



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:11 PM EDT

PDB ID : 4BC0 / pdb_00004bc0
Title : Structure of mouse acetylcholinesterase inhibited by CBDP (12-h soak) : Cresyl-phosphoserine adduct
Authors : Carletti, E.; Colletier, J.-P.; Schopfer, L.M.; Santoni, G.; Masson, P.; Lockridge, O.; Nachon, F.; Weik, M.
Deposited on : 2012-09-30
Resolution : 3.35 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

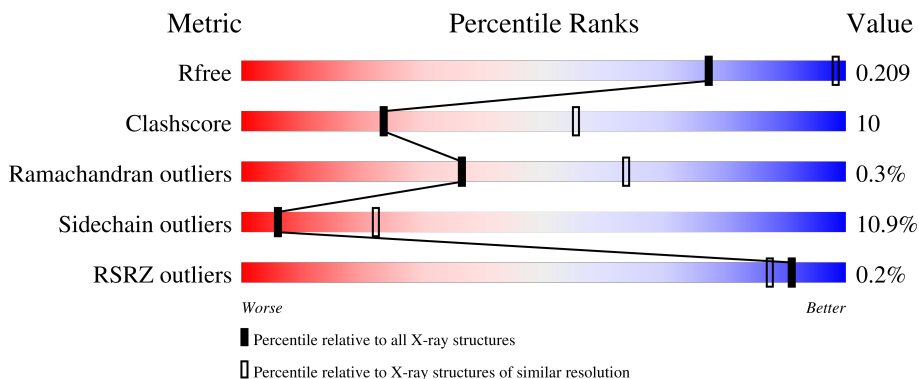
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	543	71% 25% ..
1	B	543	61% 32% 5% ..
1	C	543	73% 23% ..
1	D	543	67% 29% ..

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	NAG	D	702	X	-	-	-

2 Entry composition [i](#)

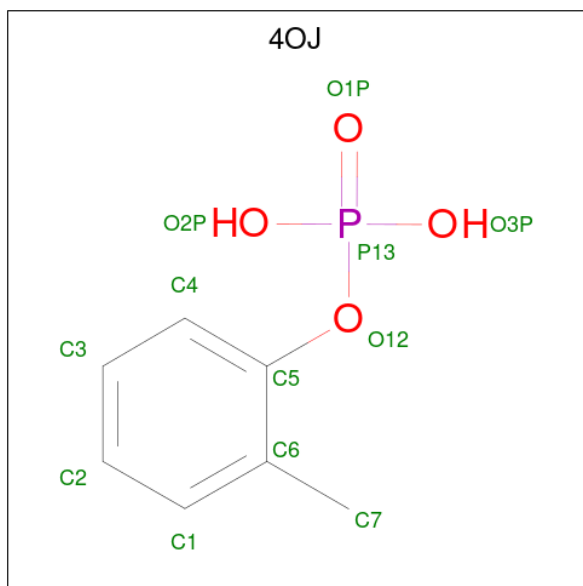
There are 6 unique types of molecules in this entry. The entry contains 17432 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	542	Total 4215	C 2702	N 733	O 766	S 14	0	0	0
1	B	539	Total 4191	C 2689	N 727	O 761	S 14	0	0	0
1	C	540	Total 4200	C 2694	N 728	O 764	S 14	0	0	0
1	D	540	Total 4200	C 2694	N 728	O 764	S 14	0	0	0

- Molecule 2 is (2-methylphenyl) dihydrogen phosphate (CCD ID: 4OJ) (formula: C₇H₉O₄P).



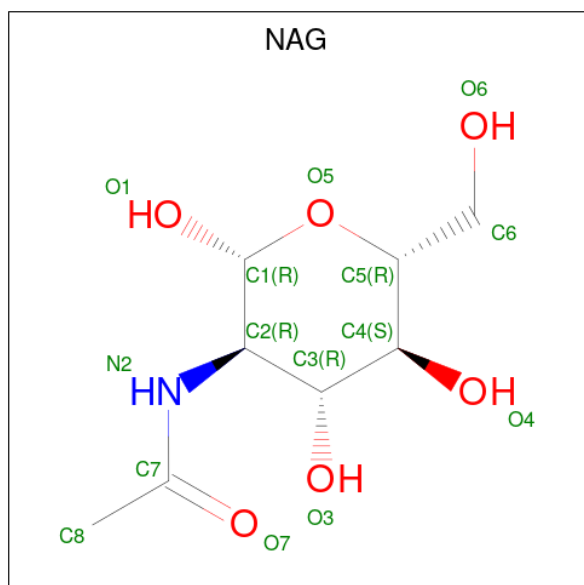
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	Total 11	C 7	O 3	P 1	0	0
2	B	1	Total 11	C 7	O 3	P 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			11	7	3	1		
2	D	1	Total	C	O	P	0	0
			11	7	3	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	5	Total Cl 5 5	0	0
5	D	3	Total Cl 3 3	0	0

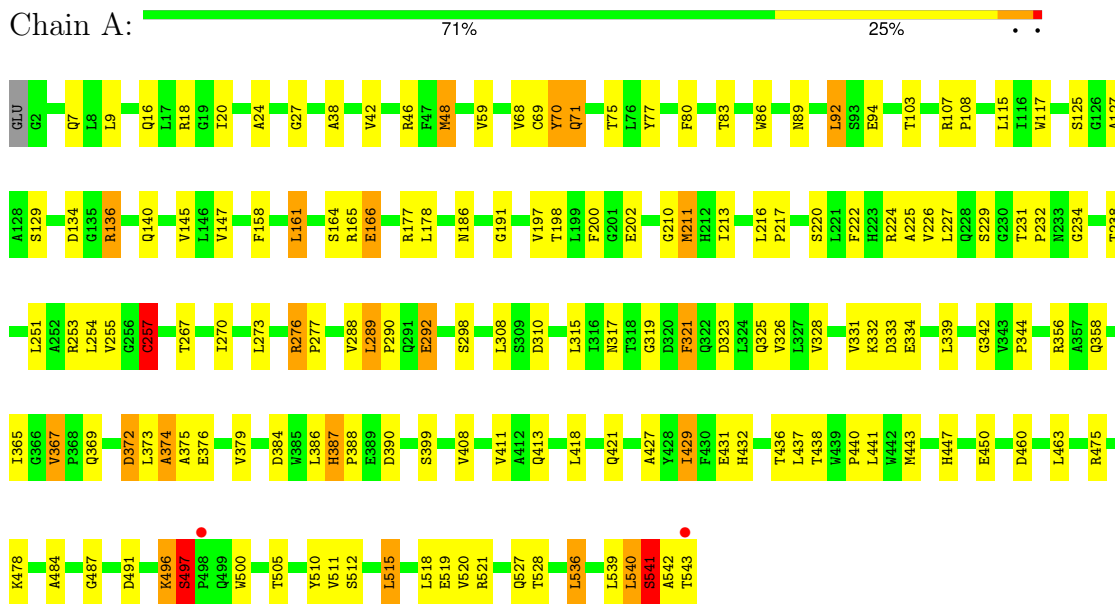
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	117	Total O 117 117	0	0
6	B	82	Total O 82 82	0	0
6	C	115	Total O 115 115	0	0
6	D	97	Total O 97 97	0	0

