



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:30 PM UTC

PDB ID : 4V3F / pdb_00004v3f
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 : 2014-10-18
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

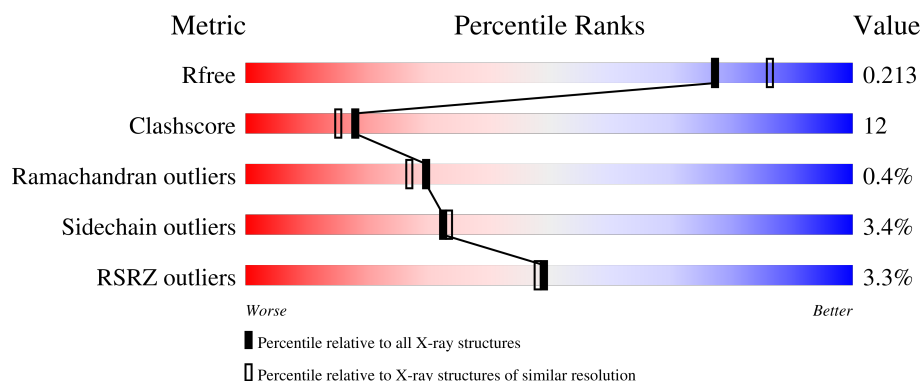
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	498	2% 78% 20% .
1	B	498	3% 73% 24% ..
1	D	498	3% 80% 18% .
2	C	497	6% 73% 25% .

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
3	IOD	B	1498	-	-	X	-
3	IOD	C	1499	-	-	X	-
4	CHT	D	1501	-	-	X	-
5	PG4	D	1502	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16235 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	495	Total	C	N	O	S	0	7	0
			3861	2475	641	726	19			
1	B	494	Total	C	N	O	S	0	11	0
			3899	2494	658	728	19			
1	D	495	Total	C	N	O	S	0	7	0
			3853	2472	640	723	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	CSO	CYS	microheterogeneity	UNP P17202
B	291	CSO	CYS	microheterogeneity	UNP P17202
D	291	CSO	CYS	microheterogeneity	UNP P17202

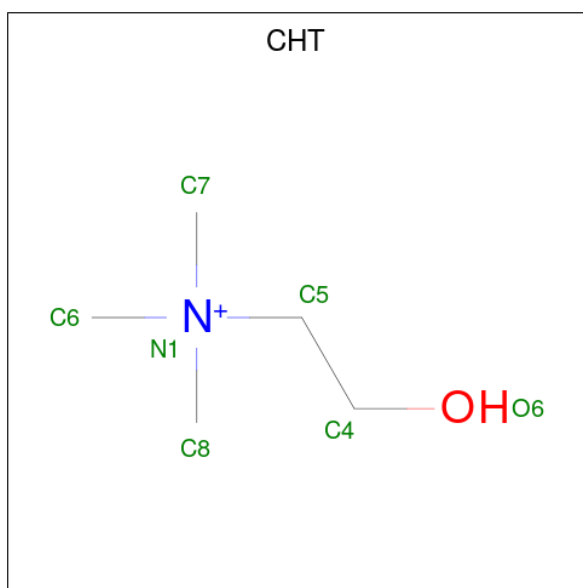
- Molecule 2 is a protein called BETAINE ALDEHYDE DEHYDROGENASE, CHLORO-PLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	495	Total	C	N	O	S	0	7	0
			3871	2478	647	729	17			

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

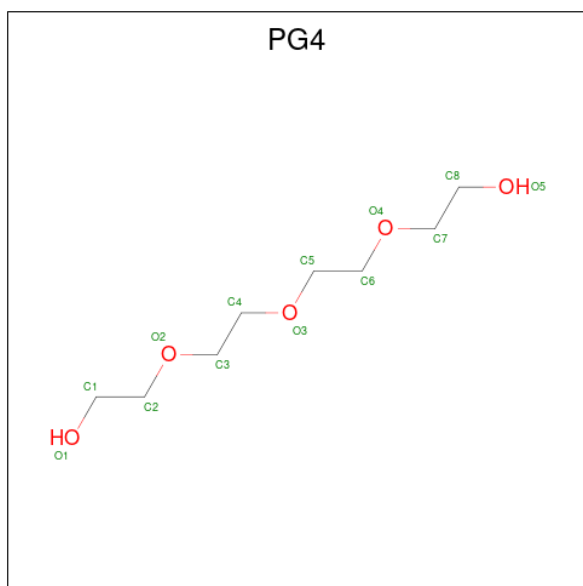
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	I	0	0
			5	5		
3	B	4	Total	I	0	0
			4	4		
3	C	3	Total	I	0	0
			3	3		
3	D	3	Total	I	0	0
			3	3		

- Molecule 4 is CHOLINE ION (CCD ID: 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		
4	D	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



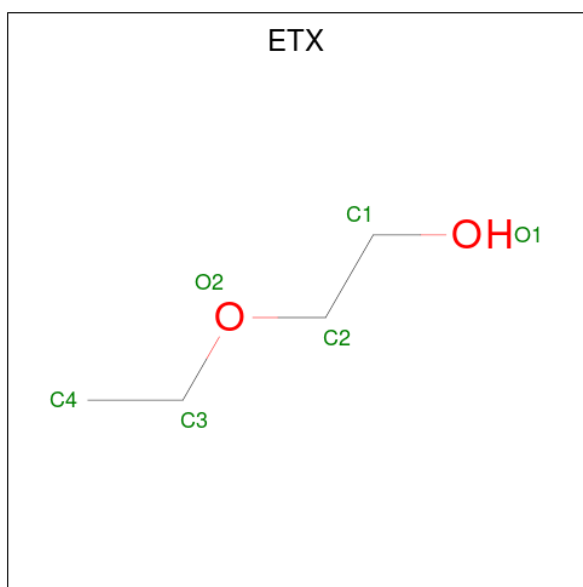
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	8	4		
5	C	1	Total	C	O	0	0
			12	8	4		
5	D	1	Total	C	O	0	0
			12	8	4		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is 2-ETHOXYETHANOL (CCD ID: ETX) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	4	2		

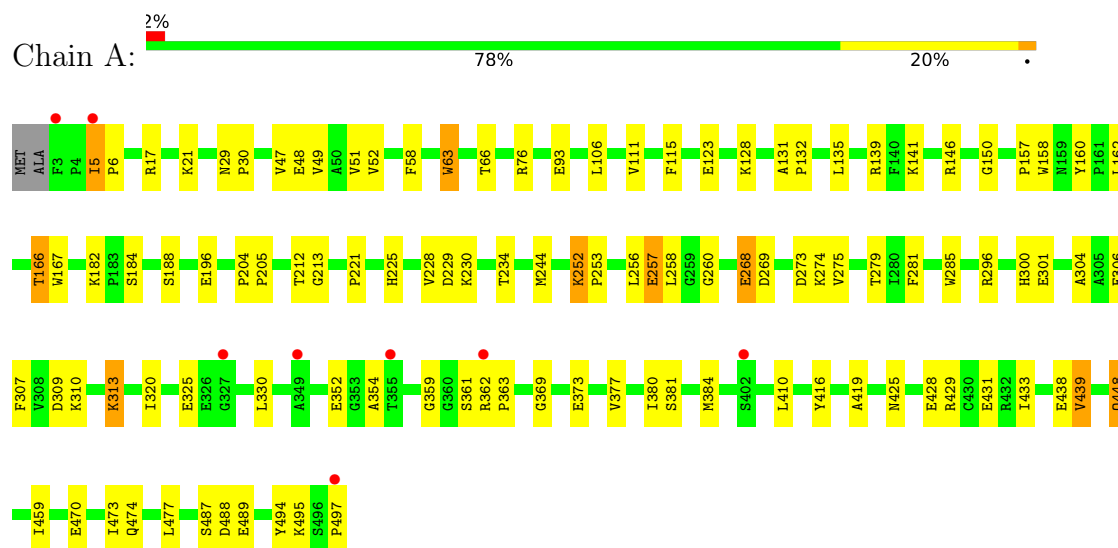
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	189	Total	O	0	0
			189	189		
8	B	130	Total	O	0	0
			130	130		
8	C	163	Total	O	0	0
			163	163		
8	D	179	Total	O	0	0
			179	179		

