



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:57 AM UTC

PDB ID : 1YW0 / pdb_00001yw0
Title : Crystal structure of the tryptophan 2,3-dioxygenase from *Xanthomonas campestris*. Northeast Structural Genomics Target XcR13.
Authors : Vorobiev, S.M.; Abashidze, M.; Forouhar, F.; Kuzin, A.; Xiao, R.; Ciano, M.; Aton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-02-16
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

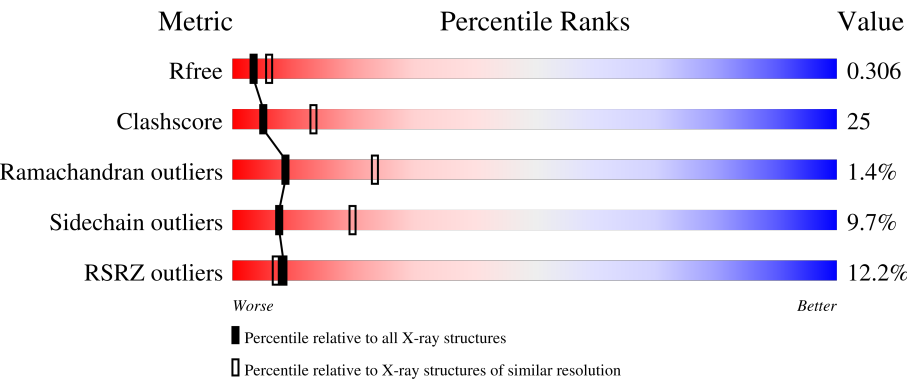
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	276	8% 47% 34% 6% • 12%
1	B	276	14% 47% 34% 6% • 12%
1	C	276	11% 50% 29% 7% • 12%
1	D	276	10% 47% 34% 5% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8274 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 tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	Se	0	0	0
			2043	1316	358	362	2	5			
1	B	242	Total	C	N	O	S	Se	0	0	0
			2035	1312	356	360	2	5			
1	C	243	Total	C	N	O	S	Se	0	0	0
			2043	1316	358	362	2	5			
1	D	243	Total	C	N	O	S	Se	0	0	0
			2040	1315	357	361	2	5			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	MSE	MET	modified residue	UNP Q8PDA8
A	114	MSE	MET	modified residue	UNP Q8PDA8
A	145	MSE	MET	modified residue	UNP Q8PDA8
A	241	MSE	MET	modified residue	UNP Q8PDA8
A	245	MSE	MET	modified residue	UNP Q8PDA8
B	49	MSE	MET	modified residue	UNP Q8PDA8
B	114	MSE	MET	modified residue	UNP Q8PDA8
B	145	MSE	MET	modified residue	UNP Q8PDA8
B	241	MSE	MET	modified residue	UNP Q8PDA8
B	245	MSE	MET	modified residue	UNP Q8PDA8
C	49	MSE	MET	modified residue	UNP Q8PDA8
C	114	MSE	MET	modified residue	UNP Q8PDA8
C	145	MSE	MET	modified residue	UNP Q8PDA8
C	241	MSE	MET	modified residue	UNP Q8PDA8
C	245	MSE	MET	modified residue	UNP Q8PDA8
D	49	MSE	MET	modified residue	UNP Q8PDA8
D	114	MSE	MET	modified residue	UNP Q8PDA8
D	145	MSE	MET	modified residue	UNP Q8PDA8
D	241	MSE	MET	modified residue	UNP Q8PDA8
D	245	MSE	MET	modified residue	UNP Q8PDA8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

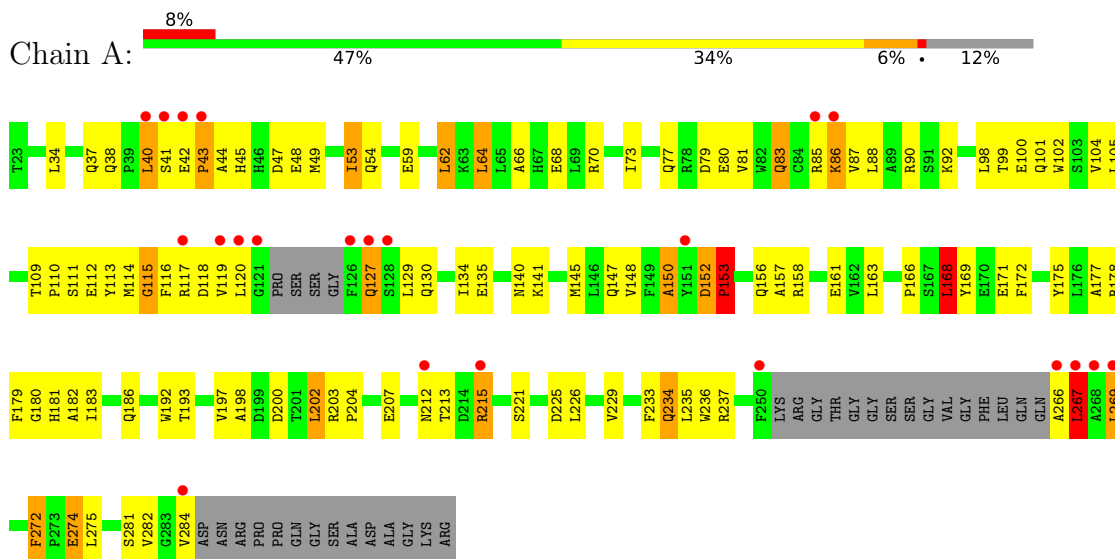
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total 31	O 31	0	0
3	B	25	Total 25	O 25	0	0
3	C	20	Total 20	O 20	0	0
3	D	29	Total 29	O 29	0	0

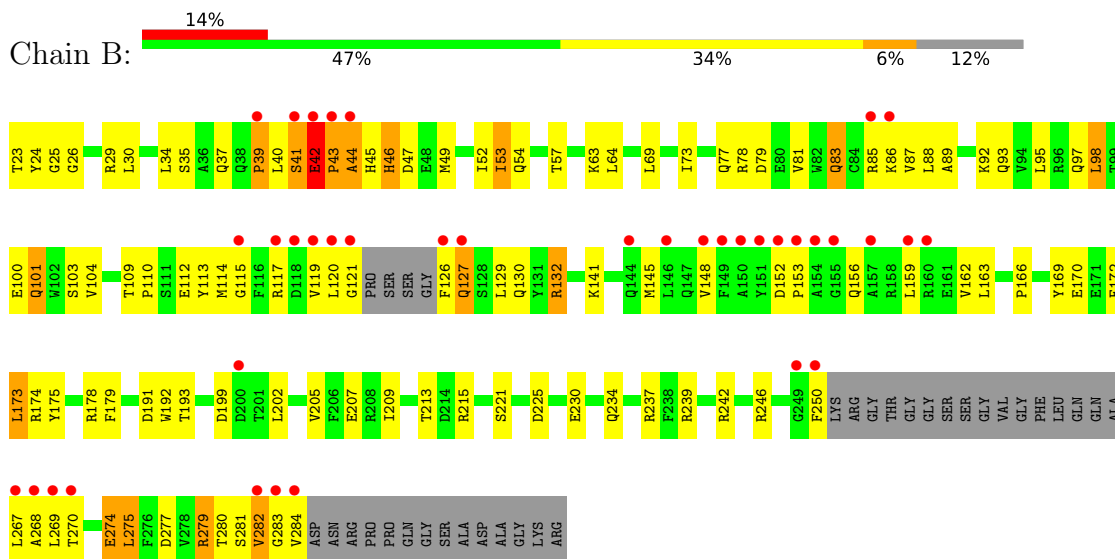
3 Residue-property plots

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.

