



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 03:01 AM UTC

PDB ID : 2C44 / pdb_00002c44
Title : Crystal Structure of E. coli Tryptophanase
Authors : Ku, S.-Y.; Yip, P.; Howell, P.L.
Deposited on : 2005-10-15
Resolution : 2.80 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

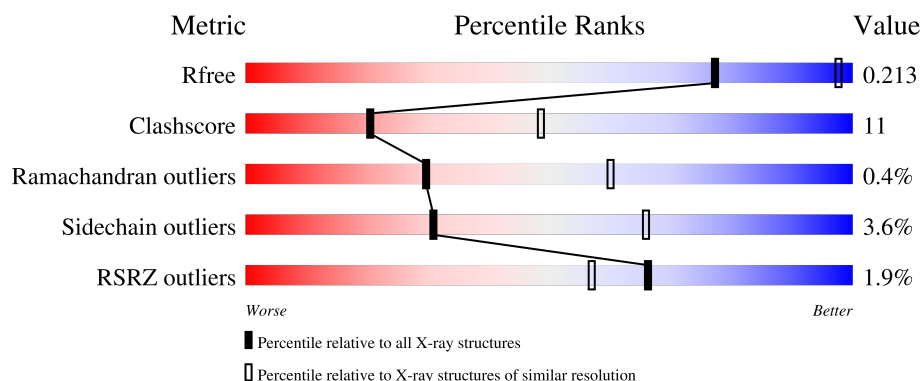
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	471	5% 75% 20% ..
1	B	471	76% 19% ..
1	C	471	76% 20% ..
1	D	471	5% 75% 19% ..

2 Entry composition [i](#)

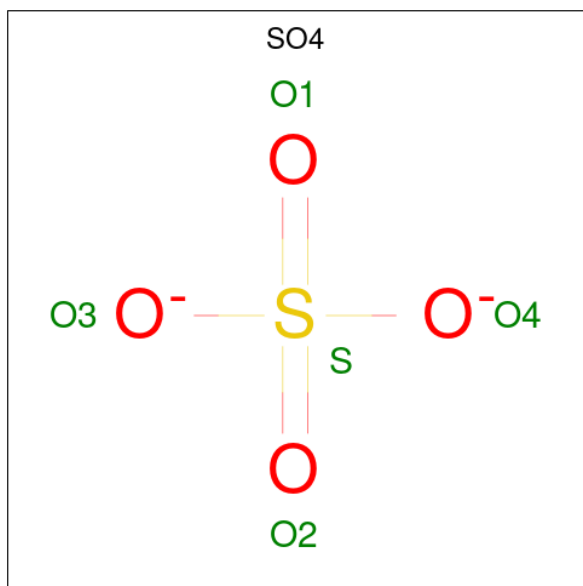
There are 4 unique types of molecules in this entry. The entry contains 14846 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRYPTOPHANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	1
			3570	2278	599	671	22			
1	B	467	Total	C	N	O	S	0	0	0
			3584	2288	604	670	22			
1	C	468	Total	C	N	O	S	0	0	0
			3584	2288	605	669	22			
1	D	467	Total	C	N	O	S	0	0	1
			3544	2258	598	666	22			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	K	0	0
			2	2		
3	B	1	Total	K	0	0
			1	1		
3	C	2	Total	K	0	0
			2	2		
3	D	1	Total	K	0	0
			1	1		

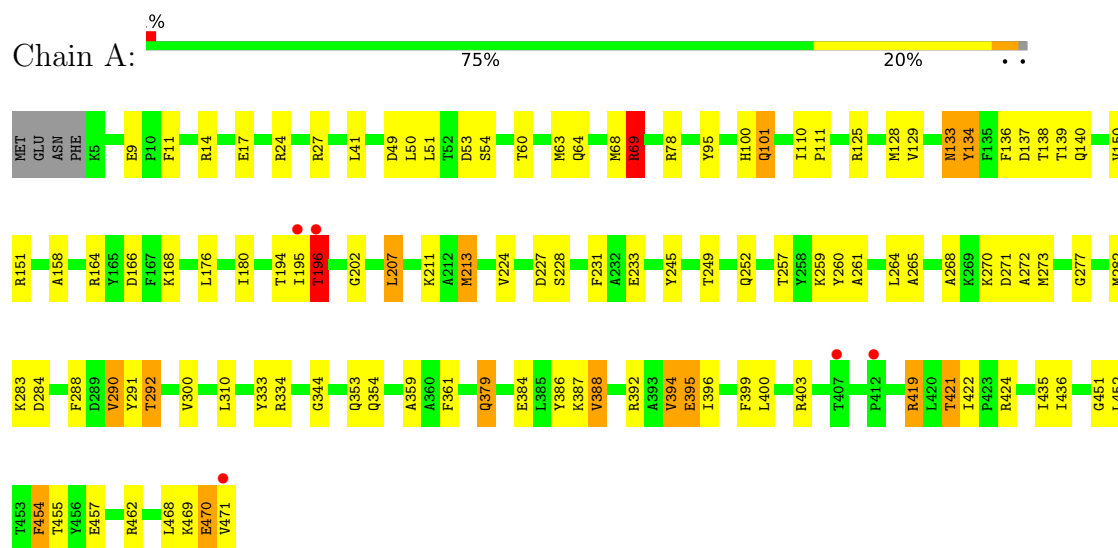
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		
4	B	143	Total	O	0	0
			143	143		
4	C	125	Total	O	0	0
			125	125		
4	D	120	Total	O	0	0
			120	120		

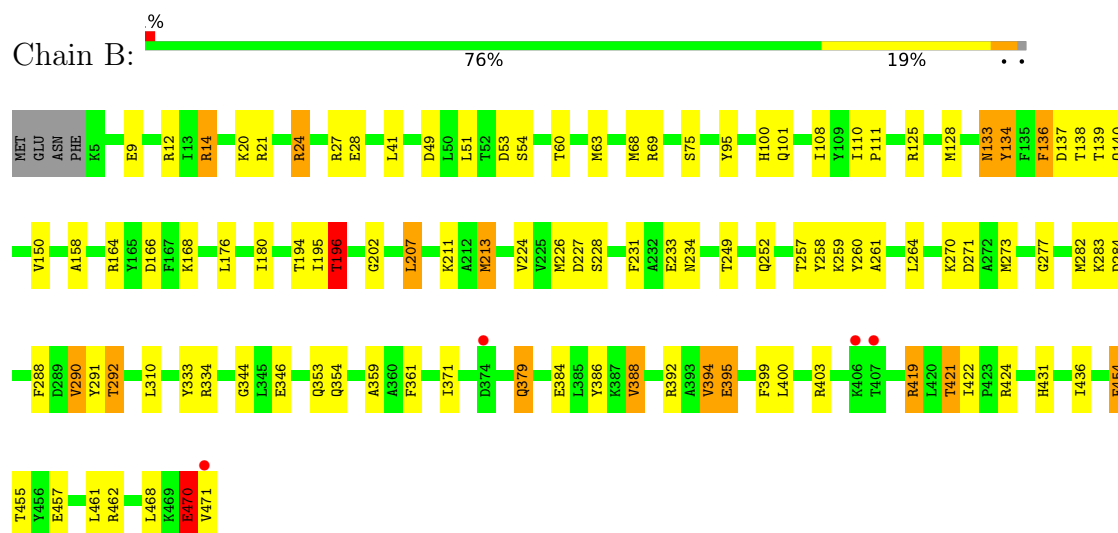
3 Residue-property plots

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.

