



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 04:03 AM UTC

PDB ID : 3W XK / pdb_00003wxk
Title : Crystal structure of trypanosoma brucei gambiense glycerol kinase in complex with glycerol
Authors : Balogun, E.O.; Inaoka, D.K.; Shiba, T.; Kido, Y.; Tsuge, C.; Nara, T.; Aoki, T.; Honma, T.; Tanaka, A.; Inoue, M.; Matsuoka, S.; Michels, P.A.M.; Kita, K.; Harada, S.
Deposited on : 2014-08-01
Resolution : 2.37 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

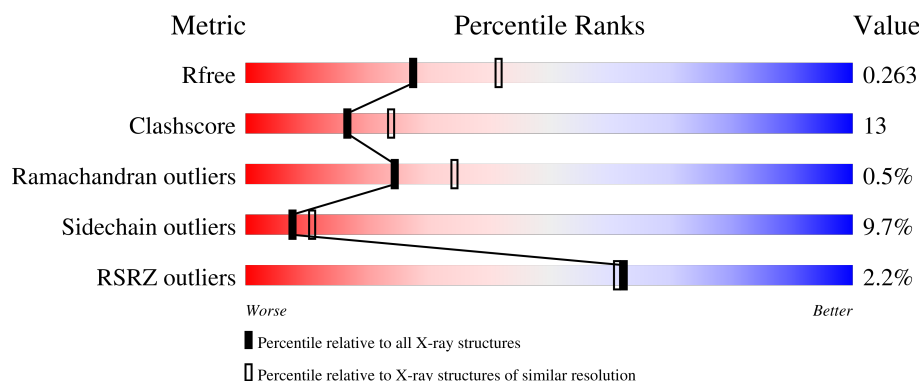
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	518	0% 70% 24% 6%
1	B	518	2% 71% 24%
1	C	518	3% 69% 25% 5%
1	D	518	3% 72% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16111 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	B	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	C	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	D	513	Total	C	N	O	S	0	1	0
			3962	2502	695	732	33			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP D3KVM3
A	-4	ILE	-	expression tag	UNP D3KVM3
A	-3	ASP	-	expression tag	UNP D3KVM3
A	-2	PRO	-	expression tag	UNP D3KVM3
A	-1	PHE	-	expression tag	UNP D3KVM3
A	0	THR	-	expression tag	UNP D3KVM3
B	-5	GLY	-	expression tag	UNP D3KVM3
B	-4	ILE	-	expression tag	UNP D3KVM3
B	-3	ASP	-	expression tag	UNP D3KVM3
B	-2	PRO	-	expression tag	UNP D3KVM3
B	-1	PHE	-	expression tag	UNP D3KVM3
B	0	THR	-	expression tag	UNP D3KVM3
C	-5	GLY	-	expression tag	UNP D3KVM3
C	-4	ILE	-	expression tag	UNP D3KVM3
C	-3	ASP	-	expression tag	UNP D3KVM3
C	-2	PRO	-	expression tag	UNP D3KVM3
C	-1	PHE	-	expression tag	UNP D3KVM3
C	0	THR	-	expression tag	UNP D3KVM3
D	-5	GLY	-	expression tag	UNP D3KVM3
D	-4	ILE	-	expression tag	UNP D3KVM3
D	-3	ASP	-	expression tag	UNP D3KVM3

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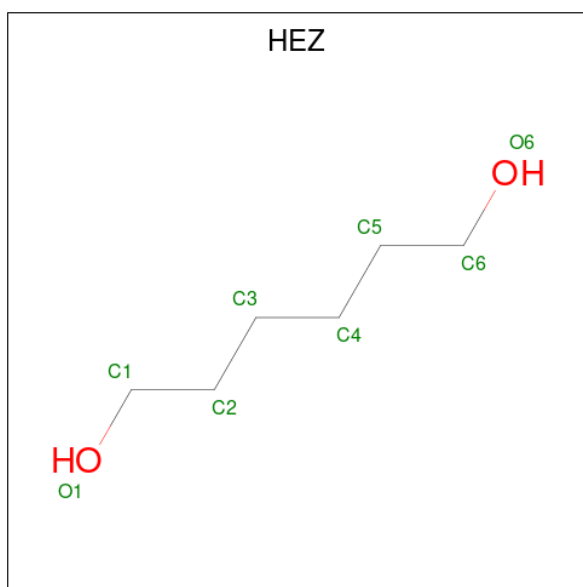
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PRO	-	expression tag	UNP D3KVM3
D	-1	PHE	-	expression tag	UNP D3KVM3
D	0	THR	-	expression tag	UNP D3KVM3

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is HEXANE-1,6-DIOL (CCD ID: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		

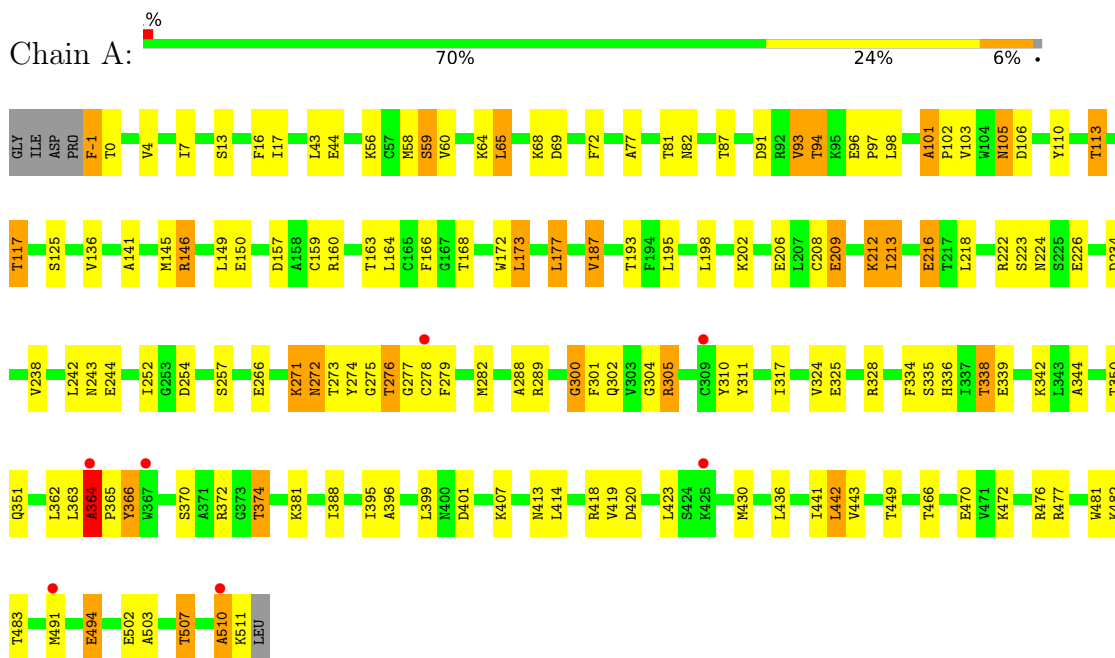
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	52	Total	O	0	0
			52	52		
4	C	50	Total	O	0	0
			50	50		
4	D	50	Total	O	0	0
			50	50		

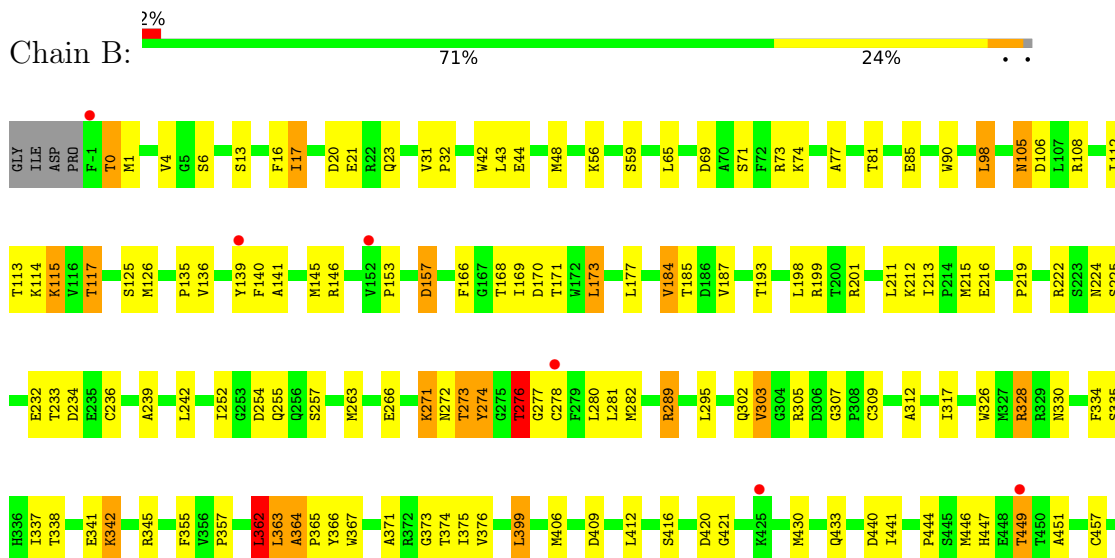
3 Residue-property plots [i](#)

