D:490:PRO:C	2.54	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
2:C:191:CYS:C	2:C:193:GLU:N	2.67	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:319:LYS:NZ	2:C:325:GLU:CD	2.69	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:270:VAL:HB	1:B:275:VAL:HG21	1.92	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
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
2:C:317:ASN:OD1	2:C:317:ASN:C	2.56	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:105:VAL:C	2:C:107:ASP:N	2.71	0.48
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
1:A:438:GLU:C	1:A:459:ILE:HD11	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:TYR:O	2:C:161:PRO:C	2.57	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
2:C:81:LYS:O	2:C:82:ILE:C	2.56	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:427:LEU:C	2:C:429:ARG:H	2.22	0.48
2:C:32:THR:O	2:C:33:GLU:HB2	2.13	0.47
2:C:99:LYS:O	2:C:100:PRO:C	2.57	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
2:C:24:ARG:HE	2:C:38:ASP:CG	2.23	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:269:ASP:O	2:C:425:ASN:CG	2.58	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:365:HIS:CD2	2:C:365:HIS:C	2.93	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:447:SER:O	1:A:448:GLN:HB2	2.16	0.44
2:C:81:LYS:HZ1	2:C:85:LYS:CD	2.26	0.44
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
2:C:438:GLU:C	2:C:459:ILE:HD11	2.43	0.44
1:A:488:ASP:OD1	1:A:488:ASP:O	2.35	0.44
2:C:244:MET:HE1	3:D:252:LYS:O	2.18	0.44
2:C:252:LYS:HB2	2:C:252:LYS:HE3	1.71	0.44
2:C:315:THR:C	2:C:317:ASN:H	2.24	0.44
3:D:496:SER:C	10:D:2177:HOH:O	2.60	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
3:D:367:LYS:C	3:D:368:LYS:HD2	2.42	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
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)
1:B:364[A]:GLU:H	1:B:364[A]:GLU:CD	2.23	0.44
2:C:277:GLU:O	2:C:278:TRP:C	2.58	0.44
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:218:ALA:C	3:D:221:PRO:HD2	2.43	0.44
3:D:443:TRP:CZ2	3:D:448:GLN:HA	2.53	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
2:C:83:THR:O	2:C:84:GLU:C	2.61	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:193:GLU:O	2:C:194:PHE:C	2.61	0.43
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:313:LYS:O	2:C:314:TRP:C	2.61	0.43
2:C:315:THR:CA	2:C:318:ILE:HD13	2.47	0.43
2:C:89:PHE:C	2:C:91:LYS:N	2.76	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:100:PRO:HD2	2:C:103:GLU:CD	2.43	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:195:GLY:O	2:C:196:GLU:C	2.61	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
3:D:218:ALA:O	3:D:221:PRO:HD2	2.18	0.43
2:C:74:TYR:HE2	2:C:202:GLY:C	2.27	0.43
2:C:467:GLU:HB3	2:C:468:LEU:HD13	2.01	0.43
2:C:414:THR:O	2:C:460:LYS:NZ	2.47	0.43
2:C:308:VAL:O	2:C:309:ASP:C	2.58	0.43
3:D:12:ILE:HG21	3:D:49:VAL:HG12	2.00	0.43
3:D:490:PRO:C	3:D:492:GLY:H	2.27	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:278:TRP:C	2:C:281:PHE:CD2	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:343:MET:HE2	2:C:346:ILE:HD12	2.00	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:244:MET:HE1	1:B:252:LYS:O	2.20	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
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
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
2:C:317:ASN:CG	2:C:318:ILE:CD1	2.81	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:11:PHE:C	2:C:12:ILE:HG13	2.46	0.41
2:C:313:LYS:HD2	2:C:313:LYS:HA	1.83	0.41
2:C:95:ILE:HG23	2:C:324:PHE:HZ	1.85	0.41
2:C:191:CYS:C	2:C:193:GLU:H	2.29	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:100:PRO:O	2:C:101:PHE:C	2.63	0.41
2:C:305:ALA:O	2:C:308:VAL:HG22	2.20	0.41
2:C:277:GLU:C	2:C:281:PHE:CD2	2.97	0.41
2:C:488:ASP:C	2:C:489:GLU:HG2	2.46	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:92:LEU:HD12	2:C:92:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:285:TRP:CD1	2:C:286:THR:H	2.39	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
2:C:430:CYS:C	2:C:432:ARG:N	2.76	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:309:ASP:O	2:C:310:LYS:C	2.63	0.40
2:C:322:ASP:OD1	2:C:324:PHE:HB2	2.20	0.40
3:D:76:ARG:HH12	3:D:123:GLU:CD	2.24	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
2:C:253:PRO:HB3	3:D:464:PHE:CG	2.57	0.40
2:C:271:ASP:OD1	2:C:271:ASP:C	2.65	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