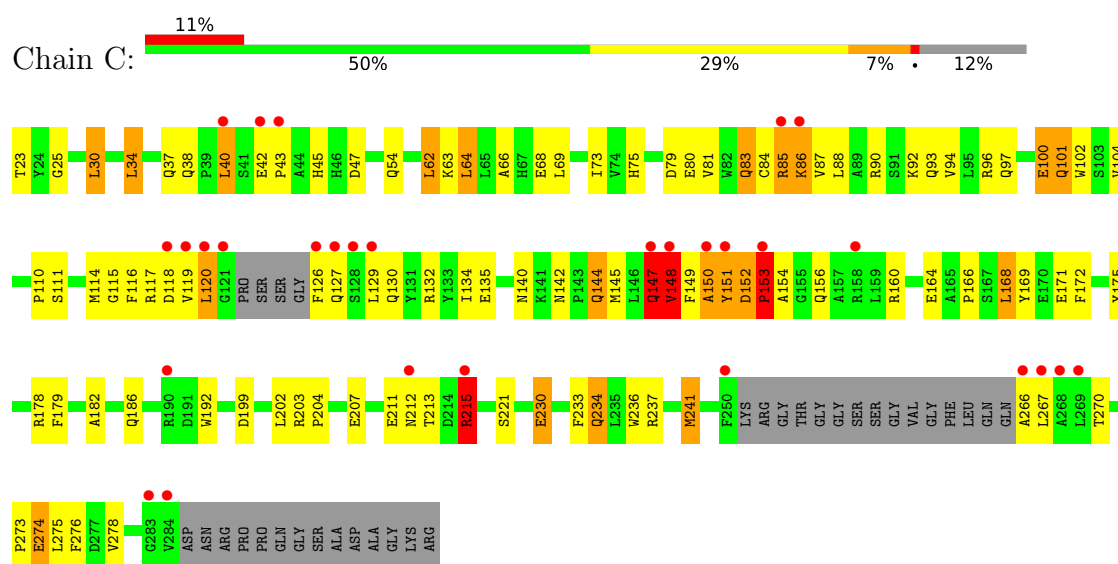
• Molecule 1: tryptophan 2,3-dioxygenase



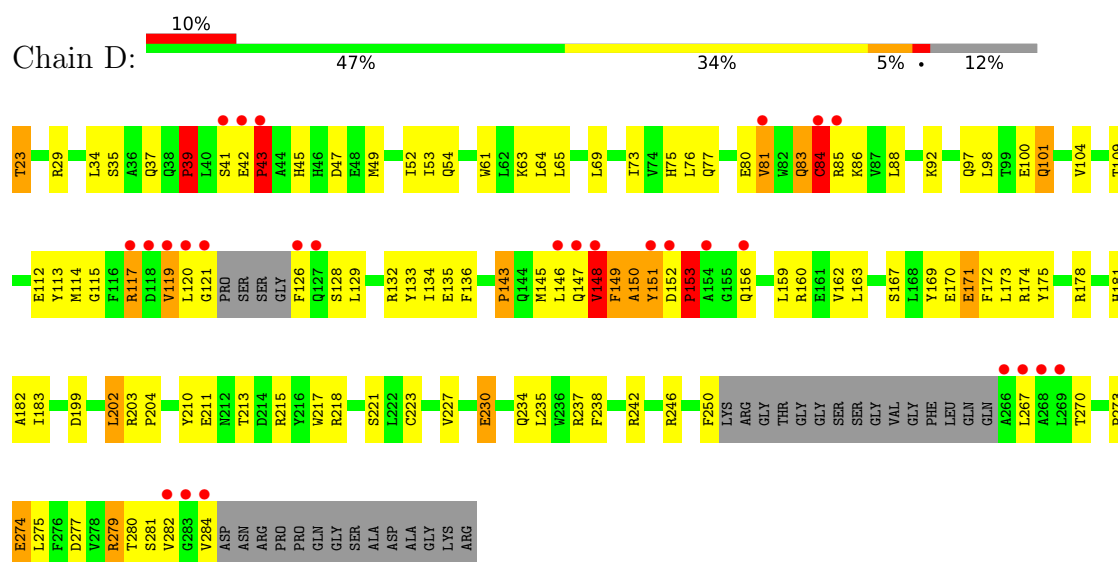
• Molecule 1: tryptophan 2,3-dioxygenase



• Molecule 1: tryptophan 2,3-dioxygenase



• Molecule 1: tryptophan 2,3-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.70Å 110.22Å 149.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.32 – 2.70 29.32 – 2.70	Depositor EDS
% Data completeness (in resolution range)	81.8 (29.32-2.70) 84.9 (29.32-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.294 0.262 , 0.306	Depositor DCC
R_{free} test set	2795 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8274	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.1917e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG

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	0.65	1/2090 (0.0%)	1.10	20/2825 (0.7%)
1	B	0.57	2/2082 (0.1%)	1.14	17/2814 (0.6%)
1	C	0.70	2/2090 (0.1%)	1.11	18/2825 (0.6%)
1	D	0.73	6/2087 (0.3%)	1.16	23/2821 (0.8%)
All	All	0.66	11/8349 (0.1%)	1.13	78/11285 (0.7%)

