



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:23 PM UTC

PDB ID : 3N4Q / pdb_00003n4q
Title : Human cytomegalovirus terminase nuclease domain, Mn soaked
Authors : Nadal, M.; Mas, P.J.; Blanco, A.G.; Arnan, C.; Sola, M.; Hart, D.J.; Coll, M.
Deposited on : 2010-05-22
Resolution : 3.20 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
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

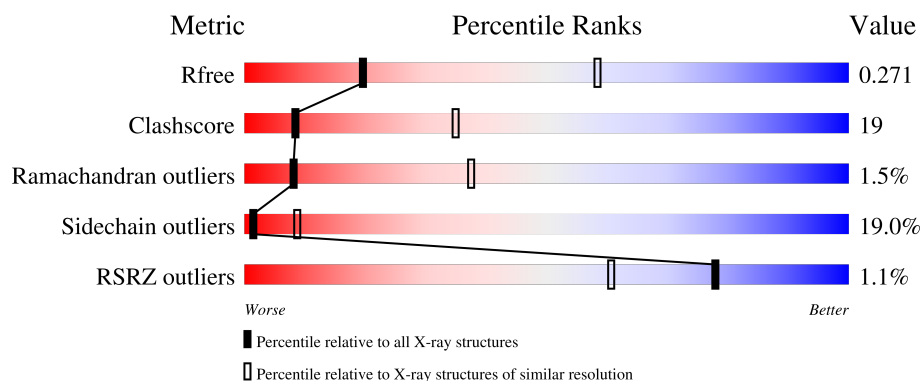
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	279	2% 46% 24% 7% 23%
1	B	279	41% 32% 6% 21%
1	C	279	2% 44% 25% 9% 22%
1	D	279	2% 45% 24% 8% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7056 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 TERMINASE SUBUNIT UL89 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1736	1113	292	325	6			
1	B	221	Total	C	N	O	S	0	0	0
			1775	1137	301	331	6			
1	C	219	Total	C	N	O	S	0	0	0
			1755	1126	293	330	6			
1	D	214	Total	C	N	O	S	0	0	0
			1722	1104	290	322	6			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	MET	-	expression tag	UNP P16732
A	397	GLY	-	expression tag	UNP P16732
A	398	HIS	-	expression tag	UNP P16732
A	399	HIS	-	expression tag	UNP P16732
A	400	HIS	-	expression tag	UNP P16732
A	401	HIS	-	expression tag	UNP P16732
A	402	HIS	-	expression tag	UNP P16732
A	403	HIS	-	expression tag	UNP P16732
A	404	ASP	-	expression tag	UNP P16732
A	405	TYR	-	expression tag	UNP P16732
A	406	ASP	-	expression tag	UNP P16732
A	407	ILE	-	expression tag	UNP P16732
A	408	PRO	-	expression tag	UNP P16732
A	409	THR	-	expression tag	UNP P16732
A	410	THR	-	expression tag	UNP P16732
A	411	GLU	-	expression tag	UNP P16732
A	412	ASN	-	expression tag	UNP P16732
A	413	LEU	-	expression tag	UNP P16732
A	414	TYR	-	expression tag	UNP P16732
A	415	PHE	-	expression tag	UNP P16732
A	416	GLN	-	expression tag	UNP P16732

