



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:24 PM UTC

PDB ID : 3UYS / pdb_00003uys
Title : Crystal structure of apo human ck1d
Authors : Huang, X.
Deposited on : 2011-12-06
Resolution : 2.30 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

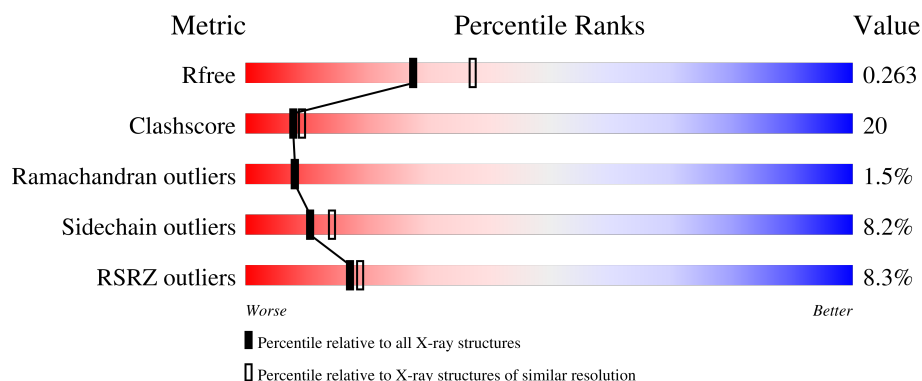
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	296	 8% 59% 29% 6% • 5%
1	B	296	 8% 56% 30% 5% • 6%
1	C	296	 7% 62% 30% • •
1	D	296	 9% 54% 35% 7% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9619 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.

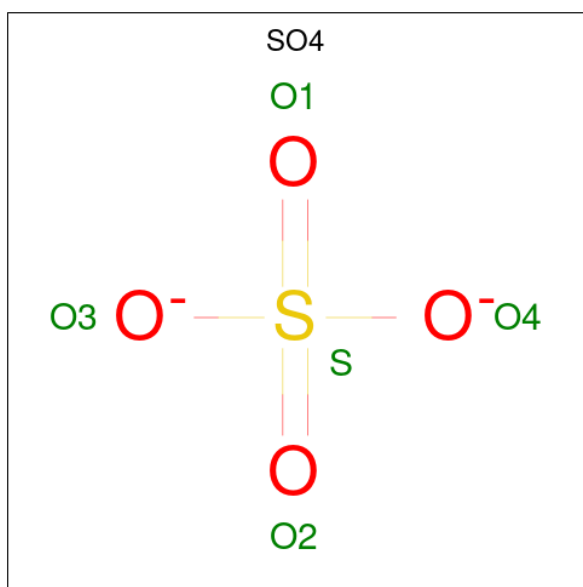
- Molecule 1 is a protein called Casein kinase I isoform delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2271	1459	390	408	14			
1	B	279	Total	C	N	O	S	0	0	0
			2267	1454	394	405	14			
1	C	286	Total	C	N	O	S	0	0	0
			2265	1454	388	409	14			
1	D	284	Total	C	N	O	S	0	0	0
			2293	1471	396	412	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P48730
A	0	SER	-	expression tag	UNP P48730
B	-1	GLY	-	expression tag	UNP P48730
B	0	SER	-	expression tag	UNP P48730
C	-1	GLY	-	expression tag	UNP P48730
C	0	SER	-	expression tag	UNP P48730
D	-1	GLY	-	expression tag	UNP P48730
D	0	SER	-	expression tag	UNP P48730

- 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		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		
3	B	118	Total	O	0	0
			118	118		

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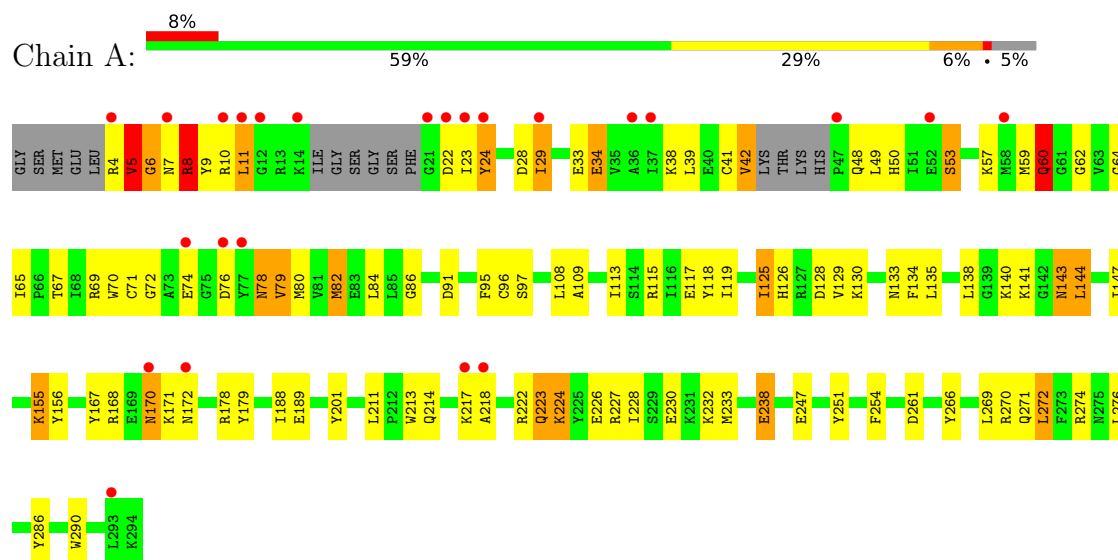
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	126	Total 126	O 126	0	0
3	D	109	Total 109	O 109	0	0

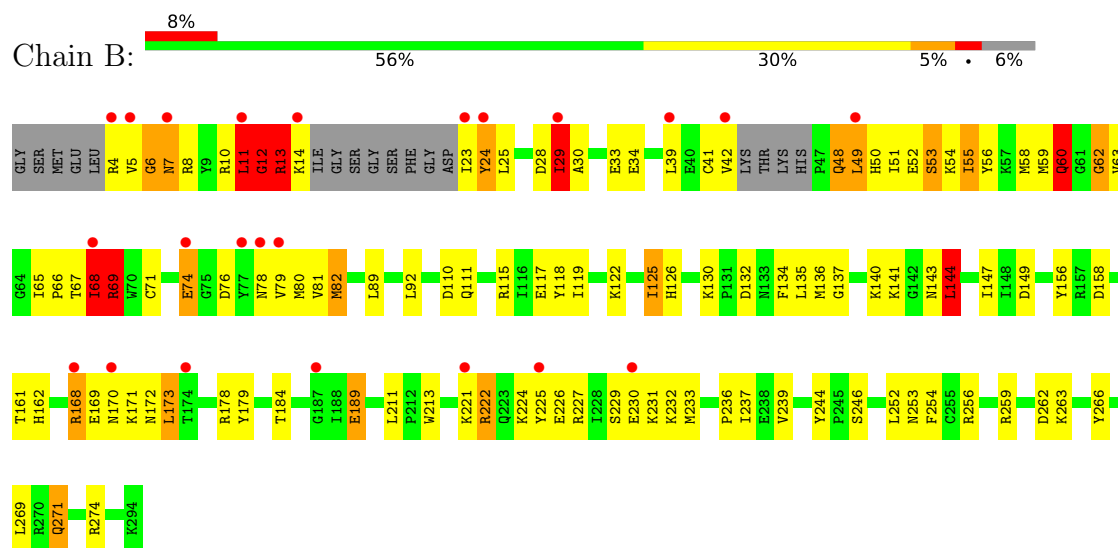
3 Residue-property plots

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: Casein kinase I isoform delta