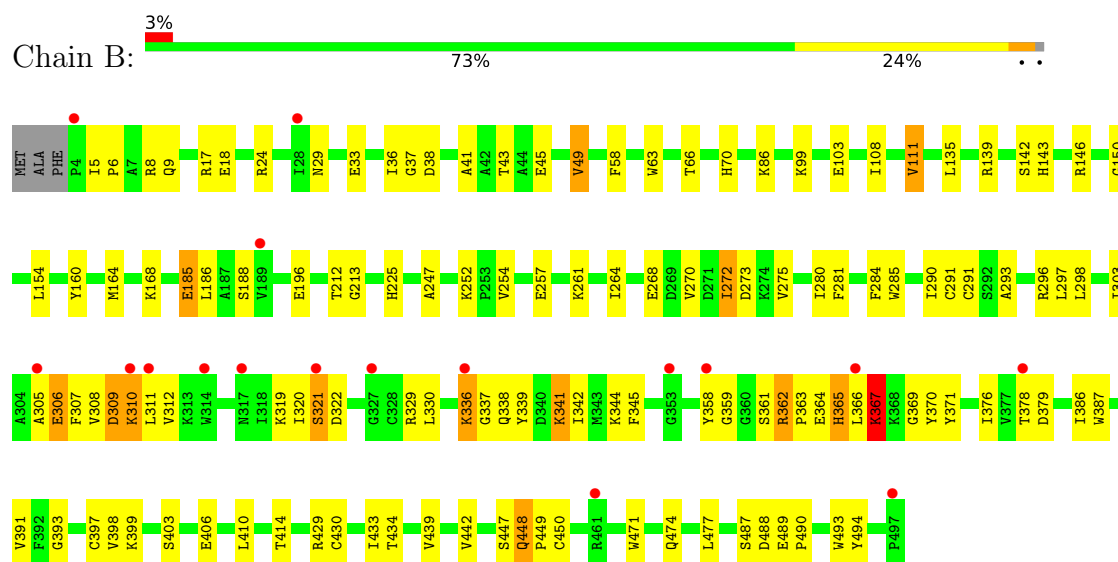
3 Residue-property plots

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.

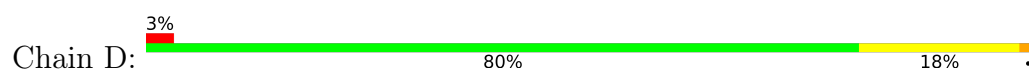
• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

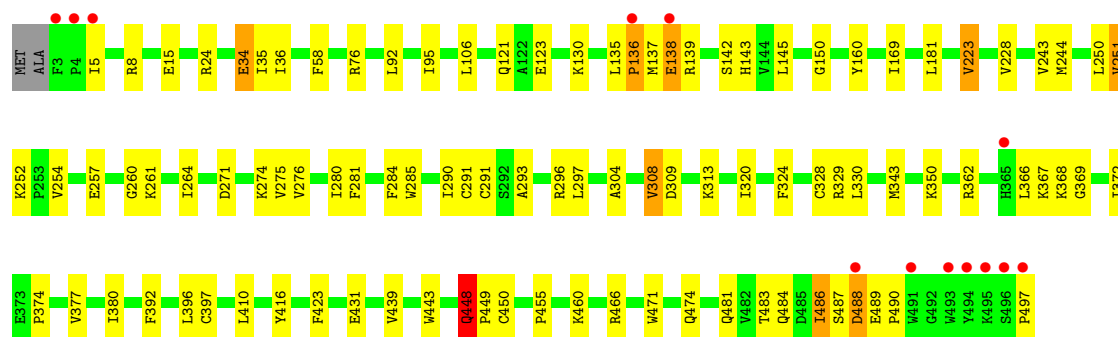


• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

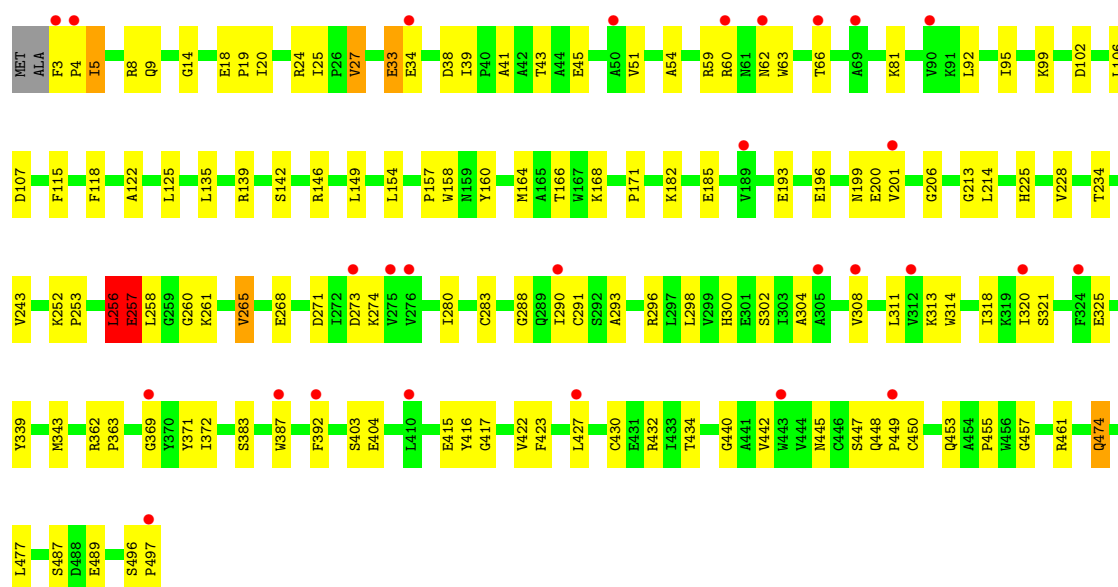


• Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC





• Molecule 2: 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	69.44Å 82.26Å 88.52Å 79.44° 84.89° 77.32°	Depositor
Resolution (Å)	28.97 – 2.00 28.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (28.97-2.00) 96.0 (28.97-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.196 , 0.211 0.199 , 0.213	Depositor DCC
R_{free} test set	5969 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.0	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	0.95	EDS
Total number of atoms	16235	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.58	1/3946 (0.0%)	0.87	8/5366 (0.1%)
1	B	0.54	0/3983	0.89	7/5412 (0.1%)
1	D	0.60	0/3939	0.91	7/5359 (0.1%)
2	C	0.53	0/3946	0.91	10/5364 (0.2%)
All	All	0.56	1/15814 (0.0%)	0.90	32/21501 (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	D	0	1
2	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	TRP	C-O	-6.25	1.16	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	497	PRO	N-CA-CB	8.36	112.19	103.00
1	D	448	GLN	CA-C-N	-8.33	111.16	119.90
1	D	448	GLN	C-N-CA	-8.33	111.16	119.90
1	B	272	ILE	N-CA-C	8.14	118.92	110.62
1	B	367	LYS	N-CA-C	7.97	119.97	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	256	LEU	O-C-N	7.10	131.62	123.31
1	A	494	TYR	CA-C-N	-6.88	112.50	122.19
1	A	494	TYR	C-N-CA	-6.88	112.50	122.19
1	A	497	PRO	N-CA-CB	6.75	110.42	103.00
1	D	250	LEU	O-C-N	-6.66	114.34	122.34
1	D	497	PRO	N-CA-CB	6.63	110.30	103.00
2	C	62	ASN	N-CA-C	6.43	118.37	111.36
1	B	362	ARG	O-C-N	-6.31	116.20	121.38
1	A	135	LEU	CA-C-N	6.14	126.03	119.28
1	A	135	LEU	C-N-CA	6.14	126.03	119.28
1	B	365	HIS	CA-C-N	-6.07	114.20	122.95
1	B	365	HIS	C-N-CA	-6.07	114.20	122.95
2	C	34	GLU	O-C-N	-5.95	116.29	123.13
1	B	361	SER	CA-C-N	5.87	129.22	120.83
1	B	361	SER	C-N-CA	5.87	129.22	120.83
1	D	488	ASP	CA-C-N	5.42	128.18	120.49
1	D	488	ASP	C-N-CA	5.42	128.18	120.49
2	C	257[A]	GLU	CA-C-N	5.31	131.12	122.67
2	C	257[A]	GLU	C-N-CA	5.31	131.12	122.67
2	C	257[B]	GLU	CA-C-N	5.31	131.12	122.67
2	C	257[B]	GLU	C-N-CA	5.31	131.12	122.67
2	C	33	GLU	CA-C-N	5.24	129.38	122.30
2	C	33	GLU	C-N-CA	5.24	129.38	122.30
1	D	448	GLN	N-CA-C	5.23	121.37	109.81
1	A	448	GLN	O-C-N	-5.11	115.44	121.32
1	A	252	LYS	CA-C-N	-5.08	114.72	119.85
1	A	252	LYS	C-N-CA	-5.08	114.72	119.85