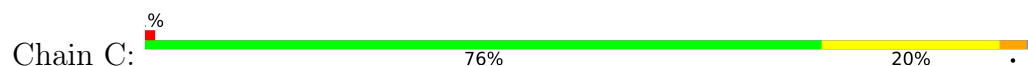
• Molecule 1: TRYPTOPHANASE

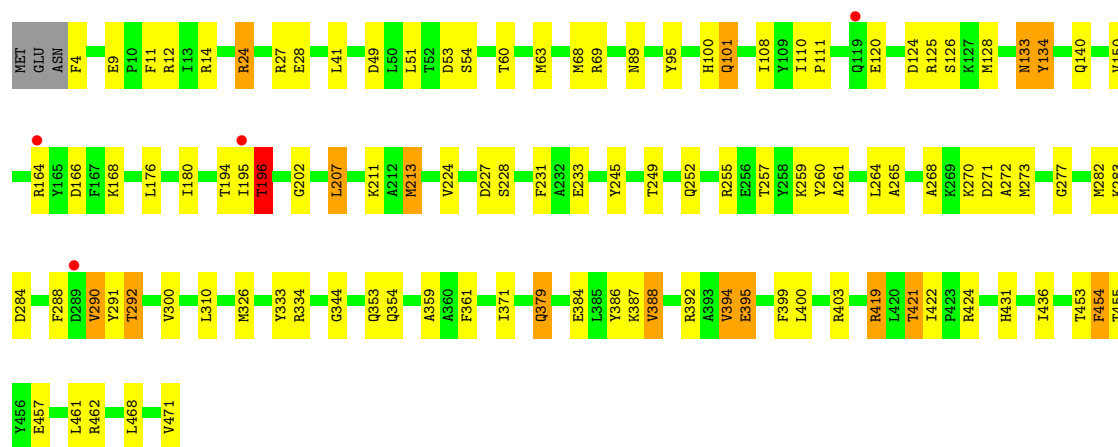


• Molecule 1: TRYPTOPHANASE

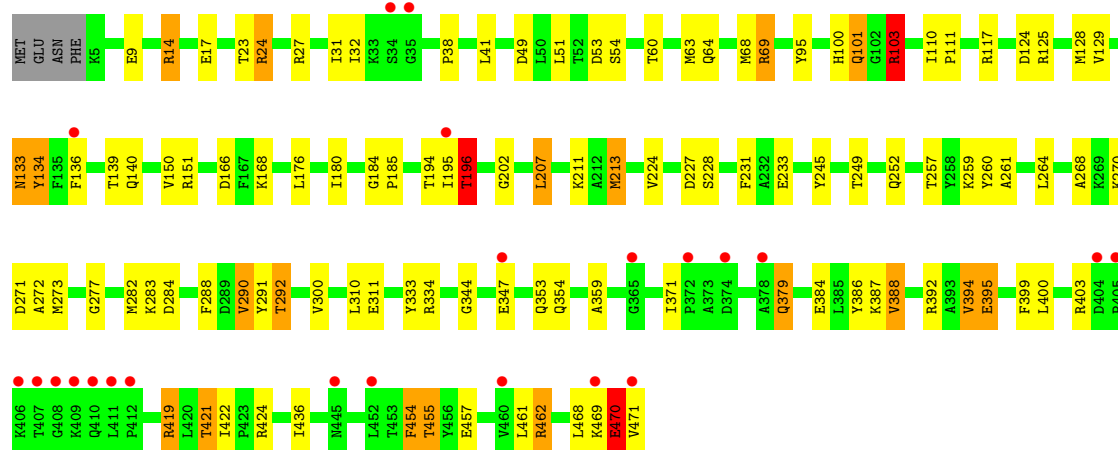
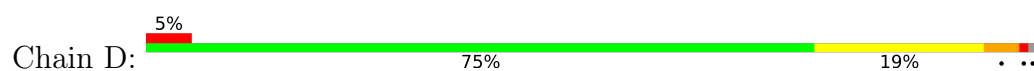


• Molecule 1: TRYPTOPHANASE





• Molecule 1: TRYPTOPHANASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	215.51Å 215.51Å 107.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.80 152.39 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.3 (500.00-2.80) 99.8 (152.39-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.64 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.196 , 0.220 0.192 , 0.213	Depositor DCC
R_{free} test set	3141 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14846	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: SO4, 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	0.44	1/3648 (0.0%)	1.04	21/4952 (0.4%)
1	B	0.41	0/3662	1.00	17/4967 (0.3%)
1	C	0.42	0/3662	1.01	17/4968 (0.3%)
1	D	0.44	1/3622 (0.0%)	1.05	25/4920 (0.5%)
All	All	0.43	2/14594 (0.0%)	1.02	80/19807 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	GLU	C-N	-5.75	1.25	1.33
1	D	470	GLU	C-N	-5.35	1.25	1.33