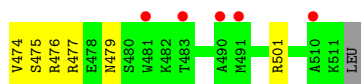
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycerol kinase

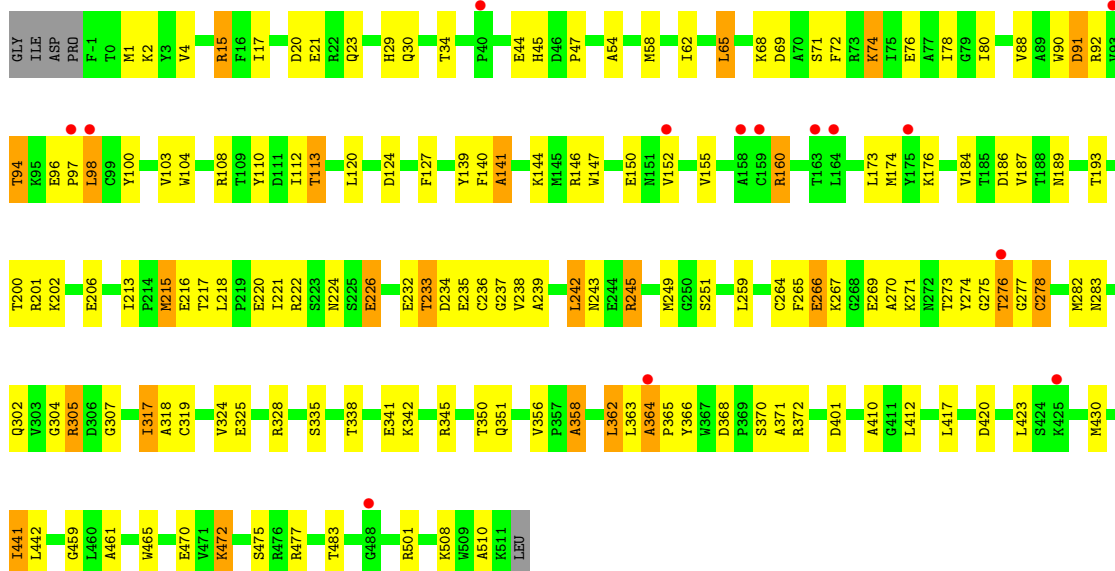


• Molecule 1: Glycerol kinase

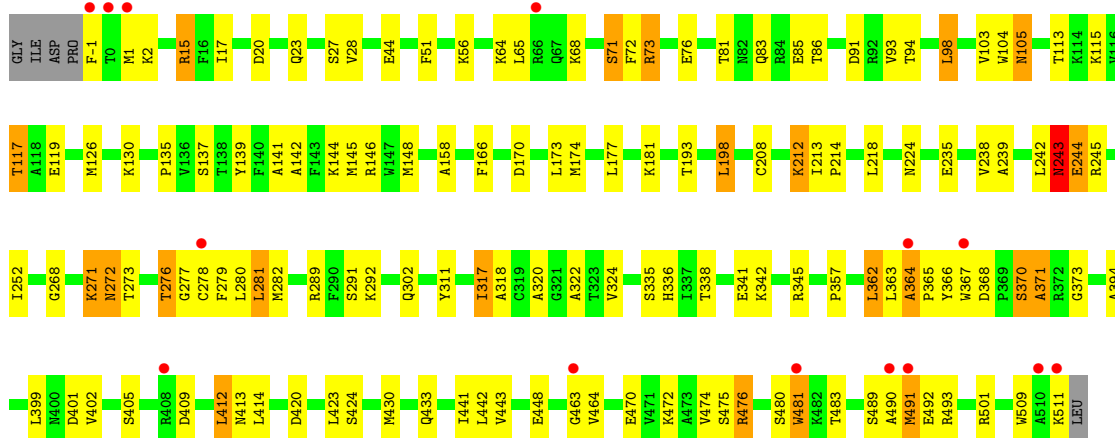




• Molecule 1: Glycerol kinase



• Molecule 1: Glycerol kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.48Å 122.14Å 154.51Å 90.00° 90.76° 90.00°	Depositor
Resolution (Å)	30.00 – 2.37 30.00 – 2.37	Depositor EDS
% Data completeness (in resolution range)	90.3 (30.00-2.37) 93.6 (30.00-2.37)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.190 , 0.251 0.206 , 0.263	Depositor DCC
R_{free} test set	4415 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-l	Xtriage
Reported twinning fraction	0.914 for H, K, L 0.086 for -h,-k,l	Depositor
Outliers	0 of 88201 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16111	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.14	11/4039 (0.3%)	1.15	14/5465 (0.3%)
1	B	1.18	16/4039 (0.4%)	1.14	13/5465 (0.2%)
1	C	1.32	11/4039 (0.3%)	1.12	18/5465 (0.3%)
1	D	1.09	7/4047 (0.2%)	1.08	5/5476 (0.1%)
All	All	1.19	45/16164 (0.3%)	1.13	50/21871 (0.2%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17	ILE	C-O	-7.96	1.15	1.24
1	C	112	ILE	CA-CB	-6.93	1.45	1.54
1	A	503	ALA	CA-CB	-6.43	1.43	1.53
1	C	221	ILE	C-O	-6.39	1.17	1.24
1	B	371	ALA	CA-CB	-6.16	1.43	1.53
1	C	358	ALA	CA-CB	-6.09	1.45	1.52
1	B	373	GLY	C-O	-6.03	1.18	1.24
1	B	17	ILE	CA-C	-5.94	1.45	1.52
1	D	83	GLN	C-O	-5.85	1.17	1.23
1	B	13	SER	C-O	-5.83	1.17	1.23
1	B	451	ALA	CA-CB	-5.78	1.44	1.53
1	B	376	VAL	C-O	-5.67	1.17	1.23
1	C	34	THR	C-O	-5.61	1.17	1.23
1	B	274	TYR	C-O	-5.57	1.17	1.24
1	D	322	ALA	CA-CB	-5.55	1.44	1.53
1	A	364	ALA	C-N	5.53	1.38	1.33
1	B	273	THR	C-O	-5.52	1.17	1.24
1	A	395	ILE	CA-CB	5.51	1.60	1.54
1	A	310	TYR	C-O	-5.47	1.17	1.24
1	A	279	PHE	C-O	-5.46	1.17	1.24
1	A	272	ASN	C-O	-5.43	1.17	1.24
1	B	444	PRO	C-O	-5.35	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	LEU	C-O	-5.34	1.17	1.24
1	C	304	GLY	C-O	-5.32	1.17	1.24
1	C	278	CYS	C-O	-5.31	1.18	1.23
1	C	62	ILE	C-O	-5.31	1.18	1.24
1	D	371	ALA	C-O	-5.28	1.17	1.23
1	D	276	THR	C-O	-5.26	1.18	1.24
1	A	304	GLY	C-O	-5.24	1.17	1.23
1	B	6	SER	C-O	-5.21	1.17	1.24
1	A	271	LYS	C-O	-5.20	1.17	1.23
1	A	96	GLU	C-O	-5.19	1.18	1.24
1	B	44	GLU	C-O	-5.19	1.17	1.23
1	B	375	ILE	C-O	-5.18	1.18	1.24
1	A	310	TYR	CA-C	-5.16	1.46	1.52
1	D	272	ASN	C-O	-5.15	1.18	1.24
1	B	374	THR	C-O	-5.14	1.17	1.23
1	B	48	MET	C-O	-5.12	1.18	1.24
1	C	371	ALA	C-O	-5.11	1.17	1.23
1	D	281	LEU	C-O	-5.11	1.17	1.24
1	D	373	GLY	C-O	-5.08	1.17	1.23
1	C	220	GLU	C-O	-5.08	1.17	1.23
1	C	368	ASP	C-O	-5.04	1.17	1.24
1	C	110	TYR	C-O	-5.03	1.18	1.24
1	A	300	GLY	C-O	-5.03	1.17	1.23