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Chain	Residue	Modelled	Actual	Comment	Reference
A	417	GLY	-	expression tag	UNP P16732
B	396	MET	-	expression tag	UNP P16732
B	397	GLY	-	expression tag	UNP P16732
B	398	HIS	-	expression tag	UNP P16732
B	399	HIS	-	expression tag	UNP P16732
B	400	HIS	-	expression tag	UNP P16732
B	401	HIS	-	expression tag	UNP P16732
B	402	HIS	-	expression tag	UNP P16732
B	403	HIS	-	expression tag	UNP P16732
B	404	ASP	-	expression tag	UNP P16732
B	405	TYR	-	expression tag	UNP P16732
B	406	ASP	-	expression tag	UNP P16732
B	407	ILE	-	expression tag	UNP P16732
B	408	PRO	-	expression tag	UNP P16732
B	409	THR	-	expression tag	UNP P16732
B	410	THR	-	expression tag	UNP P16732
B	411	GLU	-	expression tag	UNP P16732
B	412	ASN	-	expression tag	UNP P16732
B	413	LEU	-	expression tag	UNP P16732
B	414	TYR	-	expression tag	UNP P16732
B	415	PHE	-	expression tag	UNP P16732
B	416	GLN	-	expression tag	UNP P16732
B	417	GLY	-	expression tag	UNP P16732
C	396	MET	-	expression tag	UNP P16732
C	397	GLY	-	expression tag	UNP P16732
C	398	HIS	-	expression tag	UNP P16732
C	399	HIS	-	expression tag	UNP P16732
C	400	HIS	-	expression tag	UNP P16732
C	401	HIS	-	expression tag	UNP P16732
C	402	HIS	-	expression tag	UNP P16732
C	403	HIS	-	expression tag	UNP P16732
C	404	ASP	-	expression tag	UNP P16732
C	405	TYR	-	expression tag	UNP P16732
C	406	ASP	-	expression tag	UNP P16732
C	407	ILE	-	expression tag	UNP P16732
C	408	PRO	-	expression tag	UNP P16732
C	409	THR	-	expression tag	UNP P16732
C	410	THR	-	expression tag	UNP P16732
C	411	GLU	-	expression tag	UNP P16732
C	412	ASN	-	expression tag	UNP P16732
C	413	LEU	-	expression tag	UNP P16732
C	414	TYR	-	expression tag	UNP P16732

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Chain	Residue	Modelled	Actual	Comment	Reference
C	415	PHE	-	expression tag	UNP P16732
C	416	GLN	-	expression tag	UNP P16732
C	417	GLY	-	expression tag	UNP P16732
D	396	MET	-	expression tag	UNP P16732
D	397	GLY	-	expression tag	UNP P16732
D	398	HIS	-	expression tag	UNP P16732
D	399	HIS	-	expression tag	UNP P16732
D	400	HIS	-	expression tag	UNP P16732
D	401	HIS	-	expression tag	UNP P16732
D	402	HIS	-	expression tag	UNP P16732
D	403	HIS	-	expression tag	UNP P16732
D	404	ASP	-	expression tag	UNP P16732
D	405	TYR	-	expression tag	UNP P16732
D	406	ASP	-	expression tag	UNP P16732
D	407	ILE	-	expression tag	UNP P16732
D	408	PRO	-	expression tag	UNP P16732
D	409	THR	-	expression tag	UNP P16732
D	410	THR	-	expression tag	UNP P16732
D	411	GLU	-	expression tag	UNP P16732
D	412	ASN	-	expression tag	UNP P16732
D	413	LEU	-	expression tag	UNP P16732
D	414	TYR	-	expression tag	UNP P16732
D	415	PHE	-	expression tag	UNP P16732
D	416	GLN	-	expression tag	UNP P16732
D	417	GLY	-	expression tag	UNP P16732

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

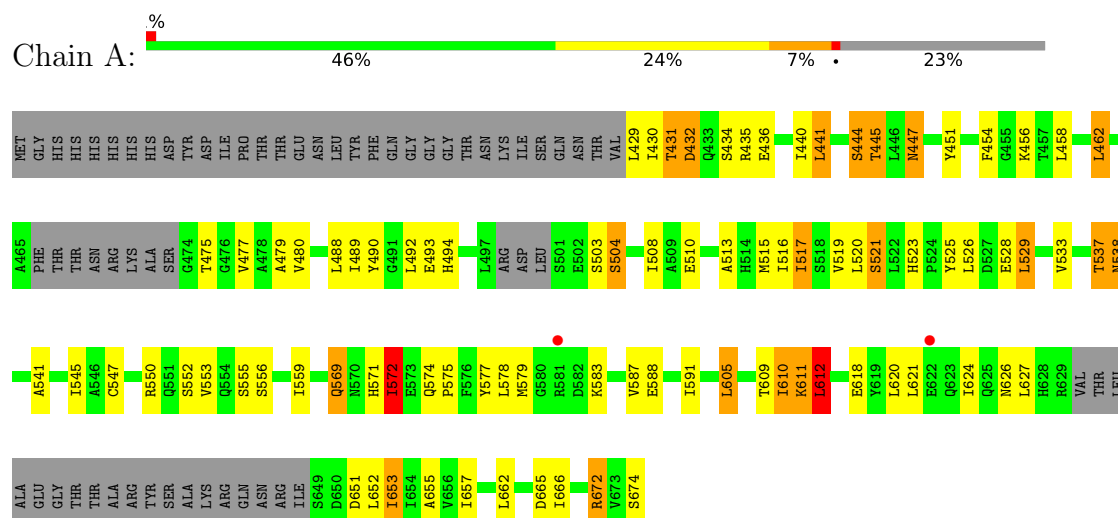
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total 11	O 11	0	0
4	B	17	Total 17	O 17	0	0
4	C	15	Total 15	O 15	0	0
4	D	13	Total 13	O 13	0	0