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	462	ARG	NE-CZ-NH2	11.72	129.75	119.20
1	D	462	ARG	NE-CZ-NH1	-10.79	110.72	121.50
1	A	69	ARG	NE-CZ-NH2	-10.75	109.53	119.20
1	A	24	ARG	NE-CZ-NH2	-10.24	109.98	119.20
1	A	69	ARG	CD-NE-CZ	10.02	138.43	124.40
1	A	24	ARG	CD-NE-CZ	9.58	137.82	124.40
1	A	455	THR	N-CA-C	-9.43	102.88	114.75
1	C	455	THR	N-CA-C	-9.31	103.02	114.75
1	D	455	THR	N-CA-C	-9.21	102.86	114.56
1	A	69	ARG	NE-CZ-NH1	9.06	130.56	121.50
1	B	455	THR	N-CA-C	-9.05	103.07	114.56
1	A	24	ARG	NE-CZ-NH1	8.73	130.23	121.50
1	D	103	ARG	NE-CZ-NH2	-8.67	111.40	119.20
1	B	228	SER	N-CA-C	8.35	122.78	112.59
1	D	462	ARG	CD-NE-CZ	8.28	135.99	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	SER	N-CA-C	8.26	122.66	112.59
1	D	388	VAL	N-CA-C	8.25	119.03	110.36
1	C	388	VAL	N-CA-C	8.17	118.27	110.42
1	D	228	SER	N-CA-C	8.02	122.37	112.59
1	A	228	SER	N-CA-C	7.93	122.26	112.59
1	A	388	VAL	N-CA-C	7.74	117.85	110.42
1	B	470	GLU	N-CA-C	7.65	120.91	110.35
1	D	103	ARG	NE-CZ-NH1	7.41	128.91	121.50
1	C	284	ASP	N-CA-C	7.28	117.62	108.45
1	B	388	VAL	N-CA-C	7.27	117.40	110.42
1	D	353	GLN	N-CA-C	-7.27	100.25	110.50
1	D	133	ASN	N-CA-C	-7.19	103.77	112.54
1	C	353	GLN	N-CA-C	-7.13	100.45	110.50
1	A	284	ASP	N-CA-C	7.08	117.37	108.45
1	C	462	ARG	N-CA-C	7.06	119.88	111.33
1	A	353	GLN	N-CA-C	-7.03	100.58	110.50
1	B	422	ILE	N-CA-C	7.01	114.49	107.55
1	D	284	ASP	N-CA-C	6.96	117.22	108.45
1	A	422	ILE	N-CA-C	6.91	114.39	107.55
1	C	422	ILE	N-CA-C	6.84	114.32	107.55
1	A	462	ARG	N-CA-C	6.82	119.58	111.33
1	B	166	ASP	N-CA-C	6.78	118.67	111.28
1	C	273	MET	N-CA-C	6.74	121.08	112.86
1	B	462	ARG	N-CA-C	6.74	119.48	111.33
1	A	166	ASP	N-CA-C	6.70	118.58	111.28
1	C	166	ASP	N-CA-C	6.69	118.57	111.28
1	B	353	GLN	N-CA-C	-6.68	101.07	110.50
1	A	133	ASN	N-CA-C	-6.63	104.45	112.54
1	B	273	MET	N-CA-C	6.61	120.93	112.86
1	C	133	ASN	N-CA-C	-6.57	104.53	112.54
1	D	422	ILE	N-CA-C	6.55	114.04	107.55
1	D	166	ASP	N-CA-C	6.54	118.41	111.28
1	D	462	ARG	N-CA-C	6.49	119.19	111.33
1	B	133	ASN	N-CA-C	-6.49	104.62	112.54
1	D	103	ARG	CD-NE-CZ	6.45	133.43	124.40
1	A	273	MET	N-CA-C	6.43	120.70	112.86
1	D	273	MET	N-CA-C	6.33	120.58	112.86
1	C	196	THR	N-CA-C	-6.28	97.43	110.80
1	D	196	THR	N-CA-C	-6.20	97.59	110.80
1	B	284	ASP	N-CA-C	6.16	117.23	108.74
1	C	259	LYS	N-CA-C	-6.09	105.81	113.18
1	B	196	THR	N-CA-C	-6.04	97.93	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	454	PHE	N-CA-C	6.04	118.56	110.35
1	B	454	PHE	N-CA-C	6.01	118.53	110.35
1	A	196	THR	N-CA-C	-5.99	98.04	110.80
1	B	136	PHE	N-CA-C	-5.93	102.70	110.53
1	B	259	LYS	N-CA-C	-5.88	106.07	113.18
1	A	259	LYS	N-CA-C	-5.84	106.12	113.18
1	D	259	LYS	N-CA-C	-5.80	106.16	113.18
1	A	454	PHE	N-CA-C	5.76	118.18	110.35
1	C	454	PHE	N-CA-C	5.75	118.17	110.35
1	C	101	GLN	N-CA-C	5.51	115.12	107.73
1	D	32	ILE	N-CA-C	-5.51	105.35	110.53
1	D	101	GLN	N-CA-C	5.31	114.85	107.73
1	C	371	ILE	N-CA-C	5.29	113.69	107.77
1	C	69	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	B	69	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	B	371	ILE	N-CA-C	5.14	113.52	107.77
1	D	69	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	D	371	ILE	CA-C-N	5.12	125.04	119.76
1	D	371	ILE	C-N-CA	5.12	125.04	119.76
1	A	101	GLN	N-CA-C	5.12	114.59	107.73
1	C	265	ALA	N-CA-C	-5.08	100.63	108.90
1	D	24	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	A	265	ALA	N-CA-C	-5.02	100.71	108.90

There are no chirality outliers.

There are no planarity outliers.

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	3570	0	3432	83	0
1	B	3584	0	3463	76	0
1	C	3584	0	3459	81	0
1	D	3544	0	3372	90	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	0	0	0
2	D	10	0	0	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	130	0	0	3	0
4	B	143	0	0	2	0
4	C	125	0	0	5	0
4	D	120	0	0	10	0
All	All	14846	0	13726	315	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 11.