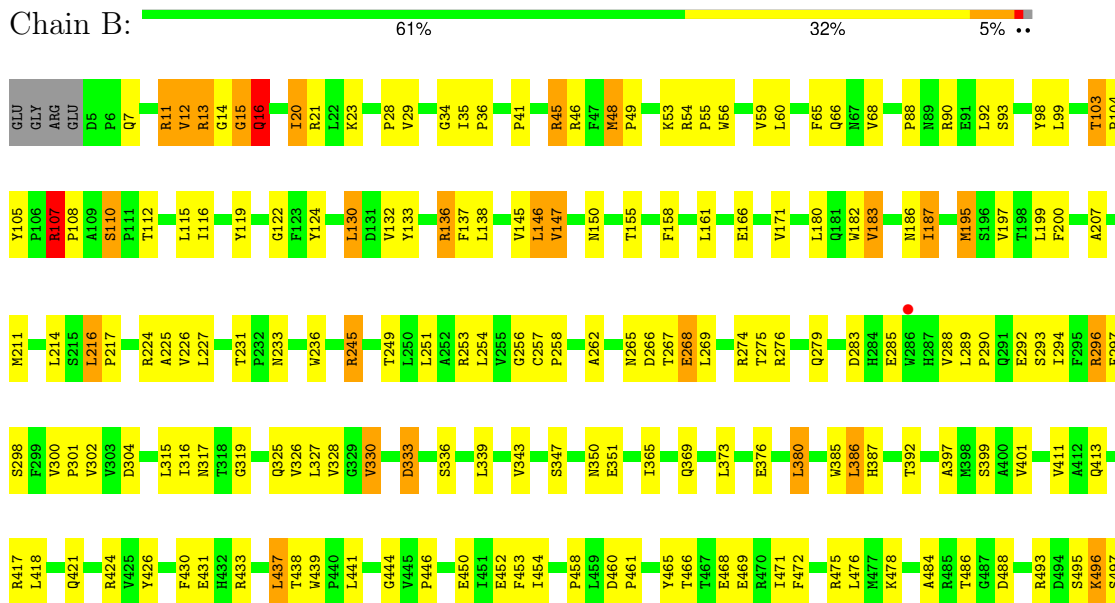
3 Residue-property plots

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: ACETYLCHOLINESTERASE



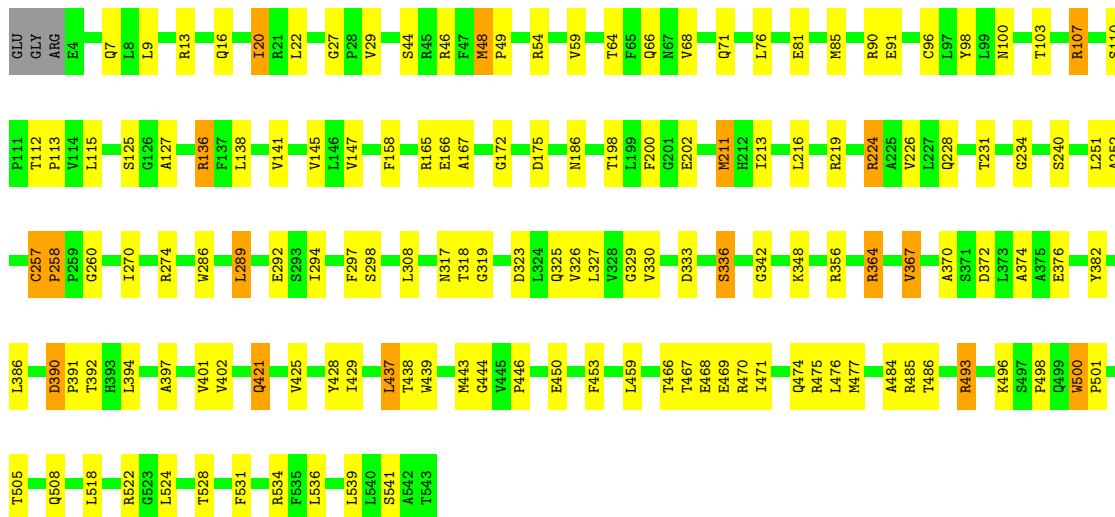
• Molecule 1: ACETYLCHOLINESTERASE





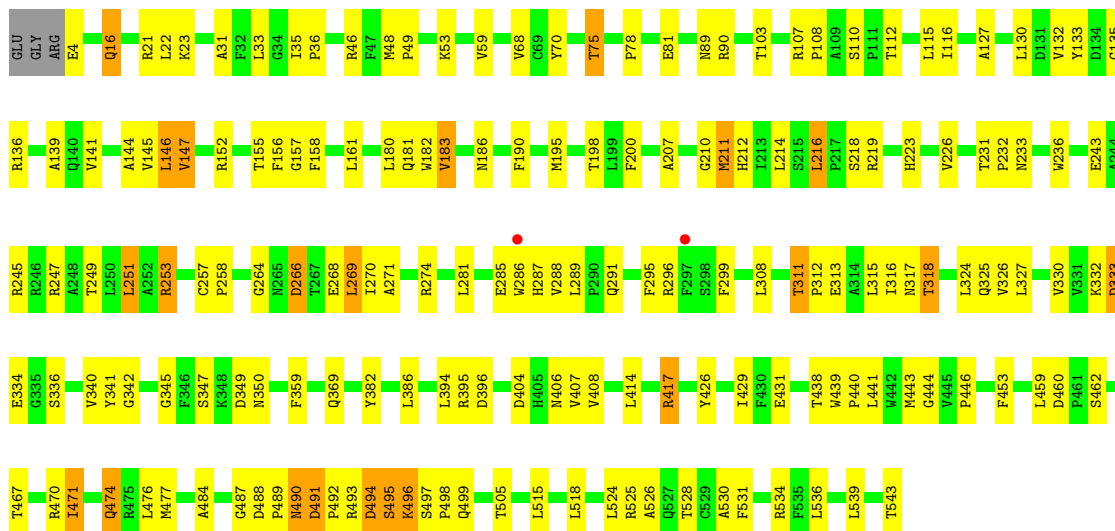
- Molecule 1: ACETYLCHOLINESTERASE

Chain C: 73% 23%



- Molecule 1: ACETYLCHOLINESTERASE

Chain D: 67% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.94Å 174.04Å 225.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.62 – 3.35 48.62 – 3.35	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.62-3.35) 96.6 (48.62-3.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 3.33Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.162 , 0.208 0.165 , 0.209	Depositor DCC
R_{free} test set	2265 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	94.9	Xtrriage
Anisotropy	0.018	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17432	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: 4OJ, NAG, SO4, CL

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	0.60	0/4341	1.12	31/5931 (0.5%)
1	B	0.56	1/4317 (0.0%)	1.05	16/5900 (0.3%)
1	C	0.62	0/4326	1.13	27/5912 (0.5%)
1	D	0.57	0/4326	1.06	21/5912 (0.4%)
All	All	0.59	1/17310 (0.0%)	1.09	95/23655 (0.4%)

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	4
1	B	0	1
1	C	0	3
1	D	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	528	THR	CA-CB	5.12	1.62	1.53