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	VAL	N-CA-C	8.44	119.07	111.81
1	A	101	ALA	CA-C-N	-8.41	111.10	119.76
1	A	101	ALA	C-N-CA	-8.41	111.10	119.76
1	C	242	LEU	N-CA-C	-8.11	96.86	109.76
1	B	362	LEU	N-CA-C	7.87	123.36	112.04
1	B	276	THR	N-CA-C	7.13	119.05	111.28
1	B	412	LEU	N-CA-C	6.95	118.33	108.74
1	A	276	THR	N-CA-C	6.87	118.77	111.28
1	C	140	PHE	N-CA-C	6.81	120.11	110.50
1	C	218	LEU	N-CA-C	6.78	119.20	110.39
1	B	242	LEU	N-CA-C	-6.64	101.76	110.53
1	C	94	THR	N-CA-C	-6.49	104.62	112.54
1	A	507	THR	N-CA-C	6.46	121.17	113.28
1	A	13	SER	N-CA-C	6.30	117.44	108.74
1	D	363	LEU	CB-CA-C	-6.30	106.52	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	ILE	N-CA-C	6.22	117.08	108.12
1	B	449	THR	N-CA-C	6.21	118.05	111.28
1	C	356	VAL	CB-CA-C	-6.13	103.80	111.04
1	C	141	ALA	N-CA-C	5.98	117.80	111.28
1	C	276	THR	N-CA-C	5.87	117.68	111.28
1	A	82	ASN	N-CA-C	5.84	117.95	109.07
1	A	300	GLY	N-CA-C	5.82	119.54	112.49
1	B	242	LEU	CA-C-N	-5.75	112.55	122.79
1	B	242	LEU	C-N-CA	-5.75	112.55	122.79
1	C	236	CYS	N-CA-C	-5.61	106.02	112.86
1	A	510	ALA	N-CA-C	5.58	118.37	110.50
1	D	181	LYS	N-CA-C	5.54	117.40	111.36
1	C	218	LEU	CA-C-N	5.53	125.50	120.03
1	C	218	LEU	C-N-CA	5.53	125.50	120.03
1	A	59	SER	N-CA-C	5.48	117.69	111.11
1	C	68	LYS	N-CA-C	5.35	119.96	113.38
1	B	13	SER	N-CA-C	5.34	116.26	108.14
1	D	318	ALA	N-CA-C	5.34	116.90	111.14
1	A	351	GLN	CB-CA-C	-5.30	104.07	111.80
1	C	221	ILE	CB-CA-C	-5.28	103.75	110.98
1	A	187	VAL	CB-CA-C	-5.24	104.04	112.16
1	C	307	GLY	CA-C-N	5.21	125.13	119.76
1	C	307	GLY	C-N-CA	5.21	125.13	119.76
1	D	276	THR	N-CA-C	5.15	116.89	111.28
1	B	374	THR	N-CA-C	5.14	117.81	109.06
1	B	140	PHE	N-CA-C	5.12	118.05	110.48
1	C	150	GLU	N-CA-C	5.11	117.75	111.82
1	C	152	VAL	CA-C-N	5.11	124.55	119.24
1	C	152	VAL	C-N-CA	5.11	124.55	119.24
1	C	113	THR	N-CA-C	-5.09	105.73	111.28
1	A	254	ASP	N-CA-C	5.09	116.51	111.07
1	A	7	ILE	CB-CA-C	-5.08	105.13	111.08
1	B	16	PHE	CA-C-N	-5.06	115.96	122.99
1	B	16	PHE	C-N-CA	-5.06	115.96	122.99
1	D	443	VAL	N-CA-C	5.04	113.00	107.60

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	3957	0	3970	105	0
1	B	3957	0	3970	90	0
1	C	3957	0	3970	103	0
1	D	3962	0	3976	110	0
2	A	12	0	16	1	0
2	B	6	0	8	1	0
2	C	12	0	16	2	0
2	D	12	0	16	1	0
3	B	16	0	28	4	0
3	C	8	0	14	0	0
3	D	8	0	14	0	0
4	A	52	0	0	7	0
4	B	52	0	0	3	0
4	C	50	0	0	6	0
4	D	50	0	0	2	0
All	All	16111	0	15998	409	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 13.