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166[B]	THR	Mainchain
2	C	256	LEU	Mainchain
1	D	396	LEU	Mainchain

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	3861	0	3839	81	0
1	B	3899	0	3899	127	0
1	D	3853	0	3848	68	0
2	C	3871	0	3857	100	0
3	A	5	0	0	2	0
3	B	4	0	0	4	0
3	C	3	0	0	4	0
3	D	3	0	0	1	0
4	A	7	0	12	4	0
4	B	7	0	12	5	0
4	D	7	0	12	6	0
5	A	12	0	15	0	0
5	C	12	0	15	0	0
5	D	12	0	15	10	0
6	B	6	0	8	0	0
6	D	6	0	8	3	0
7	C	6	0	10	0	0
8	A	189	0	0	9	0
8	B	130	0	0	6	0
8	C	163	0	0	7	0
8	D	179	0	0	2	0
All	All	16235	0	15550	375	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (375) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LYS:HD2	1:B:370:TYR:CE1	1.17	1.63
1:B:336:LYS:CD	1:B:370:TYR:HE1	1.10	1.55
1:B:336:LYS:CD	1:B:370:TYR:CE1	1.80	1.49
2:C:81:LYS:NZ	2:C:200:GLU:HB3	1.49	1.27
1:A:487:SER:O	1:A:488:ASP:OD1	1.54	1.23
1:B:450[B]:CYS:HB2	4:B:1501:CHT:C4	1.78	1.14
1:B:337:GLY:O	1:B:341:LYS:HE2	1.56	1.06
2:C:321:SER:HB2	2:C:325:GLU:OE1	1.55	1.05
1:B:336:LYS:CD	1:B:370:TYR:CZ	2.38	1.05
1:B:336:LYS:HD3	1:B:370:TYR:CE1	1.92	1.01
1:B:336:LYS:CG	1:B:370:TYR:CE1	2.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LYS:HG2	1:B:370:TYR:CZ	2.00	0.96
1:D:121:GLN:NE2	8:D:2071:HOH:O	2.00	0.95
2:C:81:LYS:HZ2	2:C:200:GLU:HB3	1.32	0.94
1:B:303:ILE:C	1:B:306:GLU:OE1	2.11	0.92
2:C:81:LYS:HZ3	2:C:200:GLU:HB3	1.15	0.92
2:C:81:LYS:NZ	2:C:200:GLU:CB	2.33	0.92
1:A:115:PHE:CE2	1:A:166[B]:THR:HG23	2.04	0.91
1:B:336:LYS:HD3	1:B:370:TYR:CZ	2.05	0.90
1:B:146[B]:ARG:NH1	8:B:2063:HOH:O	2.05	0.89
1:B:336:LYS:HD3	1:B:370:TYR:OH	1.70	0.89
2:C:81:LYS:NZ	2:C:200:GLU:C	2.30	0.89
1:B:362:ARG:NH2	1:B:369:GLY:O	2.06	0.89
1:B:336:LYS:CG	1:B:370:TYR:CZ	2.59	0.86
1:A:487:SER:O	1:A:488:ASP:CG	2.19	0.85
2:C:81:LYS:HZ2	2:C:200:GLU:CB	1.89	0.85
2:C:474:GLN:NE2	3:C:1499:IOD:I	2.80	0.85
1:B:261:LYS:O	1:B:296:ARG:NH1	2.09	0.84
2:C:158:TRP:CZ2	2:C:392:PHE:HE2	1.97	0.83
2:C:257[A]:GLU:OE2	2:C:291:CSO:OD	1.96	0.83
1:A:111:VAL:HG13	1:A:166[A]:THR:HG21	1.62	0.82
2:C:24:ARG:NE	2:C:38:ASP:OD2	2.11	0.82
2:C:81:LYS:NZ	2:C:200:GLU:O	2.13	0.81
1:D:8:ARG:O	1:D:24:ARG:NH2	2.11	0.81
2:C:403:SER:OG	8:C:2134:HOH:O	2.00	0.78
1:D:138:GLU:OE2	8:D:2076:HOH:O	2.01	0.78
1:B:337:GLY:O	1:B:341:LYS:CE	2.32	0.77
2:C:81:LYS:HZ2	2:C:200:GLU:C	1.92	0.76
1:A:196:GLU:OE2	8:A:2010:HOH:O	2.02	0.76
2:C:268:GLU:CD	2:C:302:SER:OG	2.29	0.76
2:C:268:GLU:OE2	2:C:300:HIS:CE1	2.39	0.76
1:A:296:ARG:NH2	1:A:410:LEU:O	2.18	0.76
2:C:362:ARG:NH2	2:C:369:GLY:O	2.18	0.76
2:C:102:ASP:O	2:C:106:LEU:HD12	1.86	0.74
1:B:336:LYS:HD2	1:B:370:TYR:CD1	2.14	0.73
1:A:139:ARG:NH2	1:A:489:GLU:O	2.22	0.73
1:A:268:GLU:CD	1:A:268:GLU:H	1.98	0.71
1:D:466:ARG:HG2	5:D:1502:PG4:H71	1.71	0.71
1:B:434:THR:HG22	1:B:442:VAL:HG11	1.73	0.71
1:B:378:THR:HG22	1:B:379:ASP:H	1.56	0.70
1:A:474:GLN:HG3	8:A:2181:HOH:O	1.91	0.70
2:C:185:GLU:HG3	2:C:214:LEU:HD23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:268:GLU:OE1	2:C:302:SER:OG	2.10	0.69
1:B:336:LYS:CD	1:B:370:TYR:OH	2.38	0.68
2:C:18:GLU:HG2	2:C:19:PRO:HD2	1.74	0.68
1:A:115:PHE:CE2	1:A:166[B]:THR:CG2	2.77	0.68
1:D:449:PRO:HA	6:D:1503:GOL:H31	1.73	0.68
1:B:261:LYS:HG3	1:B:296:ARG:HH11	1.59	0.68
2:C:268:GLU:CD	2:C:302:SER:HG	2.02	0.68
2:C:158:TRP:CZ2	2:C:392:PHE:CE2	2.81	0.67
2:C:434:THR:HG22	2:C:442:VAL:HG11	1.75	0.67
1:B:365:HIS:CD2	1:B:366:LEU:CD1	2.77	0.67
1:D:34:GLU:HG2	1:D:36:ILE:HG23	1.77	0.67
1:A:268:GLU:OE1	1:A:300:HIS:ND1	2.28	0.67
2:C:321:SER:CB	2:C:325:GLU:OE1	2.41	0.65
2:C:474:GLN:N	2:C:474:GLN:OE1	2.28	0.65
1:B:280:ILE:HG23	1:B:284:PHE:HD2	1.62	0.65
1:A:228:VAL:O	1:A:252:LYS:NZ	2.25	0.65
1:A:162:LEU:O	1:A:166[A]:THR:HG23	1.96	0.64
1:B:303:ILE:O	1:B:306:GLU:OE1	2.14	0.64
1:B:430:CYS:O	1:B:434:THR:HG23	1.97	0.64
1:D:450:CYS:H	6:D:1503:GOL:C3	2.08	0.64
1:B:303:ILE:CA	1:B:306:GLU:OE1	2.45	0.64
1:D:450:CYS:H	6:D:1503:GOL:H32	1.62	0.64
1:B:273:ASP:OD1	1:B:310:LYS:CD	2.45	0.64
1:A:279:THR:HG21	1:A:307:PHE:HZ	1.63	0.63
2:C:455:PRO:O	1:D:481:GLN:NE2	2.31	0.63
2:C:81:LYS:HZ3	2:C:200:GLU:CB	2.02	0.63
1:A:431:GLU:HG3	3:B:1498:IOD:I	2.69	0.63
1:D:362:ARG:NH2	1:D:369:GLY:O	2.32	0.62
1:B:270:VAL:HB	1:B:275:VAL:HG21	1.80	0.62
1:D:380:ILE:HG13	1:D:397[B]:CYS:HB2	1.82	0.62
1:B:365:HIS:C	1:B:366:LEU:HD12	2.23	0.62