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	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	42	GLU	CA-C	-12.34	1.37	1.52
1	C	212	ASN	CA-C	9.80	1.64	1.53
1	D	149	PHE	CA-C	-8.87	1.42	1.53
1	A	267	LEU	CA-CB	-7.80	1.42	1.53
1	D	42	GLU	C-O	7.55	1.31	1.24
1	C	213	THR	N-CA	6.05	1.53	1.46
1	D	43	PRO	N-CD	-5.82	1.39	1.47
1	B	43	PRO	CA-C	5.80	1.60	1.52
1	D	148	VAL	CA-C	-5.24	1.46	1.52
1	B	42	GLU	CA-CB	-5.24	1.45	1.53
1	D	151	TYR	CA-C	-5.09	1.46	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	PRO	CA-N-CD	-17.13	88.02	112.00
1	D	42	GLU	C-N-CD	-12.68	92.71	120.60
1	B	43	PRO	N-CA-C	-12.66	86.40	112.47
1	A	267	LEU	N-CA-CB	-12.41	89.69	110.16
1	D	42	GLU	CA-C-O	12.04	134.06	120.34
1	B	268	ALA	N-CA-C	-11.87	96.60	114.64
1	D	42	GLU	CA-C-N	10.73	152.75	127.00
1	D	42	GLU	C-N-CA	10.73	152.75	127.00
1	B	42	GLU	CB-CA-C	9.82	129.51	110.17
1	A	266	ALA	CB-CA-C	9.44	124.66	110.50
1	C	152	ASP	N-CA-CB	-9.40	98.57	110.79
1	A	81	VAL	N-CA-C	8.88	118.91	110.30
1	B	81	VAL	N-CA-C	8.61	118.69	110.42
1	C	81	VAL	N-CA-C	8.59	118.67	110.42
1	C	85	ARG	N-CA-C	-8.40	103.03	113.28
1	C	152	ASP	CA-C-N	-8.39	109.35	119.84
1	C	152	ASP	C-N-CA	-8.39	109.35	119.84
1	D	81	VAL	N-CA-C	8.26	118.35	110.42
1	B	42	GLU	CA-C-N	-8.05	109.77	119.84
1	B	42	GLU	C-N-CA	-8.05	109.77	119.84
1	D	43	PRO	N-CA-CB	-7.98	93.83	102.60
1	C	87	VAL	N-CA-C	-7.79	105.89	113.53
1	D	39	PRO	CA-N-CD	-7.56	101.41	112.00
1	D	213	THR	N-CA-C	7.01	119.77	111.71
1	B	42	GLU	C-N-CD	-6.97	96.43	125.00
1	B	44	ALA	N-CA-C	6.81	120.18	109.96
1	A	153	PRO	CA-N-CD	-6.77	102.52	112.00
1	D	153	PRO	CA-N-CD	-6.65	102.69	112.00
1	C	30	LEU	N-CA-C	6.61	119.31	111.71
1	D	149	PHE	N-CA-C	-6.60	101.65	111.81
1	A	87	VAL	N-CA-C	-6.56	95.69	109.34
1	B	101	GLN	N-CA-C	6.46	119.13	111.71
1	D	42	GLU	N-CA-CB	6.42	122.31	111.39
1	C	147	GLN	N-CA-C	-6.30	102.66	110.41
1	A	150	ALA	CA-C-N	-6.24	111.88	122.11
1	A	150	ALA	C-N-CA	-6.24	111.88	122.11
1	A	168	LEU	N-CA-C	-6.13	104.51	111.07
1	A	272	PHE	CA-C-N	6.06	127.42	119.84
1	A	272	PHE	C-N-CA	6.06	127.42	119.84
1	C	179	PHE	N-CA-C	6.05	119.90	111.56
1	C	153	PRO	CA-N-CD	-5.99	103.61	112.00
1	B	46	HIS	N-CA-C	5.98	117.60	111.14
1	B	41	SER	CA-C-N	-5.98	107.21	121.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	SER	C-N-CA	-5.98	107.21	121.80
1	D	101	GLN	N-CA-C	5.94	119.62	112.38
1	A	118	ASP	CA-C-N	-5.91	115.16	121.84
1	A	118	ASP	C-N-CA	-5.91	115.16	121.84
1	A	267	LEU	CA-C-N	5.90	130.69	122.79
1	A	267	LEU	C-N-CA	5.90	130.69	122.79
1	D	135	GLU	N-CA-C	-5.81	105.03	111.36
1	D	43	PRO	CA-CB-CG	-5.78	93.03	104.00
1	B	42	GLU	CA-C-O	-5.75	112.28	120.16
1	A	115	GLY	N-CA-C	5.74	119.84	112.83
1	C	168	LEU	N-CA-C	-5.71	104.96	111.07
1	A	269	LEU	N-CA-C	-5.70	101.53	110.36
1	D	151	TYR	N-CA-C	5.69	120.75	113.18
1	C	151	TYR	N-CA-CB	5.66	119.58	110.42
1	D	275	LEU	N-CA-C	-5.64	105.21	111.36
1	C	154	ALA	N-CA-C	-5.63	105.06	111.14
1	A	179	PHE	N-CA-C	5.62	118.08	110.88
1	D	35	SER	N-CA-C	-5.62	104.64	113.02
1	C	153	PRO	N-CA-C	5.49	123.77	112.47
1	C	267	LEU	O-C-N	5.48	129.09	122.68
1	D	148	VAL	CB-CA-C	-5.45	102.35	111.29
1	A	180	GLY	N-CA-C	5.37	123.00	115.43
1	C	150	ALA	O-C-N	5.32	129.25	122.39
1	D	84	CYS	CA-C-O	5.31	125.92	119.38
1	C	101	GLN	N-CA-C	5.27	118.49	111.75
1	D	150	ALA	CA-C-N	-5.27	107.25	122.15
1	D	150	ALA	C-N-CA	-5.27	107.25	122.15
1	D	128	SER	N-CA-C	5.18	117.18	108.73
1	B	213	THR	N-CA-C	5.17	118.69	112.38
1	C	215	ARG	CA-CB-CG	-5.12	103.86	114.10
1	A	86	LYS	N-CA-C	5.03	119.57	112.72
1	A	267	LEU	O-C-N	5.02	128.94	123.22
1	B	179	PHE	N-CA-C	5.01	118.70	112.59
1	B	35	SER	N-CA-C	-5.01	105.88	112.94
1	D	171	GLU	N-CA-C	-5.00	106.43	112.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	42	GLU	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2043	0	1998	109	0
1	B	2035	0	1989	100	0
1	C	2043	0	1998	120	0
1	D	2040	0	1994	116	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	0	1	0
3	B	25	0	0	1	0
3	C	20	0	0	0	0
3	D	29	0	0	2	0
All	All	8274	0	7979	400	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 25.