All (409) 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:C:364:ALA:CB	1:C:365:PRO:HD2	1.63	1.28
1:B:364:ALA:HB1	1:B:365:PRO:CD	1.64	1.27
1:C:364:ALA:HB1	1:C:365:PRO:CD	1.64	1.27
1:B:420:ASP:OD1	1:B:449:THR:HG21	1.40	1.21
1:B:364:ALA:CB	1:B:365:PRO:HD2	1.70	1.18
1:A:336:HIS:CD2	1:A:338:THR:HB	1.78	1.17
1:D:282:MET:HE2	1:D:414:LEU:HD12	1.15	1.15
1:C:305:ARG:HH11	1:C:305:ARG:HG2	1.11	1.13
1:D:364:ALA:CB	1:D:365:PRO:CD	2.26	1.12
1:D:364:ALA:CB	1:D:365:PRO:HD3	1.79	1.12
1:D:73:ARG:H	1:D:73:ARG:HD3	0.99	1.09
1:D:364:ALA:HB1	1:D:365:PRO:HD3	1.12	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ALA:CB	1:A:365:PRO:HD3	1.83	1.09
1:D:282:MET:HE2	1:D:414:LEU:CD1	1.81	1.08
1:D:243:ASN:HD22	1:D:244:GLU:N	1.50	1.07
1:A:364:ALA:HB1	1:A:365:PRO:HD3	1.08	1.07
1:D:280:LEU:HD12	1:D:399:LEU:HD12	1.37	1.06
1:B:139:TYR:CE2	3:B:603:HEZ:H31	1.90	1.05
1:D:73:ARG:HD3	1:D:73:ARG:N	1.69	1.04
1:B:364:ALA:HB1	1:B:365:PRO:HD2	1.05	1.04
1:C:91:ASP:OD1	1:C:94:THR:HG23	1.59	1.02
1:A:336:HIS:HD2	1:A:338:THR:HB	1.15	1.01
1:B:278:CYS:SG	1:B:399:LEU:HD11	2.01	1.00
1:C:305:ARG:HH11	1:C:305:ARG:CG	1.75	1.00
1:B:362:LEU:O	1:B:363:LEU:HB2	1.58	0.99
1:A:224:ASN:HD22	1:A:302:GLN:H	1.02	0.99
1:C:364:ALA:HA	4:C:749:HOH:O	1.63	0.97
1:D:364:ALA:HB1	1:D:365:PRO:CD	1.92	0.96
1:D:282:MET:CE	1:D:414:LEU:CD1	2.44	0.95
1:A:466:THR:HA	4:A:726:HOH:O	1.67	0.95
1:D:278:CYS:HB3	1:D:317:ILE:HG12	1.49	0.94
1:A:206:GLU:HB2	4:A:709:HOH:O	1.67	0.93
1:A:364:ALA:HB1	1:A:365:PRO:CD	1.97	0.93
1:A:157:ASP:O	1:A:160:ARG:HB3	1.69	0.92
1:A:224:ASN:ND2	1:A:302:GLN:H	1.67	0.92
1:C:364:ALA:HB1	1:C:365:PRO:HD2	0.92	0.91
1:A:150:GLU:HG2	1:C:202:LYS:HE3	1.53	0.91
1:A:305:ARG:HG3	1:A:305:ARG:HH11	1.34	0.91
1:D:282:MET:CE	1:D:414:LEU:HD12	2.00	0.91
1:D:476:ARG:HH21	1:D:481:TRP:HH2	1.19	0.90
1:D:278:CYS:CB	1:D:317:ILE:HG12	2.01	0.90
1:D:364:ALA:HB3	1:D:365:PRO:CD	1.97	0.90
1:B:341:GLU:O	1:B:345:ARG:HG3	1.73	0.89
1:A:226:GLU:OE1	1:A:305:ARG:HD2	1.73	0.89
1:A:364:ALA:CB	1:A:365:PRO:CD	2.50	0.89
1:D:364:ALA:HB3	1:D:365:PRO:HD2	1.54	0.89
1:D:367:TRP:HE3	4:D:747:HOH:O	1.58	0.87
1:B:399:LEU:HD23	1:B:433:GLN:OE1	1.73	0.87
1:A:336:HIS:HD2	1:A:338:THR:CB	1.87	0.86
1:C:224:ASN:HD22	1:C:302:GLN:H	1.25	0.85
1:D:105:ASN:HD22	1:D:105:ASN:H	1.23	0.84
1:A:278:CYS:SG	1:A:399:LEU:HD21	2.18	0.84
1:C:184:VAL:HG11	1:C:222:ARG:NH1	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ARG:HH11	1:A:305:ARG:CG	1.91	0.82
1:A:336:HIS:CD2	1:A:338:THR:H	1.98	0.82
1:D:280:LEU:CD1	1:D:399:LEU:HD12	2.10	0.82
1:B:224:ASN:HD22	1:B:302:GLN:H	1.24	0.81
1:B:362:LEU:O	1:B:363:LEU:CB	2.29	0.79
1:D:113:THR:O	1:D:117:THR:HG22	1.83	0.79
1:D:243:ASN:ND2	1:D:244:GLU:N	2.30	0.79
1:B:420:ASP:OD1	1:B:449:THR:CG2	2.29	0.79
1:A:374:THR:HG21	1:A:507:THR:HG22	1.64	0.78
1:C:184:VAL:CG1	1:C:222:ARG:HH11	1.96	0.78
1:A:336:HIS:CD2	1:A:338:THR:CB	2.62	0.78
1:D:73:ARG:N	1:D:73:ARG:CD	2.47	0.77
1:A:60:VAL:O	1:A:64:LYS:HG3	1.83	0.77
1:D:476:ARG:NH2	1:D:481:TRP:HH2	1.83	0.76
1:D:145:MET:HE2	1:D:166:PHE:HB3	1.68	0.75
1:C:160:ARG:HH11	1:C:160:ARG:HB2	1.52	0.75
1:B:141:ALA:HB3	1:B:193:THR:HA	1.69	0.74
1:C:184:VAL:CG1	1:C:222:ARG:NH1	2.50	0.74
1:B:146:ARG:NH1	1:B:212:LYS:HG3	2.02	0.74
1:A:336:HIS:HD2	1:A:338:THR:H	1.33	0.74
1:C:184:VAL:HG11	1:C:222:ARG:HH11	1.52	0.74
1:A:43:LEU:HD23	1:A:105:ASN:HD21	1.53	0.74
1:C:160:ARG:HH11	1:C:160:ARG:CB	2.01	0.73
1:D:73:ARG:H	1:D:73:ARG:CD	1.91	0.73
1:A:325:GLU:OE2	1:A:328:ARG:NH1	2.22	0.73
1:A:374:THR:CG2	1:A:507:THR:HG22	2.18	0.73
1:B:364:ALA:CB	1:B:365:PRO:CD	2.30	0.72
1:B:145:MET:HE2	1:B:166:PHE:HB3	1.71	0.72
1:C:341:GLU:OE2	1:C:345:ARG:NH2	2.22	0.71
1:C:341:GLU:O	1:C:345:ARG:HG3	1.90	0.70
1:A:372:ARG:O	1:A:374:THR:HG22	1.91	0.70
1:D:282:MET:CE	1:D:414:LEU:HD11	2.19	0.70
1:D:276:THR:N	1:D:277:GLY:HA3	2.07	0.70
1:A:272:ASN:ND2	1:A:278:CYS:SG	2.60	0.70
1:C:160:ARG:HH11	1:C:160:ARG:CG	2.05	0.69
1:A:226:GLU:CD	1:A:305:ARG:HD2	2.18	0.69
1:B:364:ALA:HB1	1:B:365:PRO:HD3	1.71	0.69
1:D:278:CYS:HB3	1:D:317:ILE:CG1	2.22	0.69
1:D:336:HIS:HD2	1:D:338:THR:OG1	1.75	0.69
1:B:1:MET:SD	1:B:21:GLU:HG2	2.33	0.68
1:A:91:ASP:OD1	1:A:94:THR:HG23	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:HE22	1:C:475:SER:HB2	1.58	0.68
1:B:224:ASN:ND2	1:B:302:GLN:H	1.91	0.68
1:D:243:ASN:HD22	1:D:244:GLU:H	1.42	0.68
1:D:224:ASN:HD22	1:D:302:GLN:H	1.42	0.67
1:A:150:GLU:HG3	4:A:750:HOH:O	1.94	0.66
1:C:305:ARG:CG	1:C:305:ARG:NH1	2.44	0.65
1:C:266:GLU:O	1:C:269:GLU:HG3	1.97	0.65
1:D:105:ASN:H	1:D:105:ASN:ND2	1.95	0.65
1:C:305:ARG:HG2	1:C:305:ARG:NH1	1.95	0.65
1:A:244:GLU:OE1	1:A:244:GLU:N	2.30	0.65
1:C:317:ILE:HD12	1:C:318:ALA:N	2.12	0.65
1:C:364:ALA:CB	1:C:365:PRO:CD	2.30	0.65
1:C:29:HIS:HD2	4:C:742:HOH:O	1.80	0.64
1:D:413[A]:ASN:ND2	1:D:414:LEU:H	1.95	0.64
1:A:274:TYR:HB3	1:A:423:LEU:HB2	1.79	0.64
1:B:184:VAL:HG11	1:B:222:ARG:HD2	1.79	0.64
1:D:243:ASN:ND2	1:D:243:ASN:C	2.56	0.64
1:C:147:TRP:O	1:C:147:TRP:CE3	2.51	0.64
1:A:336:HIS:HD2	1:A:338:THR:N	1.96	0.63
1:D:413[A]:ASN:HD22	1:D:414:LEU:H	1.46	0.63
1:A:242:LEU:O	1:A:243:ASN:HB3	1.99	0.63
1:A:305:ARG:CG	1:A:305:ARG:NH1	2.56	0.63
1:B:4:VAL:HG23	1:B:77:ALA:O	1.99	0.62
1:D:489:SER:OG	1:D:491:MET:HB3	1.99	0.62
3:B:602:HEZ:H32	4:B:702:HOH:O	1.99	0.62
1:D:317:ILE:HD11	1:D:320:ALA:HB2	1.81	0.62
1:B:43:LEU:HD23	1:B:105:ASN:HD21	1.65	0.62
1:C:1:MET:HA	1:C:21:GLU:OE2	1.98	0.62
1:B:364:ALA:HB3	1:B:365:PRO:HD2	1.75	0.62
1:C:215:MET:O	1:C:216:GLU:C	2.42	0.62
1:D:243:ASN:HD22	1:D:243:ASN:C	2.07	0.62
1:C:317:ILE:CD1	1:C:319:CYS:H	2.13	0.62
1:D:23:GLN:HE22	1:D:475:SER:HB2	1.65	0.61
1:D:278:CYS:SG	1:D:399:LEU:HD11	2.40	0.61
1:B:117:THR:HG21	4:B:723:HOH:O	2.00	0.61
1:B:56:LYS:HG3	1:B:236:CYS:SG	2.41	0.61
1:A:-1:PHE:HD1	1:A:0:THR:H	1.47	0.61
1:D:51:PHE:CE2	1:D:235:GLU:HG3	2.36	0.61
1:D:509:TRP:C	1:D:511:LYS:H	2.08	0.61
1:B:420:ASP:CG	1:B:449:THR:HG21	2.23	0.60
1:B:363:LEU:HA	1:B:367:TRP:HD1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:HIS:O	1:C:47:PRO:HD3	2.00	0.60
1:C:276:THR:N	1:C:277:GLY:HA3	2.16	0.60
1:C:233:THR:OG1	1:C:234:ASP:N	2.30	0.60