All (315) 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:60:THR:H	1:B:63:MET:HE3	1.34	0.91
1:D:60:THR:H	1:D:63:MET:HE3	1.36	0.91
1:C:60:THR:H	1:C:63:MET:HE3	1.36	0.90
1:A:60:THR:H	1:A:63:MET:HE3	1.37	0.90
1:D:51:LEU:HD12	1:D:394:VAL:HG13	1.58	0.85
1:A:51:LEU:HD12	1:A:394:VAL:HG13	1.59	0.84
1:B:51:LEU:HD12	1:B:394:VAL:HG13	1.59	0.84
1:A:51:LEU:HB2	1:A:392:ARG:HD3	1.60	0.83
1:A:452:LEU:HD23	1:A:471:VAL:N	1.93	0.83
1:C:51:LEU:HD12	1:C:394:VAL:HG13	1.59	0.82
1:D:51:LEU:HB2	1:D:392:ARG:HD3	1.62	0.81
1:B:51:LEU:HB2	1:B:392:ARG:HD3	1.61	0.80
1:C:51:LEU:HB2	1:C:392:ARG:HD3	1.62	0.79
1:B:470:GLU:O	1:B:471:VAL:HG12	1.85	0.76
1:A:379:GLN:HG2	1:A:395:GLU:HG2	1.68	0.76
1:D:129:VAL:HG11	1:D:151:ARG:HD3	1.68	0.75
1:D:379:GLN:HG2	1:D:395:GLU:HG2	1.69	0.75
1:B:471:VAL:HG23	4:B:2061:HOH:O	1.87	0.75
1:C:379:GLN:HG2	1:C:395:GLU:HG2	1.70	0.73
1:B:379:GLN:HG2	1:B:395:GLU:HG2	1.70	0.72
1:A:359:ALA:HB2	1:A:421:THR:HA	1.73	0.70
1:B:60:THR:N	1:B:63:MET:HE3	2.06	0.70
1:D:136:PHE:HB2	1:D:139:THR:OG1	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:ALA:HB2	1:D:421:THR:HA	1.74	0.70
1:D:424:ARG:HD3	4:D:2115:HOH:O	1.90	0.70
1:C:60:THR:N	1:C:63:MET:HE3	2.07	0.70
1:A:60:THR:N	1:A:63:MET:HE3	2.08	0.69
1:B:359:ALA:HB2	1:B:421:THR:HA	1.73	0.69
1:C:359:ALA:HB2	1:C:421:THR:HA	1.74	0.69
1:D:213:MET:HE1	1:D:224:VAL:HG21	1.75	0.69
1:A:69:ARG:NH2	1:D:69:ARG:NH2	2.41	0.69
1:D:60:THR:N	1:D:63:MET:HE3	2.06	0.68
1:D:103:ARG:HD2	2:D:500:SO4:O2	1.95	0.66
1:C:213:MET:HE1	1:C:224:VAL:HG21	1.77	0.66
1:C:196:THR:HG21	4:C:2057:HOH:O	1.94	0.66
1:B:213:MET:HE1	1:B:224:VAL:HG21	1.78	0.66
1:A:69:ARG:NH2	1:D:69:ARG:HH22	1.94	0.66
1:A:69:ARG:HH21	1:D:69:ARG:HH22	1.44	0.65
1:B:419:ARG:HD3	1:B:421:THR:HG23	1.78	0.65
1:A:213:MET:HE1	1:A:224:VAL:HG21	1.78	0.65
1:D:419:ARG:HD3	1:D:421:THR:HG23	1.79	0.64
1:D:213:MET:HE1	1:D:224:VAL:CG2	2.28	0.64
1:C:419:ARG:HD3	1:C:421:THR:HG23	1.80	0.64
1:B:400:LEU:C	1:B:400:LEU:HD23	2.24	0.63
1:D:38:PRO:HA	4:D:2013:HOH:O	1.98	0.63
1:A:213:MET:HE1	1:A:224:VAL:CG2	2.29	0.63
1:A:419:ARG:HD3	1:A:421:THR:HG23	1.80	0.63
1:C:213:MET:HE1	1:C:224:VAL:CG2	2.29	0.62
1:C:195:ILE:O	1:C:196:THR:HB	2.00	0.62
1:D:136:PHE:HE1	1:D:194:THR:HG23	1.64	0.62
1:C:164:ARG:HG2	1:C:164:ARG:HH21	1.65	0.61
1:B:213:MET:HE1	1:B:224:VAL:CG2	2.30	0.61
1:C:400:LEU:HD23	1:C:400:LEU:C	2.25	0.61
1:B:195:ILE:O	1:B:196:THR:HB	2.00	0.60
1:A:400:LEU:HD23	1:A:400:LEU:C	2.26	0.59
1:D:49:ASP:OD2	1:D:392:ARG:HD2	2.03	0.59
1:D:264:LEU:C	1:D:264:LEU:HD12	2.28	0.59
1:D:400:LEU:C	1:D:400:LEU:HD23	2.27	0.58
1:D:38:PRO:HG3	4:D:2013:HOH:O	2.01	0.58
1:D:195:ILE:HG21	1:D:231:PHE:HA	1.86	0.58
1:A:195:ILE:O	1:A:196:THR:HB	2.04	0.57
1:A:49:ASP:OD2	1:A:392:ARG:HD2	2.04	0.57
1:C:24:ARG:O	1:C:28:GLU:HG2	2.04	0.57
1:C:24:ARG:HD2	1:C:28:GLU:OE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:THR:HG21	4:D:2066:HOH:O	2.04	0.57
1:B:195:ILE:HG21	1:B:231:PHE:HA	1.85	0.57
1:B:24:ARG:HD2	1:B:28:GLU:OE1	2.04	0.57
1:B:471:VAL:OXT	1:B:471:VAL:HG13	2.04	0.57
1:C:49:ASP:OD2	1:C:392:ARG:HD2	2.05	0.57
1:C:164:ARG:HG2	1:C:164:ARG:NH2	2.19	0.56
1:C:195:ILE:HG21	1:C:231:PHE:HA	1.86	0.56
1:C:277:GLY:HA2	1:C:310:LEU:HD21	1.87	0.56
1:B:264:LEU:C	1:B:264:LEU:HD12	2.31	0.56
1:B:49:ASP:OD2	1:B:392:ARG:HD2	2.05	0.56
1:D:100:HIS:CD2	1:D:101:GLN:HG2	2.41	0.56
1:C:264:LEU:HD12	1:C:264:LEU:C	2.31	0.55
1:C:53:ASP:OD2	1:C:424:ARG:NH2	2.39	0.55
1:D:195:ILE:CG2	1:D:231:PHE:HA	2.36	0.55
1:D:53:ASP:OD2	1:D:424:ARG:NH2	2.40	0.55
1:A:195:ILE:HG21	1:A:231:PHE:HA	1.87	0.55
1:B:195:ILE:CG2	1:B:231:PHE:HA	2.37	0.55
1:A:110:ILE:HB	1:A:111:PRO:HD3	1.89	0.55
1:B:54:SER:HB2	1:B:270:LYS:HE3	1.89	0.55
1:B:100:HIS:CD2	1:B:101:GLN:HG2	2.42	0.55
1:D:277:GLY:HA2	1:D:310:LEU:HD21	1.89	0.55
1:D:195:ILE:O	1:D:196:THR:HB	2.05	0.54
1:A:264:LEU:C	1:A:264:LEU:HD12	2.31	0.54
1:D:110:ILE:HB	1:D:111:PRO:HD3	1.90	0.54
1:A:133:ASN:O	1:A:134:TYR:HB2	2.07	0.54
1:A:54:SER:HB2	1:A:270:LYS:HE3	1.90	0.54
1:C:195:ILE:CG2	1:C:231:PHE:HA	2.37	0.54
1:C:395:GLU:CD	1:C:399:PHE:HB3	2.32	0.54
1:B:110:ILE:HB	1:B:111:PRO:HD3	1.89	0.53
1:B:395:GLU:CD	1:B:399:PHE:HB3	2.32	0.53
1:A:195:ILE:CG2	1:A:231:PHE:HA	2.38	0.53
1:B:133:ASN:O	1:B:134:TYR:HB2	2.08	0.53
1:C:453:THR:CG2	1:C:471:VAL:HG12	2.38	0.53
1:A:233:GLU:HG3	1:A:271:ASP:OD2	2.08	0.53
1:C:54:SER:HB2	1:C:270:LYS:HE3	1.90	0.53
1:A:100:HIS:CD2	1:A:101:GLN:HG2	2.43	0.53
1:A:395:GLU:CD	1:A:399:PHE:HB3	2.33	0.53
1:D:133:ASN:O	1:D:134:TYR:HB2	2.08	0.53
1:C:110:ILE:HB	1:C:111:PRO:HD3	1.90	0.52
1:B:277:GLY:HA2	1:B:310:LEU:HD21	1.90	0.52
1:A:277:GLY:HA2	1:A:310:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ALA:CB	1:A:421:THR:HA	2.39	0.52
1:D:31:ILE:CD1	4:D:2013:HOH:O	2.57	0.52