2:C:496:SER:O	8:C:2163:HOH:O	2.16	0.62
2:C:228:VAL:O	2:C:252:LYS:HE3	2.00	0.62
1:B:273:ASP:OD1	1:B:310:LYS:HD2	2.00	0.62
1:D:304:ALA:O	1:D:308:VAL:HG12	2.00	0.61
1:B:303:ILE:HA	1:B:306:GLU:CD	2.26	0.61
1:A:269:ASP:O	1:A:425:ASN:ND2	2.29	0.60
1:B:365:HIS:CD2	1:B:366:LEU:HD11	2.36	0.60
1:B:291[B]:CSO:SG	4:B:1501:CHT:H82	2.42	0.60
1:B:303:ILE:HA	1:B:306:GLU:OE1	2.02	0.60
2:C:298:LEU:HD21	2:C:387:TRP:HH2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LYS:HB2	1:B:310:LYS:NZ	2.17	0.59
1:A:268:GLU:OE1	1:A:268:GLU:N	2.34	0.59
2:C:404:GLU:OE2	2:C:432:ARG:NH2	2.35	0.59
2:C:234:THR:HG23	2:C:257[B]:GLU:HG3	1.85	0.59
1:A:158:TRP:CD1	1:A:184:SER:HG	2.21	0.59
1:B:5:ILE:HD11	1:B:37:GLY:HA3	1.83	0.59
1:A:63:TRP:O	1:A:66:THR:HG22	2.03	0.58
1:A:273:ASP:OD1	1:A:310:LYS:HE2	2.03	0.58
1:A:320:ILE:HG12	1:A:330:LEU:HD23	1.86	0.58
2:C:160:TYR:HB2	2:C:164:MET:HG2	1.86	0.57
1:A:301:GLU:HA	1:A:304:ALA:HB2	1.87	0.57
1:D:343:MET:HE2	1:D:372:ILE:HG12	1.85	0.57
2:C:5:ILE:HD11	2:C:95:ILE:HG21	1.87	0.57
1:B:58:PHE:CE2	1:B:150:GLY:HA2	2.40	0.57
1:D:320:ILE:HD11	1:D:374:PRO:HD3	1.86	0.57
2:C:146[A]:ARG:NH1	8:C:2058:HOH:O	2.38	0.57
1:D:260:GLY:HA2	1:D:416:TYR:CD1	2.39	0.57
1:B:336:LYS:CG	1:B:370:TYR:OH	2.53	0.56
2:C:430:CYS:O	2:C:434:THR:HG23	2.06	0.56
1:A:51:VAL:HG21	1:A:225:HIS:NE2	2.21	0.56
2:C:158:TRP:CH2	2:C:392:PHE:CE2	2.93	0.56
1:A:474:GLN:HG2	3:A:1501:IOD:I	2.75	0.56
2:C:158:TRP:CH2	2:C:392:PHE:HE2	2.23	0.55
2:C:273:ASP:OD1	2:C:314:TRP:NE1	2.39	0.55
1:D:460:LYS:N	5:D:1502:PG4:H22	2.20	0.55
1:B:225:HIS:O	1:B:252:LYS:NZ	2.39	0.55
2:C:20:ILE:HD12	2:C:45:GLU:HB3	1.86	0.55
1:B:160:TYR:HB2	1:B:164:MET:HG2	1.89	0.55
1:A:158:TRP:HD1	1:A:184:SER:HG	1.53	0.55
1:B:268:GLU:HA	1:B:303:ILE:HD13	1.89	0.55
1:D:291[A]:CSO:SG	4:D:1501:CHT:H62	2.46	0.55
1:B:135:LEU:HD11	1:B:142:SER:HB2	1.89	0.55
1:B:303:ILE:HA	1:B:306:GLU:OE2	2.06	0.55
2:C:146[A]:ARG:HD3	3:C:1499:IOD:I	2.77	0.55
1:A:167:TRP:HH2	4:A:1502:CHT:HC52	1.71	0.54
2:C:260:GLY:HA2	2:C:416:TYR:CD1	2.43	0.54
2:C:63:TRP:O	2:C:66[A]:THR:HG22	2.07	0.54
2:C:290:ILE:HB	2:C:293:ALA:HB2	1.88	0.54
1:D:142:SER:OG	1:D:483:THR:HG22	2.07	0.54
1:D:160:TYR:OH	4:D:1501:CHT:H81	2.07	0.54
1:D:296:ARG:NH2	1:D:410:LEU:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:474:GLN:CD	3:C:1499:IOD:I	3.21	0.54
1:B:447:SER:C	1:B:449[B]:PRO:HD3	2.32	0.54
2:C:25[B]:ILE:HD13	2:C:41:ALA:HB2	1.90	0.54
1:D:309:ASP:C	1:D:309:ASP:OD1	2.50	0.54
1:D:330:LEU:HD22	1:D:374:PRO:HG3	1.90	0.54
1:A:274:LYS:HG2	1:B:490:PRO:HA	1.90	0.54
1:B:319:LYS:HG2	1:B:321:SER:OG	2.08	0.54
2:C:271:ASP:CG	2:C:274:LYS:HG2	2.34	0.53
2:C:99:LYS:NZ	2:C:107:ASP:OD2	2.40	0.53
2:C:253:PRO:HD3	5:D:1502:PG4:C1	2.39	0.53
1:D:139:ARG:HG3	1:D:487:SER:HB3	1.91	0.53
1:A:146:ARG:NH2	8:A:2076:HOH:O	2.40	0.53
1:A:275:VAL:O	1:A:279:THR:HG23	2.08	0.53
1:B:273:ASP:OD1	1:B:310:LYS:HE2	2.08	0.53
1:A:5:ILE:HG12	1:A:6:PRO:N	2.23	0.53
1:B:336:LYS:HD2	1:B:370:TYR:HE1	0.38	0.53
2:C:146[A]:ARG:HG2	2:C:477:LEU:HD13	1.90	0.53
1:B:290:ILE:HB	1:B:293:ALA:HB2	1.91	0.52
2:C:81:LYS:HD2	2:C:201:VAL:CG1	2.39	0.52
1:A:17:ARG:NH2	8:A:2008:HOH:O	2.42	0.52
1:B:63:TRP:O	1:B:66:THR:HG22	2.10	0.52
2:C:157:PRO:HD2	2:C:164:MET:HB3	1.92	0.52
1:A:268:GLU:OE1	1:A:300:HIS:CG	2.63	0.51
1:B:298:LEU:HD21	1:B:387:TRP:HH2	1.75	0.51
1:B:365:HIS:CG	1:B:366:LEU:HD12	2.45	0.51
1:A:256:LEU:HB3	1:A:258:LEU:HD21	1.92	0.51
1:D:328:CYS:O	1:D:329:ARG:NH1	2.44	0.51
1:B:337:GLY:C	1:B:341:LYS:HE2	2.32	0.51
1:B:363:PRO:HG2	1:B:371:TYR:HB3	1.92	0.50
1:D:136:PRO:HG2	1:D:137:MET:H	1.77	0.50
1:D:291[A]:CSO:OD	4:D:1501:CHT:H61	2.10	0.50
4:B:1501:CHT:O6	4:B:1501:CHT:H62	2.10	0.50
1:B:143:HIS:CE1	3:B:1498:IOD:I	3.35	0.50
1:B:342:ILE:HD13	1:B:393:GLY:HA3	1.94	0.49
2:C:8:ARG:HH12	2:C:196[A]:GLU:HB2	1.76	0.49
1:D:160:TYR:CZ	4:D:1501:CHT:H81	2.46	0.49
2:C:339:TYR:OH	2:C:362:ARG:NH1	2.46	0.49
1:D:228:VAL:O	1:D:252:LYS:HE2	2.11	0.49
1:D:488:ASP:OD1	1:D:488:ASP:O	2.30	0.49
1:B:273:ASP:OD1	1:B:310:LYS:CE	2.60	0.49
1:B:345:PHE:HD2	1:B:391:VAL:HG13	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:TYR:CD1	1:B:359:GLY:N	2.81	0.49
2:C:27:VAL:HG13	2:C:38:ASP:N	2.28	0.49
2:C:487:SER:HB2	2:C:489:GLU:HG3	1.94	0.49
1:D:251[A]:VAL:HG12	1:D:251[A]:VAL:O	2.13	0.49
1:B:139[B]:ARG:HG3	1:B:487:SER:HB3	1.93	0.49