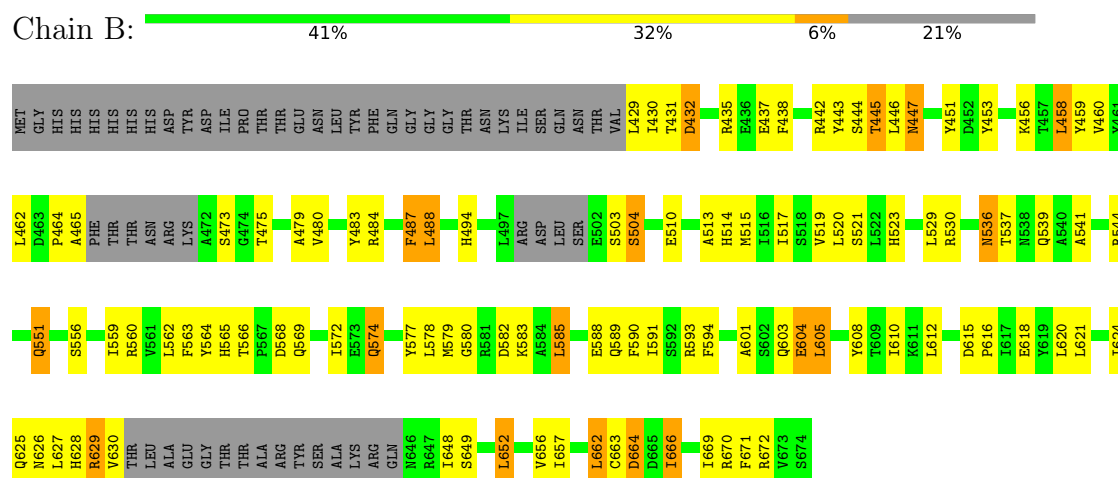
3 Residue-property plots

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.

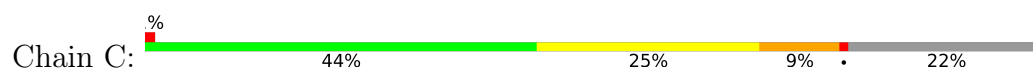
• Molecule 1: TERMINASE SUBUNIT UL89 PROTEIN