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	257	CYS	CA-C-N	-15.65	104.26	120.38
1	C	257	CYS	C-N-CA	-15.65	104.26	120.38
1	D	497	SER	N-CA-C	-13.80	92.24	108.25
1	A	374	ALA	N-CA-C	-9.98	99.22	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	CYS	CA-C-N	-9.65	110.44	120.38
1	A	257	CYS	C-N-CA	-9.65	110.44	120.38
1	B	107	ARG	CA-C-N	-8.96	111.39	120.98
1	B	107	ARG	C-N-CA	-8.96	111.39	120.98
1	A	387	HIS	CA-C-N	8.13	127.77	119.56
1	A	387	HIS	C-N-CA	8.13	127.77	119.56
1	A	497	SER	N-CA-C	7.55	126.49	109.81
1	B	158	PHE	N-CA-C	7.51	123.37	113.30
1	A	500	TRP	CA-C-N	7.51	128.12	120.38
1	A	500	TRP	C-N-CA	7.51	128.12	120.38
1	D	236	TRP	N-CA-C	7.49	122.60	113.38
1	C	390	ASP	CA-C-N	7.47	126.74	118.97
1	C	390	ASP	C-N-CA	7.47	126.74	118.97
1	A	289	LEU	CA-C-N	7.38	126.65	118.97
1	A	289	LEU	C-N-CA	7.38	126.65	118.97
1	A	158	PHE	N-CA-C	7.18	122.92	113.30
1	D	289	LEU	CA-C-N	7.17	127.50	119.32
1	D	289	LEU	C-N-CA	7.17	127.50	119.32
1	A	186	ASN	N-CA-C	7.16	122.19	113.17
1	D	158	PHE	N-CA-C	7.01	122.70	113.30
1	B	298	SER	N-CA-C	7.00	119.56	111.02
1	B	530	ALA	N-CA-C	-6.96	103.46	112.23
1	C	234	GLY	CA-C-N	6.95	126.20	118.97
1	C	234	GLY	C-N-CA	6.95	126.20	118.97
1	C	367	VAL	CA-C-N	6.93	126.54	119.19
1	C	367	VAL	C-N-CA	6.93	126.54	119.19
1	A	234	GLY	CA-C-N	6.92	126.73	119.05
1	A	234	GLY	C-N-CA	6.92	126.73	119.05
1	C	71	GLN	N-CA-C	6.82	117.58	108.38
1	C	493	ARG	N-CA-C	6.80	122.41	113.30
1	B	257	CYS	N-CA-C	6.74	118.56	110.07
1	B	11	ARG	N-CA-C	6.58	119.72	111.24
1	B	488	ASP	CA-C-N	6.51	126.14	119.56
1	B	488	ASP	C-N-CA	6.51	126.14	119.56
1	B	186	ASN	N-CA-C	6.49	121.35	113.17
1	C	167	ALA	CA-C-N	6.48	126.41	119.28
1	C	167	ALA	C-N-CA	6.48	126.41	119.28
1	A	390	ASP	CA-C-N	6.38	125.80	118.85
1	A	390	ASP	C-N-CA	6.38	125.80	118.85
1	C	500	TRP	CA-C-N	6.38	126.95	120.38
1	C	500	TRP	C-N-CA	6.38	126.95	120.38
1	D	186	ASN	N-CA-C	6.33	121.95	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	289	LEU	CA-C-N	6.22	125.63	118.85
1	C	289	LEU	C-N-CA	6.22	125.63	118.85
1	C	186	ASN	N-CA-C	6.22	121.03	113.38
1	C	158	PHE	N-CA-C	6.19	121.60	113.30
1	A	321	PHE	N-CA-C	6.15	120.48	112.92
1	D	342	GLY	CA-C-N	-6.14	118.17	122.59
1	D	342	GLY	C-N-CA	-6.14	118.17	122.59
1	A	541	SER	N-CA-C	6.03	120.92	112.72
1	B	256	GLY	N-CA-C	5.90	121.12	113.27
1	A	161	LEU	CA-C-N	5.88	126.22	119.93
1	A	161	LEU	C-N-CA	5.88	126.22	119.93
1	D	349	ASP	N-CA-C	5.88	118.92	111.69
1	D	266	ASP	N-CA-C	-5.87	104.83	112.23
1	D	112	THR	CA-C-N	5.85	125.78	119.76
1	D	112	THR	C-N-CA	5.85	125.78	119.76
1	C	27	GLY	CA-C-N	-5.84	114.54	120.85
1	C	27	GLY	C-N-CA	-5.84	114.54	120.85
1	C	96	CYS	N-CA-C	5.83	122.22	114.12
1	B	293	SER	N-CA-C	5.80	117.89	109.07
1	A	367	VAL	CA-C-N	5.79	125.40	119.56
1	A	367	VAL	C-N-CA	5.79	125.40	119.56
1	A	125	SER	N-CA-C	5.73	116.12	108.38
1	B	16	GLN	N-CA-C	5.68	118.47	110.23
1	C	508	GLN	N-CA-C	5.52	119.25	111.52
1	A	460	ASP	CA-C-N	5.49	125.14	119.05
1	A	460	ASP	C-N-CA	5.49	125.14	119.05
1	B	236	TRP	N-CA-C	5.46	120.10	113.38
1	C	298	SER	N-CA-C	5.44	117.29	111.36
1	A	27	GLY	CA-C-N	-5.42	113.07	119.84
1	A	27	GLY	C-N-CA	-5.42	113.07	119.84
1	C	76	LEU	N-CA-C	5.40	116.85	111.07
1	D	495	SER	N-CA-C	-5.39	106.75	113.38
1	D	285	GLU	CA-C-N	-5.34	114.87	122.77
1	D	285	GLU	C-N-CA	-5.34	114.87	122.77
1	D	497	SER	CA-C-N	-5.34	114.06	119.83
1	D	497	SER	C-N-CA	-5.34	114.06	119.83
1	D	406	ASN	N-CA-C	5.29	118.19	111.69
1	A	292	GLU	N-CA-C	-5.28	101.83	109.59
1	D	431	GLU	N-CA-C	5.27	119.82	113.17
1	A	276	ARG	CA-C-N	5.27	125.19	119.76
1	A	276	ARG	C-N-CA	5.27	125.19	119.76
1	B	225	ALA	N-CA-C	5.23	117.90	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	ARG	CA-C-N	5.23	125.23	119.89
1	C	54	ARG	C-N-CA	5.23	125.23	119.89
1	D	526	ALA	N-CA-C	5.18	116.62	110.97
1	A	342	GLY	N-CA-C	5.17	125.43	113.18
1	B	15	GLY	N-CA-C	5.16	118.30	111.70
1	D	318	THR	N-CA-C	5.12	118.81	111.02
1	C	125	SER	N-CA-C	5.05	115.00	107.88

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	CYS	Peptide
1	A	323	ASP	Peptide
1	A	497	SER	Peptide
1	A	541	SER	Peptide
1	B	496	LYS	Peptide
1	C	258	PRO	Peptide
1	C	342	GLY	Peptide
1	C	496	LYS	Peptide
1	D	257	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4215	0	4103	84	0
1	B	4191	0	4080	122	0
1	C	4200	0	4088	56	0
1	D	4200	0	4086	90	0
2	A	11	0	7	1	0
2	B	11	0	7	0	0
2	C	11	0	7	0	0
2	D	11	0	7	0	0
3	A	14	0	13	0	0
3	B	28	0	26	1	0
3	C	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	42	0	39	1	0
4	A	25	0	0	1	0
4	B	15	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	1	0
5	C	5	0	0	0	0
5	D	3	0	0	0	0
6	A	117	0	0	8	0
6	B	82	0	0	6	0
6	C	115	0	0	6	0
6	D	97	0	0	4	0
All	All	17432	0	16476	343	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 10.