1:A:377:VAL:HG12	1:A:380:ILE:HD11	1.95	0.49
2:C:9:GLN:OE1	2:C:18:GLU:HG3	2.12	0.49
1:A:359:GLY:HA2	1:A:373:GLU:OE1	2.13	0.49
2:C:320:ILE:HD13	2:C:363:PRO:HG2	1.94	0.49
2:C:450:CSO:OD	8:C:2142:HOH:O	2.18	0.49
1:B:364:GLU:OE2	8:B:2107:HOH:O	2.20	0.49
1:D:291[A]:CSO:OD	4:D:1501:CHT:C6	2.61	0.49
1:B:43:THR:OG1	1:B:45:GLU:OE1	2.28	0.49
1:B:309:ASP:O	1:B:312:VAL:HG22	2.13	0.49
1:B:70:HIS:HE1	8:B:2021:HOH:O	1.95	0.48
1:D:130:LYS:NZ	3:D:1498:IOD:I	3.16	0.48
1:D:223[B]:VAL:O	1:D:252:LYS:NZ	2.38	0.48
1:D:460:LYS:H	5:D:1502:PG4:H22	1.77	0.48
1:A:438:GLU:C	1:A:459:ILE:HD11	2.37	0.48
1:B:307:PHE:O	1:B:311:LEU:HB2	2.13	0.48
1:B:471:TRP:O	1:B:474:GLN:HG3	2.13	0.48
1:B:139[A]:ARG:HG3	1:B:487:SER:HB3	1.95	0.48
2:C:54:ALA:HA	2:C:206:GLY:O	2.13	0.48
2:C:139:ARG:HG3	2:C:487:SER:HB3	1.95	0.48
2:C:404:GLU:OE1	2:C:432:ARG:NH1	2.46	0.48
1:D:139:ARG:NH2	1:D:489:GLU:O	2.46	0.48
2:C:185:GLU:HB3	2:C:213:GLY:O	2.13	0.48
1:A:160:TYR:CZ	4:A:1502:CHT:H71	2.48	0.48
2:C:265:VAL:HG22	2:C:422:VAL:HG23	1.94	0.48
2:C:135:LEU:HD11	2:C:142:SER:HB2	1.96	0.48
2:C:320:ILE:HD11	2:C:371:TYR:HD1	1.79	0.48
1:A:115:PHE:CZ	1:A:166[B]:THR:HG23	2.47	0.47
1:B:143:HIS:HE1	3:B:1498:IOD:I	2.67	0.47
1:B:247:ALA:HB1	1:B:252:LYS:HG3	1.96	0.47
1:A:76:ARG:HH12	1:A:123:GLU:CD	2.22	0.47
1:A:234:THR:HG23	1:A:257[A]:GLU:HB3	1.96	0.47
1:A:167:TRP:CH2	4:A:1502:CHT:HC52	2.49	0.47
1:D:275:VAL:HG22	1:D:423:PHE:CD2	2.49	0.47
1:B:448:GLN:N	1:B:449[B]:PRO:HD3	2.30	0.47
1:A:252:LYS:HB2	1:A:252:LYS:HE2	1.76	0.47
5:D:1502:PG4:H51	5:D:1502:PG4:H72	1.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:LEU:HD11	5:D:1502:PG4:H32	1.95	0.47
1:B:310:LYS:HB2	1:B:310:LYS:HZ2	1.79	0.47
2:C:283:CYS:O	2:C:288:GLY:HA2	2.15	0.47
1:D:139:ARG:HH22	1:D:490:PRO:C	2.23	0.47
1:D:362:ARG:NH1	1:D:366:LEU:O	2.46	0.47
2:C:423:PHE:CD2	2:C:445:ASN:HA	2.49	0.47
1:D:95:ILE:HG12	1:D:324:PHE:HZ	1.80	0.47
1:A:274:LYS:HE2	1:B:490:PRO:HD3	1.96	0.47
2:C:43:THR:HG23	2:C:45:GLU:H	1.80	0.47
2:C:81:LYS:NZ	2:C:200:GLU:CA	2.77	0.47
1:D:130:LYS:HG3	1:D:145:LEU:HD21	1.97	0.47
1:A:182:LYS:HE2	1:A:213:GLY:O	2.15	0.46
1:B:296:ARG:HD2	1:B:387:TRP:CE3	2.50	0.46
1:B:312:VAL:HG12	1:B:376:ILE:HD13	1.97	0.46
1:A:21:LYS:NZ	3:A:1500:IOD:I	3.17	0.46
1:B:291[A]:CSO:SG	4:B:1501:CHT:H82	2.55	0.46
1:B:448:GLN:N	1:B:449[B]:PRO:CD	2.78	0.46
1:D:58:PHE:CE1	1:D:150:GLY:HA2	2.51	0.46
1:B:337:GLY:O	1:B:341:LYS:HG2	2.16	0.46
1:B:338:GLN:O	1:B:342:ILE:HG13	2.16	0.46
1:D:135:LEU:HD11	1:D:142:SER:HB2	1.98	0.46
1:B:336:LYS:HG2	1:B:370:TYR:CE1	2.30	0.46
2:C:225:HIS:HB3	2:C:228:VAL:HG23	1.97	0.46
1:D:260:GLY:HA2	1:D:416:TYR:CG	2.50	0.46
1:A:362:ARG:NH1	1:A:369:GLY:O	2.42	0.46
1:B:24:ARG:HD3	1:B:38:ASP:OD2	2.14	0.46
2:C:308:VAL:HA	2:C:311:LEU:HB3	1.98	0.46
1:D:271:ASP:HB3	1:D:274:LYS:HD2	1.98	0.46
1:B:429:ARG:O	1:B:433:ILE:HG12	2.16	0.46
2:C:447:SER:C	2:C:449:PRO:HD3	2.40	0.46
1:D:466:ARG:NH2	5:D:1502:PG4:H62	2.31	0.46
1:B:320:ILE:HG12	1:B:330:LEU:HD23	1.96	0.46
2:C:343:MET:HE2	2:C:372:ILE:HG12	1.98	0.46
1:A:488:ASP:OD1	1:A:488:ASP:O	2.34	0.45
1:B:336:LYS:HG2	1:B:370:TYR:OH	2.10	0.45
1:D:443:TRP:CZ2	1:D:448:GLN:HA	2.51	0.45
1:B:146[B]:ARG:NH1	3:B:1499:IOD:I	3.18	0.45
1:B:9:GLN:HB3	1:B:17:ARG:O	2.16	0.45
1:B:99:LYS:HB2	1:B:103:GLU:OE1	2.16	0.45
1:B:474:GLN:HA	1:B:477:LEU:HD12	1.98	0.45
2:C:149:LEU:HD11	5:D:1502:PG4:C3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:PRO:HG3	1:D:471:TRP:CZ3	2.51	0.45
8:C:2153:HOH:O	5:D:1502:PG4:H81	2.16	0.45
1:B:341:LYS:N	1:B:341:LYS:HD3	2.32	0.45
1:B:365:HIS:CD2	1:B:366:LEU:HD12	2.51	0.45
1:D:5:ILE:HD13	1:D:92:LEU:HD22	1.98	0.45
1:D:76:ARG:NH1	1:D:123:GLU:OE2	2.32	0.45
1:A:260:GLY:HA2	1:A:416:TYR:CG	2.52	0.45
1:A:381:SER:H	1:A:384:MET:HE3	1.81	0.45
4:D:1501:CHT:H82	4:D:1501:CHT:O6	2.17	0.45
1:A:306:GLU:O	1:A:309:ASP:HB3	2.17	0.44
1:B:108:ILE:HA	1:B:111:VAL:HG13	1.99	0.44
1:D:261:LYS:HG3	1:D:296:ARG:CD	2.48	0.44
2:C:260:GLY:HA2	2:C:416:TYR:CG	2.52	0.44
1:D:471:TRP:O	1:D:474:GLN:HG3	2.17	0.44
1:A:93:GLU:OE1	1:A:93:GLU:HA	2.18	0.44
1:A:429:ARG:O	1:A:433:ILE:HG12	2.18	0.44
2:C:59:ARG:NH2	8:C:2017:HOH:O	2.49	0.44
1:B:291[B]:CSO:HB2	8:B:2089:HOH:O	2.16	0.44
1:B:297:LEU:HD23	1:B:398:VAL:HG13	1.99	0.44
1:A:188:SER:HB3	1:A:212:THR:HG21	1.99	0.44