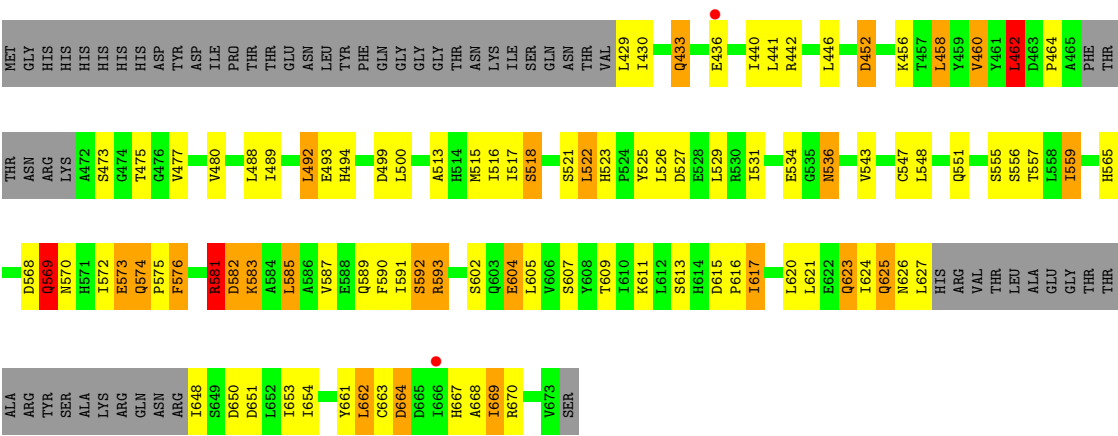


• Molecule 1: TERMINASE SUBUNIT UL89 PROTEIN

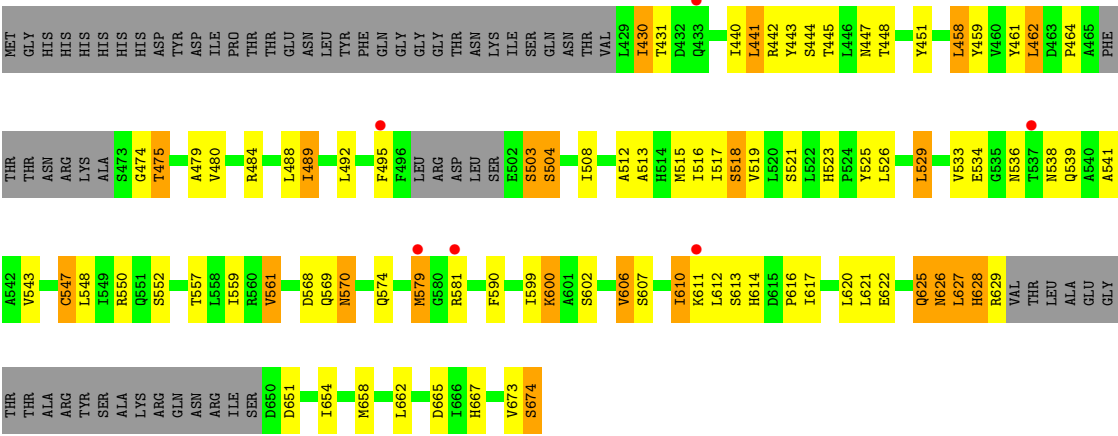


• Molecule 1: TERMINASE SUBUNIT UL89 PROTEIN





● Molecule 1: TERMINASE SUBUNIT UL89 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.70Å 88.10Å 190.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.05 – 3.20 44.05 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.6 (44.05-3.20) 90.3 (44.05-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.207 , 0.283 0.200 , 0.271	Depositor DCC
R_{free} test set	1109 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	75.1	Xtriage
Anisotropy	0.820	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 101.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.046 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7056	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: MG, MN

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	0.76	1/1770 (0.1%)	1.03	2/2399 (0.1%)
1	B	0.71	0/1809	1.04	4/2452 (0.2%)
1	C	0.73	0/1789	1.05	5/2427 (0.2%)
1	D	0.72	0/1756	1.01	4/2380 (0.2%)
All	All	0.73	1/7124 (0.0%)	1.03	15/9658 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	572	ILE	CA-CB	6.20	1.60	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	462	LEU	N-CA-C	7.82	121.23	108.26
1	C	473	SER	N-CA-C	6.99	121.75	111.34
1	C	480	VAL	N-CA-C	6.86	117.41	108.35
1	C	569	GLN	N-CA-C	-6.82	96.27	110.80
1	D	606	VAL	N-CA-C	6.79	116.49	106.85
1	A	611	LYS	N-CA-C	6.47	118.98	108.63
1	D	628	HIS	N-CA-C	6.19	116.44	108.34
1	B	559	ILE	N-CA-C	5.87	116.09	107.75
1	C	623	GLN	N-CA-C	-5.54	106.45	113.43
1	B	629	ARG	N-CA-C	5.49	117.07	111.14
1	A	559	ILE	N-CA-C	5.37	114.93	108.06
1	B	487	PHE	N-CA-C	5.33	117.58	108.90
1	D	543	VAL	N-CA-C	5.19	115.41	110.42
1	D	561	VAL	N-CA-C	5.06	115.25	108.17
1	C	462	LEU	N-CA-C	5.03	117.60	108.69

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	1736	0	1707	67	0
1	B	1775	0	1751	72	0
1	C	1755	0	1732	74	0
1	D	1722	0	1691	58	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	11	0	0	0	0
4	B	17	0	0	2	0
4	C	15	0	0	2	0
4	D	13	0	0	0	0
All	All	7056	0	6881	265	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 19.