1:C:317:ILE:HD12	1:C:319:CYS:H	1.66	0.60
1:A:105:ASN:HD22	1:A:105:ASN:H	1.50	0.60
1:C:417:LEU:HB3	1:C:441:ILE:HG13	1.83	0.60
1:C:401:ASP:CG	1:C:501:ARG:HH21	2.10	0.59
1:A:65:LEU:HD22	1:A:69:ASP:HB3	1.84	0.59
1:C:364:ALA:HB3	1:C:365:PRO:HD2	1.77	0.59
1:C:206:GLU:HB2	4:C:746:HOH:O	2.03	0.58
1:D:144:LYS:O	1:D:148:MET:HG3	2.03	0.58
1:B:272:ASN:ND2	1:B:278:CYS:SG	2.69	0.58
1:A:173:LEU:O	1:A:177:LEU:HB2	2.04	0.58
1:D:268:GLY:HA2	1:D:412:LEU:HD11	1.86	0.57
1:D:105:ASN:HD22	1:D:105:ASN:N	1.99	0.57
1:A:396:ALA:HB1	1:A:436:LEU:HD12	1.86	0.57
1:C:88:VAL:HG12	1:C:90:TRP:HE3	1.69	0.57
1:C:54:ALA:O	1:C:58:MET:HG3	2.05	0.57
1:D:481:TRP:HE3	1:D:481:TRP:O	1.88	0.57
1:C:275:GLY:HA3	2:C:601:GOL:H12	1.87	0.57
1:D:278:CYS:SG	1:D:399:LEU:HD21	2.45	0.57
1:A:224:ASN:HD22	1:A:302:GLN:N	1.87	0.56
1:B:105:ASN:HD22	1:B:105:ASN:H	1.53	0.56
1:C:358:ALA:HB2	1:C:362:LEU:HD13	1.88	0.56
1:A:146:ARG:NE	4:A:750:HOH:O	2.32	0.56
1:B:416:SER:HB2	1:B:440:ASP:O	2.06	0.55
1:B:106:ASP:OD1	1:B:108:ARG:HG2	2.06	0.55
1:D:20:ASP:C	1:D:20:ASP:OD1	2.49	0.55
1:A:110:TYR:O	1:A:113:THR:HG22	2.07	0.55
1:B:278:CYS:SG	1:B:399:LEU:CD1	2.87	0.55
1:C:477:ARG:NH2	4:C:709:HOH:O	2.39	0.55
1:D:278:CYS:HB2	1:D:317:ILE:HG12	1.88	0.54
1:A:234:ASP:HB2	4:A:752:HOH:O	2.06	0.54
1:D:242:LEU:O	1:D:243:ASN:HB3	2.05	0.54
1:C:124:ASP:O	1:C:127:PHE:HB3	2.07	0.54
1:D:424:SER:HA	1:D:430:MET:HE3	1.89	0.54
1:B:0:THR:HG22	1:B:1:MET:H	1.73	0.54
1:C:160:ARG:HB2	1:C:160:ARG:NH1	2.23	0.54
1:D:489:SER:C	1:D:493:ARG:HE	2.16	0.54
1:A:198:LEU:HD22	1:A:311:TYR:HE1	1.71	0.54
1:A:222:ARG:HD3	1:A:226:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:VAL:HG12	1:C:222:ARG:HH11	1.71	0.54
1:D:85:GLU:OE1	1:D:139:TYR:CE2	2.61	0.54
1:A:466:THR:HG23	1:A:470:GLU:OE1	2.08	0.54
1:B:328:ARG:HH11	1:B:328:ARG:CG	2.21	0.53
1:A:117:THR:HG22	1:A:136:VAL:HG11	1.90	0.53
1:A:242:LEU:O	1:A:243:ASN:CB	2.57	0.53
1:D:268:GLY:CA	1:D:412:LEU:HD11	2.38	0.53
1:C:160:ARG:HH11	1:C:160:ARG:HG2	1.71	0.53
1:A:223:SER:HB2	1:A:302:GLN:HG2	1.89	0.53
1:B:146:ARG:NH1	1:B:212:LYS:CG	2.71	0.53
1:B:328:ARG:HH11	1:B:328:ARG:HG2	1.74	0.53
1:D:336:HIS:CD2	1:D:338:THR:OG1	2.60	0.53
1:C:141:ALA:HB3	1:C:193:THR:HA	1.90	0.52
1:B:474:VAL:HG22	1:B:477:ARG:HH12	1.74	0.52
1:B:184:VAL:CG1	1:B:222:ARG:HD2	2.39	0.52
1:C:224:ASN:ND2	1:C:302:GLN:H	2.02	0.52
1:D:324:VAL:HG21	1:D:423:LEU:HD21	1.90	0.52
1:A:141:ALA:HB3	1:A:193:THR:HA	1.91	0.52
1:B:274:TYR:CZ	1:B:430:MET:HE1	2.45	0.52
1:C:232:GLU:OE1	1:C:245:ARG:NH1	2.43	0.52
1:C:273:THR:HA	1:C:420:ASP:OD2	2.10	0.52
1:B:252:ILE:HG23	1:B:257:SER:HB2	1.91	0.51
1:D:224:ASN:ND2	1:D:302:GLN:H	2.07	0.51
1:D:98:LEU:HD21	1:D:158:ALA:HB3	1.93	0.51
1:D:282:MET:HE3	1:D:414:LEU:HD11	1.93	0.51
1:B:126:MET:SD	1:B:135:PRO:HB3	2.51	0.51
1:C:160:ARG:NH1	1:C:160:ARG:HG2	2.26	0.51
1:B:125:SER:O	1:B:136:VAL:HG23	2.11	0.50
1:B:85:GLU:OE1	1:B:139:TYR:CE1	2.64	0.50
1:B:234:ASP:OD2	1:B:234:ASP:N	2.39	0.50
1:D:51:PHE:HE2	1:D:235:GLU:HG3	1.77	0.50
1:A:494:GLU:O	1:A:494:GLU:OE2	2.29	0.50
1:B:69:ASP:C	1:B:71:SER:H	2.18	0.50
1:D:72:PHE:HA	1:D:73:ARG:HH11	1.75	0.50
1:C:370:SER:HA	1:C:510:ALA:HB3	1.94	0.50
1:D:238:VAL:HG23	1:D:239:ALA:N	2.26	0.50
1:C:239:ALA:O	1:C:242:LEU:O	2.30	0.50
1:C:283:ASN:C	1:C:283:ASN:OD1	2.55	0.49
1:A:277:GLY:HA3	2:A:602:GOL:O2	2.12	0.49
1:D:115:LYS:HG3	1:D:119:GLU:OE1	2.13	0.49
1:D:271:LYS:HG2	1:D:272:ASN:N	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:ARG:NH2	1:D:481:TRP:CH2	2.71	0.49
1:C:139:TYR:O	1:C:144:LYS:HE2	2.12	0.49
1:D:279:PHE:CZ	2:D:602:GOL:H32	2.47	0.49
1:B:201:ARG:HD3	1:B:309:CYS:SG	2.53	0.49
1:D:198:LEU:HD22	1:D:311:TYR:HE1	1.77	0.49
1:A:466:THR:N	1:A:470:GLU:OE1	2.31	0.49
1:B:81:THR:OG1	1:B:254:ASP:HA	2.13	0.49
1:A:145:MET:HE2	1:A:166:PHE:HB3	1.95	0.49
1:C:267:LYS:HE3	1:C:412:LEU:HD21	1.95	0.48
1:A:209:GLU:O	1:A:212:LYS:HD2	2.12	0.48
1:B:211:LEU:O	1:B:212:LYS:HG2	2.12	0.48
1:D:280:LEU:HD12	1:D:399:LEU:CD1	2.27	0.48
1:B:274:TYR:O	1:B:421:GLY:HA3	2.13	0.48
1:C:274:TYR:HB3	1:C:423:LEU:HB2	1.96	0.48
1:B:225:SER:OG	1:B:457:CYS:O	2.20	0.48
1:D:44:GLU:HA	1:D:103:VAL:HG23	1.96	0.48
1:A:442:LEU:HB3	1:A:481:TRP:CE3	2.49	0.48
1:B:90:TRP:HA	1:B:98:LEU:HD22	1.96	0.48
1:C:91:ASP:OD1	1:C:94:THR:CG2	2.48	0.48
1:B:303:VAL:O	1:B:307:GLY:HA3	2.13	0.48
1:B:355:PHE:O	1:B:357:PRO:HD3	2.14	0.48
1:D:235:GLU:O	1:D:238:VAL:HG13	2.14	0.47
1:A:336:HIS:N	1:A:339:GLU:OE1	2.30	0.47
1:A:477:ARG:NH2	4:A:713:HOH:O	2.29	0.47
1:B:278:CYS:HG	1:B:399:LEU:HD11	1.78	0.47
1:B:282:MET:O	1:B:312:ALA:HA	2.14	0.47
1:D:71:SER:O	1:D:73:ARG:HD2	2.14	0.47
1:A:159:CYS:HB2	1:A:164:LEU:HD22	1.95	0.47
1:B:115:LYS:HE2	1:B:115:LYS:HB3	1.64	0.47
1:C:65:LEU:HD22	1:C:69:ASP:HB3	1.97	0.47
1:C:274:TYR:CE1	1:C:430:MET:HE1	2.50	0.47
1:A:274:TYR:CZ	1:A:430:MET:HE1	2.50	0.47
1:A:282:MET:HE2	1:A:414:LEU:HD13	1.97	0.47
1:C:328:ARG:HD2	1:C:335:SER:O	2.14	0.47
1:C:358:ALA:O	1:C:372:ARG:HA	2.14	0.47
1:D:433:GLN:HG2	1:D:441:ILE:HD11	1.97	0.47
1:D:509:TRP:C	1:D:511:LYS:N	2.72	0.47
1:A:198:LEU:HD22	1:A:311:TYR:CE1	2.49	0.47
1:D:357:PRO:HD3	1:D:394:ALA:HB1	1.96	0.46
1:D:15:ARG:NH2	1:D:448:GLU:OE1	2.49	0.46
1:A:419:VAL:CG2	1:A:443:VAL:HG22	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:LEU:HA	1:B:367:TRP:CD1	2.49	0.46
1:A:407:LYS:HD2	1:A:413:ASN:HA	1.97	0.46
1:B:342:LYS:HA	1:B:342:LYS:HD3	1.74	0.46
1:C:200:THR:O	1:C:201:ARG:HB2	2.15	0.46
1:A:81:THR:HA	1:A:252:ILE:O	2.16	0.46
1:A:224:ASN:ND2	1:A:302:GLN:N	2.50	0.46
1:B:271:LYS:HE3	1:B:281:LEU:HD13	1.96	0.46
1:C:92:ARG:HD3	4:C:733:HOH:O	2.16	0.46
1:D:291:SER:HA	1:D:409:ASP:OD2	2.15	0.46
1:C:184:VAL:HG12	1:C:222:ARG:NH1	2.28	0.45
1:B:276:THR:N	1:B:277:GLY:HA3	2.32	0.45
1:D:137:SER:C	1:D:139:TYR:H	2.24	0.45
1:C:176:LYS:HD2	1:C:176:LYS:HA	1.43	0.45
1:D:362:LEU:HD22	1:D:371:ALA:CB	2.46	0.45
1:A:64:LYS:O	1:A:68:LYS:HG2	2.17	0.45
1:A:366:TYR:CE1	1:A:401:ASP:OD1	2.70	0.45
1:C:324:VAL:HG21	1:C:423:LEU:HD21	1.99	0.45
1:D:271:LYS:HE2	1:D:281:LEU:HD13	1.98	0.45
1:A:430:MET:HE2	1:A:430:MET:HA	1.99	0.45
1:A:328:ARG:HB2	1:A:334:PHE:CE2	2.51	0.45