1:B:139[B]:ARG:NH2	1:B:489:GLU:O	2.51	0.44
1:B:406:GLU:O	1:B:410:LEU:HD13	2.18	0.44
1:D:95:ILE:HG12	1:D:324:PHE:CZ	2.52	0.44
1:D:377:VAL:HG12	1:D:380:ILE:HD11	1.99	0.44
1:B:308:VAL:O	1:B:312:VAL:HG13	2.18	0.43
1:B:365:HIS:CG	1:B:366:LEU:CD1	3.00	0.43
1:D:484:GLN:HG2	1:D:486:ILE:HG23	2.00	0.43
2:C:115:PHE:CE2	2:C:166:THR:HG23	2.53	0.43
1:D:252:LYS:HB2	1:D:252:LYS:HE3	1.78	0.43
1:B:5:ILE:HD12	1:B:6:PRO:O	2.18	0.43
1:D:264:ILE:HG23	1:D:297:LEU:HA	2.00	0.43
1:A:48:GLU:O	1:A:52:VAL:HG23	2.19	0.43
1:A:128:LYS:NZ	8:A:2067:HOH:O	2.36	0.43
1:B:291[A]:CSO:HB2	8:B:2089:HOH:O	2.18	0.43
2:C:27:VAL:HG12	2:C:39:ILE:HG12	1.99	0.43
1:B:45:GLU:O	1:B:49:VAL:HG13	2.18	0.43
1:B:296:ARG:NH1	1:B:414[B]:THR:HG21	2.34	0.43
1:A:229:ASP:O	1:A:253:PRO:HD2	2.19	0.43
1:B:86:LYS:HB3	1:B:86:LYS:HE2	1.83	0.43
2:C:33:GLU:HG3	2:C:369:GLY:HA2	1.99	0.43
4:A:1502:CHT:O6	4:A:1502:CHT:H73	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLU:OE1	1:B:336:LYS:NZ	2.46	0.43
1:B:41:ALA:HA	1:B:213:GLY:HA2	2.00	0.42
1:B:322:ASP:HA	1:B:371:TYR:OH	2.19	0.42
2:C:3:PHE:HE2	2:C:92:LEU:HD21	1.84	0.42
1:D:35:ILE:HD12	1:D:35:ILE:H	1.84	0.42
1:D:290:ILE:HB	1:D:293:ALA:HB2	2.00	0.42
1:A:58:PHE:CE1	1:A:150:GLY:HA2	2.55	0.42
1:B:99:LYS:HD3	1:B:103:GLU:HB3	2.01	0.42
1:A:419:ALA:HA	1:A:439:VAL:HG13	2.00	0.42
1:B:9:GLN:OE1	1:B:18:GLU:HA	2.19	0.42
1:B:154:LEU:HD22	1:B:168:LYS:HB3	2.02	0.42
1:A:131:ALA:HA	1:A:132:PRO:HD3	1.85	0.42
1:A:361:SER:HB2	8:A:2148:HOH:O	2.20	0.42
1:B:5:ILE:HG12	1:B:36:ILE:O	2.19	0.42
1:B:336:LYS:HA	1:B:339:TYR:HB3	2.00	0.42
1:A:204:PRO:HA	1:A:205:PRO:HD3	1.88	0.42
2:C:261:LYS:HE3	2:C:296:ARG:HG3	2.01	0.42
1:B:493:TRP:HD1	1:B:494:TYR:CE1	2.38	0.42
2:C:118:PHE:CE1	2:C:171:PRO:HB3	2.55	0.42
2:C:440:GLY:HA3	2:C:457:GLY:O	2.20	0.42
1:A:47:VAL:HG21	1:A:221:PRO:HB2	2.01	0.42
1:A:157:PRO:HB2	8:A:2083:HOH:O	2.20	0.42
1:A:274:LYS:NZ	1:B:488:ASP:O	2.35	0.42
1:A:488:ASP:OD1	1:A:488:ASP:C	2.60	0.42
1:B:386:ILE:HG23	1:B:397:CYS:SG	2.60	0.42
2:C:51:VAL:HG21	2:C:225:HIS:NE2	2.35	0.42
1:A:244:MET:HE1	1:B:252:LYS:O	2.19	0.42
1:A:354:ALA:HB2	1:A:384:MET:SD	2.59	0.42
1:A:470:GLU:OE1	8:A:2182:HOH:O	2.21	0.42
1:B:280:ILE:HG23	1:B:284:PHE:CD2	2.50	0.42
1:D:280:ILE:HG23	1:D:284:PHE:HD2	1.85	0.42
1:D:466:ARG:CG	5:D:1502:PG4:H71	2.46	0.42
4:B:1501:CHT:H73	4:B:1501:CHT:HC41	1.83	0.41
1:B:367:LYS:HE3	1:B:367:LYS:HB3	1.69	0.41
2:C:280:ILE:HG21	2:C:318:ILE:HD11	2.02	0.41
1:B:264:ILE:HG23	1:B:297:LEU:HA	2.03	0.41
2:C:51:VAL:HG21	2:C:225:HIS:CE1	2.55	0.41
2:C:415:GLU:HB3	2:C:461:ARG:HG3	2.02	0.41
1:B:329:ARG:HD3	1:B:329:ARG:HA	1.90	0.41
2:C:304:ALA:O	2:C:308:VAL:HG12	2.20	0.41
1:A:352:GLU:O	8:A:2146:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:SER:C	1:B:449[A]:PRO:HD3	2.45	0.41
2:C:154:LEU:HD13	2:C:168:LYS:HB3	2.02	0.41
1:D:276:VAL:O	1:D:280:ILE:HG12	2.21	0.41
1:A:281:PHE:O	1:A:285:TRP:HB3	2.21	0.41
1:B:281:PHE:O	1:B:285:TRP:HB3	2.19	0.41
3:C:1498:IOD:I	1:D:431:GLU:HG3	2.90	0.41
1:D:130:LYS:HG2	1:D:143:HIS:CE1	2.56	0.41
1:B:29:ASN:HB2	1:B:36:ILE:HD13	2.03	0.41
1:A:139:ARG:HG3	1:A:487:SER:HB3	2.03	0.41
1:B:188:SER:HB3	1:B:212:THR:HG21	2.01	0.41
1:B:399:LYS:HE3	1:B:399:LYS:HB3	1.93	0.41
2:C:256:LEU:HB3	2:C:258:LEU:HD21	2.03	0.41
1:A:76:ARG:NH1	1:A:123:GLU:OE2	2.47	0.41
1:A:158:TRP:HD1	1:A:184:SER:OG	2.02	0.41
1:B:305:ALA:HA	1:B:308:VAL:HG22	2.02	0.41
1:B:414[B]:THR:HG22	8:B:2112:HOH:O	2.19	0.41
2:C:122:ALA:O	2:C:125:LEU:HB3	2.20	0.41
2:C:258:LEU:CD1	1:D:251[A]:VAL:HG11	2.51	0.41
2:C:453:GLN:NE2	8:C:2044:HOH:O	2.37	0.41
1:D:281:PHE:O	1:D:285:TRP:HB3	2.21	0.41
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.91	0.41
2:C:257[B]:GLU:CD	2:C:257[B]:GLU:C	2.88	0.41
1:A:146:ARG:HB3	1:A:477:LEU:HD13	2.02	0.40
1:A:230:LYS:HE3	1:A:253:PRO:HB2	2.03	0.40
1:B:273:ASP:CG	1:B:310:LYS:HE2	2.46	0.40
1:A:29:ASN:HA	1:A:30:PRO:HD2	1.91	0.40
1:A:51:VAL:HG21	1:A:225:HIS:CD2	2.56	0.40
1:A:260:GLY:HA2	1:A:416:TYR:CD1	2.56	0.40
1:D:169:ILE:HD11	1:D:181:LEU:HD22	2.04	0.40
1:A:310:LYS:HA	1:A:313:LYS:HB2	2.02	0.40
2:C:14:GLY:O	2:C:199:ASN:ND2	2.44	0.40
1:D:486:ILE:H	1:D:486:ILE:HG13	1.58	0.40
1:A:362:ARG:HA	1:A:363:PRO:HD3	1.97	0.40
1:B:185:GLU:HG2	1:B:186:LEU:N	2.36	0.40
2:C:193:GLU:O	2:C:196[B]:GLU:HB3	2.21	0.40
2:C:252:LYS:O	1:D:244:MET:HE1	2.21	0.40