All (265) 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:664:ASP:HB2	4:B:18:HOH:O	1.55	1.03
1:D:464:PRO:HA	1:D:475:THR:HB	1.44	1.00
1:D:611:LYS:HB3	1:D:612:LEU:HD22	1.45	0.99
1:B:568:ASP:CG	1:B:569:GLN:H	1.77	0.91
1:A:456:LYS:HD3	1:A:525:TYR:O	1.73	0.90
1:D:430:ILE:HD12	1:D:430:ILE:H	1.40	0.85
1:C:617:ILE:HD13	1:C:617:ILE:H	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LYS:O	1:A:526:LEU:HD23	1.77	0.84
1:C:570:ASN:HD22	1:C:572:ILE:H	1.26	0.84
1:B:445:THR:HG21	1:B:523:HIS:CD2	2.13	0.83
1:A:494:HIS:H	1:A:609:THR:HG21	1.48	0.79
1:A:538:ASN:OD1	1:A:541:ALA:N	2.15	0.79
1:D:513:ALA:O	1:D:517:ILE:HG13	1.86	0.76
1:A:494:HIS:N	1:A:609:THR:HG21	2.03	0.74
1:C:464:PRO:HD2	1:C:534:GLU:HB3	1.70	0.73
1:C:446:LEU:HG	1:C:604:GLU:HG2	1.71	0.73
1:B:432:ASP:HA	1:B:435:ARG:HD3	1.69	0.73
1:A:451:TYR:HA	1:A:454:PHE:CD1	2.24	0.73
1:B:530:ARG:HH11	1:B:671:PHE:HB2	1.54	0.72
1:A:523:HIS:HB3	1:A:525:TYR:CE1	2.25	0.71
1:D:512:ALA:O	1:D:516:ILE:HD12	1.91	0.71
1:A:462:LEU:HD21	1:A:533:VAL:HG22	1.73	0.70
1:A:523:HIS:HB2	1:A:526:LEU:HD12	1.72	0.70
1:A:611:LYS:O	1:A:612:LEU:HB2	1.90	0.70
1:B:530:ARG:NH1	1:B:671:PHE:HB2	2.06	0.69
1:C:536:ASN:H	1:C:536:ASN:HD22	1.36	0.69
1:C:654:ILE:HD12	4:C:55:HOH:O	1.92	0.69
1:A:492:LEU:HD22	1:A:652:LEU:HD11	1.74	0.68
1:C:583:LYS:NZ	4:C:37:HOH:O	2.27	0.67
1:A:516:ILE:HG22	1:A:520:LEU:HD11	1.76	0.67
1:D:492:LEU:O	1:D:607:SER:HB3	1.95	0.66
1:C:581:ARG:H	1:C:581:ARG:HH11	1.43	0.66
1:D:538:ASN:HD22	1:D:541:ALA:H	1.43	0.66
1:A:550:ARG:HD3	1:A:674:SER:OG	1.96	0.66
1:B:459:TYR:CE2	1:B:530:ARG:HD2	2.31	0.66
1:A:513:ALA:HA	1:A:516:ILE:HD12	1.78	0.65
1:D:547:CYS:O	1:D:550:ARG:HB3	1.95	0.65
1:B:560:ARG:HH21	1:B:562:LEU:HD11	1.62	0.65
1:D:534:GLU:HG2	1:D:536:ASN:HD22	1.62	0.64
1:D:480:VAL:HG12	1:D:489:ILE:HA	1.79	0.63
1:B:568:ASP:CG	1:B:569:GLN:N	2.49	0.63
1:B:664:ASP:CB	4:B:18:HOH:O	2.30	0.62
1:C:494:HIS:O	1:C:609:THR:HG21	1.99	0.62
1:A:432:ASP:OD1	1:A:432:ASP:N	2.32	0.62