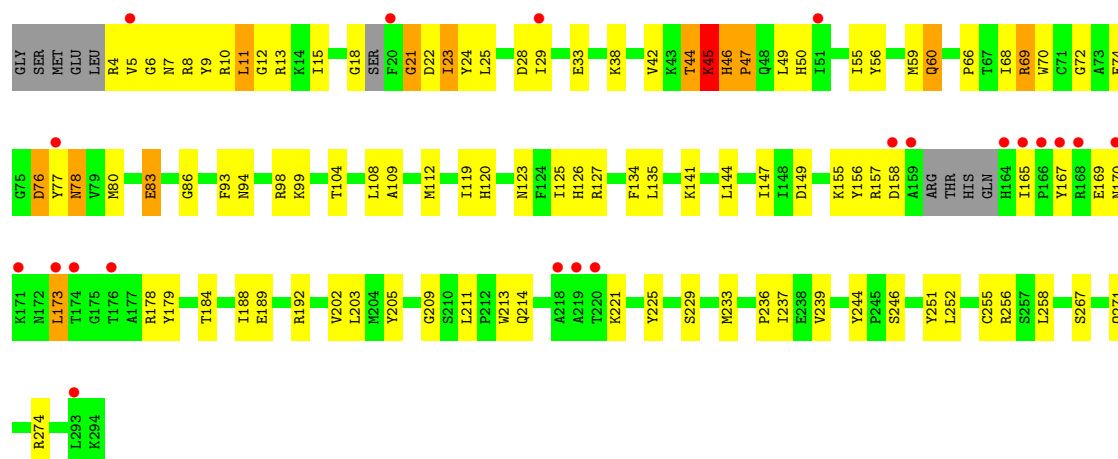


- Molecule 1: Casein kinase I isoform delta

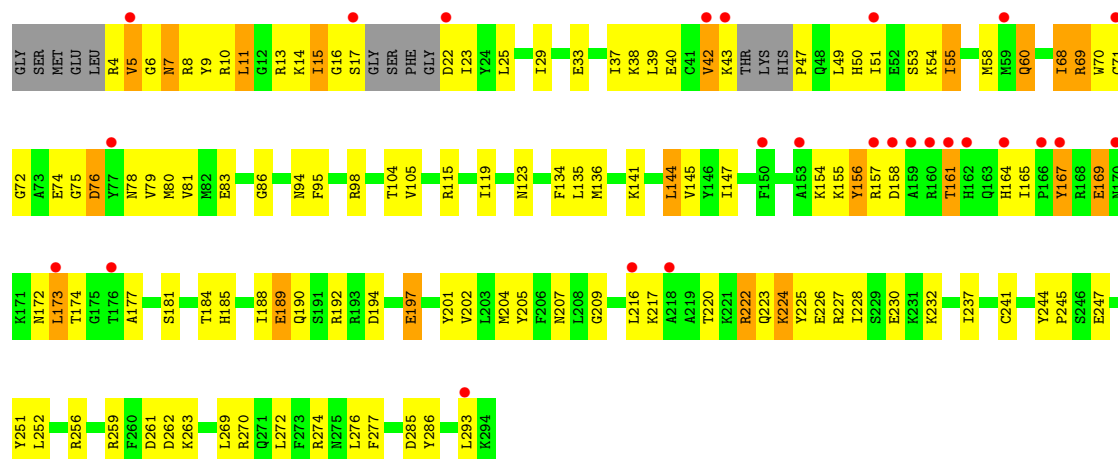


- Molecule 1: Casein kinase I isoform delta





• Molecule 1: Casein kinase I isoform delta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.77Å 85.16Å 89.12Å 70.19° 73.86° 86.15°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.30) 97.1 (50.00-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.276 0.231 , 0.263	Depositor DCC
R_{free} test set	3223 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9619	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.62	1/2322 (0.0%)	1.07	16/3123 (0.5%)
1	B	0.65	0/2317	1.13	24/3114 (0.8%)
1	C	0.62	0/2314	1.04	15/3118 (0.5%)
1	D	0.66	0/2343	1.13	18/3151 (0.6%)
All	All	0.64	1/9296 (0.0%)	1.09	73/12506 (0.6%)

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	B	0	2
1	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	233	MET	SD-CE	5.33	1.92	1.79