All (343) 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:496:LYS:HB3	1:B:497:SER:HA	1.62	0.82
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.65	0.79
1:A:496:LYS:HD2	1:A:497:SER:HB3	1.65	0.77
1:B:28:PRO:HG2	1:B:105:TYR:HB3	1.66	0.76
1:C:286:TRP:NE1	6:C:2077:HOH:O	2.19	0.75
1:A:210:GLY:HA3	1:A:232:PRO:HG3	1.69	0.75
1:D:474:GLN:HA	1:D:477:MET:HE2	1.68	0.74
1:B:319:GLY:O	1:B:421:GLN:HG2	1.88	0.73
1:A:373:LEU:HD12	1:B:538:LYS:HB3	1.73	0.71
1:D:135:GLY:HA3	1:D:146:LEU:HD22	1.72	0.70
1:B:187:ILE:N	6:B:2032:HOH:O	2.24	0.69
1:A:292:GLU:HB2	1:D:249:THR:HG21	1.73	0.69
1:A:334:GLU:OE1	6:A:2088:HOH:O	2.10	0.68
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.75	0.68
1:D:68:VAL:HG13	1:D:127:ALA:HB2	1.75	0.67
1:A:373:LEU:HA	1:A:376:GLU:HB3	1.76	0.67
1:D:488:ASP:OD1	1:D:490:ASN:ND2	2.28	0.67
1:D:249:THR:HG22	1:D:253:ARG:HH21	1.58	0.67
1:D:333:ASP:OD1	1:D:333:ASP:N	2.26	0.67
1:A:202:GLU:OE2	6:A:2060:HOH:O	2.13	0.67
1:B:258:PRO:HD3	1:B:269:LEU:HD12	1.76	0.66
1:B:211:MET:HE3	1:B:301:PRO:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ARG:NH1	6:B:2047:HOH:O	2.30	0.64
1:A:510:TYR:CZ	1:A:521:ARG:HB2	2.33	0.63
1:B:116:ILE:HD11	1:B:183:VAL:HG11	1.81	0.63
1:B:294:ILE:HG12	1:B:365:ILE:HG22	1.80	0.62
1:C:103:THR:HG22	1:C:145:VAL:HG22	1.82	0.61
1:D:226:VAL:HG22	1:D:327:LEU:HB3	1.82	0.61
1:A:70:TYR:HA	1:A:92:LEU:HD13	1.82	0.61
1:C:336:SER:HB2	1:C:443:MET:HG2	1.83	0.59
1:B:265:ASN:OD1	1:B:268:GLU:HB2	2.03	0.59
1:C:485:ARG:NH2	6:C:2052:HOH:O	2.35	0.59
1:B:54:ARG:HG2	1:B:55:PRO:HD2	1.84	0.59
1:B:147:VAL:HG21	1:B:183:VAL:HG21	1.84	0.59
1:B:265:ASN:O	6:B:2044:HOH:O	2.17	0.59
1:C:475:ARG:NH2	6:C:2107:HOH:O	2.34	0.59
1:A:103:THR:HG22	1:A:145:VAL:HG22	1.86	0.58
1:B:12:VAL:O	1:B:14:GLY:N	2.36	0.58
1:D:116:ILE:HD11	1:D:183:VAL:HG11	1.84	0.58
1:D:115:LEU:HD23	1:D:198:THR:HB	1.84	0.58
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.86	0.58
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.85	0.58
1:C:459:LEU:HD11	1:C:474:GLN:HG2	1.84	0.58
1:A:68:VAL:HG13	1:A:127:ALA:HB2	1.85	0.58
1:B:103:THR:HG22	1:B:104:PRO:HD2	1.86	0.57
1:D:161:LEU:HD12	1:D:270:ILE:HD11	1.86	0.57
1:D:36:PRO:HB2	1:D:53:LYS:HD3	1.85	0.57
1:B:46:ARG:O	1:B:274:ARG:NH1	2.37	0.57
1:D:115:LEU:HD21	1:D:484:ALA:HB2	1.87	0.57
1:D:395:ARG:NH1	1:D:395:ASP:OD1	2.38	0.57
1:A:372:ASP:N	1:A:372:ASP:OD1	2.38	0.57
1:C:364:ARG:NH2	1:C:370:ALA:O	2.37	0.56
1:B:333:ASP:OD1	1:B:333:ASP:N	2.37	0.56
1:A:331:VAL:N	1:A:334:GLU:OE2	2.34	0.56
1:D:214:LEU:HD22	1:D:315:LEU:HB2	1.87	0.56
1:D:295:PHE:O	1:D:296:ARG:NH1	2.37	0.56
1:A:161:LEU:HD12	1:A:270:ILE:HD11	1.86	0.56
1:B:183:VAL:HG22	1:B:187:ILE:HB	1.87	0.56
1:A:511:VAL:HG12	1:A:520:VAL:HG22	1.88	0.56
1:B:431:GLU:OE2	1:B:521:ARG:NH2	2.38	0.56
1:B:166:GLU:OE1	1:B:267:THR:HG22	2.06	0.56
1:B:115:LEU:HD21	1:B:484:ALA:HB2	1.87	0.55
1:C:46:ARG:HB3	1:C:274:ARG:HG2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ARG:CZ	1:B:441:LEU:HA	2.36	0.55
1:D:408:VAL:HG11	1:D:525:ARG:HG3	1.87	0.55
1:B:136:ARG:HG2	1:B:137:PHE:N	2.20	0.55
1:C:226:VAL:HG22	1:C:327:LEU:HB3	1.88	0.55
1:A:225:ALA:HB3	1:A:326:VAL:HG12	1.89	0.55
1:B:12:VAL:O	1:B:15:GLY:N	2.36	0.55
1:B:41:PRO:HA	1:B:45:ARG:HB3	1.88	0.55
1:B:426:TYR:HB3	1:B:500:TRP:NE1	2.21	0.55
1:A:166:GLU:HB3	1:A:270:ILE:HD13	1.89	0.54
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.88	0.54
1:A:332:LYS:HA	1:A:429:ILE:HD11	1.88	0.54
1:A:200:PHE:HB2	1:A:226:VAL:HB	1.88	0.54
1:C:107:ARG:HG2	1:C:107:ARG:HH11	1.72	0.54
1:D:245:ARG:NH2	1:D:266:ASP:OD2	2.41	0.54
1:A:69:CYS:O	1:A:71:GLN:NE2	2.40	0.54
1:A:332:LYS:HD3	6:A:2086:HOH:O	2.07	0.54
1:B:107:ARG:HG2	1:B:108:PRO:HD3	1.88	0.54
1:B:245:ARG:NH2	1:B:266:ASP:OD1	2.41	0.54
1:A:432:HIS:ND1	1:A:515:LEU:HD23	2.23	0.53
1:D:460:ASP:OD1	1:D:462:SER:OG	2.20	0.53
1:B:48:MET:HE2	1:B:49:PRO:HD2	1.90	0.53
1:B:296:ARG:NH1	1:B:369:GLN:OE1	2.42	0.53
1:C:7:GLN:HB2	6:C:2002:HOH:O	2.08	0.53
1:D:453:PHE:HB3	6:D:2091:HOH:O	2.07	0.53
1:D:107:ARG:HG2	1:D:108:PRO:HD2	1.90	0.53
1:B:458:PRO:HA	1:B:465:TYR:CD1	2.44	0.53
1:C:115:LEU:HD23	1:C:198:THR:HB	1.91	0.53
1:A:440:PRO:HG2	1:A:443:MET:HG3	1.90	0.52
1:D:130:LEU:HD12	1:D:133:TYR:CE2	2.44	0.52
1:D:211:MET:HG3	1:D:308:LEU:HD21	1.92	0.52
1:B:339:LEU:HD11	1:B:399:SER:HA	1.91	0.52
1:C:258:PRO:HB2	1:C:260:GLY:N	2.25	0.52
1:D:525:ARG:NH1	4:D:1544:SO4:O4	2.41	0.52
1:A:86:TRP:HB3	6:A:2028:HOH:O	2.08	0.52
1:C:382:TYR:CD2	1:C:401:VAL:HG22	2.45	0.52
1:D:539:LEU:O	1:D:543:THR:HG22	2.09	0.52
1:D:530:ALA:O	1:D:534:ARG:HB2	2.09	0.52
1:C:522:ARG:NH1	6:C:2111:HOH:O	2.41	0.52
1:B:119:TYR:HE2	1:B:150:ASN:HA	1.74	0.52
1:B:300:VAL:HB	1:B:301:PRO:HD2	1.92	0.52
1:D:231:THR:HB	1:D:233:ASN:OD1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:MET:HG2	1:A:308:LEU:HD21	1.92	0.51
1:C:318:THR:OG1	1:C:319:GLY:N	2.43	0.51
1:C:498:PRO:HG2	1:C:518:LEU:HB2	1.92	0.51
1:D:48:MET:HE3	1:D:49:PRO:HD2	1.90	0.51
1:B:65:PHE:HB2	1:B:90:ARG:NH2	2.25	0.51
1:B:413:GLN:O	1:B:417:ARG:HG2	2.11	0.51
1:C:20:ILE:HD12	1:C:22:LEU:HD23	1.92	0.51
1:A:210:GLY:HA2	1:A:213:ILE:HD12	1.92	0.51
1:B:380:LEU:HA	1:B:385:TRP:HZ2	1.74	0.51
1:D:496:LYS:HA	1:D:496:LYS:HE2	1.92	0.51
1:B:472:PHE:O	1:B:475:ARG:HB2	2.10	0.51
1:B:527:GLN:O	1:B:528:THR:HB	2.09	0.51
1:D:16:GLN:HB2	1:D:59:VAL:HG22	1.92	0.51
1:D:103:THR:HG21	1:D:190:PHE:HB3	1.91	0.51
1:A:108:PRO:HG2	1:A:191:GLY:HA3	1.93	0.51
1:B:231:THR:HB	1:B:233:ASN:OD1	2.11	0.51
1:A:115:LEU:HD21	1:A:484:ALA:HB2	1.93	0.51
1:D:494:ASP:OD1	1:D:494:ASP:N	2.43	0.50
1:A:89:ASN:OD1	1:A:129:SER:HB2	2.11	0.50
1:D:258:PRO:HD2	6:D:2062:HOH:O	2.09	0.50
1:B:249:THR:HG21	1:C:292:GLU:HB2	1.94	0.50
1:B:453:PHE:HB3	1:B:476:LEU:HD12	1.94	0.50
1:B:16:GLN:HG2	1:B:59:VAL:HG22	1.93	0.50
1:A:375:ALA:O	1:A:379:VAL:HG23	2.12	0.50
1:A:539:LEU:C	1:A:541:SER:H	2.20	0.50
1:B:433:ARG:HG3	1:B:437:LEU:HD12	1.94	0.50
1:B:536:LEU:HG	1:B:540:LEU:HD22	1.94	0.50
1:B:166:GLU:HB3	1:B:274:ARG:HH22	1.77	0.50
1:B:200:PHE:CB	1:B:226:VAL:HB	2.42	0.50
1:C:68:VAL:HG13	1:C:127:ALA:HB2	1.94	0.49
1:C:467:THR:HG22	6:C:2105:HOH:O	2.11	0.49
1:B:430:PHE:CD2	1:B:450:GLU:HB2	2.47	0.49
1:D:89:ASN:O	1:D:90:ARG:NH1	2.41	0.49
1:A:319:GLY:O	1:A:421:GLN:HG3	2.12	0.49
1:B:262:ALA:HB2	6:B:2043:HOH:O	2.13	0.49
1:C:528:THR:O	1:C:531:PHE:HB3	2.11	0.49
1:D:68:VAL:HG23	1:D:90:ARG:HB2	1.92	0.49
1:B:497:SER:HB3	1:B:498:PRO:O	2.12	0.49
1:B:452:GLU:HG3	6:B:2069:HOH:O	2.13	0.49
1:A:431:GLU:CD	1:A:521:ARG:HH12	2.20	0.49
1:B:34:GLY:HA2	1:B:98:TYR:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:VAL:HG21	1:B:136:ARG:HB2	1.94	0.49
1:A:298:SER:HB2	6:A:2072:HOH:O	2.13	0.49
1:B:279:GLN:NE2	1:B:283:ASP:OD1	2.42	0.49
1:B:326:VAL:HG12	1:B:328:VAL:HG13	1.95	0.49
1:D:31:ALA:HB1	1:D:33:LEU:HD21	1.94	0.49
1:D:286:TRP:HA	6:D:2066:HOH:O	2.13	0.49
1:B:136:ARG:HD3	1:B:137:PHE:CE1	2.48	0.48
1:B:444:GLY:O	1:B:446:PRO:HD3	2.13	0.48
1:D:22:LEU:HD13	1:D:136:ARG:HH21	1.78	0.48
1:D:70:TYR:HB3	1:D:156:PHE:CE2	2.48	0.48
1:D:155:THR:HG22	1:D:299:PHE:CE2	2.49	0.48
1:B:35:ILE:HG21	1:B:182:TRP:CZ2	2.49	0.48
1:D:210:GLY:HA3	1:D:232:PRO:HD3	1.95	0.48
1:D:317:ASN:OD1	1:D:417:ARG:NH1	2.46	0.48
1:A:387:HIS:CE1	1:B:522:ARG:HH22	2.31	0.48
1:A:475:ARG:HH21	1:A:518:LEU:HD23	1.79	0.48
1:C:224:ARG:NH2	1:C:484:ALA:O	2.43	0.48
1:D:296:ARG:HE	1:D:369:GLN:HE22	1.62	0.48
1:A:384:ASP:HA	1:B:527:GLN:OE1	2.14	0.47
1:B:373:LEU:HD23	1:B:543:THR:HG21	1.96	0.47
1:A:229:SER:HB3	1:A:447:HIS:CE1	2.50	0.47
1:B:7:GLN:HG3	1:B:105:TYR:CZ	2.50	0.47
1:D:103:THR:HG22	1:D:145:VAL:HG22	1.95	0.47
1:A:325:GLN:NE2	1:A:487:GLY:HA3	2.29	0.47
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.44	0.47
1:B:130:LEU:HB2	1:B:133:TYR:CD2	2.50	0.47
1:B:207:ALA:O	1:B:211:MET:HB2	2.13	0.47
1:B:430:PHE:CE2	1:B:450:GLU:HB2	2.50	0.47
1:D:498:PRO:HG2	1:D:518:LEU:HB2	1.95	0.47
1:C:138:LEU:HD23	1:C:477:MET:HE3	1.96	0.47
1:C:252:ALA:O	1:C:257:CYS:HB2	2.15	0.47
1:B:88:PRO:HG3	1:B:92:LEU:HD21	1.97	0.47
1:B:454:ILE:HD13	1:B:476:LEU:HB3	1.97	0.47