1:B:69:ASP:C	1:B:71:SER:N	2.74	0.45
1:C:74:LYS:HE3	1:C:76:GLU:OE2	2.16	0.45
1:C:226:GLU:CD	1:C:305:ARG:HG3	2.42	0.45
1:A:366:TYR:HE1	1:A:401:ASP:OD1	2.00	0.45
1:C:103:VAL:O	1:C:104:TRP:C	2.60	0.45
1:A:97:PRO:HD3	1:A:172:TRP:CH2	2.52	0.45
1:A:288:ALA:HB2	1:A:311:TYR:CE1	2.52	0.45
1:C:235:GLU:C	1:C:237:GLY:N	2.72	0.45
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.31	0.44
1:D:17:ILE:HD13	1:D:28:VAL:HG23	1.99	0.44
1:A:157:ASP:O	1:A:160:ARG:CB	2.53	0.44
1:C:96:GLU:HB3	1:C:97:PRO:HD2	2.00	0.44
1:C:350:THR:O	1:C:351:GLN:HB2	2.17	0.44
1:A:275:GLY:N	1:A:277:GLY:O	2.50	0.44
1:B:447:HIS:C	1:B:449:THR:H	2.23	0.44
1:C:160:ARG:CG	1:C:160:ARG:NH1	2.70	0.44
1:A:65:LEU:HD13	1:A:72:PHE:CG	2.52	0.44
1:B:171:THR:OG1	1:B:185:THR:HB	2.17	0.44
1:D:413[A]:ASN:ND2	1:D:414:LEU:N	2.63	0.44
1:A:243:ASN:OD1	1:A:244:GLU:OE1	2.36	0.44
1:B:185:THR:HG22	1:B:219:PRO:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ARG:HG3	1:C:30:GLN:HG3	1.99	0.44
1:C:80:ILE:O	1:C:251:SER:HA	2.18	0.44
1:A:91:ASP:OD2	1:A:163:THR:HG23	2.18	0.44
1:A:113:THR:O	1:A:117:THR:HG22	2.17	0.44
1:B:187:VAL:HG13	1:B:222:ARG:O	2.17	0.44
1:D:64:LYS:O	1:D:68:LYS:HG3	2.17	0.44
1:D:91:ASP:HB3	1:D:94:THR:OG1	2.17	0.44
1:D:489:SER:HA	1:D:493:ARG:HH21	1.83	0.44
1:B:153:PRO:O	1:B:157:ASP:OD1	2.36	0.44
1:C:58:MET:HE1	1:C:78:ILE:HD13	2.00	0.44
1:C:276:THR:HB	2:C:601:GOL:H2	1.99	0.44
1:C:270:ALA:HB2	1:C:282:MET:HG3	2.00	0.44
1:D:126:MET:SD	1:D:135:PRO:HB3	2.58	0.44
1:D:2:LYS:HD2	1:D:76:GLU:CD	2.42	0.43
1:A:374:THR:HG23	1:A:507:THR:HG22	1.97	0.43
1:C:90:TRP:HA	1:C:98:LEU:HD22	2.01	0.43
1:C:267:LYS:HA	1:C:283:ASN:O	2.18	0.43
1:C:20:ASP:OD1	1:C:20:ASP:C	2.60	0.43
1:B:328:ARG:HB2	1:B:334:PHE:CZ	2.52	0.43
1:C:44:GLU:HG3	1:C:100:TYR:CB	2.49	0.43
1:D:341:GLU:O	1:D:345:ARG:HG3	2.18	0.43
1:D:357:PRO:HD3	1:D:394:ALA:CB	2.49	0.43
1:B:105:ASN:HB2	3:B:602:HEZ:H11	1.99	0.43
1:B:446:MET:HB2	1:B:479:ASN:OD1	2.18	0.43
1:A:374:THR:HG21	1:A:507:THR:CG2	2.43	0.43
1:D:81:THR:HA	1:D:252:ILE:O	2.19	0.43
1:D:463:GLY:O	1:D:464:VAL:C	2.62	0.43
1:B:20:ASP:C	1:B:20:ASP:OD1	2.61	0.43
1:B:42:TRP:HA	1:B:106:ASP:OD2	2.18	0.43
1:C:249:MET:HE2	1:C:461:ALA:HB1	2.01	0.43
1:A:216:GLU:H	1:A:216:GLU:HG3	1.65	0.43
1:C:265:PHE:HD1	1:C:472:LYS:HE3	1.83	0.43
1:B:430:MET:HE2	1:B:430:MET:HA	2.01	0.42
1:A:44:GLU:HA	1:A:103:VAL:HG23	2.01	0.42
1:A:477:ARG:NH1	4:A:713:HOH:O	2.48	0.42
1:B:254:ASP:OD2	1:B:255:GLN:HG2	2.19	0.42
1:B:363:LEU:HB3	1:B:364:ALA:H	1.52	0.42
1:B:73:ARG:HG3	1:B:74:LYS:HG2	2.01	0.42
1:C:147:TRP:CE3	1:C:147:TRP:C	2.97	0.42
1:A:101:ALA:O	1:A:102:PRO:C	2.60	0.42
1:A:300:GLY:O	1:A:301:PHE:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:VAL:HG21	1:A:423:LEU:HD21	2.01	0.42
1:A:336:HIS:HD2	1:A:338:THR:CA	2.30	0.42
1:B:168:THR:OG1	1:B:170:ASP:OD1	2.33	0.42
1:D:490:ALA:O	1:D:491:MET:C	2.62	0.42
1:A:113:THR:O	1:A:117:THR:CG2	2.68	0.42
1:B:289:ARG:HG2	1:B:409:ASP:O	2.19	0.42
1:B:326:TRP:O	1:B:330:ASN:HB2	2.20	0.42
1:D:170:ASP:O	1:D:174:MET:HG3	2.20	0.42
1:D:368:ASP:OD1	1:D:370:SER:HB2	2.19	0.42
1:B:31:VAL:HG13	1:B:32:PRO:HD2	2.00	0.42
1:D:401:ASP:OD2	1:D:501:ARG:NH2	2.46	0.42
1:C:410:ALA:HB1	1:C:412:LEU:HD12	2.02	0.42
1:C:472:LYS:HD3	4:C:743:HOH:O	2.19	0.42
1:A:252:ILE:HG23	1:A:257:SER:HB2	2.02	0.41
1:D:208:CYS:HB3	1:D:213:ILE:O	2.20	0.41
1:D:212:LYS:O	1:D:214:PRO:HD3	2.19	0.41
1:A:372:ARG:HA	1:A:372:ARG:HD3	1.85	0.41
1:D:85:GLU:HB2	1:D:104:TRP:HB3	2.02	0.41
1:A:344:ALA:HB2	1:A:388:ILE:HG22	2.03	0.41
1:A:418:ARG:HD2	1:A:418:ARG:N	2.35	0.41
1:B:23:GLN:HE22	1:B:475:SER:HB2	1.85	0.41
1:C:147:TRP:O	1:C:147:TRP:CD2	2.74	0.41
1:B:233:THR:O	1:B:239:ALA:HB2	2.20	0.41
1:B:254:ASP:OD1	2:B:601:GOL:O1	2.28	0.41
1:C:44:GLU:OE1	1:C:100:TYR:HB2	2.21	0.41
1:C:47:PRO:HB2	1:C:97:PRO:HG3	2.03	0.41
1:D:213:ILE:HG21	1:D:218:LEU:HD21	2.03	0.41
1:A:117:THR:HB	1:A:125:SER:HA	2.02	0.41
1:A:420:ASP:OD1	1:A:449:THR:OG1	2.38	0.41
1:A:273:THR:HA	1:A:420:ASP:OD2	2.21	0.41
1:C:80:ILE:HD12	1:C:174:MET:HG3	2.02	0.41
1:A:208:CYS:HB3	1:A:213:ILE:O	2.20	0.41
1:B:295:LEU:HD13	1:B:406:MET:HG3	2.01	0.41
3:B:602:HEZ:O1	3:B:603:HEZ:H62	2.20	0.41
1:D:142:ALA:O	1:D:145:MET:HB2	2.21	0.41
1:B:106:ASP:OD1	4:B:725:HOH:O	2.22	0.41
1:C:325:GLU:OE2	1:C:328:ARG:NH1	2.53	0.41
1:C:459:GLY:HA3	1:C:465:TRP:CZ3	2.55	0.41
1:B:447:HIS:C	1:B:449:THR:N	2.78	0.41
1:C:108:ARG:HD3	1:C:147:TRP:CE2	2.55	0.41
1:C:186:ASP:CG	1:C:189:ASN:HD22	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:MET:O	1:C:217:THR:N	2.52	0.41
1:C:215:MET:C	1:C:217:THR:N	2.76	0.41
1:D:170:ASP:OD1	1:D:170:ASP:N	2.51	0.41
1:D:364:ALA:HB1	1:D:402:VAL:HG22	2.03	0.41
1:A:370:SER:HA	1:A:510:ALA:HB3	2.03	0.41
1:B:90:TRP:CA	1:B:98:LEU:HD22	2.51	0.41
1:B:273:THR:HG23	1:B:420:ASP:OD2	2.21	0.41
1:C:215:MET:HB3	1:C:215:MET:HE2	1.42	0.41
1:C:363:LEU:HB3	1:C:364:ALA:H	1.16	0.41
1:D:130:LYS:HA	1:D:130:LYS:HD3	1.84	0.41
1:A:-1:PHE:HD1	1:A:0:THR:N	2.16	0.40
1:A:274:TYR:CE1	1:A:430:MET:HE1	2.56	0.40
1:C:65:LEU:HD13	1:C:72:PHE:CG	2.56	0.40
1:A:146:ARG:HH12	1:A:149:LEU:HD12	1.86	0.40
1:A:195:LEU:HD13	1:A:218:LEU:HD11	2.04	0.40
1:B:447:HIS:O	1:B:449:THR:N	2.46	0.40
1:D:271:LYS:NZ	1:D:273:THR:OG1	2.41	0.40
1:A:4:VAL:HG23	1:A:77:ALA:O	2.20	0.40
1:A:16:PHE:CD2	1:A:58:MET:HA	2.57	0.40
1:C:259:LEU:CD1	1:C:264:CYS:HB2	2.51	0.40
1:B:169:ILE:O	1:B:173:LEU:HB2	2.21	0.40
1:C:108:ARG:HD3	1:C:147:TRP:CZ2	2.56	0.40
1:D:130:LYS:HD2	4:D:720:HOH:O	2.21	0.40
1:D:141:ALA:HB3	1:D:193:THR:HA	2.04	0.40
1:D:470:GLU:O	1:D:474:VAL:HG23	2.21	0.40
1:D:85:GLU:O	1:D:86:THR:C	2.63	0.40
1:D:317:ILE:O	1:D:317:ILE:HG13	2.16	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	511/518 (99%)	485 (95%)	25 (5%)	1 (0%)	43	56
1	B	511/518 (99%)	480 (94%)	27 (5%)	4 (1%)	16	23
1	C	511/518 (99%)	492 (96%)	17 (3%)	2 (0%)	30	40
1	D	512/518 (99%)	476 (93%)	33 (6%)	3 (1%)	21	30
All	All	2045/2072 (99%)	1933 (94%)	102 (5%)	10 (0%)	24	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA
1	B	364	ALA
1	C	364	ALA
1	D	364	ALA
1	B	215	MET
1	B	337	ILE
1	D	243	ASN
1	C	226	GLU
1	B	363	LEU
1	D	480	SER