There are no symmetry-related clashes.

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	498/498 (100%)	478 (96%)	19 (4%)	1 (0%)	43	42
1	B	501/498 (101%)	470 (94%)	30 (6%)	1 (0%)	43	42
1	D	498/498 (100%)	478 (96%)	16 (3%)	4 (1%)	16	11
2	C	498/497 (100%)	466 (94%)	29 (6%)	3 (1%)	21	17
All	All	1995/1991 (100%)	1892 (95%)	94 (5%)	9 (0%)	30	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	GLN
1	B	448	GLN
2	C	448	GLN
1	D	448	GLN
1	D	136	PRO
2	C	4	PRO
2	C	417	GLY
1	D	251[A]	VAL
1	D	251[B]	VAL

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%)	402 (97%)	12 (3%)	37	40
1	B	418/410 (102%)	399 (96%)	19 (4%)	24	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	414/410 (101%)	397 (96%)	17 (4%)	27	26
2	C	413/408 (101%)	400 (97%)	13 (3%)	35	37
All	All	1659/1638 (101%)	1598 (96%)	61 (4%)	32	30

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	49	VAL
1	A	141	LYS
1	A	257[A]	GLU
1	A	257[B]	GLU
1	A	268	GLU
1	A	313	LYS
1	A	325	GLU
1	A	428	GLU
1	A	439	VAL
1	A	473	ILE
1	A	495	LYS
1	B	8[A]	ARG
1	B	8[B]	ARG
1	B	49	VAL
1	B	111	VAL
1	B	185	GLU
1	B	196	GLU
1	B	254	VAL
1	B	257	GLU
1	B	272	ILE
1	B	306	GLU
1	B	309	ASP
1	B	310	LYS
1	B	321	SER
1	B	336	LYS
1	B	341	LYS
1	B	344	LYS
1	B	367	LYS
1	B	403	SER
1	B	439	VAL
2	C	5	ILE
2	C	27	VAL
2	C	60[A]	ARG

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Mol	Chain	Res	Type
2	C	60[B]	ARG
2	C	182	LYS
2	C	243	VAL
2	C	257[A]	GLU
2	C	257[B]	GLU
2	C	265	VAL
2	C	313	LYS
2	C	383	SER
2	C	427	LEU
2	C	474	GLN
1	D	15	GLU
1	D	34	GLU
1	D	106	LEU
1	D	138	GLU
1	D	223[A]	VAL
1	D	223[B]	VAL
1	D	243	VAL
1	D	254	VAL
1	D	257	GLU
1	D	308	VAL
1	D	313	LYS
1	D	350	LYS
1	D	367	LYS
1	D	368	LYS
1	D	392	PHE
1	D	439	VAL
1	D	486	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	385	GLN
1	B	143	HIS
2	C	481	GLN
1	D	70	HIS
1	D	338	GLN
1	D	385	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z > 2$
1	CSO	D	291[A]	1	3,6,7	0.71	0	1,6,8	0.02	0
2	CSO	C	450	2	3,6,7	0.66	0	1,6,8	1.27	0
2	CSO	C	291	2	3,6,7	0.72	0	1,6,8	0.67	0
1	CSO	B	291[B]	1	3,6,7	0.66	0	1,6,8	0.28	0
1	CSO	B	291[A]	1	3,6,7	0.66	0	1,6,8	0.27	0
1	CSO	A	291[A]	1	3,6,7	0.71	0	1,6,8	0.22	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
1	CSO	D	291[A]	1	-	1/1/5/7	-
2	CSO	C	450	2	-	0/1/5/7	-
2	CSO	C	291	2	-	0/1/5/7	-
1	CSO	B	291[B]	1	-	1/1/5/7	-
1	CSO	B	291[A]	1	-	0/1/5/7	-
1	CSO	A	291[A]	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	291[B]	CSO	N-CA-CB-SG
1	A	291[A]	CSO	N-CA-CB-SG
1	D	291[A]	CSO	N-CA-CB-SG