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	VAL	N-CA-C	16.99	131.56	109.30
1	D	16	GLY	N-CA-C	12.43	131.21	111.08
1	B	5	VAL	N-CA-C	11.70	124.62	109.30
1	B	24	TYR	N-CA-C	10.49	123.87	110.33
1	D	6	GLY	N-CA-C	10.20	128.38	113.48
1	D	86	GLY	CA-C-N	9.62	129.67	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	86	GLY	C-N-CA	9.62	129.67	119.76
1	D	263	LYS	N-CA-C	-9.25	98.16	109.72
1	A	11	LEU	N-CA-C	8.92	123.66	110.46
1	B	143	ASN	N-CA-C	-8.68	102.69	113.28
1	D	78	ASN	N-CA-C	-8.42	96.61	110.17
1	A	223	GLN	N-CA-C	-8.22	103.26	113.28
1	C	221	LYS	N-CA-C	-7.69	103.88	113.18
1	D	5	VAL	N-CA-C	7.66	120.46	109.51
1	C	21	GLY	N-CA-C	7.55	131.06	113.18
1	D	156	TYR	N-CA-C	-7.50	105.03	114.56
1	B	168	ARG	CB-CG-CD	7.44	128.41	111.30
1	C	209	GLY	N-CA-C	-7.24	105.25	114.37
1	D	169	GLU	N-CA-C	-6.96	99.68	108.45
1	A	86	GLY	CA-C-N	6.95	126.91	120.03
1	A	86	GLY	C-N-CA	6.95	126.91	120.03
1	C	125	ILE	N-CA-C	-6.71	98.80	108.53
1	D	223	GLN	N-CA-C	-6.71	105.07	113.18
1	B	60	GLN	N-CA-C	6.62	118.84	110.24
1	B	79	VAL	N-CA-C	6.45	117.99	108.45
1	C	78	ASN	N-CA-C	-6.31	99.42	109.76
1	A	155	LYS	N-CA-C	-6.25	101.03	110.28
1	B	78	ASN	N-CA-C	-6.23	99.55	109.76
1	A	8	ARG	N-CA-C	6.02	118.14	110.61
1	B	144	LEU	N-CA-C	6.01	120.06	109.96
1	B	11	LEU	N-CA-C	5.88	119.64	110.17
1	B	126	HIS	N-CA-C	5.88	117.69	111.28
1	D	217	LYS	N-CA-C	5.87	118.30	108.96
1	A	125	ILE	N-CA-C	-5.86	99.82	108.85
1	C	225	TYR	N-CA-C	-5.71	104.97	111.14
1	C	50	HIS	N-CA-C	-5.65	105.20	111.36
1	B	68	ILE	CA-C-N	5.65	128.12	120.44
1	B	68	ILE	C-N-CA	5.65	128.12	120.44
1	C	83	GLU	N-CA-C	-5.61	102.72	110.35
1	A	60	GLN	N-CA-C	5.56	117.46	110.24
1	A	4	ARG	CA-C-N	5.51	128.73	120.69
1	A	4	ARG	C-N-CA	5.51	128.73	120.69
1	C	77	TYR	N-CA-C	5.51	118.55	109.85
1	B	4	ARG	CA-C-N	5.49	128.70	120.69
1	B	4	ARG	C-N-CA	5.49	128.70	120.69
1	B	224	LYS	N-CA-C	-5.45	105.24	111.07
1	D	197	GLU	N-CA-C	-5.41	105.46	111.36
1	B	6	GLY	N-CA-C	5.41	126.00	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	LYS	N-CA-C	-5.41	99.28	110.80
1	D	225	TYR	N-CA-C	-5.39	105.57	111.82
1	B	67	THR	CA-C-N	-5.38	116.02	122.90
1	B	67	THR	C-N-CA	-5.38	116.02	122.90
1	D	55	ILE	N-CA-C	-5.36	105.49	110.53
1	B	62	GLY	N-CA-C	5.35	117.62	111.36
1	D	209	GLY	N-CA-C	-5.34	108.27	115.21
1	B	12	GLY	N-CA-C	5.28	125.69	113.18
1	D	185	HIS	N-CA-C	-5.28	106.10	112.54
1	C	23	ILE	N-CA-C	5.28	115.91	108.36
1	A	6	GLY	CA-C-N	5.26	131.58	121.54
1	A	6	GLY	C-N-CA	5.26	131.58	121.54
1	B	13	ARG	N-CA-C	5.26	122.00	110.80
1	D	144	LEU	N-CA-C	5.23	118.15	109.46
1	C	24	TYR	N-CA-C	5.20	117.88	109.40
1	C	86	GLY	CA-C-N	5.14	124.90	119.76
1	C	86	GLY	C-N-CA	5.14	124.90	119.76
1	B	69	ARG	N-CA-C	5.09	116.64	111.14
1	B	55	ILE	N-CA-C	-5.09	105.89	110.82
1	A	78	ASN	N-CA-C	-5.08	100.44	108.73
1	B	125	ILE	N-CA-C	-5.06	100.84	108.12
1	A	6	GLY	N-CA-C	5.04	122.84	115.08
1	C	28	ASP	N-CA-C	-5.03	99.13	107.99
1	D	83	GLU	N-CA-C	-5.03	102.94	110.23
1	A	143	ASN	N-CA-C	-5.01	106.58	113.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	244	TYR	Sidechain
1	B	6	GLY	Mainchain
1	C	244	TYR	Sidechain

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	2271	0	2239	94	0
1	B	2267	0	2249	101	0
1	C	2265	0	2206	74	0
1	D	2293	0	2263	93	0
2	A	15	0	0	2	0
2	B	15	0	0	0	0
2	C	10	0	0	2	0
2	D	10	0	0	0	0
3	A	120	0	0	10	0
3	B	118	0	0	14	0
3	C	126	0	0	4	0
3	D	109	0	0	7	0
All	All	9619	0	8957	358	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 20.