1:C:16:GLN:HB3	1:C:59:VAL:HG22	1.97	0.47
1:A:328:VAL:O	1:A:427:ALA:HA	2.15	0.47
1:B:56:TRP:NE1	1:B:60:LEU:HB2	2.30	0.47
1:D:417:ARG:HE	1:D:417:ARG:HA	1.80	0.47
1:D:207:ALA:O	1:D:211:MET:HE2	2.15	0.46
1:A:229:SER:HB3	1:A:447:HIS:HE1	1.80	0.46
1:A:344:PRO:HG3	1:D:264:GLY:HA2	1.97	0.46
1:A:48:MET:HE2	1:A:48:MET:HB3	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ARG:HD2	1:B:525:ARG:N	2.29	0.46
1:A:200:PHE:CB	1:A:226:VAL:HB	2.45	0.46
1:A:251:LEU:HB2	1:A:288:VAL:HG11	1.98	0.46
1:D:216:LEU:HD22	1:D:216:LEU:HA	1.66	0.46
1:B:226:VAL:HG22	1:B:327:LEU:HB3	1.97	0.46
1:C:81:GLU:O	1:C:85:MET:HB3	2.15	0.46
1:C:294:ILE:HD11	1:C:402:VAL:HG21	1.98	0.46
1:C:437:LEU:HD23	1:C:439:TRP:HB2	1.97	0.46
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.75	0.46
1:A:463:LEU:HD23	1:A:463:LEU:HA	1.75	0.45
1:C:390:ASP:HA	1:C:391:PRO:HD3	1.77	0.45
1:C:319:GLY:O	1:C:421:GLN:HG2	2.16	0.45
1:D:231:THR:HG22	1:D:414:LEU:HD22	1.98	0.45
1:A:413:GLN:HG3	4:A:1545:SO4:O1	2.17	0.45
1:A:443:MET:HE2	1:A:443:MET:HB3	1.83	0.45
1:A:527:GLN:NE2	1:B:385:TRP:HD1	2.13	0.45
1:B:56:TRP:HE1	1:B:60:LEU:HB2	1.80	0.45
1:B:66:GLN:HG3	1:B:98:TYR:CG	2.51	0.45
1:B:216:LEU:HD22	1:B:216:LEU:HA	1.80	0.45
1:C:29:VAL:HG21	1:C:136:ARG:HB2	1.98	0.45
1:C:66:GLN:HG3	1:C:98:TYR:CD2	2.52	0.45
1:C:213:ILE:O	1:C:219:ARG:HD3	2.16	0.45
1:A:289:LEU:O	1:D:253:ARG:NH1	2.49	0.45
1:A:356:ARG:HD2	1:A:388:PRO:O	2.16	0.45
1:B:336:SER:HA	1:B:339:LEU:HD12	1.98	0.45
1:C:48:MET:HE2	1:C:49:PRO:HD2	1.98	0.45
1:C:211:MET:HE2	1:C:308:LEU:HD11	1.99	0.45
1:A:46:ARG:NE	1:A:94:GLU:OE2	2.31	0.45
1:B:468:GLU:HA	1:B:471:ILE:HG12	1.98	0.45
1:A:166:GLU:HB2	6:A:2053:HOH:O	2.16	0.45
1:A:334:GLU:HB3	6:A:2088:HOH:O	2.17	0.45
1:B:330:VAL:HG12	1:B:411:VAL:HG21	1.98	0.45
1:D:141:VAL:HG21	1:D:477:MET:HE1	1.99	0.45
1:D:347:SER:HB3	1:D:350:ASN:OD1	2.17	0.45
1:B:36:PRO:HB2	1:B:53:LYS:HD3	2.00	0.44
1:D:312:PRO:O	1:D:316:ILE:HG12	2.16	0.44
1:A:16:GLN:HB3	1:A:59:VAL:HG22	1.99	0.44
1:C:397:ALA:O	1:C:401:VAL:HG23	2.17	0.44
1:A:115:LEU:HD23	1:A:198:THR:HB	2.00	0.44
1:B:339:LEU:HD23	1:B:343:VAL:HG21	1.98	0.44
1:B:369:GLN:HB2	6:B:2055:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:HIS:HB3	1:D:218:SER:HB3	1.99	0.44
1:A:536:LEU:O	1:A:540:LEU:HD22	2.17	0.44
1:D:251:LEU:HB2	1:D:288:VAL:HG11	1.99	0.44
1:D:268:GLU:O	1:D:271:ALA:HB3	2.17	0.44
1:B:115:LEU:HB2	1:B:146:LEU:HD12	2.00	0.44
1:D:139:ALA:HA	1:D:144:ALA:O	2.18	0.44
1:A:210:GLY:CA	1:A:232:PRO:HG3	2.44	0.44
1:B:253:ARG:NH1	1:C:289:LEU:O	2.51	0.44
1:C:100:ASN:O	1:C:147:VAL:HA	2.17	0.44
1:C:500:TRP:HA	1:C:501:PRO:HD3	1.75	0.44
1:D:311:THR:O	1:D:315:LEU:HG	2.18	0.44
1:C:364:ARG:HH12	1:C:372:ASP:HA	1.83	0.43
1:D:200:PHE:HB2	1:D:226:VAL:HB	2.00	0.43
1:D:382:TYR:OH	1:D:404:ASP:OD2	2.25	0.43
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.72	0.43
1:B:433:ARG:NH1	1:B:441:LEU:HA	2.33	0.43
1:D:200:PHE:CB	1:D:226:VAL:HB	2.48	0.43
1:D:444:GLY:O	1:D:446:PRO:HD3	2.18	0.43
1:D:471:ILE:HD12	1:D:471:ILE:HA	1.84	0.43
1:C:444:GLY:O	1:C:446:PRO:HD3	2.18	0.43
1:A:211:MET:HE3	1:A:232:PRO:HB3	2.00	0.43
1:A:227:LEU:HB2	1:A:328:VAL:HG12	2.00	0.43
1:A:512:SER:OG	1:A:519:GLU:HG2	2.18	0.43
1:B:155:THR:HG23	1:B:285:GLU:HG3	2.01	0.43
1:A:86:TRP:CD2	2:A:600:4OJ:H1	2.53	0.43
1:A:339:LEU:HD11	1:A:399:SER:HA	2.00	0.43
1:C:459:LEU:HD12	1:C:470:ARG:HG2	2.01	0.43
1:B:397:ALA:O	1:B:401:VAL:HG23	2.18	0.43
1:C:172:GLY:O	1:C:175:ASP:HB2	2.18	0.43
1:D:211:MET:HE2	1:D:211:MET:HB2	1.62	0.43
1:D:334:GLU:CD	1:D:407:VAL:HG11	2.44	0.43
1:B:528:THR:O	1:B:532:TRP:HD1	2.01	0.43
1:B:534:ARG:O	1:B:537:PRO:HG2	2.19	0.43
1:A:134:ASP:OD2	1:A:136:ARG:HB3	2.19	0.43
1:B:45:ARG:HD3	1:B:48:MET:HB2	2.00	0.42
1:B:214:LEU:HD21	1:B:316:ILE:HG23	2.00	0.42
1:C:141:VAL:HG21	1:C:459:LEU:HD23	2.00	0.42
1:A:117:TRP:HA	1:A:200:PHE:O	2.19	0.42
1:A:491:ASP:HB3	6:A:2107:HOH:O	2.18	0.42
1:A:539:LEU:O	1:A:543:THR:N	2.52	0.42
1:B:289:LEU:HA	1:B:290:PRO:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:THR:O	1:C:469:GLU:HB2	2.19	0.42
1:D:269:LEU:HD12	1:D:269:LEU:C	2.44	0.42
1:D:324:LEU:HG	1:D:326:VAL:HG23	2.01	0.42
1:D:459:LEU:HD23	1:D:470:ARG:HG2	2.01	0.42
1:B:116:ILE:HB	1:B:199:LEU:HD23	2.00	0.42
1:A:372:ASP:C	1:A:374:ALA:H	2.27	0.42
1:B:122:GLY:C	1:B:124:TYR:H	2.28	0.42
1:B:132:VAL:HG23	1:B:133:TYR:CD1	2.54	0.42
1:B:195:MET:HE2	1:B:195:MET:HB2	1.93	0.42
1:C:112:THR:HG23	1:C:113:PRO:HD2	2.01	0.42
1:C:115:LEU:HD23	1:C:115:LEU:HA	1.74	0.42
1:B:65:PHE:HB2	1:B:90:ARG:CZ	2.50	0.42
1:B:216:LEU:HB3	1:B:217:PRO:HD3	2.00	0.42
1:D:23:LYS:HA	1:D:23:LYS:HD3	1.80	0.42
1:D:528:THR:O	1:D:531:PHE:HB3	2.19	0.42
1:B:347:SER:HB3	1:B:350:ASN:OD1	2.20	0.42
1:A:38:ALA:HB2	1:A:178:LEU:HD23	2.00	0.42
1:B:20:ILE:HG12	1:B:21:ARG:N	2.35	0.42
1:D:75:THR:O	1:D:78:PRO:HD3	2.20	0.42
1:A:276:ARG:HA	1:A:277:PRO:HD3	1.91	0.42
1:A:450:GLU:OE1	1:A:450:GLU:N	2.46	0.42
1:C:374:ALA:HA	1:C:539:LEU:HD23	2.02	0.42
1:B:304:ASP:OD1	1:B:304:ASP:N	2.37	0.42
1:B:433:ARG:NH2	1:B:441:LEU:HA	2.35	0.42
1:B:510:TYR:CE1	1:B:521:ARG:HB2	2.54	0.42
1:D:152:ARG:O	1:D:157:GLY:HA3	2.20	0.42
1:A:24:ALA:HB3	1:A:140:GLN:HG3	2.02	0.41
1:A:321:PHE:CD2	1:A:418:LEU:HD23	2.55	0.41
1:A:310:ASP:H	1:A:315:LEU:HD11	1.85	0.41
1:B:214:LEU:HD23	1:B:315:LEU:HB2	2.03	0.41
1:B:386:LEU:HD22	1:B:387:HIS:CE1	2.55	0.41
1:D:426:TYR:CZ	1:D:489:PRO:HD2	2.54	0.41
1:A:197:VAL:HB	1:A:222:PHE:HA	2.02	0.41
1:C:202:GLU:HA	1:C:228:GLN:O	2.20	0.41
1:D:330:VAL:HG23	1:D:429:ILE:HG13	2.02	0.41
1:B:108:PRO:HB2	1:B:110:SER:O	2.20	0.41
1:A:77:TYR:O	1:A:80:PHE:HB3	2.20	0.41
1:A:289:LEU:HA	1:A:290:PRO:HD3	1.81	0.41
1:B:28:PRO:CG	1:B:105:TYR:HB3	2.45	0.41
1:C:68:VAL:HG23	1:C:90:ARG:HB2	2.02	0.41
1:C:329:GLY:HA3	1:C:428:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:PHE:HB3	1:C:476:LEU:HD12	2.01	0.41
1:D:345:GLY:HA2	3:D:702:NAG:H4	2.01	0.41
1:B:265:ASN:HB3	3:B:701:NAG:C8	2.50	0.41
1:B:437:LEU:HD22	1:B:439:TRP:HB2	2.03	0.41
1:C:356:ARG:HA	1:C:394:LEU:HD13	2.02	0.41
1:D:325:GLN:HG3	6:D:2074:HOH:O	2.20	0.41
1:D:340:VAL:HG23	1:D:341:TYR:CD1	2.55	0.41
1:B:138:LEU:HD21	1:B:454:ILE:O	2.21	0.41
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.85	0.41
1:A:255:VAL:HG23	1:A:257:CYS:HB2	2.02	0.41
1:B:460:ASP:HA	1:B:461:PRO:HD3	1.89	0.41
1:B:466:THR:OG1	1:B:469:GLU:HG3	2.21	0.41
1:C:437:LEU:CD2	1:C:439:TRP:HB2	2.50	0.41
1:D:147:VAL:HG21	1:D:183:VAL:CG2	2.51	0.41
1:D:359:PHE:CG	1:D:394:LEU:HD22	2.56	0.41
1:D:491:ASP:HA	1:D:492:PRO:HD3	1.83	0.41
1:D:243:GLU:HG3	1:D:247:ARG:NE	2.36	0.41
1:D:336:SER:HB2	1:D:443:MET:HG2	2.03	0.41
1:D:439:TRP:HB3	1:D:440:PRO:HD2	2.03	0.41
1:A:254:LEU:HA	1:A:254:LEU:HD23	1.74	0.40
1:B:424:ARG:HD3	1:B:426:TYR:OH	2.21	0.40
1:B:145:VAL:HG11	1:B:187:ILE:HD11	2.02	0.40
1:C:326:VAL:O	1:C:425:VAL:HA	2.21	0.40
1:D:195:MET:C	1:D:223:HIS:CE1	2.99	0.40
1:D:219:ARG:HA	1:D:219:ARG:HD2	1.78	0.40
1:A:231:THR:HG21	1:A:411:VAL:HA	2.03	0.40
1:B:326:VAL:HG21	1:B:418:LEU:HD13	2.02	0.40
1:D:325:GLN:NE2	1:D:487:GLY:HA3	2.37	0.40
1:A:339:LEU:HD23	1:A:339:LEU:HA	1.88	0.40
1:B:525:ARG:HD2	1:B:525:ARG:H	1.86	0.40
1:D:35:ILE:HG21	1:D:182:TRP:CZ2	2.56	0.40
1:D:394:LEU:HA	1:D:394:LEU:HD23	1.88	0.40
1:B:495:SER:HA	1:B:496:LYS:C	2.46	0.40
1:D:46:ARG:HB3	1:D:274:ARG:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	540/543 (99%)	510 (94%)	29 (5%)	1 (0%)	43	70
1	B	537/543 (99%)	502 (94%)	31 (6%)	4 (1%)	18	46
1	C	538/543 (99%)	512 (95%)	25 (5%)	1 (0%)	43	70
1	D	538/543 (99%)	508 (94%)	30 (6%)	0	100	100
All	All	2153/2172 (99%)	2032 (94%)	115 (5%)	6 (0%)	36	63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	ALA
1	B	13	ARG
1	B	12	VAL
1	B	526	ALA
1	C	110	SER
1	B	107	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	442/443 (100%)	395 (89%)	47 (11%)	6	23
1	B	440/443 (99%)	385 (88%)	55 (12%)	4	17
1	C	441/443 (100%)	395 (90%)	46 (10%)	7	24
1	D	441/443 (100%)	397 (90%)	44 (10%)	7	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1764/1772 (100%)	1572 (89%)	192 (11%)	6 22