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	291[A]	CSO	3	0
2	C	450	CSO	1	0
2	C	291	CSO	1	0
1	B	291[B]	CSO	2	0
1	B	291[A]	CSO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 15 are monoatomic - leaving 9 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	D	1501	1	6,6,6	2.01	1 (16%)	8,8,8	1.29	1 (12%)
6	GOL	D	1503	-	5,5,5	0.26	0	5,5,5	0.31	0
5	PG4	D	1502	-	11,11,12	0.76	0	10,10,11	0.60	0
4	CHT	A	1502	1	6,6,6	2.24	3 (50%)	8,8,8	1.75	1 (12%)
6	GOL	B	1502	-	5,5,5	0.46	0	5,5,5	0.59	0
5	PG4	A	1503	-	11,11,12	0.74	0	10,10,11	0.41	0
7	ETX	C	1501	-	5,5,5	0.36	0	4,4,4	0.41	0
4	CHT	B	1501	1	6,6,6	2.05	1 (16%)	8,8,8	1.16	1 (12%)
5	PG4	C	1500	-	11,11,12	0.74	0	10,10,11	0.41	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	D	1501	1	-	0/4/4/4	-
6	GOL	D	1503	-	-	0/4/4/4	-
5	PG4	D	1502	-	-	6/9/9/10	-
4	CHT	A	1502	1	-	1/4/4/4	-
6	GOL	B	1502	-	-	2/4/4/4	-
5	PG4	A	1503	-	-	7/9/9/10	-
7	ETX	C	1501	-	-	1/3/3/3	-
4	CHT	B	1501	1	-	0/4/4/4	-
5	PG4	C	1500	-	-	3/9/9/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1502	CHT	O6-C4	-3.97	1.21	1.42
4	B	1501	CHT	O6-C4	-3.96	1.21	1.42
4	D	1501	CHT	O6-C4	-3.71	1.23	1.42
4	A	1502	CHT	C8-N1	-2.26	1.43	1.50
4	A	1502	CHT	C7-N1	-2.15	1.43	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1502	CHT	C8-N1-C5	3.18	122.55	109.91
4	D	1501	CHT	C8-N1-C5	2.32	119.12	109.91
4	B	1501	CHT	C8-N1-C5	2.14	118.43	109.91

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1502	GOL	O1-C1-C2-O2
5	D	1502	PG4	C5-C6-O4-C7
6	B	1502	GOL	O1-C1-C2-C3
5	C	1500	PG4	O3-C5-C6-O4
4	A	1502	CHT	O6-C4-C5-N1
5	C	1500	PG4	O4-C7-C8-O5
5	D	1502	PG4	C8-C7-O4-C6

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Mol	Chain	Res	Type	Atoms
7	C	1501	ETX	C1-C2-O2-C3
5	D	1502	PG4	C6-C5-O3-C4
5	A	1503	PG4	O4-C7-C8-O5
5	D	1502	PG4	O4-C7-C8-O5
5	C	1500	PG4	C8-C7-O4-C6
5	A	1503	PG4	C5-C6-O4-C7
5	A	1503	PG4	C8-C7-O4-C6
5	A	1503	PG4	C1-C2-O2-C3
5	A	1503	PG4	C4-C3-O2-C2
5	A	1503	PG4	O2-C3-C4-O3
5	D	1502	PG4	O3-C5-C6-O4
5	A	1503	PG4	O3-C5-C6-O4
5	D	1502	PG4	C4-C3-O2-C2

There are no ring outliers.

5 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1501	CHT	6	0
6	D	1503	GOL	3	0
5	D	1502	PG4	10	0
4	A	1502	CHT	4	0
4	B	1501	CHT	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	494/498 (99%)	0.07	8 (1%) 70 70	11, 34, 63, 103	6 (1%)
1	B	493/498 (98%)	0.29	17 (3%) 48 47	14, 40, 69, 84	10 (2%)
1	D	494/498 (99%)	0.05	13 (2%) 57 56	10, 31, 57, 108	6 (1%)
2	C	493/497 (99%)	0.64	28 (5%) 29 28	18, 41, 59, 105	7 (1%)
All	All	1974/1991 (99%)	0.26	66 (3%) 49 48	10, 37, 65, 108	29 (1%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	3	PHE	5.2
1	A	3	PHE	4.3
2	C	497	PRO	4.1
1	D	3	PHE	3.9
1	A	497	PRO	3.8
1	D	497	PRO	3.7
1	D	138	GLU	3.6
1	A	5	ILE	3.6
2	C	427	LEU	3.5
1	D	4	PRO	3.3
2	C	312	VAL	3.2
1	D	136	PRO	3.0
1	B	321	SER	3.0
1	D	496	SER	2.9
1	B	366	LEU	2.9
2	C	305	ALA	2.9
1	B	336	LYS	2.9
1	D	493	TRP	2.8
1	B	4	PRO	2.8
1	B	358	TYR	2.6
2	C	410	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	491	TRP	2.6
1	D	488	ASP	2.5
2	C	189	VAL	2.5
2	C	4	PRO	2.5
1	B	310	LYS	2.5
1	B	327	GLY	2.5
2	C	308	VAL	2.4
1	B	305	ALA	2.4
2	C	369	GLY	2.4
2	C	273	ASP	2.4
1	D	5	ILE	2.4
1	B	311	LEU	2.3
2	C	60[A]	ARG	2.3
1	A	349	ALA	2.3
2	C	320	ILE	2.3
2	C	90	VAL	2.3
2	C	387	TRP	2.3
1	B	497	PRO	2.3
2	C	290	ILE	2.3
1	B	353	GLY	2.2
1	D	494	TYR	2.2
1	B	28	ILE	2.2
2	C	449	PRO	2.2
2	C	324	PHE	2.2
1	A	362	ARG	2.2
1	B	189	VAL	2.2
2	C	50	ALA	2.2
2	C	392	PHE	2.1
2	C	66[A]	THR	2.1
2	C	34	GLU	2.1
2	C	62	ASN	2.1
1	A	402	SER	2.1
2	C	276	VAL	2.1
2	C	69	ALA	2.1
1	B	378	THR	2.1
1	B	314	TRP	2.1
1	D	365	HIS	2.1
1	B	317	ASN	2.1
2	C	275	VAL	2.1
2	C	443	TRP	2.1
1	D	495	LYS	2.0
1	A	327	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	355	THR	2.0
1	B	461[A]	ARG	2.0
2	C	201	VAL	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
2	CSO	C	450	7/8	0.82	0.12	44,54,57,71	0
2	CSO	C	291	7/8	0.88	0.10	31,37,53,59	0
1	CSO	B	291[A]	7/8	0.89	0.12	30,30,36,37	7
1	CSO	B	291[B]	7/8	0.89	0.12	30,30,36,37	7
1	CSO	A	291[A]	7/8	0.94	0.08	16,21,34,35	7
1	CSO	D	291[A]	7/8	0.95	0.06	20,22,30,33	7

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
6	GOL	D	1503	6/6	0.74	0.16	48,59,61,63	0
7	ETX	C	1501	6/6	0.76	0.17	54,59,69,73	0
6	GOL	B	1502	6/6	0.77	0.17	49,55,56,63	0
4	CHT	A	1502	7/7	0.84	0.13	20,25,33,36	7
4	CHT	D	1501	7/7	0.86	0.14	22,24,31,31	7
5	PG4	D	1502	12/13	0.87	0.11	16,30,43,46	0
4	CHT	B	1501	7/7	0.87	0.14	27,32,36,37	7
5	PG4	A	1503	12/13	0.89	0.11	19,35,41,49	0
5	PG4	C	1500	12/13	0.92	0.10	26,40,53,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IOD	A	1500	1/1	0.94	0.07	43,43,43,43	1
3	IOD	A	1498	1/1	0.94	0.07	49,49,49,49	1
3	IOD	B	1499	1/1	0.95	0.06	39,39,39,39	1
3	IOD	D	1500	1/1	0.96	0.05	37,37,37,37	1
3	IOD	B	1500	1/1	0.97	0.05	53,53,53,53	1
3	IOD	D	1498	1/1	0.97	0.05	42,42,42,42	1
3	IOD	B	502	1/1	0.97	0.05	46,46,46,46	1
3	IOD	A	1499	1/1	0.97	0.04	42,42,42,42	1
3	IOD	C	1499	1/1	0.98	0.04	44,44,44,44	1
3	IOD	B	1498	1/1	0.98	0.04	38,38,38,38	1
3	IOD	A	1501	1/1	0.98	0.04	41,41,41,41	1
3	IOD	A	501	1/1	0.98	0.04	41,41,41,41	1
3	IOD	C	1498	1/1	0.99	0.03	41,41,41,41	1
3	IOD	D	1499	1/1	0.99	0.03	43,43,43,43	1
3	IOD	C	503	1/1	0.99	0.03	42,42,42,42	1

6.5 Other polymers

There are no such residues in this entry.