All (358) 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:222:ARG:HH11	1:B:222:ARG:HG2	1.00	1.09
1:A:60:GLN:HE21	1:A:60:GLN:HA	1.25	1.01
1:B:23:ILE:HG22	1:B:24:TYR:H	1.20	1.00
1:A:170:ASN:O	1:B:222:ARG:NH1	1.97	0.97
1:B:222:ARG:HH11	1:B:222:ARG:CG	1.77	0.96
1:C:141:LYS:HD2	1:C:144:LEU:HD12	1.46	0.96
1:A:223:GLN:O	1:A:227:ARG:HG3	1.66	0.95
1:D:69:ARG:HH11	1:D:69:ARG:HB3	1.32	0.93
1:B:222:ARG:HG2	1:B:222:ARG:NH1	1.84	0.92
1:B:59:MET:HA	3:B:1495:HOH:O	1.70	0.91
1:B:122:LYS:HG3	3:B:1495:HOH:O	1.70	0.90
1:B:74:GLU:HB2	3:B:333:HOH:O	1.72	0.90
1:B:23:ILE:HG22	1:B:24:TYR:N	1.82	0.88
1:C:69:ARG:HH11	1:C:69:ARG:HB3	1.36	0.87
1:B:256:ARG:HD2	3:B:299:HOH:O	1.75	0.86
1:C:5:VAL:HG23	1:C:9:TYR:HB2	1.59	0.84
1:C:45:LYS:C	1:C:47:PRO:HD2	2.05	0.80
1:B:13:ARG:CG	1:B:13:ARG:HH11	1.97	0.78
1:D:5:VAL:HG23	1:D:9:TYR:HB2	1.64	0.78
1:D:68:ILE:HD12	1:D:68:ILE:O	1.84	0.77
1:A:95:PHE:HB3	3:A:1293:HOH:O	1.84	0.76
1:D:23:ILE:HD11	1:D:38:LYS:HE2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:MET:HE3	1:B:82:MET:HE3	1.69	0.74
1:A:60:GLN:HA	1:A:60:GLN:NE2	1.98	0.74
1:C:271:GLN:NE2	1:C:274:ARG:NH1	2.37	0.73
1:A:140:LYS:H	1:A:140:LYS:HD2	1.54	0.72
1:D:237:ILE:HD13	1:D:252:LEU:HB3	1.70	0.71
1:A:5:VAL:O	1:A:9:TYR:HB2	1.88	0.71
1:B:13:ARG:HH11	1:B:13:ARG:HG3	1.55	0.71
1:C:33:GLU:OE1	1:C:69:ARG:NH2	2.24	0.71
1:C:156:TYR:O	1:C:165:ILE:HG23	1.91	0.71
1:A:39:LEU:CD2	1:A:79:VAL:HG12	2.20	0.71
1:C:271:GLN:NE2	1:C:274:ARG:HH12	1.89	0.70
1:D:47:PRO:HB3	3:D:336:HOH:O	1.89	0.70
1:B:54:LYS:O	1:B:58:MET:HG3	1.91	0.70
1:D:55:ILE:HA	1:D:58:MET:HE3	1.74	0.70
1:C:69:ARG:HH11	1:C:69:ARG:CB	2.04	0.70
1:C:49:LEU:HD11	1:C:80:MET:HE2	1.74	0.69
1:B:23:ILE:CG2	1:B:24:TYR:N	2.55	0.69
1:B:221:LYS:HE3	1:B:225:TYR:OH	1.92	0.69
1:C:44:THR:OG1	1:C:45:LYS:N	2.22	0.69
1:C:46:HIS:N	1:C:47:PRO:HD2	2.07	0.69
1:B:237:ILE:HD12	1:B:253:ASN:OD1	1.91	0.69
1:B:172:ASN:HD22	1:B:222:ARG:HH22	1.40	0.69
1:D:123:ASN:OD1	1:D:157:ARG:NE	2.23	0.69
1:A:238:GLU:HG3	3:A:300:HOH:O	1.92	0.68
1:C:165:ILE:HD12	1:C:189:GLU:OE1	1.93	0.68
1:A:80:MET:HE3	1:A:82:MET:SD	2.34	0.68
1:D:40:GLU:HA	3:D:314:HOH:O	1.95	0.67
1:A:60:GLN:HE21	1:A:60:GLN:CA	1.95	0.67
1:D:188:ILE:HD11	3:D:308:HOH:O	1.95	0.67
1:D:173:LEU:HD22	1:D:184:THR:HG22	1.77	0.66
1:C:70:TRP:CH2	1:C:72:GLY:HA3	2.31	0.65
1:D:181:SER:HB2	1:D:197:GLU:OE1	1.97	0.65
1:A:70:TRP:HZ3	1:A:79:VAL:CG2	2.11	0.64
1:B:236:PRO:HG2	1:B:239:VAL:HG23	1.79	0.64
1:B:259:ARG:NH1	1:B:262:ASP:OD1	2.29	0.64
1:C:271:GLN:HE22	1:C:274:ARG:NH1	1.95	0.64
1:B:8:ARG:O	1:B:29:ILE:HG22	1.98	0.64
1:B:226:GLU:O	1:B:230:GLU:HG2	1.98	0.64
1:B:130:LYS:HE3	1:B:132:ASP:HB2	1.77	0.64
1:C:46:HIS:N	1:C:47:PRO:CD	2.60	0.64
1:A:64:GLY:HA3	1:A:115:ARG:NE	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:HG23	1:A:9:TYR:HB2	1.80	0.63
1:B:137:GLY:HA3	1:B:141:LYS:O	1.99	0.63
1:A:217:LYS:O	1:A:227:ARG:NH1	2.30	0.63
1:B:13:ARG:HG3	1:B:13:ARG:NH1	2.13	0.63
1:D:11:LEU:HD11	1:D:39:LEU:HD11	1.81	0.63
1:A:254:PHE:CD2	1:A:269:LEU:HD21	2.34	0.62
1:A:39:LEU:HD22	1:A:79:VAL:HG12	1.81	0.62
1:A:53:SER:O	1:A:57:LYS:HG3	2.00	0.62
1:A:226:GLU:O	1:A:230:GLU:HG2	1.99	0.62
1:A:22:ASP:C	1:A:23:ILE:HD12	2.25	0.61
1:D:69:ARG:HH11	1:D:69:ARG:CB	2.11	0.61
1:D:167:TYR:HD1	1:D:167:TYR:O	1.83	0.61
1:A:42:VAL:HG23	1:A:78:ASN:ND2	2.15	0.61
1:D:190:GLN:HA	1:D:194:ASP:OD2	2.00	0.61
1:B:119:ILE:CD1	1:B:147:ILE:HD13	2.31	0.61
1:D:154:LYS:HZ3	1:D:189:GLU:CD	2.09	0.61
1:D:204:MET:HE2	1:D:241:CYS:HA	1.81	0.61
1:A:6:GLY:C	1:A:8:ARG:H	2.06	0.61
1:C:18:GLY:C	3:C:307:HOH:O	2.43	0.61
1:A:119:ILE:CD1	1:A:147:ILE:HD13	2.31	0.61
1:D:167:TYR:O	1:D:167:TYR:CD1	2.53	0.61
1:C:202:VAL:O	1:C:205:TYR:HB3	2.01	0.60
1:B:236:PRO:HG2	1:B:239:VAL:CG2	2.32	0.60
1:B:259:ARG:HG3	1:B:262:ASP:OD2	2.01	0.60
1:A:10:ARG:NH1	3:A:719:HOH:O	2.34	0.60
1:C:120:HIS:CG	1:C:192:ARG:HG2	2.36	0.60
1:B:33:GLU:OE1	1:B:69:ARG:NH2	2.33	0.59
1:D:43:LYS:NZ	3:D:337:HOH:O	2.34	0.59
1:A:213:TRP:CE2	1:A:232:LYS:HE2	2.37	0.59
1:B:92:LEU:HD11	1:B:136:MET:HG2	1.84	0.59
1:B:118:TYR:CE2	3:B:1495:HOH:O	2.52	0.59
1:B:173:LEU:HD12	1:B:184:THR:HG22	1.85	0.59
1:B:227:ARG:HG3	1:B:227:ARG:HH11	1.68	0.59
1:D:154:LYS:HG2	1:D:155:LYS:O	2.03	0.59
1:B:119:ILE:HD11	1:B:147:ILE:HD13	1.85	0.58
1:B:13:ARG:O	1:B:14:LYS:C	2.46	0.58
1:A:141:LYS:HD2	1:A:144:LEU:HD22	1.84	0.58
1:C:229:SER:O	1:C:233:MET:HG3	2.04	0.58
1:D:70:TRP:CH2	1:D:72:GLY:HA3	2.38	0.58
1:A:271:GLN:OE1	1:A:274:ARG:NH1	2.37	0.58
1:A:223:GLN:HG2	3:A:732:HOH:O	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:MET:HE3	1:B:119:ILE:HG23	1.86	0.57
1:C:78:ASN:OD1	3:C:759:HOH:O	2.16	0.57
1:C:236:PRO:HG2	1:C:239:VAL:CG2	2.35	0.57
1:C:13:ARG:NH1	1:C:13:ARG:HB3	2.19	0.57
1:B:110:ASP:CG	1:B:274:ARG:HH22	2.12	0.57
1:A:91:ASP:O	1:A:95:PHE:CD2	2.58	0.57
1:D:154:LYS:NZ	1:D:189:GLU:CD	2.62	0.57
1:C:108:LEU:O	1:C:112:MET:HG3	2.05	0.56
1:A:119:ILE:HD12	1:A:147:ILE:HD13	1.86	0.56
1:D:49:LEU:HD11	1:D:80:MET:HE2	1.87	0.56
1:B:171:LYS:NZ	1:B:189:GLU:OE2	2.38	0.56
1:C:167:TYR:HB3	3:C:337:HOH:O	2.05	0.56
1:D:123:ASN:O	1:D:155:LYS:HG2	2.06	0.56
1:D:156:TYR:CZ	1:D:192:ARG:HD3	2.40	0.56
1:A:247:GLU:HG3	1:A:272:LEU:CD2	2.36	0.56
1:C:4:ARG:CB	1:C:9:TYR:O	2.54	0.55