All (400) 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:150:ALA:CB	1:C:156:GLN:HE22	1.32	1.41
1:C:150:ALA:HA	1:C:156:GLN:NE2	1.56	1.20
1:C:150:ALA:CB	1:C:156:GLN:NE2	2.02	1.19
1:C:215:ARG:O	1:C:215:ARG:HD2	1.40	1.18
1:C:150:ALA:CA	1:C:156:GLN:NE2	2.11	1.14
1:C:215:ARG:HD2	1:C:215:ARG:C	1.52	1.11
1:C:150:ALA:HB2	1:C:156:GLN:HE22	1.04	1.09
1:C:150:ALA:HA	1:C:156:GLN:HE21	0.91	1.06
1:C:241:MSE:CE	1:C:266:ALA:HB2	1.84	1.06
1:C:241:MSE:HE1	1:C:266:ALA:HB2	1.39	1.05
1:C:150:ALA:HB2	1:C:156:GLN:NE2	1.68	1.04
1:A:40:LEU:HD13	1:A:119:VAL:CG2	1.87	1.04
1:C:86:LYS:O	1:C:86:LYS:HG3	1.56	1.01
1:C:83:GLN:HE21	1:C:83:GLN:H	1.09	0.99
1:C:150:ALA:CA	1:C:156:GLN:HE21	1.73	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLN:H	1:B:83:GLN:HE21	1.07	0.94
1:A:83:GLN:H	1:A:83:GLN:HE21	1.01	0.94
1:D:83:GLN:H	1:D:83:GLN:HE21	1.03	0.92
1:A:40:LEU:HD13	1:A:119:VAL:HG22	1.54	0.90
1:A:112:GLU:CD	1:D:86:LYS:NZ	2.30	0.89
1:A:40:LEU:HD13	1:A:119:VAL:HG21	1.53	0.89
1:C:150:ALA:O	1:C:153:PRO:HD3	1.71	0.89
1:A:37:GLN:HE21	1:D:63:LYS:HZ3	1.20	0.88
1:C:215:ARG:C	1:C:215:ARG:CD	2.46	0.85
1:D:203:ARG:HH11	1:D:281:SER:HB3	1.42	0.83
1:A:112:GLU:CD	1:D:86:LYS:HZ3	1.84	0.83
1:C:40:LEU:HD13	1:C:119:VAL:CG2	2.07	0.83
1:C:85:ARG:CZ	1:C:221:SER:HB3	2.09	0.83
1:C:117:ARG:O	1:C:120:LEU:HB2	1.78	0.83
1:C:42:GLU:HB3	1:C:43:PRO:HD3	1.61	0.83
1:A:112:GLU:OE2	1:D:86:LYS:NZ	2.13	0.82
1:D:83:GLN:H	1:D:83:GLN:NE2	1.78	0.81
1:C:150:ALA:HB1	1:C:156:GLN:HE22	1.41	0.81
1:C:215:ARG:O	1:C:215:ARG:CD	2.27	0.81
1:A:234:GLN:HE21	1:A:234:GLN:HA	1.46	0.80
1:B:41:SER:HB2	1:B:44:ALA:HA	1.60	0.80
1:D:149:PHE:O	1:D:151:TYR:N	2.15	0.80
1:C:40:LEU:HD13	1:C:119:VAL:HG21	1.63	0.79
1:A:54:GLN:HE21	1:A:105:LEU:HB2	1.48	0.79
1:B:83:GLN:H	1:B:83:GLN:NE2	1.80	0.79
1:C:241:MSE:HE3	1:C:266:ALA:HB2	1.63	0.78
1:B:47:ASP:OD2	1:B:112:GLU:HB3	1.81	0.78
1:A:38:GLN:HG3	1:D:29:ARG:NH2	1.99	0.78
1:D:175:TYR:HA	1:D:178:ARG:NH1	1.98	0.78
1:D:148:VAL:HG22	1:D:148:VAL:O	1.85	0.77
1:C:45:HIS:HD2	1:C:47:ASP:H	1.32	0.77
1:A:109:THR:HG23	1:D:86:LYS:HZ1	1.50	0.77
1:C:241:MSE:CE	1:C:266:ALA:CB	2.64	0.75
1:D:53:ILE:HD12	1:D:54:GLN:N	2.02	0.75
1:A:37:GLN:HG2	1:A:49:MSE:HE1	1.68	0.74
1:A:145:MSE:O	1:A:148:VAL:HG12	1.87	0.74
1:B:73:ILE:O	1:B:77:GLN:HG3	1.87	0.74
1:C:234:GLN:HA	1:C:234:GLN:HE21	1.54	0.73
1:C:83:GLN:H	1:C:83:GLN:NE2	1.83	0.73
1:B:120:LEU:HG	1:B:121:GLY:H	1.54	0.72
1:A:83:GLN:H	1:A:83:GLN:NE2	1.84	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD22	1:A:269:LEU:HG	1.72	0.71
1:C:150:ALA:C	1:C:153:PRO:HD3	2.16	0.71
1:D:41:SER:HB3	1:D:43:PRO:O	1.91	0.71
1:A:83:GLN:HE21	1:A:83:GLN:N	1.83	0.71
1:D:203:ARG:HH12	1:D:280:THR:HG22	1.55	0.70
1:B:175:TYR:HA	1:B:178:ARG:NH1	2.06	0.70
1:C:85:ARG:NH1	1:C:221:SER:HB3	2.05	0.70
1:D:65:LEU:HD23	1:D:134:ILE:HD13	1.72	0.70
1:B:109:THR:HG23	1:C:86:LYS:HZ1	1.55	0.69
1:B:199:ASP:HB3	1:B:202:LEU:HD23	1.74	0.69
1:A:86:LYS:HG2	1:A:86:LYS:O	1.90	0.69
1:A:111:SER:HA	1:A:114:MSE:HE2	1.75	0.69
1:A:42:GLU:HB3	1:A:43:PRO:HD3	1.73	0.68
1:D:234:GLN:HE21	1:D:234:GLN:HA	1.56	0.68
1:A:37:GLN:HE21	1:D:63:LYS:NZ	1.90	0.68
1:B:23:THR:HG22	1:B:26:GLY:H	1.57	0.68
1:A:64:LEU:HG	1:D:53:ILE:HG12	1.76	0.68
1:C:116:PHE:O	1:C:119:VAL:HG12	1.93	0.68
1:C:241:MSE:HE1	1:C:266:ALA:CB	2.22	0.67
1:A:109:THR:HG23	1:D:86:LYS:NZ	2.08	0.67
1:B:63:LYS:HZ3	1:C:37:GLN:HE21	1.43	0.67
1:B:39:PRO:HG3	1:B:52:ILE:HD12	1.76	0.67
1:A:175:TYR:HA	1:A:178:ARG:NH1	2.09	0.67
1:C:101:GLN:O	1:C:104:VAL:HG12	1.95	0.66
1:C:75:HIS:HB2	1:C:84:CYS:HB2	1.77	0.66
1:B:103:SER:HB3	1:C:93:GLN:NE2	2.11	0.66
1:A:233:PHE:HE1	1:A:237:ARG:HH11	1.44	0.66
1:C:75:HIS:CB	1:C:84:CYS:HB2	2.25	0.66
1:B:53:ILE:HD11	1:C:64:LEU:HG	1.78	0.66
1:D:274:GLU:H	1:D:274:GLU:CD	2.04	0.65
1:C:40:LEU:HD13	1:C:119:VAL:HG22	1.79	0.65
1:A:49:MSE:HE3	1:A:53:ILE:CG2	2.27	0.65
1:A:101:GLN:O	1:A:104:VAL:HG12	1.96	0.65
1:B:279:ARG:HD3	1:D:246:ARG:O	1.97	0.65
1:C:172:PHE:O	1:C:175:TYR:HB3	1.96	0.64
1:D:120:LEU:HD23	1:D:121:GLY:N	2.12	0.64
1:C:54:GLN:HE22	1:C:101:GLN:HB3	1.62	0.64
1:D:153:PRO:HA	1:D:156:GLN:HG2	1.78	0.64
1:A:49:MSE:HE3	1:A:53:ILE:HG22	1.79	0.64
1:B:29:ARG:CZ	1:C:38:GLN:HG3	2.27	0.64
1:B:53:ILE:CD1	1:C:64:LEU:HG	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:GLN:HA	1:D:234:GLN:NE2	2.12	0.64
1:B:207:GLU:OE1	1:B:284:VAL:HG21	1.98	0.63
1:A:150:ALA:HA	1:A:156:GLN:NE2	2.13	0.63
1:A:113:TYR:CE1	1:A:117:ARG:HD3	2.34	0.63
1:D:273:PRO:HG2	1:D:274:GLU:OE1	1.99	0.63
1:B:145:MSE:O	1:B:148:VAL:HG22	1.97	0.63
1:D:83:GLN:HE21	1:D:83:GLN:N	1.86	0.63
1:B:109:THR:CG2	1:C:86:LYS:HZ1	2.13	0.62
1:B:39:PRO:HD3	1:B:52:ILE:HD13	1.82	0.62
1:D:237:ARG:HH21	1:D:267:LEU:HA	1.64	0.62
1:A:112:GLU:CD	1:D:86:LYS:HZ1	2.03	0.61
1:B:42:GLU:O	1:B:42:GLU:HG3	1.99	0.61
1:C:233:PHE:HE1	1:C:237:ARG:HH11	1.46	0.61
1:B:113:TYR:CE1	1:B:117:ARG:HD3	2.35	0.61
1:D:202:LEU:HD23	1:D:274:GLU:HG3	1.82	0.61
1:C:88:LEU:O	1:C:92:LYS:HG3	2.01	0.61
1:B:127:GLN:CD	1:B:127:GLN:H	2.09	0.60
1:A:169:TYR:OH	1:A:274:GLU:HG2	2.01	0.60
1:B:63:LYS:NZ	1:C:37:GLN:HE21	2.00	0.60
1:B:141:LYS:HD2	1:B:163:LEU:HD12	1.83	0.60
1:A:59:GLU:HG3	1:A:130:GLN:HE21	1.65	0.60
1:C:241:MSE:HE3	1:C:266:ALA:CB	2.30	0.59
1:C:42:GLU:CB	1:C:43:PRO:HD3	2.31	0.59
1:B:109:THR:OG1	1:B:112:GLU:HG3	2.02	0.59
1:D:237:ARG:HB3	1:D:267:LEU:HD21	1.82	0.59
1:B:54:GLN:HE22	1:B:101:GLN:HG2	1.67	0.59
1:B:282:VAL:HG22	1:B:282:VAL:O	2.03	0.59
1:D:152:ASP:OD2	1:D:152:ASP:N	2.32	0.59
1:D:277:ASP:O	1:D:280:THR:HG22	2.03	0.59
1:B:237:ARG:HH22	1:B:269:LEU:HB2	1.66	0.59
1:A:130:GLN:NE2	1:D:34:LEU:HD21	2.17	0.59
1:C:147:GLN:O	1:C:148:VAL:HG12	2.03	0.59
1:B:277:ASP:O	1:B:280:THR:HG22	2.03	0.58
1:D:170:GLU:O	1:D:174:ARG:HG3	2.03	0.58
1:D:132:ARG:HH11	1:D:132:ARG:HG2	1.69	0.58
1:B:39:PRO:HD3	1:B:52:ILE:CD1	2.34	0.58
1:D:211:GLU:HG3	1:D:282:VAL:HG23	1.84	0.58