1:D:233:GLU:HG3	1:D:271:ASP:OD2	2.09	0.52
1:C:100:HIS:CD2	1:C:101:GLN:HG2	2.44	0.52
1:D:38:PRO:CA	4:D:2013:HOH:O	2.55	0.52
1:D:468:LEU:HD12	1:D:468:LEU:N	2.24	0.52
1:A:53:ASP:OD2	1:A:424:ARG:NH2	2.43	0.52
1:D:344:GLY:HA3	1:D:436:ILE:HD13	1.92	0.52
1:A:344:GLY:HA3	1:A:436:ILE:HD13	1.91	0.51
1:B:53:ASP:OD2	1:B:424:ARG:NH2	2.44	0.51
1:C:133:ASN:O	1:C:134:TYR:HB2	2.10	0.51
1:D:23:THR:HA	4:D:2010:HOH:O	2.10	0.51
1:D:51:LEU:CD1	1:D:394:VAL:HG13	2.38	0.51
1:D:419:ARG:HD3	1:D:421:THR:OG1	2.11	0.51
1:D:395:GLU:CD	1:D:399:PHE:HB3	2.35	0.51
1:B:359:ALA:CB	1:B:421:THR:HA	2.40	0.51
1:C:233:GLU:HG3	1:C:271:ASP:OD2	2.10	0.51
1:A:468:LEU:N	1:A:468:LEU:HD12	2.26	0.51
1:D:54:SER:HB2	1:D:270:LYS:HE3	1.93	0.51
1:D:359:ALA:CB	1:D:421:THR:HA	2.39	0.51
1:B:468:LEU:HD12	1:B:468:LEU:N	2.26	0.50
1:D:249:THR:OG1	1:D:252:GLN:HG3	2.12	0.50
1:C:468:LEU:N	1:C:468:LEU:HD12	2.26	0.50
1:D:344:GLY:O	1:D:347:GLU:CG	2.60	0.50
1:B:334:ARG:HH21	1:B:424:ARG:NH1	2.09	0.50
1:D:469:LYS:HG2	1:D:470:GLU:H	1.76	0.50
1:A:9:GLU:HG3	1:A:333:TYR:CZ	2.47	0.50
1:C:125:ARG:HA	1:C:128:MET:HE2	1.94	0.50
1:B:95:TYR:HB3	1:B:291:TYR:CD2	2.47	0.49
1:C:359:ALA:CB	1:C:421:THR:HA	2.40	0.49
1:B:233:GLU:HG3	1:B:271:ASP:OD2	2.12	0.49
1:B:346:GLU:HG3	4:B:2104:HOH:O	2.13	0.49
1:A:140:GLN:HG3	1:A:150:VAL:HG21	1.95	0.49
1:B:51:LEU:CD1	1:B:394:VAL:HG13	2.39	0.49
1:B:68:MET:HE1	1:D:68:MET:HE1	1.94	0.49
1:A:249:THR:OG1	1:A:252:GLN:HG3	2.13	0.49
1:B:125:ARG:HA	1:B:128:MET:HE2	1.94	0.49
1:B:164:ARG:HA	1:B:354:GLN:OE1	2.13	0.48
1:D:41:LEU:HD11	4:D:2013:HOH:O	2.13	0.48
1:C:461:LEU:HD12	1:D:300:VAL:HG22	1.96	0.48
1:D:9:GLU:HG3	1:D:333:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:GLU:HA	4:D:2090:HOH:O	2.13	0.48
1:C:9:GLU:HG3	1:C:333:TYR:CZ	2.49	0.48
1:C:140:GLN:HG3	1:C:150:VAL:HG21	1.96	0.48
1:D:419:ARG:HD3	1:D:421:THR:CG2	2.43	0.48
1:D:455:THR:HG21	1:D:469:LYS:HB2	1.95	0.48
1:A:68:MET:HE3	1:D:64:GLN:HG2	1.96	0.48
1:B:261:ALA:O	1:B:283:LYS:HE3	2.13	0.48
1:D:124:ASP:HA	4:D:2045:HOH:O	2.12	0.48
1:C:51:LEU:CD1	1:C:394:VAL:HG13	2.39	0.48
1:A:196:THR:HG21	4:A:2113:HOH:O	2.14	0.48
1:A:207:LEU:HD11	1:A:257:THR:HA	1.95	0.48
1:C:344:GLY:HA3	1:C:436:ILE:HD13	1.95	0.48
1:A:68:MET:HE1	1:C:68:MET:HE1	1.96	0.48
1:B:140:GLN:HG3	1:B:150:VAL:HG21	1.96	0.47
1:B:344:GLY:HA3	1:B:436:ILE:HD13	1.94	0.47
1:B:400:LEU:HD23	1:B:400:LEU:O	2.14	0.47
1:C:261:ALA:O	1:C:283:LYS:HE3	2.14	0.47
1:D:261:ALA:O	1:D:283:LYS:HE3	2.13	0.47
1:C:207:LEU:HD11	1:C:257:THR:HA	1.96	0.47
1:A:78:ARG:NH1	4:A:2032:HOH:O	2.47	0.47
1:B:12:ARG:HH11	1:D:17:GLU:CD	2.23	0.47
1:B:207:LEU:HD11	1:B:257:THR:HA	1.96	0.47
1:D:344:GLY:O	1:D:347:GLU:HG3	2.14	0.47
1:A:419:ARG:HD3	1:A:421:THR:OG1	2.15	0.47
1:B:211:LYS:HG2	1:B:260:TYR:CZ	2.50	0.47
1:C:95:TYR:HB3	1:C:291:TYR:CD2	2.50	0.47
1:C:334:ARG:HH21	1:C:424:ARG:NH1	2.13	0.47
1:D:140:GLN:HG3	1:D:150:VAL:HG21	1.97	0.47
1:D:207:LEU:HD11	1:D:257:THR:HA	1.97	0.47
1:A:334:ARG:HH21	1:A:424:ARG:NH1	2.13	0.47
1:A:419:ARG:HD3	1:A:421:THR:CG2	2.45	0.47
1:C:211:LYS:HG2	1:C:260:TYR:CZ	2.49	0.47
1:A:17:GLU:CD	1:C:12:ARG:HH11	2.23	0.46
1:B:9:GLU:HG3	1:B:333:TYR:CZ	2.49	0.46
1:B:431:HIS:CE1	1:D:9:GLU:HB2	2.50	0.46
1:B:249:THR:OG1	1:B:252:GLN:HG3	2.15	0.46
1:B:419:ARG:HD3	1:B:421:THR:OG1	2.16	0.46
1:D:196:THR:HG23	1:D:202:GLY:HA2	1.98	0.46
1:A:27:ARG:HG2	1:A:386:TYR:CZ	2.51	0.46
1:C:419:ARG:HD3	1:C:421:THR:OG1	2.15	0.46
1:A:125:ARG:HA	1:A:128:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LYS:HE3	1:C:354:GLN:OE1	2.16	0.46
1:C:249:THR:OG1	1:C:252:GLN:HG3	2.15	0.46
1:A:261:ALA:O	1:A:283:LYS:HE3	2.14	0.46
1:D:400:LEU:HD23	1:D:400:LEU:O	2.16	0.46
1:A:400:LEU:HD23	1:A:400:LEU:O	2.16	0.45
1:A:95:TYR:HB3	1:A:291:TYR:CD2	2.51	0.45
1:A:300:VAL:HG22	1:B:461:LEU:HD12	1.98	0.45
1:D:27:ARG:NH1	1:D:387:LYS:O	2.39	0.45
1:A:129:VAL:HG11	1:A:151:ARG:HG3	1.98	0.45
1:A:195:ILE:HD13	1:A:195:ILE:HA	1.75	0.45
1:A:136:PHE:HB2	1:A:139:THR:OG1	2.17	0.45
1:C:400:LEU:HD23	1:C:400:LEU:O	2.16	0.45
1:D:384:GLU:O	1:D:388:VAL:HG23	2.16	0.45
1:C:89:ASN:O	1:C:255:ARG:NH2	2.50	0.45
1:D:41:LEU:O	1:D:392:ARG:NH2	2.50	0.45
1:C:4:PHE:N	4:C:2001:HOH:O	2.49	0.45
1:A:469:LYS:O	1:A:470:GLU:HB3	2.17	0.45
1:B:288:PHE:O	1:B:292:THR:HG23	2.17	0.45
1:D:288:PHE:O	1:D:292:THR:HG23	2.17	0.45
1:A:27:ARG:NH1	1:A:387:LYS:O	2.48	0.45
1:A:288:PHE:O	1:A:292:THR:HG23	2.16	0.44
1:B:176:LEU:O	1:B:180:ILE:HG13	2.17	0.44
1:A:41:LEU:O	1:A:392:ARG:NH2	2.51	0.44
1:A:64:GLN:HG2	1:D:68:MET:HE3	1.99	0.44
1:A:69:ARG:HH21	1:D:69:ARG:NH2	2.08	0.44
1:A:164:ARG:HA	1:A:354:GLN:OE1	2.17	0.44
1:A:168:LYS:HE3	1:A:354:GLN:OE1	2.17	0.44
1:A:196:THR:HG23	1:A:202:GLY:HA2	2.00	0.44
1:A:395:GLU:O	1:A:396:ILE:HD13	2.17	0.44
1:B:282:MET:HE2	1:B:290:VAL:HG23	1.99	0.44