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	421/425 (99%)	372 (88%)	49 (12%)	5	7
1	B	421/425 (99%)	383 (91%)	38 (9%)	9	13
1	C	421/425 (99%)	384 (91%)	37 (9%)	9	14
1	D	422/425 (99%)	383 (91%)	39 (9%)	8	12
All	All	1685/1700 (99%)	1522 (90%)	163 (10%)	8	11

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	PHE

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Mol	Chain	Res	Type
1	A	17	ILE
1	A	56	LYS
1	A	59	SER
1	A	65	LEU
1	A	87	THR
1	A	93	VAL
1	A	94	THR
1	A	98	LEU
1	A	105	ASN
1	A	106	ASP
1	A	113	THR
1	A	117	THR
1	A	146	ARG
1	A	168	THR
1	A	173	LEU
1	A	177	LEU
1	A	187	VAL
1	A	202	LYS
1	A	209	GLU
1	A	212	LYS
1	A	213	ILE
1	A	216	GLU
1	A	238	VAL
1	A	266	GLU
1	A	271	LYS
1	A	276	THR
1	A	289	ARG
1	A	305	ARG
1	A	317	ILE
1	A	335	SER
1	A	338	THR
1	A	342	LYS
1	A	350	THR
1	A	362	LEU
1	A	363	LEU
1	A	366	TYR
1	A	374	THR
1	A	381	LYS
1	A	441	ILE
1	A	442	LEU
1	A	472	LYS
1	A	476	ARG

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Mol	Chain	Res	Type
1	A	482	LYS
1	A	483	THR
1	A	491	MET
1	A	494	GLU
1	A	502	GLU
1	A	511	LYS
1	B	0	THR
1	B	17	ILE
1	B	59	SER
1	B	65	LEU
1	B	98	LEU
1	B	105	ASN
1	B	112	ILE
1	B	113	THR
1	B	114	LYS
1	B	115	LYS
1	B	117	THR
1	B	157	ASP
1	B	173	LEU
1	B	177	LEU
1	B	184	VAL
1	B	198	LEU
1	B	199	ARG
1	B	213	ILE
1	B	216	GLU
1	B	232	GLU
1	B	263	MET
1	B	266	GLU
1	B	271	LYS
1	B	276	THR
1	B	289	ARG
1	B	303	VAL
1	B	305	ARG
1	B	317	ILE
1	B	328	ARG
1	B	335	SER
1	B	338	THR
1	B	342	LYS
1	B	362	LEU
1	B	366	TYR
1	B	399	LEU
1	B	441	ILE

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Mol	Chain	Res	Type
1	B	476	ARG
1	B	501	ARG
1	C	2	LYS
1	C	4	VAL
1	C	15	ARG
1	C	17	ILE
1	C	65	LEU
1	C	71	SER
1	C	74	LYS
1	C	91	ASP
1	C	98	LEU
1	C	113	THR
1	C	120	LEU
1	C	146	ARG
1	C	155	VAL
1	C	160	ARG
1	C	173	LEU
1	C	187	VAL
1	C	213	ILE
1	C	215	MET
1	C	233	THR
1	C	238	VAL
1	C	243	ASN
1	C	245	ARG
1	C	266	GLU
1	C	271	LYS
1	C	278	CYS
1	C	305	ARG
1	C	317	ILE
1	C	338	THR
1	C	342	LYS
1	C	362	LEU
1	C	366	TYR
1	C	441	ILE
1	C	442	LEU
1	C	470	GLU
1	C	472	LYS
1	C	483	THR
1	C	508	LYS
1	D	-1	PHE
1	D	1	MET
1	D	15	ARG