1:D:237:ILE:HD13	1:D:252:LEU:CB	2.35	0.55
1:B:89:LEU:HD23	1:B:92:LEU:HD12	1.88	0.55
1:A:140:LYS:HD2	1:A:140:LYS:N	2.20	0.55
1:D:4:ARG:CB	1:D:10:ARG:HA	2.37	0.55
1:A:64:GLY:HA3	1:A:115:ARG:HE	1.72	0.55
1:D:94:ASN:OD1	1:D:98:ARG:NH1	2.39	0.55
1:C:93:PHE:O	1:C:98:ARG:HA	2.07	0.54
1:D:141:LYS:HD2	1:D:144:LEU:HD12	1.89	0.54
1:D:136:MET:SD	1:D:145:VAL:HG22	2.47	0.54
1:D:285:ASP:O	1:D:286:TYR:HB2	2.08	0.54
1:A:23:ILE:C	1:A:24:TYR:CD1	2.86	0.54
1:B:23:ILE:N	1:B:23:ILE:HD12	2.23	0.54
1:C:119:ILE:HD11	1:C:147:ILE:HD13	1.90	0.54
1:B:161:THR:O	1:B:162:HIS:HB2	2.07	0.54
1:A:71:CYS:HB3	3:A:354:HOH:O	2.07	0.54
1:C:237:ILE:HD13	1:C:252:LEU:HB3	1.88	0.54
1:D:222:ARG:O	1:D:222:ARG:HG2	2.06	0.54
1:A:178:ARG:HD2	1:A:179:TYR:CZ	2.43	0.53
1:A:223:GLN:CG	3:A:732:HOH:O	2.55	0.53
1:B:48:GLN:O	1:B:49:LEU:C	2.50	0.53
1:B:134:PHE:C	1:B:135:LEU:HD12	2.34	0.53
1:C:55:ILE:O	1:C:59:MET:HG2	2.09	0.53
1:C:123:ASN:OD1	1:C:157:ARG:NE	2.39	0.53
1:A:10:ARG:HB2	1:A:29:ILE:HD12	1.91	0.53
1:C:256:ARG:NH2	3:C:953:HOH:O	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ARG:CB	1:C:10:ARG:HA	2.39	0.52
1:A:24:TYR:CD1	1:A:24:TYR:N	2.77	0.52
1:C:94:ASN:OD1	1:C:98:ARG:NH1	2.41	0.52
1:B:56:TYR:CE1	1:B:66:PRO:HG2	2.44	0.52
1:A:141:LYS:O	1:A:144:LEU:HB2	2.10	0.52
1:A:214:GLN:HG3	2:A:295:SO4:O4	2.09	0.52
1:B:252:LEU:O	1:B:256:ARG:HG3	2.09	0.52
1:A:126:HIS:CE1	1:A:128:ASP:HB3	2.44	0.52
1:B:34:GLU:HG2	3:B:1357:HOH:O	2.09	0.52
1:D:98:ARG:NH2	1:D:205:TYR:OH	2.41	0.52
1:B:222:ARG:O	1:B:226:GLU:HG2	2.10	0.52
1:C:134:PHE:C	1:C:135:LEU:HD12	2.35	0.52
1:C:141:LYS:CD	1:C:144:LEU:HD12	2.30	0.52
1:D:23:ILE:CD1	1:D:38:LYS:HG3	2.40	0.52
1:D:247:GLU:HG2	1:D:276:LEU:HB2	1.92	0.51
1:D:269:LEU:O	1:D:272:LEU:HB2	2.10	0.51
1:B:51:ILE:O	1:B:52:GLU:C	2.52	0.51
1:B:221:LYS:HE3	1:B:225:TYR:CZ	2.46	0.51
1:B:28:ASP:O	1:B:30:ALA:N	2.44	0.51
1:C:46:HIS:O	1:C:47:PRO:C	2.53	0.51
1:D:22:ASP:O	1:D:38:LYS:HA	2.11	0.51
1:B:50:HIS:O	1:B:53:SER:HB3	2.11	0.51
1:B:69:ARG:HB2	1:B:81:VAL:O	2.10	0.51
1:A:49:LEU:HD23	1:A:78:ASN:O	2.11	0.50
1:D:154:LYS:NZ	1:D:189:GLU:OE1	2.43	0.50
1:A:59:MET:HB3	1:A:65:ILE:HG21	1.91	0.50
1:B:23:ILE:CG2	1:B:24:TYR:H	1.97	0.50
1:D:169:GLU:OE1	3:D:308:HOH:O	2.19	0.50
1:A:218:ALA:HB3	1:A:224:LYS:HE3	1.93	0.50
1:D:53:SER:OG	1:D:71:CYS:SG	2.68	0.50
1:C:11:LEU:HD23	1:C:12:GLY:H	1.76	0.50
1:D:60:GLN:HE21	1:D:60:GLN:HA	1.77	0.50
1:D:167:TYR:OH	1:D:188:ILE:HD12	2.12	0.50
1:B:110:ASP:OD1	1:B:274:ARG:NH2	2.45	0.49
1:B:254:PHE:CD2	1:B:269:LEU:HD21	2.48	0.49
1:C:271:GLN:HE22	1:C:274:ARG:HH12	1.56	0.49
1:C:156:TYR:CE1	1:C:157:ARG:HD3	2.47	0.49
1:B:178:ARG:HD2	1:B:179:TYR:CZ	2.47	0.49
1:D:174:THR:O	1:D:174:THR:HG23	2.12	0.49
1:C:5:VAL:O	1:C:9:TYR:HB2	2.12	0.49
1:A:74:GLU:HB2	3:A:414:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ILE:HD12	1:C:23:ILE:N	2.28	0.49
1:A:70:TRP:CH2	1:A:72:GLY:HA3	2.47	0.49
1:A:218:ALA:CB	1:A:224:LYS:HE3	2.43	0.49
1:D:226:GLU:O	1:D:230:GLU:HG2	2.13	0.49
1:A:22:ASP:O	1:A:38:LYS:HA	2.13	0.49
1:D:216:LEU:HD13	1:D:227:ARG:HB3	1.95	0.48
1:C:173:LEU:HG	1:C:184:THR:HG22	1.94	0.48
1:D:5:VAL:CG2	1:D:9:TYR:HB2	2.39	0.48
1:B:256:ARG:HB3	3:B:299:HOH:O	2.13	0.48
1:C:120:HIS:ND1	1:C:192:ARG:HG2	2.28	0.48
1:B:227:ARG:HG3	1:B:227:ARG:NH1	2.28	0.48
1:B:52:GLU:O	1:B:55:ILE:N	2.40	0.48
1:B:229:SER:OG	1:B:233:MET:CE	2.62	0.48
1:D:204:MET:CE	1:D:241:CYS:HA	2.44	0.48
1:B:246:SER:HB2	3:B:375:HOH:O	2.12	0.48
1:A:168:ARG:NH1	3:A:307:HOH:O	2.46	0.47
1:B:119:ILE:HD11	1:B:147:ILE:HG21	1.94	0.47
1:B:263:LYS:HE2	3:B:310:HOH:O	2.14	0.47
1:D:33:GLU:OE1	1:D:69:ARG:NH2	2.47	0.47
1:D:158:ASP:HA	3:D:1307:HOH:O	2.13	0.47
1:A:167:TYR:O	1:A:168:ARG:HD3	2.14	0.47
1:B:92:LEU:HD11	1:B:136:MET:CG	2.44	0.47
1:B:56:TYR:HB3	1:B:68:ILE:CD1	2.45	0.47
1:B:60:GLN:CA	1:B:60:GLN:HE21	2.27	0.47
1:A:6:GLY:C	1:A:8:ARG:N	2.73	0.47
1:B:62:GLY:HA3	1:B:118:TYR:CZ	2.50	0.47
1:D:13:ARG:HG3	1:D:13:ARG:HH11	1.80	0.47
1:D:49:LEU:HA	1:D:49:LEU:HD12	1.58	0.47
1:D:115:ARG:O	1:D:119:ILE:HG13	2.15	0.47
1:C:141:LYS:HD2	1:C:144:LEU:CD1	2.33	0.47
1:D:154:LYS:NZ	1:D:189:GLU:OE2	2.48	0.47
1:B:237:ILE:HG13	1:B:256:ARG:NH2	2.30	0.46
1:C:104:THR:O	1:C:108:LEU:HG	2.15	0.46
1:B:222:ARG:NH1	1:B:222:ARG:CG	2.50	0.46
1:D:50:HIS:CB	3:D:305:HOH:O	2.63	0.46
1:D:202:VAL:O	1:D:205:TYR:HB3	2.16	0.46
1:D:274:ARG:O	1:D:277:PHE:HB3	2.15	0.46
1:A:8:ARG:NH1	1:A:28:ASP:OD1	2.49	0.46
1:C:274:ARG:NH2	2:C:295:SO4:O3	2.48	0.46
1:C:5:VAL:HG23	1:C:9:TYR:CB	2.38	0.46
1:B:271:GLN:OE1	1:B:271:GLN:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ALA:HB2	1:C:203:LEU:HD21	1.98	0.46
1:C:126:HIS:O	1:C:127:ARG:HB2	2.15	0.46
1:D:4:ARG:CB	1:D:9:TYR:O	2.63	0.46
1:D:60:GLN:HE21	1:D:60:GLN:CA	2.29	0.46
1:A:70:TRP:CZ3	1:A:79:VAL:CG2	2.95	0.46
3:A:428:HOH:O	1:D:167:TYR:HE2	1.98	0.46
1:B:173:LEU:CD1	1:B:184:THR:HG22	2.45	0.46
1:A:270:ARG:NH2	2:A:297:SO4:O2	2.33	0.46
1:B:213:TRP:CE2	1:B:232:LYS:HE2	2.51	0.46
1:C:15:ILE:HG21	1:C:25:LEU:HB2	1.97	0.46
1:C:44:THR:O	1:C:45:LYS:HB2	2.16	0.45
1:C:123:ASN:HB2	1:C:155:LYS:NZ	2.31	0.45
1:D:134:PHE:C	1:D:135:LEU:HD12	2.41	0.45
1:B:11:LEU:HD11	1:B:39:LEU:HD11	1.98	0.45
1:C:158:ASP:CB	1:D:161:THR:HG21	2.47	0.45
1:C:255:CYS:HA	1:C:258:LEU:HD12	1.98	0.45