1:A:54:GLN:HE22	1:A:104:VAL:HG13	1.69	0.58
1:C:93:GLN:HA	1:C:93:GLN:OE1	2.03	0.58
1:A:41:SER:HB2	1:A:48:GLU:OE1	2.04	0.58
1:C:68:GLU:CD	1:C:90:ARG:HD2	2.29	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PHE:C	1:D:151:TYR:N	2.61	0.57
1:B:85:ARG:HG3	1:B:225:ASP:OD2	2.04	0.57
1:C:93:GLN:HE22	1:C:96:ARG:HH21	1.53	0.57
1:C:111:SER:HA	1:C:114:MSE:HE2	1.86	0.57
1:A:110:PRO:O	1:A:114:MSE:HG3	2.04	0.57
1:B:83:GLN:HE21	1:B:83:GLN:N	1.90	0.57
1:D:81:VAL:O	1:D:85:ARG:HB2	2.03	0.57
1:C:149:PHE:C	1:C:151:TYR:H	2.12	0.57
1:C:150:ALA:O	1:C:153:PRO:CD	2.49	0.57
1:A:54:GLN:NE2	1:A:105:LEU:HB2	2.19	0.57
1:B:45:HIS:CE1	1:B:115:GLY:HA3	2.39	0.57
1:B:85:ARG:CZ	1:B:221:SER:HB2	2.35	0.57
1:A:59:GLU:HG3	1:A:130:GLN:NE2	2.20	0.56
1:C:230:GLU:O	1:C:234:GLN:HG2	2.05	0.56
1:D:199:ASP:HB3	1:D:202:LEU:HD22	1.87	0.56
1:C:152:ASP:O	1:C:153:PRO:C	2.47	0.56
1:C:80:GLU:HB3	1:C:83:GLN:NE2	2.20	0.56
1:C:85:ARG:NH1	1:C:221:SER:CB	2.69	0.56
1:A:37:GLN:NE2	1:D:63:LYS:NZ	2.52	0.56
1:A:45:HIS:HD2	1:A:47:ASP:H	1.52	0.56
1:B:117:ARG:HD2	1:B:117:ARG:O	2.04	0.56
1:B:113:TYR:CZ	1:B:117:ARG:HD3	2.41	0.56
1:C:169:TYR:OH	1:C:274:GLU:HG2	2.06	0.56
1:D:148:VAL:O	1:D:148:VAL:CG2	2.54	0.56
1:A:49:MSE:O	1:A:53:ILE:HG23	2.06	0.55
1:A:181:HIS:O	1:A:183:ILE:HD12	2.05	0.55
1:D:149:PHE:C	1:D:151:TYR:H	2.13	0.55
1:A:45:HIS:CD2	1:A:47:ASP:H	2.24	0.55
1:D:203:ARG:HH12	1:D:280:THR:CG2	2.18	0.55
1:B:175:TYR:HA	1:B:178:ARG:HH12	1.72	0.55
1:D:145:MSE:O	1:D:148:VAL:HG12	2.07	0.55
1:B:41:SER:CB	1:B:44:ALA:HA	2.34	0.54
1:B:132:ARG:HG2	1:B:145:MSE:HG2	1.89	0.54
1:D:109:THR:OG1	1:D:112:GLU:HG3	2.07	0.54
1:A:86:LYS:O	1:A:86:LYS:CG	2.56	0.54
1:C:83:GLN:HE21	1:C:83:GLN:N	1.92	0.54
1:C:241:MSE:HE3	1:C:266:ALA:N	2.23	0.53
1:D:85:ARG:CZ	1:D:221:SER:HB3	2.38	0.53
1:C:132:ARG:HG2	1:C:145:MSE:HG2	1.89	0.53
1:A:42:GLU:CB	1:A:43:PRO:HD3	2.39	0.53
1:C:241:MSE:HE3	1:C:266:ALA:CA	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ILE:HD12	1:D:53:ILE:C	2.34	0.53
1:A:79:ASP:OD2	1:A:178:ARG:NH1	2.42	0.53
1:C:202:LEU:HD23	1:C:274:GLU:HG3	1.91	0.53
1:A:212:ASN:O	1:A:213:THR:C	2.52	0.52
1:A:281:SER:O	1:A:284:VAL:HG12	2.09	0.52
1:B:39:PRO:HG3	1:B:52:ILE:CD1	2.39	0.52
1:A:109:THR:CG2	1:D:86:LYS:NZ	2.73	0.52
1:A:102:TRP:HE1	1:A:236:TRP:CD1	2.28	0.52
1:B:49:MSE:HG3	1:B:53:ILE:CD1	2.40	0.52
1:C:102:TRP:HE1	1:C:236:TRP:CD1	2.28	0.51
1:C:23:THR:HG22	1:C:25:GLY:H	1.74	0.51
1:B:109:THR:CG2	1:C:86:LYS:NZ	2.73	0.51
1:A:274:GLU:CD	1:A:274:GLU:H	2.16	0.51
1:B:29:ARG:NH2	1:C:38:GLN:HG3	2.25	0.51
1:B:170:GLU:O	1:B:174:ARG:HG3	2.10	0.51
1:A:37:GLN:NE2	1:D:63:LYS:HZ3	1.96	0.50
1:A:175:TYR:HA	1:A:178:ARG:HH12	1.75	0.50
1:B:63:LYS:HB2	1:B:130:GLN:HE22	1.76	0.50
1:C:117:ARG:HA	1:C:120:LEU:HD22	1.93	0.50
1:B:88:LEU:O	1:B:92:LYS:HG3	2.11	0.50
1:B:93:GLN:OE1	1:B:93:GLN:HA	2.11	0.50
1:B:239:ARG:HH11	1:D:235:LEU:HD11	1.76	0.50
1:A:54:GLN:NE2	1:A:104:VAL:HG13	2.26	0.50
1:C:79:ASP:OD2	1:C:178:ARG:NH1	2.42	0.50
1:B:169:TYR:O	1:B:172:PHE:HB3	2.11	0.50
1:C:135:GLU:HG2	1:C:140:ASN:HD22	1.76	0.50
1:D:117:ARG:O	1:D:119:VAL:HG22	2.12	0.50
1:A:45:HIS:CE1	1:A:115:GLY:HA3	2.47	0.50
1:A:42:GLU:HB3	1:A:43:PRO:CD	2.40	0.50
1:A:172:PHE:O	1:A:175:TYR:HB3	2.10	0.50
1:D:129:LEU:HD22	1:D:159:LEU:HD11	1.93	0.50
1:B:49:MSE:O	1:B:53:ILE:HG12	2.12	0.50
1:A:42:GLU:OE1	1:A:43:PRO:HD3	2.12	0.50
1:B:250:PHE:HE1	1:D:277:ASP:HA	1.77	0.50
1:A:234:GLN:HA	1:A:234:GLN:NE2	2.22	0.49
1:B:97:GLN:HE22	1:C:100:GLU:HB3	1.77	0.49
1:D:85:ARG:O	1:D:86:LYS:C	2.54	0.49
1:A:147:GLN:NE2	1:A:147:GLN:HA	2.27	0.49
1:D:23:THR:N	3:D:557:HOH:O	2.45	0.49
1:A:203:ARG:O	1:A:207:GLU:HB2	2.13	0.49
1:B:29:ARG:NH1	1:C:38:GLN:HG3	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:HIS:HB2	1:D:84:CYS:HB2	1.94	0.49
1:C:119:VAL:HG22	1:C:119:VAL:O	2.12	0.49
1:B:25:GLY:HA2	1:B:30:LEU:HD12	1.95	0.49
1:C:66:ALA:HB2	1:C:134:ILE:HD11	1.94	0.49
1:D:274:GLU:HA	1:D:277:ASP:HB2	1.95	0.49
1:C:45:HIS:CE1	1:C:115:GLY:HA3	2.48	0.49
1:D:113:TYR:CE1	1:D:117:ARG:HG2	2.47	0.49
1:B:159:LEU:O	1:B:162:VAL:HG12	2.13	0.48
1:A:212:ASN:ND2	1:A:215:ARG:HB2	2.28	0.48
1:B:279:ARG:HD3	1:D:246:ARG:C	2.39	0.48
1:D:114:MSE:HA	1:D:117:ARG:HD2	1.94	0.48
1:D:119:VAL:HG23	1:D:120:LEU:H	1.78	0.48
1:D:203:ARG:NH1	1:D:280:THR:CG2	2.77	0.48
1:B:78:ARG:O	1:B:79:ASP:HB2	2.14	0.48
1:B:53:ILE:O	1:B:57:THR:HG23	2.14	0.48
1:B:234:GLN:HA	1:B:234:GLN:HE21	1.78	0.48
1:D:113:TYR:O	1:D:117:ARG:HG3	2.13	0.48
1:B:114:MSE:HE3	1:D:284:VAL:HG22	1.95	0.48
1:D:143:PRO:HG3	1:D:163:LEU:HD21	1.96	0.48
1:B:267:LEU:HD23	1:B:267:LEU:N	2.29	0.48
1:A:157:ALA:O	1:A:161:GLU:HG3	2.13	0.47
1:C:142:ASN:OD1	1:C:144:GLN:HB2	2.15	0.47
1:D:146:LEU:HD13	1:D:160:ARG:NH2	2.29	0.47
1:B:49:MSE:HG3	1:B:53:ILE:HD13	1.97	0.47
1:D:76:LEU:HG	1:D:84:CYS:SG	2.54	0.47
1:B:34:LEU:HA	1:B:37:GLN:HE22	1.79	0.47
1:C:83:GLN:C	1:C:86:LYS:H	2.21	0.47
1:A:70:ARG:NH2	1:A:158:ARG:HH21	2.13	0.47
1:B:103:SER:HB3	1:C:93:GLN:HE22	1.79	0.47
1:C:30:LEU:O	1:C:34:LEU:HB2	2.13	0.47
1:C:102:TRP:HE1	1:C:236:TRP:HD1	1.63	0.47
1:C:110:PRO:O	1:C:114:MSE:HG3	2.14	0.47
1:C:207:GLU:O	1:C:211:GLU:HG3	2.15	0.47
1:C:274:GLU:CD	1:C:274:GLU:H	2.19	0.47
1:A:267:LEU:CD2	1:A:269:LEU:HG	2.43	0.47
1:C:75:HIS:HB3	1:C:84:CYS:HB2	1.95	0.47
1:A:80:GLU:HB3	1:A:83:GLN:NE2	2.30	0.47
1:B:242:ARG:CZ	1:D:234:GLN:HG3	2.45	0.47
1:C:241:MSE:CE	1:C:266:ALA:N	2.78	0.47
1:D:80:GLU:HB3	1:D:83:GLN:CD	2.39	0.47
1:C:93:GLN:HE22	1:C:96:ARG:NH2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:HIS:HB2	1:A:183:ILE:CD1	2.45	0.47
1:B:152:ASP:N	1:B:153:PRO:HD3	2.29	0.47
1:D:97:GLN:O	1:D:101:GLN:HB2	2.14	0.47
1:D:132:ARG:HE	1:D:145:MSE:HE3	1.80	0.47
1:B:230:GLU:O	1:B:234:GLN:HG2	2.15	0.46
1:D:175:TYR:HA	1:D:178:ARG:HH12	1.77	0.46
1:B:46:HIS:HD2	1:B:47:ASP:OD1	1.97	0.46
1:C:147:GLN:C	1:C:149:PHE:H	2.23	0.46
1:C:166:PRO:HG3	1:C:192:TRP:CE2	2.51	0.46