5.3.1 Protein backbone

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%)	43	35
1	B	502/497 (101%)	474 (94%)	26 (5%)	2 (0%)	30	20
2	C	492/497 (99%)	447 (91%)	40 (8%)	5 (1%)	12	5
3	D	492/497 (99%)	474 (96%)	16 (3%)	2 (0%)	30	20
All	All	1984/1988 (100%)	1877 (95%)	97 (5%)	10 (0%)	24	14

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%)	406 (98%)	8 (2%)	50	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	417/410 (102%)	404 (97%)	13 (3%)	35	26
2	C	408/409 (100%)	369 (90%)	39 (10%)	8	2
3	D	408/408 (100%)	393 (96%)	15 (4%)	30	20
All	All	1647/1637 (101%)	1572 (95%)	75 (5%)	24	12

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	230	LYS
1	A	257	GLU
1	A	264	ILE
1	A	274	LYS
1	A	310	LYS
1	A	319	LYS
1	A	495	LYS
1	B	95	ILE
1	B	111	VAL
1	B	182	LYS
1	B	254	VAL
1	B	257	GLU
1	B	264	ILE
1	B	290	ILE
1	B	318	ILE
1	B	326	GLU
1	B	448	GLN
1	B	483[A]	THR
1	B	483[B]	THR
1	B	495	LYS
2	C	21	LYS
2	C	22	LYS
2	C	27	VAL
2	C	35	ILE
2	C	48	GLU
2	C	62	ASN
2	C	75	LEU
2	C	85	LYS
2	C	91	LYS
2	C	93	GLU
2	C	99	LYS
2	C	160	TYR

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Mol	Chain	Res	Type
2	C	182	LYS
2	C	185	GLU
2	C	193	GLU
2	C	196	GLU
2	C	200	GLU
2	C	270	VAL
2	C	280	ILE
2	C	286	THR
2	C	290	ILE
2	C	306	GLU
2	C	311	LEU
2	C	318	ILE
2	C	364	GLU
2	C	367	LYS
2	C	368	LYS
2	C	392	PHE
2	C	398	VAL
2	C	400	THR
2	C	422	VAL
2	C	427	LEU
2	C	428	GLU
2	C	429	ARG
2	C	435	LYS
2	C	439	VAL
2	C	446	CYS
2	C	450	CYS
2	C	474	GLN
3	D	5	ILE
3	D	15	GLU
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	473[A]	ILE
3	D	473[B]	ILE
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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	B	23	ASN
2	C	61	ASN
2	C	88	HIS
2	C	474	GLN
3	D	199	ASN

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	$\# Z > 2$
3	CSO	D	450	3	3,6,7	0.82	0	1,6,8	0.72	0
3	CSO	D	291	3	3,6,7	1.03	0	1,6,8	1.22	0
2	CSO	C	291	2	3,6,7	0.56	0	1,6,8	0.35	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
3	CSO	D	450	3	-	0/1/5/7	-
3	CSO	D	291	3	-	0/1/5/7	-
2	CSO	C	291	2	-	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 oligosaccharides 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	$\# Z > 2$
7	PG4	B	1498	-	11,11,12	0.76	0	10,10,11	0.44	0
4	CHT	B	1497	1	6,6,6	2.01	1 (16%)	8,8,8	1.11	1 (12%)
4	CHT	A	1497	1	6,6,6	2.00	1 (16%)	8,8,8	1.21	1 (12%)
5	ETX	A	1498	-	5,5,5	0.44	0	4,4,4	0.31	0
8	AE3	C	1497	-	8,8,8	0.72	0	7,7,7	0.37	0
5	ETX	D	1498	-	5,5,5	0.38	0	4,4,4	0.49	0
9	GOL	D	1500	-	5,5,5	0.36	0	5,5,5	0.33	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
7	PG4	B	1498	-	-	6/9/9/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHT	B	1497	1	-	1/4/4/4	-
4	CHT	A	1497	1	-	0/4/4/4	-
5	ETX	A	1498	-	-	2/3/3/3	-
8	AE3	C	1497	-	-	2/6/6/6	-
5	ETX	D	1498	-	-	1/3/3/3	-
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	-3.87	1.22	1.42
4	A	1497	CHT	O6-C4	-3.75	1.23	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1497	CHT	C8-N1-C5	2.36	119.29	109.91
4	B	1497	CHT	C8-N1-C5	2.06	118.10	109.91

There are no chirality outliers.