1:D:23:ILE:HD11	1:D:38:LYS:CE	2.42	0.45
1:B:80:MET:HE3	1:B:82:MET:CE	2.44	0.45
1:D:37:ILE:HG12	1:D:81:VAL:HG22	1.98	0.45
1:B:34:GLU:CG	3:B:1357:HOH:O	2.63	0.45
1:B:115:ARG:HH21	1:B:144:LEU:HD23	1.81	0.45
1:B:110:ASP:OD1	1:B:274:ARG:NH1	2.49	0.45
1:C:120:HIS:CE1	1:C:192:ARG:HG2	2.52	0.44
1:D:251:TYR:CD1	1:D:251:TYR:C	2.95	0.44
1:C:12:GLY:HA3	1:C:25:LEU:O	2.17	0.44
1:C:56:TYR:CE1	1:C:66:PRO:HG2	2.52	0.44
1:D:259:ARG:HG3	1:D:262:ASP:OD2	2.18	0.44
1:B:60:GLN:HE21	1:B:60:GLN:N	2.15	0.44
1:B:117:GLU:HB2	1:B:266:TYR:CD1	2.53	0.44
1:C:5:VAL:CG2	1:C:9:TYR:HB2	2.37	0.44
1:C:11:LEU:HD23	1:C:12:GLY:N	2.32	0.44
1:A:49:LEU:CD2	1:A:78:ASN:O	2.65	0.44
1:B:56:TYR:CB	1:B:68:ILE:CD1	2.96	0.44
1:D:156:TYR:CZ	1:D:157:ARG:HD3	2.53	0.44
1:A:50:HIS:CD2	1:A:50:HIS:C	2.95	0.44
1:B:211:LEU:HD13	1:B:213:TRP:CZ2	2.53	0.44
1:C:56:TYR:O	1:C:60:GLN:NE2	2.51	0.44
1:D:42:VAL:HG22	1:D:76:ASP:C	2.42	0.44
1:D:74:GLU:O	1:D:75:GLY:C	2.61	0.44
1:D:105:VAL:HG21	1:D:207:ASN:OD1	2.18	0.44
1:D:164:HIS:CD2	1:D:261:ASP:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ARG:NH1	1:A:28:ASP:OD2	2.51	0.43
1:A:286:TYR:CD1	1:A:286:TYR:N	2.83	0.43
1:A:34:GLU:HB3	1:A:84:LEU:HD22	1.98	0.43
1:A:38:LYS:HG2	1:A:49:LEU:HD13	1.99	0.43
1:A:126:HIS:HE1	1:A:128:ASP:HB3	1.83	0.43
1:A:251:TYR:C	1:A:251:TYR:CD1	2.96	0.43
1:B:55:ILE:HD11	3:B:1251:HOH:O	2.18	0.43
1:A:140:LYS:H	1:A:140:LYS:CD	2.24	0.43
1:D:201:TYR:OH	1:D:256:ARG:NH1	2.51	0.43
1:B:158:ASP:O	1:B:162:HIS:HA	2.19	0.43
1:D:161:THR:O	1:D:161:THR:OG1	2.35	0.43
1:B:111:GLN:O	1:B:115:ARG:HG2	2.17	0.43
1:C:251:TYR:CD1	1:C:251:TYR:C	2.96	0.43
1:B:140:LYS:H	1:B:140:LYS:HD2	1.83	0.43
1:A:188:ILE:HG22	1:A:189:GLU:N	2.33	0.43
1:B:60:GLN:CA	1:B:60:GLN:NE2	2.81	0.43
1:A:5:VAL:CG2	1:A:9:TYR:HB2	2.46	0.43
1:A:69:ARG:O	1:A:70:TRP:HB2	2.18	0.43
1:A:96:CYS:O	1:A:97:SER:HB2	2.19	0.43
1:A:226:GLU:CD	1:B:227:ARG:HH22	2.27	0.43
1:A:60:GLN:NE2	1:A:60:GLN:CA	2.68	0.43
1:B:168:ARG:HG3	1:B:169:GLU:N	2.34	0.43
1:C:211:LEU:HD13	1:C:213:TRP:CZ2	2.54	0.43
1:D:154:LYS:HE2	1:D:165:ILE:HD13	1.99	0.43
1:A:50:HIS:CD2	1:A:50:HIS:O	2.72	0.42
1:A:125:ILE:HG23	1:A:156:TYR:CD2	2.53	0.42
1:A:129:VAL:HG13	1:A:134:PHE:HE2	1.84	0.42
1:B:259:ARG:CD	3:B:564:HOH:O	2.67	0.42
1:D:177:ALA:O	1:D:232:LYS:NZ	2.49	0.42
1:A:70:TRP:HZ3	1:A:79:VAL:HG22	1.84	0.42
1:A:224:LYS:O	1:A:228:ILE:HG13	2.19	0.42
1:A:247:GLU:HG2	1:A:276:LEU:HB2	2.01	0.42
1:A:84:LEU:HG	1:A:138:LEU:HD11	2.01	0.42
1:A:109:ALA:O	1:A:113:ILE:HG13	2.18	0.42
1:A:218:ALA:CB	1:A:224:LYS:HB2	2.50	0.42
1:D:29:ILE:O	1:D:29:ILE:CG2	2.68	0.42
1:D:270:ARG:O	1:D:274:ARG:HG3	2.19	0.42
1:B:230:GLU:HB3	3:B:352:HOH:O	2.18	0.42
1:A:143:ASN:HD22	1:A:286:TYR:HD2	1.68	0.42
1:A:201:TYR:OH	3:A:740:HOH:O	2.21	0.42
1:B:56:TYR:CG	1:B:68:ILE:CD1	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ILE:HG23	1:B:156:TYR:CD2	2.54	0.42
1:B:12:GLY:O	1:B:13:ARG:HB2	2.19	0.42
1:D:95:PHE:CE2	1:D:293:LEU:HD13	2.55	0.42
1:A:33:GLU:OE1	1:A:69:ARG:NH2	2.52	0.42
1:A:130:LYS:HE2	1:A:133:ASN:HD21	1.85	0.42
1:D:72:GLY:O	1:D:79:VAL:HG12	2.19	0.41
1:A:134:PHE:C	1:A:135:LEU:HD12	2.44	0.41
1:A:178:ARG:HG2	1:A:211:LEU:HD12	2.02	0.41
1:B:229:SER:OG	1:B:233:MET:HE2	2.19	0.41
1:C:6:GLY:C	1:C:8:ARG:H	2.28	0.41
1:D:70:TRP:HZ3	1:D:79:VAL:CG1	2.33	0.41
1:A:62:GLY:HA3	1:A:118:TYR:CZ	2.54	0.41
1:B:65:ILE:HG13	1:B:118:TYR:CE2	2.55	0.41
1:C:69:ARG:HH11	1:C:69:ARG:CG	2.32	0.41
1:C:169:GLU:CD	1:C:188:ILE:HD13	2.45	0.41
1:D:167:TYR:CZ	1:D:188:ILE:HD12	2.55	0.41
1:D:172:ASN:O	1:D:173:LEU:C	2.62	0.41
1:B:63:VAL:HG12	1:B:144:LEU:HD21	2.02	0.41
1:C:236:PRO:HG2	1:C:239:VAL:HG23	2.01	0.41
1:D:17:SER:O	1:D:23:ILE:HD13	2.20	0.41
1:B:125:ILE:HG13	1:B:125:ILE:O	2.19	0.41
1:D:220:THR:C	1:D:222:ARG:H	2.28	0.41
1:D:224:LYS:HB2	1:D:224:LYS:HE3	1.88	0.41
1:A:5:VAL:O	1:A:5:VAL:HG23	2.20	0.41
1:A:117:GLU:HB2	1:A:266:TYR:CD1	2.56	0.41
1:A:171:LYS:HD2	1:A:189:GLU:OE1	2.21	0.41
1:D:38:LYS:HD2	1:D:49:LEU:HD11	2.01	0.41
1:A:108:LEU:HD21	1:A:290:TRP:HH2	1.86	0.41
1:C:23:ILE:HD11	1:C:38:LYS:HE2	2.02	0.41
1:C:178:ARG:HD2	1:C:179:TYR:CZ	2.56	0.41
1:D:169:GLU:OE1	1:D:188:ILE:CD1	2.69	0.41
1:D:228:ILE:O	1:D:232:LYS:HB2	2.21	0.41
1:D:60:GLN:OE1	1:D:68:ILE:HG13	2.21	0.41
1:B:56:TYR:HB3	1:B:68:ILE:HD12	2.02	0.40
1:C:42:VAL:HB	1:C:76:ASP:O	2.21	0.40
1:C:66:PRO:HA	1:C:83:GLU:OE2	2.21	0.40
1:A:60:GLN:OE1	1:A:67:THR:HA	2.20	0.40
1:A:270:ARG:HB3	1:A:274:ARG:NH2	2.36	0.40
1:B:71:CYS:HB3	3:B:323:HOH:O	2.20	0.40
1:B:171:LYS:HB3	1:B:171:LYS:HE2	1.73	0.40
1:C:44:THR:HG1	1:C:46:HIS:H	1.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:GLN:HG3	2:C:296:SO4:O4	2.20	0.40
1:D:23:ILE:HD12	1:D:38:LYS:HG3	2.03	0.40
1:D:134:PHE:CE1	1:D:147:ILE:HD12	2.56	0.40
1:D:141:LYS:CD	1:D:144:LEU:HD12	2.50	0.40
1:A:24:TYR:N	1:A:24:TYR:HD1	2.18	0.40
1:A:170:ASN:ND2	1:B:221:LYS:HE2	2.36	0.40
1:C:13:ARG:CB	1:C:13:ARG:HH11	2.34	0.40
1:D:244:TYR:HB3	1:D:245:PRO:CD	2.52	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	275/296 (93%)	259 (94%)	14 (5%)	2 (1%)	18	23
1	B	273/296 (92%)	250 (92%)	17 (6%)	6 (2%)	5	4
1	C	280/296 (95%)	257 (92%)	17 (6%)	6 (2%)	5	4
1	D	278/296 (94%)	253 (91%)	22 (8%)	3 (1%)	11	13
All	All	1106/1184 (93%)	1019 (92%)	70 (6%)	17 (2%)	8	8