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	9	LEU
1	A	18	ARG
1	A	20	ILE
1	A	42	VAL
1	A	48	MET
1	A	70	TYR
1	A	71	GLN
1	A	75	THR
1	A	83	THR
1	A	92	LEU
1	A	107	ARG
1	A	136	ARG
1	A	147	VAL
1	A	164	SER
1	A	165	ARG
1	A	166	GLU
1	A	211	MET
1	A	216	LEU
1	A	220	SER
1	A	224	ARG
1	A	238	THR
1	A	253	ARG
1	A	257	CYS
1	A	267	THR
1	A	273	LEU
1	A	317	ASN
1	A	333	ASP
1	A	358	GLN
1	A	365	ILE
1	A	367	VAL
1	A	369	GLN
1	A	372	ASP
1	A	386	LEU
1	A	408	VAL
1	A	429	ILE
1	A	436	THR

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Mol	Chain	Res	Type
1	A	437	LEU
1	A	438	THR
1	A	441	LEU
1	A	478	LYS
1	A	496	LYS
1	A	505	THR
1	A	515	LEU
1	A	528	THR
1	A	536	LEU
1	A	540	LEU
1	B	11	ARG
1	B	13	ARG
1	B	16	GLN
1	B	20	ILE
1	B	23	LYS
1	B	45	ARG
1	B	48	MET
1	B	93	SER
1	B	99	LEU
1	B	103	THR
1	B	110	SER
1	B	112	THR
1	B	130	LEU
1	B	136	ARG
1	B	146	LEU
1	B	147	VAL
1	B	171	VAL
1	B	180	LEU
1	B	183	VAL
1	B	187	ILE
1	B	195	MET
1	B	197	VAL
1	B	216	LEU
1	B	245	ARG
1	B	251	LEU
1	B	268	GLU
1	B	275	THR
1	B	288	VAL
1	B	292	GLU
1	B	296	ARG
1	B	297	PHE
1	B	302	VAL