1:D:282:MET:HE2	1:D:290:VAL:HG23	1.99	0.44
1:B:403:ARG:NH1	1:B:457:GLU:OE2	2.51	0.44
1:D:211:LYS:HG2	1:D:260:TYR:CZ	2.51	0.44
1:D:334:ARG:HH21	1:D:424:ARG:NH1	2.16	0.44
1:B:20:LYS:HG2	1:B:21:ARG:N	2.32	0.44
1:B:419:ARG:HD3	1:B:421:THR:CG2	2.44	0.44
1:C:282:MET:HE2	1:C:290:VAL:HG23	1.99	0.44
1:C:288:PHE:O	1:C:292:THR:HG23	2.18	0.44
1:C:300:VAL:HG22	1:D:461:LEU:HD12	1.99	0.44
1:C:419:ARG:HD3	1:C:421:THR:CG2	2.46	0.44
1:D:27:ARG:HG2	1:D:386:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:PHE:CD2	1:A:457:GLU:HB2	2.53	0.44
1:D:454:PHE:CD2	1:D:457:GLU:HB2	2.53	0.44
1:C:288:PHE:O	1:C:291:TYR:HB3	2.17	0.44
1:D:95:TYR:HB3	1:D:291:TYR:CD2	2.52	0.44
1:B:196:THR:HG23	1:B:202:GLY:HA2	2.00	0.43
1:C:403:ARG:NH1	1:C:457:GLU:OE2	2.51	0.43
1:C:453:THR:HG22	1:C:471:VAL:HG12	1.99	0.43
1:C:124:ASP:OD1	1:C:126:SER:OG	2.30	0.43
1:C:27:ARG:NH1	1:C:387:LYS:O	2.44	0.43
1:C:384:GLU:O	1:C:388:VAL:HG23	2.18	0.43
1:D:125:ARG:HA	1:D:128:MET:HE2	1.99	0.43
1:B:168:LYS:HE3	1:B:354:GLN:OE1	2.19	0.43
1:B:41:LEU:O	1:B:392:ARG:NH2	2.52	0.43
1:B:137:ASP:OD2	1:B:138:THR:N	2.52	0.43
1:C:27:ARG:HG2	1:C:386:TYR:CZ	2.54	0.43
1:D:403:ARG:NH1	1:D:457:GLU:OE2	2.52	0.43
1:A:9:GLU:HB2	1:C:431:HIS:CE1	2.54	0.43
1:A:60:THR:HG23	1:A:63:MET:CE	2.49	0.43
1:A:137:ASP:OD2	1:A:138:THR:N	2.52	0.43
1:A:282:MET:HE2	1:A:290:VAL:HG23	2.00	0.42
1:A:403:ARG:NH1	1:A:457:GLU:OE2	2.52	0.42
1:B:136:PHE:HB2	1:B:139:THR:OG1	2.18	0.42
1:A:207:LEU:HD23	1:A:245:TYR:CZ	2.54	0.42
1:A:361:PHE:CE2	1:A:419:ARG:HG3	2.55	0.42
1:B:384:GLU:O	1:B:388:VAL:HG23	2.18	0.42
1:C:454:PHE:CD2	1:C:457:GLU:HB2	2.54	0.42
1:A:268:ALA:O	1:A:272:ALA:HB3	2.18	0.42
1:B:194:THR:HA	1:B:227:ASP:HB3	2.01	0.42
1:C:268:ALA:O	1:C:272:ALA:HB3	2.19	0.42
1:A:158:ALA:HA	1:A:168:LYS:HB3	2.02	0.42
1:D:176:LEU:O	1:D:180:ILE:HG13	2.19	0.42
1:A:51:LEU:CD1	1:A:394:VAL:HG13	2.38	0.42
1:A:211:LYS:HG2	1:A:260:TYR:CZ	2.53	0.42
1:A:50:LEU:HD11	1:A:435:ILE:HD13	2.02	0.42
1:A:451:GLY:O	1:A:470:GLU:HG2	2.20	0.42
1:B:195:ILE:HD13	1:B:195:ILE:HA	1.76	0.42
1:C:176:LEU:O	1:C:180:ILE:HG13	2.20	0.42
1:D:344:GLY:O	1:D:347:GLU:HG2	2.20	0.42
1:C:95:TYR:HA	4:C:2038:HOH:O	2.20	0.42
1:D:268:ALA:O	1:D:272:ALA:HB3	2.20	0.42
1:A:469:LYS:O	1:A:471:VAL:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:PHE:CE2	1:B:419:ARG:HG3	2.55	0.41
1:C:125:ARG:CA	1:C:128:MET:HE2	2.50	0.41
1:D:49:ASP:OD2	1:D:392:ARG:CD	2.68	0.41
1:D:168:LYS:HE3	1:D:354:GLN:OE1	2.20	0.41
1:B:361:PHE:CZ	1:B:419:ARG:HG3	2.55	0.41
1:A:194:THR:HA	1:A:227:ASP:HB3	2.01	0.41
1:C:164:ARG:HA	1:C:354:GLN:OE1	2.20	0.41
1:C:196:THR:HG23	1:C:202:GLY:HA2	2.02	0.41
1:D:469:LYS:HG2	1:D:470:GLU:N	2.35	0.41
1:D:469:LYS:O	1:D:471:VAL:N	2.53	0.41
1:A:361:PHE:CZ	1:A:419:ARG:HG3	2.56	0.41
1:C:120:GLU:CB	4:C:2041:HOH:O	2.69	0.41
1:D:194:THR:HA	1:D:227:ASP:HB3	2.02	0.41
1:B:14:ARG:NE	1:B:14:ARG:HA	2.35	0.41
1:C:41:LEU:O	1:C:392:ARG:NH2	2.53	0.41
1:C:207:LEU:HD23	1:C:245:TYR:CZ	2.56	0.41
1:D:207:LEU:HD23	1:D:245:TYR:CZ	2.55	0.41
1:A:9:GLU:C	1:A:11:PHE:H	2.28	0.41
1:A:49:ASP:OD2	1:A:392:ARG:CD	2.69	0.41
1:A:452:LEU:CD2	1:A:471:VAL:N	2.76	0.41
1:C:326:MET:HE3	4:C:2063:HOH:O	2.19	0.41
1:B:27:ARG:HG2	1:B:386:TYR:CZ	2.56	0.41
1:B:158:ALA:HA	1:B:168:LYS:HB3	2.02	0.41
1:B:288:PHE:O	1:B:291:TYR:HB3	2.20	0.41
1:B:400:LEU:C	1:B:400:LEU:CD2	2.93	0.41
1:B:454:PHE:CD2	1:B:457:GLU:HB2	2.56	0.41
1:C:60:THR:OG1	1:C:63:MET:HG3	2.21	0.41
1:C:211:LYS:HE2	1:C:260:TYR:OH	2.21	0.41
1:C:361:PHE:CZ	1:C:419:ARG:HG3	2.56	0.41
1:C:361:PHE:CE2	1:C:419:ARG:HG3	2.56	0.41
1:C:9:GLU:C	1:C:11:PHE:H	2.28	0.41
1:D:14:ARG:HA	1:D:14:ARG:NE	2.36	0.41
1:D:117:ARG:HG3	1:D:117:ARG:HH11	1.86	0.41
1:D:288:PHE:O	1:D:291:TYR:HB3	2.21	0.41
1:B:108:ILE:O	1:B:111:PRO:HD2	2.22	0.40
1:C:108:ILE:O	1:C:111:PRO:HD2	2.21	0.40
1:A:176:LEU:O	1:A:180:ILE:HG13	2.20	0.40
1:A:384:GLU:O	1:A:388:VAL:HG23	2.20	0.40
1:B:195:ILE:HG23	1:B:234:ASN:CB	2.52	0.40
1:B:211:LYS:HE2	1:B:260:TYR:OH	2.22	0.40
1:C:194:THR:HA	1:C:227:ASP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2013:HOH:O	1:B:75:SER:HB3	2.21	0.40
1:B:125:ARG:CA	1:B:128:MET:HE2	2.52	0.40
1:D:184:GLY:HA2	1:D:185:PRO:HD2	1.95	0.40
1:B:226:MET:HG2	1:B:258:TYR:CE1	2.57	0.40
1:C:195:ILE:HD13	1:C:195:ILE:HA	1.76	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	465/471 (99%)	441 (95%)	22 (5%)	2 (0%)	30	60
1	B	465/471 (99%)	446 (96%)	17 (4%)	2 (0%)	30	60
1	C	466/471 (99%)	445 (96%)	19 (4%)	2 (0%)	30	60
1	D	465/471 (99%)	442 (95%)	21 (4%)	2 (0%)	30	60
All	All	1861/1884 (99%)	1774 (95%)	79 (4%)	8 (0%)	30	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	TYR
1	B	134	TYR
1	C	134	TYR
1	D	134	TYR
1	B	196	THR
1	C	196	THR
1	A	196	THR
1	D	196	THR