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	ARG
1	B	29	ILE
1	C	45	LYS
1	B	149	ASP
1	C	21	GLY
1	A	222	ARG
1	B	7	ASN

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Mol	Chain	Res	Type
1	B	49	LEU
1	D	7	ASN
1	A	170	ASN
1	C	149	ASP
1	C	246	SER
1	D	167	TYR
1	B	12	GLY
1	C	47	PRO
1	D	15	ILE
1	C	46	HIS

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	240/259 (93%)	218 (91%)	22 (9%)	8	11
1	B	241/259 (93%)	218 (90%)	23 (10%)	8	10
1	C	234/259 (90%)	220 (94%)	14 (6%)	17	25
1	D	242/259 (93%)	223 (92%)	19 (8%)	11	15
All	All	957/1036 (92%)	879 (92%)	78 (8%)	10	14

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	7	ASN
1	A	8	ARG
1	A	11	LEU
1	A	24	TYR
1	A	29	ILE
1	A	34	GLU
1	A	41	CYS
1	A	42	VAL
1	A	48	GLN
1	A	53	SER

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Mol	Chain	Res	Type
1	A	60	GLN
1	A	76	ASP
1	A	79	VAL
1	A	82	MET
1	A	144	LEU
1	A	155	LYS
1	A	172	ASN
1	A	224	LYS
1	A	238	GLU
1	A	261	ASP
1	A	272	LEU
1	B	7	ASN
1	B	10	ARG
1	B	11	LEU
1	B	13	ARG
1	B	25	LEU
1	B	29	ILE
1	B	41	CYS
1	B	42	VAL
1	B	48	GLN
1	B	53	SER
1	B	60	GLN
1	B	68	ILE
1	B	69	ARG
1	B	74	GLU
1	B	76	ASP
1	B	82	MET
1	B	144	LEU
1	B	170	ASN
1	B	173	LEU
1	B	189	GLU
1	B	222	ARG
1	B	231	LYS
1	B	271	GLN
1	C	7	ASN
1	C	11	LEU
1	C	22	ASP
1	C	29	ILE
1	C	44	THR
1	C	60	GLN
1	C	68	ILE
1	C	69	ARG