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Mol	Chain	Res	Type
1	D	27	SER
1	D	56	LYS
1	D	65	LEU
1	D	71	SER
1	D	73	ARG
1	D	93	VAL
1	D	98	LEU
1	D	105	ASN
1	D	117	THR
1	D	146	ARG
1	D	173	LEU
1	D	177	LEU
1	D	198	LEU
1	D	212	LYS
1	D	243	ASN
1	D	244	GLU
1	D	245	ARG
1	D	271	LYS
1	D	289	ARG
1	D	292	LYS
1	D	317	ILE
1	D	335	SER
1	D	342	LYS
1	D	362	LEU
1	D	366	TYR
1	D	370	SER
1	D	405	SER
1	D	412	LEU
1	D	420	ASP
1	D	442	LEU
1	D	472	LYS
1	D	476	ARG
1	D	481	TRP
1	D	483	THR
1	D	491	MET
1	D	492	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	36	HIS

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Mol	Chain	Res	Type
1	A	39	HIS
1	A	105	ASN
1	A	151	ASN
1	A	224	ASN
1	A	272	ASN
1	A	293	HIS
1	A	302	GLN
1	A	336	HIS
1	B	23	GLN
1	B	30	GLN
1	B	105	ASN
1	B	151	ASN
1	B	224	ASN
1	B	243	ASN
1	B	351	GLN
1	C	23	GLN
1	C	35	GLN
1	C	36	HIS
1	C	105	ASN
1	C	224	ASN
1	C	272	ASN
1	C	302	GLN
1	C	336	HIS
1	C	351	GLN
1	C	393	GLN
1	D	23	GLN
1	D	151	ASN
1	D	224	ASN
1	D	243	ASN
1	D	336	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

11 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	$\# Z > 2$
3	HEZ	C	603	-	7,7,7	0.53	0	6,6,6	0.47	0
3	HEZ	B	603	-	7,7,7	0.52	0	6,6,6	0.29	0
2	GOL	B	601	-	5,5,5	0.58	0	5,5,5	0.97	0
2	GOL	A	602	-	5,5,5	0.47	0	5,5,5	0.36	0
2	GOL	A	601	-	5,5,5	0.51	0	5,5,5	0.48	0
2	GOL	C	602	-	5,5,5	0.45	0	5,5,5	0.50	0
3	HEZ	D	603	-	7,7,7	0.51	0	6,6,6	0.34	0
3	HEZ	B	602	-	7,7,7	0.50	0	6,6,6	0.40	0
2	GOL	C	601	-	5,5,5	0.33	0	5,5,5	0.36	0
2	GOL	D	602	-	5,5,5	0.28	0	5,5,5	0.69	0
2	GOL	D	601	-	5,5,5	0.35	0	5,5,5	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEZ	C	603	-	-	3/5/5/5	-
3	HEZ	B	603	-	-	4/5/5/5	-
2	GOL	B	601	-	-	3/4/4/4	-
2	GOL	A	602	-	-	4/4/4/4	-
2	GOL	A	601	-	-	2/4/4/4	-
2	GOL	C	602	-	-	4/4/4/4	-
3	HEZ	D	603	-	-	5/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEZ	B	602	-	-	4/5/5/5	-
2	GOL	C	601	-	-	0/4/4/4	-
2	GOL	D	602	-	-	0/4/4/4	-
2	GOL	D	601	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	GOL	O1-C1-C2-C3
2	A	602	GOL	C1-C2-C3-O3
2	C	602	GOL	O1-C1-C2-C3
2	C	602	GOL	C1-C2-C3-O3
2	A	602	GOL	O2-C2-C3-O3
2	C	602	GOL	O2-C2-C3-O3
2	A	601	GOL	O1-C1-C2-C3
2	B	601	GOL	C1-C2-C3-O3
2	A	602	GOL	O1-C1-C2-O2
3	C	603	HEZ	C1-C2-C3-C4
3	B	603	HEZ	C3-C4-C5-C6
3	C	603	HEZ	C2-C3-C4-C5
3	B	602	HEZ	C4-C5-C6-O6
3	D	603	HEZ	C4-C5-C6-O6
3	B	602	HEZ	C1-C2-C3-C4
3	D	603	HEZ	C2-C3-C4-C5
3	B	603	HEZ	C2-C3-C4-C5
3	B	602	HEZ	O1-C1-C2-C3
2	C	602	GOL	O1-C1-C2-O2
3	D	603	HEZ	O1-C1-C2-C3
3	D	603	HEZ	C3-C4-C5-C6
3	B	602	HEZ	C2-C3-C4-C5
2	B	601	GOL	O1-C1-C2-O2
3	C	603	HEZ	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-O2
2	B	601	GOL	O2-C2-C3-O3
3	B	603	HEZ	O1-C1-C2-C3
3	B	603	HEZ	C4-C5-C6-O6
3	D	603	HEZ	C1-C2-C3-C4

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	HEZ	2	0
2	B	601	GOL	1	0
2	A	602	GOL	1	0
3	B	602	HEZ	3	0
2	C	601	GOL	2	0
2	D	602	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/518 (99%)	0.13	7 (1%) 73 72	33, 49, 63, 72	1 (0%)
1	B	513/518 (99%)	0.29	11 (2%) 63 62	30, 53, 69, 87	1 (0%)
1	C	513/518 (99%)	0.27	14 (2%) 56 56	32, 51, 68, 75	1 (0%)
1	D	513/518 (99%)	0.23	14 (2%) 56 56	31, 51, 69, 84	2 (0%)
All	All	2052/2072 (99%)	0.23	46 (2%) 62 61	30, 51, 67, 87	5 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	510	ALA	4.8
1	A	278	CYS	4.8
1	D	278	CYS	4.6
1	B	278	CYS	4.5
1	D	511	LYS	3.7
1	B	425	LYS	3.6
1	C	158	ALA	3.5
1	B	510	ALA	3.5
1	C	175	TYR	3.2
1	B	449	THR	3.2
1	B	481	TRP	3.1
1	C	98	LEU	2.9
1	D	491	MET	2.8
1	C	425	LYS	2.6
1	A	309	CYS	2.6
1	D	-1	PHE	2.5
1	B	152	VAL	2.5
1	C	152	VAL	2.5
1	D	481	TRP	2.5
1	A	425	LYS	2.4
1	C	159	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	367	TRP	2.4
1	A	510	ALA	2.4
1	B	490	ALA	2.3
1	A	491	MET	2.3
1	D	490	ALA	2.3
1	C	276	THR	2.3
1	D	408	ARG	2.3
1	C	93	VAL	2.3
1	B	139	TYR	2.3
1	A	364	ALA	2.3
1	D	367	TRP	2.2
1	C	40	PRO	2.2
1	D	0	THR	2.2
1	C	163	THR	2.1
1	B	-1	PHE	2.1
1	C	97	PRO	2.1
1	B	483	THR	2.1
1	C	364	ALA	2.1
1	D	364	ALA	2.1
1	C	164	LEU	2.1
1	C	488	GLY	2.1
1	D	463	GLY	2.1
1	D	66	ARG	2.0
1	B	491	MET	2.0
1	D	1	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	HEZ	C	603	8/8	0.68	0.17	49,51,52,53	0
3	HEZ	D	603	8/8	0.79	0.16	52,56,57,58	0
3	HEZ	B	602	8/8	0.80	0.17	63,66,67,67	0
2	GOL	A	602	6/6	0.80	0.13	58,60,63,65	0
2	GOL	D	602	6/6	0.80	0.15	60,61,61,62	0
2	GOL	C	601	6/6	0.82	0.12	72,73,74,75	0
3	HEZ	B	603	8/8	0.85	0.17	58,62,63,64	0
2	GOL	C	602	6/6	0.89	0.12	50,58,61,65	0
2	GOL	D	601	6/6	0.93	0.10	38,40,43,45	0
2	GOL	A	601	6/6	0.93	0.09	58,59,60,63	0
2	GOL	B	601	6/6	0.94	0.08	31,34,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.