1:C:230:GLU:O	1:C:230:GLU:HG3	2.15	0.46
1:B:23:THR:HG22	1:B:25:GLY:N	2.30	0.46
1:A:85:ARG:CZ	1:A:221:SER:HB3	2.46	0.46
1:B:23:THR:CG2	1:B:24:TYR:N	2.79	0.46
1:D:153:PRO:HA	1:D:156:GLN:HE21	1.81	0.46
1:A:34:LEU:C	1:A:37:GLN:HE22	2.24	0.46
1:A:104:VAL:HG11	1:D:61:TRP:CH2	2.51	0.46
1:D:39:PRO:HD3	1:D:52:ILE:CD1	2.46	0.46
1:D:81:VAL:HG21	1:D:218:ARG:HD3	1.97	0.46
1:D:129:LEU:CD2	1:D:159:LEU:HD11	2.46	0.46
1:D:73:ILE:O	1:D:77:GLN:HG3	2.16	0.45
1:A:99:THR:HG21	1:A:235:LEU:HG	1.98	0.45
1:D:169:TYR:O	1:D:172:PHE:HB3	2.16	0.45
1:A:203:ARG:N	1:A:204:PRO:HD2	2.31	0.45
1:D:80:GLU:HB3	1:D:83:GLN:NE2	2.31	0.45
1:B:63:LYS:NZ	1:C:37:GLN:NE2	2.65	0.45
1:C:160:ARG:O	1:C:164:GLU:HG3	2.17	0.45
1:D:203:ARG:N	1:D:204:PRO:HD2	2.31	0.45
1:C:97:GLN:O	1:C:101:GLN:HG3	2.16	0.45
1:A:112:GLU:OE2	1:D:86:LYS:CE	2.65	0.45
1:A:168:LEU:CD1	1:A:226:LEU:HD21	2.46	0.45
1:B:45:HIS:CD2	1:B:47:ASP:H	2.35	0.45
1:C:149:PHE:C	1:C:151:TYR:N	2.74	0.45
1:D:119:VAL:O	1:D:120:LEU:HB2	2.16	0.45
1:D:136:PHE:CE2	1:D:163:LEU:HD13	2.52	0.45
1:D:167:SER:OG	1:D:170:GLU:HG3	2.17	0.45
1:B:45:HIS:ND1	1:B:115:GLY:HA3	2.31	0.45
1:B:246:ARG:O	1:D:279:ARG:NH2	2.36	0.45
1:C:68:GLU:OE2	1:C:90:ARG:HD2	2.17	0.45
1:C:129:LEU:HB2	1:C:149:PHE:CE2	2.52	0.45
1:A:109:THR:CG2	1:D:86:LYS:HZ2	2.30	0.45
1:A:147:GLN:HA	1:A:147:GLN:HE21	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:HB3	1:B:126:PHE:CE1	2.52	0.44
1:B:191:ASP:OD2	1:B:193:THR:HB	2.17	0.44
1:C:62:LEU:HD13	1:C:62:LEU:HA	1.88	0.44
1:B:169:TYR:O	1:B:173:LEU:HD22	2.17	0.44
1:D:210:TYR:OH	1:D:279:ARG:NH1	2.50	0.44
1:B:86:LYS:O	1:B:89:ALA:N	2.50	0.44
1:C:270:THR:HG23	1:C:273:PRO:HG3	1.99	0.44
1:C:275:LEU:O	1:C:278:VAL:HG12	2.16	0.44
1:A:116:PHE:O	1:A:119:VAL:HG12	2.17	0.44
1:A:152:ASP:O	1:A:152:ASP:CG	2.61	0.44
1:B:129:LEU:C	1:B:129:LEU:HD13	2.43	0.44
1:B:169:TYR:OH	1:B:274:GLU:HG2	2.18	0.44
1:D:85:ARG:NH2	1:D:221:SER:HB3	2.33	0.44
1:A:225:ASP:O	1:A:229:VAL:HG23	2.18	0.44
1:B:109:THR:HG23	1:C:86:LYS:NZ	2.28	0.44
1:D:203:ARG:HH11	1:D:281:SER:CB	2.22	0.44
1:D:234:GLN:HE21	1:D:234:GLN:CA	2.20	0.44
1:B:127:GLN:HE21	1:B:127:GLN:C	2.25	0.44
1:A:202:LEU:HD23	1:A:274:GLU:HG3	1.99	0.43
1:C:132:ARG:CG	1:C:145:MSE:HG2	2.47	0.43
1:D:129:LEU:C	1:D:129:LEU:HD13	2.43	0.43
1:D:181:HIS:O	1:D:183:ILE:HG12	2.18	0.43
1:D:47:ASP:HA	3:D:588:HOH:O	2.18	0.43
1:D:146:LEU:O	1:D:148:VAL:N	2.51	0.43
1:A:112:GLU:OE1	1:D:86:LYS:NZ	2.37	0.43
1:B:86:LYS:O	1:B:87:VAL:C	2.59	0.43
1:C:203:ARG:N	1:C:204:PRO:HD2	2.33	0.43
1:D:88:LEU:O	1:D:92:LYS:HG3	2.18	0.43
1:D:282:VAL:HG13	1:D:282:VAL:O	2.18	0.43
1:A:53:ILE:C	1:A:53:ILE:HD12	2.43	0.43
1:D:132:ARG:HG2	1:D:132:ARG:NH1	2.32	0.43
1:C:80:GLU:HB3	1:C:83:GLN:CD	2.44	0.43
1:C:116:PHE:O	1:C:119:VAL:CG1	2.66	0.43
1:C:130:GLN:O	1:C:134:ILE:HD13	2.19	0.43
1:D:133:TYR:CZ	1:D:162:VAL:HG21	2.54	0.43
1:A:38:GLN:HG3	1:D:29:ARG:HH22	1.80	0.43
1:B:172:PHE:O	1:B:175:TYR:HB3	2.19	0.43
1:D:45:HIS:CE1	1:D:115:GLY:HA3	2.53	0.43
1:A:181:HIS:HB2	1:A:183:ILE:HD11	2.00	0.43
1:B:95:LEU:HA	1:B:98:LEU:HD23	2.00	0.43
1:B:85:ARG:HA	1:B:88:LEU:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PRO:O	1:B:114:MSE:HG3	2.19	0.42
1:D:73:ILE:HG23	1:D:171:GLU:HG3	2.01	0.42
1:B:234:GLN:HA	1:B:234:GLN:NE2	2.34	0.42
1:A:73:ILE:O	1:A:77:GLN:HG3	2.19	0.42
1:C:64:LEU:HD13	1:C:94:VAL:HG21	2.02	0.42
1:B:166:PRO:HG3	1:B:192:TRP:CE2	2.54	0.42
1:C:230:GLU:HG2	1:C:276:PHE:CE1	2.53	0.42
1:C:233:PHE:CE1	1:C:237:ARG:HD3	2.54	0.42
1:B:170:GLU:HA	1:B:173:LEU:HD23	2.02	0.42
1:D:75:HIS:CB	1:D:84:CYS:HB2	2.50	0.42
1:A:62:LEU:HD12	1:A:134:ILE:HG13	2.02	0.42
1:A:88:LEU:O	1:A:92:LYS:HG3	2.19	0.42
1:C:83:GLN:O	1:C:86:LYS:N	2.47	0.42
1:C:149:PHE:HA	1:C:151:TYR:CE1	2.55	0.42
1:D:217:TRP:CZ2	1:D:218:ARG:CZ	3.02	0.42
1:A:66:ALA:O	1:A:70:ARG:HG3	2.19	0.42
1:B:153:PRO:HA	1:B:156:GLN:HB3	2.02	0.42
1:C:149:PHE:HA	1:C:151:TYR:CD1	2.55	0.42
1:A:53:ILE:HD12	1:A:53:ILE:O	2.19	0.42
1:A:152:ASP:N	1:A:153:PRO:CD	2.82	0.42
1:B:205:VAL:O	1:B:209:ILE:HG13	2.19	0.41
1:D:238:PHE:O	1:D:242:ARG:HG2	2.20	0.41
1:A:177:ALA:HA	1:A:183:ILE:HD13	2.02	0.41
1:A:42:GLU:CB	1:A:43:PRO:CD	2.97	0.41
1:A:64:LEU:HG	1:D:53:ILE:CG1	2.47	0.41
1:A:169:TYR:O	1:A:172:PHE:HB3	2.20	0.41
1:B:281:SER:C	1:B:283:GLY:H	2.27	0.41
1:A:62:LEU:HD13	1:A:62:LEU:HA	1.89	0.41
1:A:127:GLN:NE2	1:A:127:GLN:N	2.68	0.41
1:B:24:TYR:HB2	1:C:126:PHE:HA	2.02	0.41
1:C:40:LEU:HD12	1:C:40:LEU:H	1.85	0.41
1:D:47:ASP:OD2	1:D:112:GLU:HB3	2.20	0.41
1:D:223:CYS:O	1:D:227:VAL:HG23	2.21	0.41
1:A:40:LEU:CD1	1:A:119:VAL:HG22	2.37	0.41
1:D:120:LEU:HD23	1:D:121:GLY:C	2.46	0.41
1:A:85:ARG:HG3	3:A:522:HOH:O	2.19	0.41
1:A:135:GLU:HG2	1:A:140:ASN:HB3	2.03	0.41
1:A:237:ARG:HH22	1:A:269:LEU:HB2	1.84	0.41
1:A:272:PHE:HB3	1:A:275:LEU:HD12	2.03	0.41
1:A:73:ILE:HG23	1:A:171:GLU:HG3	2.03	0.41
1:A:80:GLU:HB3	1:A:83:GLN:CD	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:PRO:HG3	1:A:192:TRP:CE2	2.56	0.41
1:A:197:VAL:O	1:A:198:ALA:C	2.64	0.41
1:B:37:GLN:HE21	1:C:63:LYS:NZ	2.19	0.41
1:C:199:ASP:HB3	1:C:202:LEU:HD22	2.02	0.41
1:D:34:LEU:HA	1:D:37:GLN:HE22	1.86	0.41
1:D:230:GLU:O	1:D:234:GLN:HG2	2.21	0.41
1:A:141:LYS:HE2	1:A:163:LEU:HA	2.01	0.40
1:D:49:MSE:O	1:D:53:ILE:HG13	2.21	0.40
1:B:23:THR:N	3:B:563:HOH:O	2.53	0.40
1:D:199:ASP:O	1:D:202:LEU:HB2	2.20	0.40
1:A:177:ALA:CA	1:A:183:ILE:HD13	2.52	0.40
1:B:275:LEU:HD12	1:B:275:LEU:HA	1.91	0.40
1:D:151:TYR:O	1:D:153:PRO:HD2	2.21	0.40
1:A:68:GLU:CD	1:A:90:ARG:HD2	2.47	0.40
1:B:109:THR:HG21	1:C:86:LYS:NZ	2.36	0.40
1:C:73:ILE:HG23	1:C:171:GLU:HG3	2.03	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	237/276 (86%)	220 (93%)	13 (6%)	4 (2%)	7	19
1	B	236/276 (86%)	213 (90%)	21 (9%)	2 (1%)	16	37
1	C	237/276 (86%)	219 (92%)	16 (7%)	2 (1%)	16	37
1	D	237/276 (86%)	214 (90%)	18 (8%)	5 (2%)	5	15
All	All	947/1104 (86%)	866 (91%)	68 (7%)	13 (1%)	9	23