All (12) 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

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1498	PG4	1	0
4	B	1497	CHT	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

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, 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%)	-0.08	3 (0%) 85 90	13, 38, 67, 97	7 (1%)
1	B	493/497 (99%)	0.21	11 (2%) 62 71	14, 48, 79, 118	11 (2%)
2	C	491/497 (98%)	1.04	72 (14%) 6 7	24, 68, 109, 194	3 (0%)
3	D	491/497 (98%)	0.06	19 (3%) 43 53	12, 40, 78, 183	3 (0%)
All	All	1968/1988 (98%)	0.31	105 (5%) 32 41	12, 46, 92, 194	24 (1%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	281	PHE	8.9
2	C	90	VAL	5.4
1	B	496	SER	5.2
2	C	446	CYS	4.6
3	D	487	SER	4.6
2	C	427	LEU	4.5
2	C	110	ASP	4.2
1	B	4	PRO	4.2
2	C	104	ALA	4.1
2	C	105	VAL	4.0
2	C	305	ALA	3.9
3	D	490	PRO	3.9
1	B	318	ILE	3.9
2	C	192	LEU	3.8
3	D	486	ILE	3.8
3	D	494	TYR	3.7
2	C	282	GLY	3.7
1	B	383	SER	3.5
2	C	320	ILE	3.5
2	C	285	TRP	3.5
2	C	201	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
3	D	65	ALA	3.4
2	C	308	VAL	3.3
2	C	106	LEU	3.3
2	C	84	GLU	3.2
3	D	493	TRP	3.2
2	C	283	CYS	3.2
2	C	91	LYS	3.2
3	D	127	GLY	3.2
2	C	36	ILE	3.2
2	C	300	HIS	3.2
3	D	363	PRO	3.1
2	C	280	ILE	3.0
2	C	276	VAL	3.0
2	C	317	ASN	3.0
3	D	492	GLY	2.9
1	A	4	PRO	2.9
2	C	199	ASN	2.9
2	C	496	SER	2.9
2	C	365	HIS	2.8
2	C	451	PHE	2.8
2	C	378	THR	2.8
3	D	137	MET	2.8
2	C	270	VAL	2.8
2	C	324	PHE	2.7
2	C	301	GLU	2.7
2	C	77	ALA	2.7
2	C	328	CYS	2.7
2	C	450	CYS	2.7
1	A	496	SER	2.7
2	C	363	PRO	2.7
2	C	5	ILE	2.7
2	C	278	TRP	2.6
1	B	299	VAL	2.6
3	D	491	TRP	2.6
2	C	108	ILE	2.6
1	B	305	ALA	2.6
2	C	267	PHE	2.6
2	C	284	PHE	2.5
2	C	366	LEU	2.5
2	C	303	ILE	2.5
2	C	93	GLU	2.5
2	C	198	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	402	SER	2.4
2	C	137	MET	2.4
1	A	309	ASP	2.4
2	C	190	THR	2.4
2	C	88	HIS	2.4
2	C	80	ALA	2.4
3	D	7	ALA	2.4
1	B	161	PRO	2.4
2	C	101	PHE	2.3
3	D	5	ILE	2.3
3	D	131	ALA	2.3
2	C	100	PRO	2.3
2	C	272	ILE	2.3
2	C	94	THR	2.3
2	C	288	GLY	2.3
2	C	189	VAL	2.3
1	B	495	LYS	2.3
3	D	483	THR	2.3
2	C	429	ARG	2.2
2	C	7	ALA	2.2
3	D	4	PRO	2.2
2	C	376	ILE	2.2
2	C	367	LYS	2.2
3	D	485	ASP	2.2
2	C	355	THR	2.1
2	C	37	GLY	2.1
2	C	304	ALA	2.1
1	B	403	SER	2.1
2	C	286	THR	2.1
2	C	275	VAL	2.1
2	C	426	ASP	2.1
3	D	383	SER	2.1
2	C	316	LYS	2.1
1	B	35	ILE	2.0
2	C	194	PHE	2.0
2	C	200	GLU	2.0
2	C	353	GLY	2.0
2	C	312	VAL	2.0
2	C	87	ASP	2.0
2	C	103	GLU	2.0
2	C	290	ILE	2.0
3	D	66	THR	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, 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	B-factors(Å ²)	Q<0.9
3	CSO	D	450	7/8	0.86	0.12	38,43,61,89	0
2	CSO	C	291	7/8	0.88	0.11	54,59,75,80	0
3	CSO	D	291	7/8	0.93	0.09	29,30,62,92	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
9	GOL	D	1500	6/6	0.70	0.18	54,60,62,63	0
5	ETX	D	1498	6/6	0.75	0.19	55,63,66,68	0
8	AE3	C	1497	9/9	0.86	0.12	50,53,56,59	0
5	ETX	A	1498	6/6	0.87	0.10	57,58,60,62	0
4	CHT	B	1497	7/7	0.89	0.12	59,60,65,66	7
7	PG4	B	1498	12/13	0.89	0.10	35,40,48,51	0
6	K	B	1499	1/1	0.90	0.10	45,45,45,45	1
4	CHT	A	1497	7/7	0.91	0.13	53,55,61,61	7
6	K	D	1499	1/1	0.95	0.07	43,43,43,43	1
6	K	C	1498	1/1	0.95	0.07	48,48,48,48	1
6	K	A	1499	1/1	0.97	0.04	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.