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Mol	Chain	Res	Type
1	C	74	GLU
1	C	76	ASP
1	C	99	LYS
1	C	170	ASN
1	C	173	LEU
1	C	267	SER
1	D	7	ASN
1	D	8	ARG
1	D	11	LEU
1	D	14	LYS
1	D	15	ILE
1	D	25	LEU
1	D	42	VAL
1	D	51	ILE
1	D	54	LYS
1	D	60	GLN
1	D	68	ILE
1	D	69	ARG
1	D	76	ASP
1	D	104	THR
1	D	161	THR
1	D	173	LEU
1	D	189	GLU
1	D	222	ARG
1	D	224	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	50	HIS
1	A	78	ASN
1	A	133	ASN
1	A	163	GLN
1	A	170	ASN
1	A	172	ASN
1	B	7	ASN
1	B	60	GLN
1	B	78	ASN
1	B	170	ASN
1	B	172	ASN
1	B	271	GLN

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Mol	Chain	Res	Type
1	B	291	ASN
1	C	7	ASN
1	C	78	ASN
1	C	143	ASN
1	C	172	ASN
1	C	271	GLN
1	D	7	ASN
1	D	78	ASN
1	D	163	GLN
1	D	170	ASN
1	D	172	ASN
1	D	190	GLN
1	D	214	GLN
1	D	223	GLN

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](#)

10 ligands 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	$\# Z > 2$
2	SO4	B	295	-	4,4,4	0.92	0	6,6,6	0.31	0
2	SO4	B	297	-	4,4,4	0.69	0	6,6,6	0.84	0
2	SO4	D	295	-	4,4,4	0.62	0	6,6,6	0.55	0
2	SO4	A	295	-	4,4,4	0.74	0	6,6,6	0.49	0
2	SO4	B	296	-	4,4,4	0.80	0	6,6,6	0.47	0
2	SO4	C	295	-	4,4,4	0.81	0	6,6,6	0.28	0
2	SO4	C	296	-	4,4,4	0.60	0	6,6,6	1.04	0
2	SO4	A	297	-	4,4,4	1.08	0	6,6,6	0.30	0
2	SO4	D	296	-	4,4,4	0.75	0	6,6,6	0.40	0
2	SO4	A	296	-	4,4,4	0.83	0	6,6,6	0.56	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	295	SO4	1	0
2	C	295	SO4	1	0
2	C	296	SO4	1	0
2	A	297	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	281/296 (94%)	0.56	24 (8%) 16 18	34, 49, 79, 87	1 (0%)
1	B	279/296 (94%)	0.61	23 (8%) 17 19	31, 48, 76, 83	1 (0%)
1	C	286/296 (96%)	0.50	21 (7%) 21 23	32, 47, 81, 91	1 (0%)
1	D	284/296 (95%)	0.61	26 (9%) 14 16	33, 50, 84, 95	1 (0%)
All	All	1130/1184 (95%)	0.57	94 (8%) 17 19	31, 48, 80, 95	4 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	167	TYR	5.3
1	D	293	LEU	4.1
1	C	167	TYR	4.0
1	A	22	ASP	4.0
1	C	77	TYR	4.0
1	D	158	ASP	3.7
1	D	77	TYR	3.7
1	D	17	SER	3.7
1	B	39	LEU	3.7
1	D	5	VAL	3.6
1	D	161	THR	3.6
1	A	21	GLY	3.6
1	C	170	ASN	3.6
1	D	159	ALA	3.5
1	C	159	ALA	3.4
1	D	162	HIS	3.4
1	B	170	ASN	3.3
1	C	166	PRO	3.3
1	A	23	ILE	3.2
1	C	165	ILE	3.2
1	B	5	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	23	ILE	3.2
1	C	158	ASP	3.2
1	C	171	LYS	3.2
1	A	11	LEU	3.2
1	D	42	VAL	3.2
1	C	20	PHE	3.1
1	A	12	GLY	3.1
1	A	29	ILE	3.1
1	C	176	THR	3.0
1	B	7	ASN	3.0
1	D	166	PRO	3.0
1	B	42	VAL	2.9
1	B	174	THR	2.9
1	A	293	LEU	2.9
1	D	170	ASN	2.9
1	C	5	VAL	2.9
1	A	37	ILE	2.9
1	B	168	ARG	2.8
1	D	176	THR	2.8
1	A	24	TYR	2.8
1	B	49	LEU	2.7
1	A	77	TYR	2.6
1	A	7	ASN	2.6
1	B	74	GLU	2.6
1	A	74	GLU	2.6
1	B	24	TYR	2.6
1	C	293	LEU	2.5
1	D	153	ALA	2.5
1	A	58	MET	2.5
1	D	218	ALA	2.5
1	A	218	ALA	2.4
1	D	43	LYS	2.4
1	D	164	HIS	2.4
1	B	68	ILE	2.3
1	B	4	ARG	2.3
1	B	11	LEU	2.3
1	D	22	ASP	2.3
1	B	187	GLY	2.3
1	B	14	LYS	2.3
1	B	78	ASN	2.3
1	B	225	TYR	2.3
1	A	14	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	173	LEU	2.3
1	A	76	ASP	2.3
1	B	77	TYR	2.3
1	A	36	ALA	2.3
1	B	29	ILE	2.3
1	C	168	ARG	2.2
1	D	160	ARG	2.2
1	C	164	HIS	2.2
1	D	51	ILE	2.2
1	A	52	GLU	2.2
1	C	220	THR	2.2
1	D	157	ARG	2.2
1	A	4	ARG	2.1
1	C	51	ILE	2.1
1	B	230	GLU	2.1
1	C	174	THR	2.1
1	B	221	LYS	2.1
1	C	173	LEU	2.1
1	C	219	ALA	2.1
1	A	217	LYS	2.1
1	D	59	MET	2.1
1	B	79	VAL	2.1
1	D	150	PHE	2.1
1	D	71	CYS	2.0
1	A	170	ASN	2.0
1	A	172	ASN	2.0
1	D	216	LEU	2.0
1	C	29	ILE	2.0
1	A	47	PRO	2.0
1	A	10	ARG	2.0
1	C	218	ALA	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(Å ²)	Q<0.9
2	SO4	A	297	5/5	0.70	0.11	104,104,104,105	0
2	SO4	A	296	5/5	0.81	0.10	77,78,78,79	0
2	SO4	B	296	5/5	0.85	0.08	86,87,88,88	0
2	SO4	B	297	5/5	0.85	0.11	102,102,103,103	0
2	SO4	C	296	5/5	0.89	0.10	65,67,67,71	0
2	SO4	D	295	5/5	0.90	0.11	68,70,70,72	0
2	SO4	A	295	5/5	0.92	0.10	62,64,64,65	0
2	SO4	C	295	5/5	0.93	0.09	54,56,57,57	0
2	SO4	B	295	5/5	0.94	0.10	55,56,58,58	0
2	SO4	D	296	5/5	0.95	0.07	58,60,60,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.