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	148	VAL
1	D	150	ALA
1	B	282	VAL
1	D	148	VAL
1	D	182	ALA
1	A	182	ALA
1	C	182	ALA
1	D	147	GLN
1	D	117	ARG
1	A	44	ALA
1	A	43	PRO
1	B	119	VAL
1	A	282	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/234 (92%)	195 (90%)	21 (10%)	8	20
1	B	215/234 (92%)	196 (91%)	19 (9%)	9	23
1	C	216/234 (92%)	194 (90%)	22 (10%)	7	18
1	D	215/234 (92%)	193 (90%)	22 (10%)	7	18
All	All	862/936 (92%)	778 (90%)	84 (10%)	8	20

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	53	ILE
1	A	62	LEU
1	A	64	LEU
1	A	83	GLN
1	A	98	LEU
1	A	100	GLU
1	A	120	LEU
1	A	127	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	129	LEU
1	A	152	ASP
1	A	153	PRO
1	A	168	LEU
1	A	186	GLN
1	A	193	THR
1	A	200	ASP
1	A	202	LEU
1	A	215	ARG
1	A	234	GLN
1	A	267	LEU
1	A	274	GLU
1	B	39	PRO
1	B	40	LEU
1	B	42	GLU
1	B	43	PRO
1	B	53	ILE
1	B	64	LEU
1	B	69	LEU
1	B	83	GLN
1	B	98	LEU
1	B	100	GLU
1	B	104	VAL
1	B	127	GLN
1	B	132	ARG
1	B	173	LEU
1	B	215	ARG
1	B	270	THR
1	B	274	GLU
1	B	275	LEU
1	B	279	ARG
1	C	34	LEU
1	C	40	LEU
1	C	62	LEU
1	C	64	LEU
1	C	69	LEU
1	C	83	GLN
1	C	86	LYS
1	C	100	GLU
1	C	118	ASP
1	C	120	LEU
1	C	127	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	144	GLN
1	C	147	GLN
1	C	148	VAL
1	C	153	PRO
1	C	168	LEU
1	C	186	GLN
1	C	215	ARG
1	C	230	GLU
1	C	234	GLN
1	C	241	MSE
1	C	274	GLU
1	D	23	THR
1	D	39	PRO
1	D	43	PRO
1	D	64	LEU
1	D	69	LEU
1	D	83	GLN
1	D	84	CYS
1	D	98	LEU
1	D	100	GLU
1	D	104	VAL
1	D	119	VAL
1	D	126	PHE
1	D	143	PRO
1	D	153	PRO
1	D	173	LEU
1	D	202	LEU
1	D	215	ARG
1	D	230	GLU
1	D	250	PHE
1	D	270	THR
1	D	274	GLU
1	D	279	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	37	GLN
1	A	38	GLN
1	A	45	HIS
1	A	54	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	67	HIS
1	A	83	GLN
1	A	127	GLN
1	A	130	GLN
1	A	147	GLN
1	A	212	ASN
1	A	234	GLN
1	B	32	GLN
1	B	37	GLN
1	B	38	GLN
1	B	45	HIS
1	B	46	HIS
1	B	83	GLN
1	B	97	GLN
1	B	127	GLN
1	B	130	GLN
1	B	156	GLN
1	B	188	GLN
1	B	232	GLN
1	B	234	GLN
1	C	32	GLN
1	C	37	GLN
1	C	38	GLN
1	C	45	HIS
1	C	67	HIS
1	C	83	GLN
1	C	101	GLN
1	C	127	GLN
1	C	130	GLN
1	C	140	ASN
1	C	144	GLN
1	C	156	GLN
1	C	232	GLN
1	C	234	GLN
1	D	32	GLN
1	D	37	GLN
1	D	38	GLN
1	D	45	HIS
1	D	83	GLN
1	D	93	GLN
1	D	97	GLN
1	D	140	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	156	GLN
1	D	234	GLN