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	360/391 (92%)	348 (97%)	12 (3%)	33	69
1	B	362/391 (93%)	349 (96%)	13 (4%)	31	66
1	C	361/391 (92%)	349 (97%)	12 (3%)	33	69
1	D	352/391 (90%)	337 (96%)	15 (4%)	26	60
All	All	1435/1564 (92%)	1383 (96%)	52 (4%)	31	66

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	69	ARG
1	A	196	THR
1	A	207	LEU
1	A	213	MET
1	A	290	VAL
1	A	292	THR
1	A	379	GLN
1	A	394	VAL
1	A	395	GLU
1	A	419	ARG
1	A	421	THR
1	B	14	ARG
1	B	24	ARG
1	B	196	THR
1	B	207	LEU
1	B	213	MET
1	B	290	VAL
1	B	292	THR
1	B	379	GLN
1	B	394	VAL
1	B	395	GLU
1	B	419	ARG
1	B	421	THR

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Mol	Chain	Res	Type
1	B	470	GLU
1	C	14	ARG
1	C	24	ARG
1	C	196	THR
1	C	207	LEU
1	C	213	MET
1	C	290	VAL
1	C	292	THR
1	C	379	GLN
1	C	394	VAL
1	C	395	GLU
1	C	419	ARG
1	C	421	THR
1	D	14	ARG
1	D	24	ARG
1	D	103	ARG
1	D	196	THR
1	D	207	LEU
1	D	213	MET
1	D	290	VAL
1	D	292	THR
1	D	379	GLN
1	D	394	VAL
1	D	395	GLU
1	D	419	ARG
1	D	421	THR
1	D	462	ARG
1	D	470	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	301	GLN
1	A	337	GLN
1	A	339	GLN
1	A	379	GLN
1	A	441	HIS
1	A	448	ASN
1	B	301	GLN
1	B	339	GLN
1	B	379	GLN