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Mol	Chain	Res	Type
1	B	317	ASN
1	B	330	VAL
1	B	333	ASP
1	B	351	GLU
1	B	376	GLU
1	B	380	LEU
1	B	386	LEU
1	B	392	THR
1	B	437	LEU
1	B	438	THR
1	B	478	LYS
1	B	486	THR
1	B	493	ARG
1	B	505	THR
1	B	511	VAL
1	B	515	LEU
1	B	518	LEU
1	B	524	LEU
1	B	525	ARG
1	B	527	GLN
1	B	528	THR
1	B	529	CYS
1	B	540	LEU
1	C	9	LEU
1	C	13	ARG
1	C	20	ILE
1	C	44	SER
1	C	48	MET
1	C	64	THR
1	C	91	GLU
1	C	107	ARG
1	C	136	ARG
1	C	165	ARG
1	C	166	GLU
1	C	200	PHE
1	C	211	MET
1	C	216	LEU
1	C	224	ARG
1	C	231	THR
1	C	240	SER
1	C	251	LEU
1	C	270	ILE

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Mol	Chain	Res	Type
1	C	297	PHE
1	C	317	ASN
1	C	323	ASP
1	C	325	GLN
1	C	330	VAL
1	C	333	ASP
1	C	336	SER
1	C	348	LYS
1	C	364	ARG
1	C	367	VAL
1	C	376	GLU
1	C	386	LEU
1	C	392	THR
1	C	421	GLN
1	C	429	ILE
1	C	437	LEU
1	C	438	THR
1	C	450	GLU
1	C	468	GLU
1	C	471	ILE
1	C	486	THR
1	C	493	ARG
1	C	505	THR
1	C	524	LEU
1	C	534	ARG
1	C	536	LEU
1	C	541	SER
1	D	4	GLU
1	D	16	GLN
1	D	21	ARG
1	D	75	THR
1	D	81	GLU
1	D	110	SER
1	D	132	VAL
1	D	146	LEU
1	D	147	VAL
1	D	180	LEU
1	D	181	GLN
1	D	183	VAL
1	D	211	MET
1	D	216	LEU
1	D	251	LEU