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 ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	238/276 (86%)	0.40	22 (9%) 14 12	4, 19, 53, 78	0
1	B	237/276 (85%)	0.67	38 (16%) 5 4	3, 22, 68, 96	0
1	C	238/276 (86%)	0.48	29 (12%) 8 7	5, 18, 56, 91	0
1	D	238/276 (86%)	0.60	27 (11%) 10 8	4, 22, 65, 88	0
All	All	951/1104 (86%)	0.54	116 (12%) 8 7	3, 20, 63, 96	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	266	ALA	11.3
1	B	284	VAL	8.8
1	D	284	VAL	7.8
1	C	284	VAL	7.4
1	B	151	TYR	6.0
1	B	120	LEU	6.0
1	C	127	GLN	5.8
1	A	266	ALA	5.8
1	A	151	TYR	5.6
1	B	42	GLU	5.5
1	B	267	LEU	5.4
1	C	43	PRO	5.2
1	D	126	PHE	5.1
1	A	126	PHE	5.0
1	C	151	TYR	4.9
1	B	119	VAL	4.9
1	C	126	PHE	4.8
1	D	119	VAL	4.8
1	A	127	GLN	4.7
1	B	117	ARG	4.7
1	D	120	LEU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	268	ALA	4.3
1	D	266	ALA	4.3
1	B	127	GLN	4.3
1	A	121	GLY	4.2
1	D	151	TYR	4.2
1	B	250	PHE	4.1
1	A	267	LEU	4.0
1	C	148	VAL	4.0
1	B	121	GLY	4.0
1	A	120	LEU	4.0
1	B	152	ASP	3.9
1	C	120	LEU	3.9
1	D	121	GLY	3.9
1	B	154	ALA	3.9
1	B	118	ASP	3.9
1	D	267	LEU	3.8
1	B	126	PHE	3.8
1	C	128	SER	3.8
1	A	43	PRO	3.7
1	B	44	ALA	3.7
1	D	148	VAL	3.7
1	B	268	ALA	3.6
1	D	147	GLN	3.6
1	C	153	PRO	3.6
1	D	154	ALA	3.6
1	B	41	SER	3.6
1	B	150	ALA	3.5
1	C	150	ALA	3.5
1	C	267	LEU	3.5
1	B	155	GLY	3.4
1	D	283	GLY	3.4
1	B	43	PRO	3.3
1	D	117	ARG	3.3
1	C	86	LYS	3.3
1	A	212	ASN	3.3
1	C	212	ASN	3.3
1	A	119	VAL	3.2
1	B	283	GLY	3.1
1	D	43	PRO	3.1
1	D	85	ARG	3.1
1	A	250	PHE	3.1
1	B	39	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	86	LYS	3.0
1	C	118	ASP	3.0
1	C	250	PHE	3.0
1	B	148	VAL	2.9
1	B	153	PRO	2.9
1	B	146	LEU	2.9
1	C	85	ARG	2.9
1	B	200	ASP	2.9
1	D	268	ALA	2.8
1	C	121	GLY	2.8
1	B	115	GLY	2.7
1	C	119	VAL	2.7
1	D	156	GLN	2.7
1	C	268	ALA	2.7
1	A	41	SER	2.6
1	A	269	LEU	2.6
1	D	146	LEU	2.6
1	D	42	GLU	2.6
1	A	215	ARG	2.5
1	B	85	ARG	2.5
1	A	42	GLU	2.5
1	D	127	GLN	2.5
1	B	144	GLN	2.5
1	C	215	ARG	2.4
1	A	128	SER	2.4
1	C	283	GLY	2.4
1	A	40	LEU	2.4
1	B	269	LEU	2.4
1	A	284	VAL	2.4
1	D	84	CYS	2.3
1	B	160	ARG	2.3
1	B	157	ALA	2.3
1	C	129	LEU	2.3
1	C	158	ARG	2.2
1	D	118	ASP	2.2
1	C	40	LEU	2.2
1	D	282	VAL	2.2
1	D	269	LEU	2.2
1	D	81	VAL	2.2
1	A	86	LYS	2.2
1	D	152	ASP	2.2
1	B	149	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	269	LEU	2.1
1	C	42	GLU	2.1
1	B	270	THR	2.1
1	C	147	GLN	2.1
1	B	159	LEU	2.1
1	C	190	ARG	2.1
1	A	117	ARG	2.0
1	D	41	SER	2.0
1	B	249	GLY	2.0
1	A	85	ARG	2.0
1	B	282	VAL	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	MG	A	406	1/1	0.91	0.08	19,19,19,19	0
2	MG	B	405	1/1	0.92	0.07	13,13,13,13	0
2	MG	C	407	1/1	0.92	0.29	20,20,20,20	0
2	MG	D	402	1/1	0.94	0.09	14,14,14,14	0
2	MG	B	404	1/1	0.95	0.16	15,15,15,15	0
2	MG	C	400	1/1	0.95	0.16	5,5,5,5	0
2	MG	B	403	1/1	0.96	0.08	15,15,15,15	0
2	MG	A	401	1/1	0.96	0.10	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.