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Mol	Chain	Res	Type
1	B	441	HIS
1	B	448	ASN
1	C	64	GLN
1	C	339	GLN
1	C	379	GLN
1	C	441	HIS
1	C	448	ASN
1	D	101	GLN
1	D	339	GLN
1	D	379	GLN
1	D	441	HIS
1	D	448	ASN

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 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	$\# Z > 2$
2	SO4	C	501	-	4,4,4	1.11	0	6,6,6	1.28	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	500	-	4,4,4	1.18	0	6,6,6	1.28	1 (16%)
2	SO4	B	501	-	4,4,4	1.16	0	6,6,6	1.30	1 (16%)
2	SO4	A	501	-	4,4,4	1.20	0	6,6,6	1.30	1 (16%)
2	SO4	D	501	-	4,4,4	1.08	0	6,6,6	1.29	1 (16%)
2	SO4	B	500	-	4,4,4	1.12	0	6,6,6	1.30	1 (16%)
2	SO4	C	500	-	4,4,4	1.19	0	6,6,6	1.26	1 (16%)
2	SO4	D	500	-	4,4,4	1.15	0	6,6,6	1.33	1 (16%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	SO4	O4-S-O3	2.92	124.63	108.54
2	B	501	SO4	O4-S-O3	2.86	124.32	108.54
2	B	500	SO4	O4-S-O3	2.86	124.31	108.54
2	A	501	SO4	O4-S-O3	2.85	124.28	108.54
2	C	501	SO4	O4-S-O3	2.83	124.12	108.54
2	D	501	SO4	O4-S-O3	2.82	124.11	108.54
2	A	500	SO4	O4-S-O3	2.80	124.00	108.54
2	C	500	SO4	O4-S-O3	2.77	123.80	108.54

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
2	D	500	SO4	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	467/471 (99%)	-0.25	5 (1%) 78 70	6, 12, 24, 35	0
1	B	467/471 (99%)	-0.17	4 (0%) 81 74	6, 12, 24, 34	0
1	C	468/471 (99%)	-0.21	4 (0%) 81 74	6, 13, 24, 35	0
1	D	467/471 (99%)	0.07	23 (4%) 35 27	6, 12, 25, 36	0
All	All	1869/1884 (99%)	-0.14	36 (1%) 66 57	6, 12, 24, 36	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	VAL	11.3
1	D	471	VAL	6.3
1	D	374	ASP	3.7
1	D	407	THR	3.3
1	D	409	LYS	3.1
1	D	412	PRO	3.0
1	A	407	THR	2.9
1	B	374	ASP	2.9
1	D	405	PRO	2.9
1	D	410	GLN	2.7
1	B	471	VAL	2.7
1	D	136	PHE	2.7
1	B	407	THR	2.6
1	D	347	GLU	2.6
1	C	289	ASP	2.6
1	A	412	PRO	2.5
1	D	365	GLY	2.5
1	C	119	GLN	2.5
1	D	460	VAL	2.5
1	D	195	ILE	2.5
1	D	469	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	164	ARG	2.4
1	A	195	ILE	2.4
1	D	408	GLY	2.3
1	D	372	PRO	2.3
1	D	378	ALA	2.2
1	B	406	LYS	2.2
1	D	406	LYS	2.2
1	D	404	ASP	2.2
1	D	445	ASN	2.2
1	D	452	LEU	2.1
1	C	195	ILE	2.1
1	D	35	GLY	2.1
1	D	411	LEU	2.1
1	D	34	SER	2.0
1	A	196	THR	2.0

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($\text{\AA}^2$)	Q<0.9
2	SO4	D	501	5/5	0.93	0.13	50,51,53,56	0
2	SO4	B	501	5/5	0.97	0.10	25,28,30,32	0
2	SO4	C	501	5/5	0.97	0.10	22,25,30,31	0
2	SO4	A	501	5/5	0.97	0.12	23,24,26,33	0
3	K	A	1472	1/1	0.97	0.03	19,19,19,19	0
3	K	B	1472	1/1	0.97	0.04	27,27,27,27	0
3	K	C	1473	1/1	0.97	0.05	19,19,19,19	0
3	K	D	1471	1/1	0.97	0.04	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	500	5/5	0.98	0.07	11,14,16,17	0
2	SO4	B	500	5/5	0.98	0.06	22,24,25,26	0
3	K	C	1472	1/1	0.98	0.05	13,13,13,13	0
2	SO4	A	500	5/5	0.98	0.07	11,11,15,15	0
3	K	A	1471	1/1	0.98	0.05	18,18,18,18	0
2	SO4	D	500	5/5	0.99	0.06	11,16,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.