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Mol	Chain	Res	Type
1	D	253	ARG
1	D	269	LEU
1	D	281	LEU
1	D	287	HIS
1	D	291	GLN
1	D	311	THR
1	D	313	GLU
1	D	318	THR
1	D	332	LYS
1	D	333	ASP
1	D	386	LEU
1	D	417	ARG
1	D	438	THR
1	D	441	LEU
1	D	467	THR
1	D	471	ILE
1	D	474	GLN
1	D	476	LEU
1	D	490	ASN
1	D	491	ASP
1	D	493	ARG
1	D	494	ASP
1	D	495	SER
1	D	496	LYS
1	D	499	GLN
1	D	505	THR
1	D	515	LEU
1	D	524	LEU
1	D	536	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	HIS
1	B	100	ASN
1	B	317	ASN
1	B	393	HIS
1	B	474	GLN
1	C	287	HIS
1	D	284	HIS
1	D	387	HIS
1	D	393	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 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
3	NAG	D	703	1	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
4	SO4	B	1544	-	4,4,4	0.22	0	6,6,6	0.31	0
3	NAG	B	701	1	14,14,15	0.47	0	17,19,21	2.24	5 (29%)
4	SO4	A	1545	-	4,4,4	0.23	0	6,6,6	0.16	0
2	4OJ	C	600	1	8,11,12	0.67	0	10,14,17	1.06	1 (10%)
3	NAG	D	701	1	14,14,15	0.54	0	17,19,21	1.26	2 (11%)
4	SO4	D	1544	-	4,4,4	0.26	0	6,6,6	0.29	0
2	4OJ	A	600	1	8,11,12	0.74	0	10,14,17	1.06	1 (10%)
4	SO4	A	1546	-	4,4,4	0.23	0	6,6,6	0.17	0
3	NAG	C	701	-	14,14,15	0.41	0	17,19,21	1.25	2 (11%)
4	SO4	A	1548	-	4,4,4	0.30	0	6,6,6	0.17	0
3	NAG	B	702	1	14,14,15	0.61	0	17,19,21	1.59	2 (11%)
4	SO4	D	1546	-	4,4,4	0.28	0	6,6,6	0.11	0
3	NAG	D	702	1	14,14,15	1.05	1 (7%)	17,19,21	2.03	5 (29%)
3	NAG	A	701	1	14,14,15	0.52	0	17,19,21	0.96	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	1544	-	4,4,4	0.27	0	6,6,6	0.12	0
4	SO4	B	1545	-	4,4,4	0.26	0	6,6,6	0.17	0
4	SO4	C	1546	-	4,4,4	0.28	0	6,6,6	0.38	0
4	SO4	D	1545	-	4,4,4	0.26	0	6,6,6	0.14	0
4	SO4	A	1547	-	4,4,4	0.24	0	6,6,6	0.24	0
2	4OJ	B	600	1	8,11,12	0.58	0	10,14,17	1.20	1 (10%)
4	SO4	C	1547	-	4,4,4	0.22	0	6,6,6	0.26	0
4	SO4	B	1546	-	4,4,4	0.24	0	6,6,6	0.11	0
2	4OJ	D	600	1	8,11,12	0.74	0	10,14,17	1.15	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4OJ	A	600	1	-	0/2/4/5	0/1/1/1
2	4OJ	B	600	1	-	0/2/4/5	0/1/1/1
3	NAG	D	702	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1
3	NAG	D	703	1	-	3/6/23/26	0/1/1/1
3	NAG	B	701	1	-	5/6/23/26	0/1/1/1
2	4OJ	C	600	1	-	0/2/4/5	0/1/1/1
2	4OJ	D	600	1	-	0/2/4/5	0/1/1/1
3	NAG	C	701	-	-	2/6/23/26	0/1/1/1
3	NAG	D	701	1	-	4/6/23/26	0/1/1/1
3	NAG	B	702	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	NAG	C1-C2	3.09	1.56	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	NAG	C1-O5-C5	5.10	119.03	112.19
3	D	702	NAG	C2-N2-C7	5.09	129.72	122.90
3	B	702	NAG	C1-O5-C5	4.48	118.19	112.19
3	B	701	NAG	C4-C3-C2	-3.94	105.24	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	NAG	O5-C1-C2	-3.74	105.51	111.29
3	D	701	NAG	C1-O5-C5	3.63	117.05	112.19
3	D	703	NAG	C1-O5-C5	3.59	117.00	112.19
3	B	701	NAG	C1-C2-N2	3.48	115.92	110.43
3	D	702	NAG	C1-O5-C5	3.34	116.67	112.19
3	D	702	NAG	O5-C1-C2	-3.32	106.16	111.29
3	B	701	NAG	C2-N2-C7	3.24	127.24	122.90
3	C	701	NAG	C1-O5-C5	3.19	116.46	112.19
2	D	600	4OJ	O12-C5-C6	2.80	120.93	118.49
2	B	600	4OJ	O12-C5-C6	2.67	120.81	118.49
2	C	600	4OJ	O12-C5-C6	2.55	120.70	118.49
3	B	702	NAG	O5-C1-C2	-2.51	107.40	111.29
3	D	702	NAG	C4-C3-C2	2.46	114.63	111.02
3	D	701	NAG	O5-C5-C6	2.37	112.27	107.66
2	A	600	4OJ	O12-C5-C6	2.31	120.50	118.49
3	A	701	NAG	O5-C1-C2	-2.29	107.75	111.29
3	D	702	NAG	O7-C7-C8	-2.24	118.07	122.05
3	A	701	NAG	C2-N2-C7	-2.23	119.91	122.90
3	C	701	NAG	C4-C3-C2	-2.08	107.97	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	702	NAG	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	NAG	C1-C2-N2-C7
3	B	701	NAG	C8-C7-N2-C2
3	B	701	NAG	O7-C7-N2-C2
3	B	702	NAG	C8-C7-N2-C2
3	B	702	NAG	O7-C7-N2-C2
3	D	702	NAG	C3-C2-N2-C7
3	D	702	NAG	C8-C7-N2-C2
3	D	702	NAG	O7-C7-N2-C2
3	A	701	NAG	C8-C7-N2-C2
3	A	701	NAG	O7-C7-N2-C2
3	D	703	NAG	C8-C7-N2-C2
3	D	703	NAG	O7-C7-N2-C2
3	D	701	NAG	O5-C5-C6-O6
3	B	701	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	D	701	NAG	C8-C7-N2-C2
3	C	701	NAG	C8-C7-N2-C2
3	C	701	NAG	O7-C7-N2-C2
3	D	701	NAG	O7-C7-N2-C2
3	B	702	NAG	C4-C5-C6-O6
3	D	701	NAG	C4-C5-C6-O6
3	D	703	NAG	O5-C5-C6-O6
3	D	702	NAG	O5-C5-C6-O6
3	B	701	NAG	C4-C5-C6-O6
3	B	702	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	NAG	1	0
4	A	1545	SO4	1	0
4	D	1544	SO4	1	0
2	A	600	4OJ	1	0
3	D	702	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	542/543 (99%)	-0.90	2 (0%) 88 81	16, 35, 75, 135	2 (0%)
1	B	539/543 (99%)	-0.66	1 (0%) 91 87	24, 61, 106, 152	0
1	C	540/543 (99%)	-0.97	0 100 100	13, 30, 71, 145	1 (0%)
1	D	540/543 (99%)	-0.89	2 (0%) 88 81	20, 43, 87, 123	1 (0%)
All	All	2161/2172 (99%)	-0.86	5 (0%) 91 87	13, 40, 94, 152	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	THR	2.6
1	B	286	TRP	2.5
1	D	297	PHE	2.4
1	D	286	TRP	2.3
1	A	498	PRO	2.2

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

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

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
3	NAG	D	703	14/15	0.62	0.15	115,127,131,133	0
3	NAG	C	701	14/15	0.66	0.16	102,104,105,106	14
3	NAG	B	702	14/15	0.67	0.12	61,97,104,106	0
3	NAG	D	702	14/15	0.69	0.13	84,92,95,96	0
3	NAG	B	701	14/15	0.78	0.11	85,91,95,97	0
4	SO4	B	1545	5/5	0.79	0.12	127,127,128,129	0
4	SO4	A	1548	5/5	0.84	0.14	120,121,122,123	0
3	NAG	A	701	14/15	0.84	0.09	102,113,115,115	0
3	NAG	D	701	14/15	0.86	0.10	91,100,105,108	0
4	SO4	D	1546	5/5	0.86	0.10	119,120,120,121	0
4	SO4	A	1545	5/5	0.89	0.10	113,113,115,117	0
4	SO4	B	1546	5/5	0.90	0.16	126,127,127,128	0
4	SO4	B	1544	5/5	0.90	0.07	79,84,85,85	0
4	SO4	D	1545	5/5	0.91	0.14	118,120,120,121	0
4	SO4	A	1546	5/5	0.91	0.12	112,112,112,114	0
5	CL	C	3002	1/1	0.91	0.14	57,57,57,57	0
5	CL	C	3001	1/1	0.92	0.07	57,57,57,57	0
5	CL	D	3001	1/1	0.92	0.06	54,54,54,54	0
4	SO4	C	1547	5/5	0.93	0.17	100,104,105,106	0
4	SO4	D	1544	5/5	0.94	0.08	63,64,65,69	0
4	SO4	A	1547	5/5	0.94	0.17	100,101,102,102	0
4	SO4	C	1546	5/5	0.95	0.07	63,65,66,69	0
4	SO4	A	1544	5/5	0.95	0.05	82,83,84,84	0
5	CL	D	3002	1/1	0.95	0.09	66,66,66,66	0
2	4OJ	D	600	11/12	0.97	0.12	32,61,73,73	0
5	CL	D	3000	1/1	0.97	0.07	61,61,61,61	0
5	CL	C	3000	1/1	0.98	0.04	44,44,44,44	0
2	4OJ	A	600	11/12	0.98	0.11	35,75,83,84	0
2	4OJ	B	600	11/12	0.98	0.11	35,78,84,86	0
2	4OJ	C	600	11/12	0.98	0.10	23,55,61,61	0
5	CL	C	1544	1/1	0.98	0.06	42,42,42,42	0
5	CL	C	1545	1/1	0.98	0.04	51,51,51,51	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.