1:C:581:ARG:H	1:C:581:ARG:NH1	1.97	0.62
1:C:527:ASP:HA	1:C:559:ILE:HD11	1.82	0.61
1:B:565:HIS:HA	1:B:574:GLN:O	2.00	0.61
1:D:629:ARG:HE	1:D:629:ARG:HA	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:615:ASP:OD1	1:C:616:PRO:HD2	2.01	0.60
1:C:494:HIS:O	1:C:609:THR:CG2	2.50	0.60
1:C:565:HIS:HB3	1:C:573:GLU:HB3	1.84	0.60
1:A:528:GLU:HG2	1:A:529:LEU:H	1.66	0.60
1:B:588:GLU:HG3	1:C:592:SER:HB3	1.84	0.60
1:C:662:LEU:C	1:C:664:ASP:H	2.08	0.60
1:B:589:GLN:HG2	1:B:593:ARG:HE	1.66	0.59
1:A:440:ILE:HG22	1:B:447:ASN:HB3	1.83	0.59
1:C:589:GLN:O	1:C:593:ARG:HG3	2.01	0.59
1:C:617:ILE:O	1:C:621:LEU:HD12	2.03	0.59
1:A:462:LEU:HB3	1:A:477:VAL:HG22	1.85	0.58
1:B:604:GLU:CD	1:B:604:GLU:H	2.11	0.58
1:B:577:TYR:HE1	1:B:579:MET:HA	1.68	0.58
1:B:443:TYR:CD1	1:B:488:LEU:HD21	2.38	0.58
1:D:610:ILE:HG21	1:D:616:PRO:HA	1.86	0.57
1:D:462:LEU:HD21	1:D:533:VAL:HG22	1.85	0.57
1:D:611:LYS:HB3	1:D:612:LEU:CD2	2.28	0.57
1:A:462:LEU:N	1:A:462:LEU:HD23	2.20	0.57
1:B:605:LEU:C	1:B:605:LEU:HD12	2.30	0.56
1:C:477:VAL:HG12	1:C:515:MET:HE1	1.87	0.56
1:D:610:ILE:O	1:D:610:ILE:HG22	2.05	0.56
1:C:494:HIS:C	1:C:609:THR:HG21	2.30	0.56
1:A:430:ILE:HD13	1:A:624:ILE:CG2	2.35	0.56
1:A:515:MET:O	1:A:519:VAL:HG23	2.05	0.56
1:A:493:GLU:HA	1:A:609:THR:CG2	2.36	0.56
1:C:464:PRO:HA	1:C:475:THR:HG23	1.86	0.56
1:C:462:LEU:HD12	1:C:464:PRO:HD3	1.86	0.56
1:D:568:ASP:CG	1:D:569:GLN:H	2.14	0.56
1:D:622:GLU:O	1:D:626:ASN:ND2	2.38	0.56
1:A:588:GLU:HA	1:A:591:ILE:HD12	1.87	0.55
1:A:493:GLU:HA	1:A:609:THR:HG21	1.88	0.55
1:B:487:PHE:HE2	1:B:593:ARG:HH11	1.54	0.55
1:B:536:ASN:OD1	1:B:579:MET:N	2.36	0.55
1:C:573:GLU:C	1:C:574:GLN:HE21	2.14	0.55
1:C:624:ILE:C	1:C:626:ASN:H	2.14	0.55
1:D:442:ARG:NH1	1:D:617:ILE:HD13	2.22	0.54
1:A:572:ILE:HD12	1:A:574:GLN:OE1	2.08	0.54
1:B:615:ASP:O	1:B:616:PRO:C	2.50	0.54
1:C:607:SER:O	1:C:611:LYS:HB2	2.08	0.54
1:C:489:ILE:HG21	1:C:492:LEU:HD21	1.89	0.54
1:A:653:ILE:O	1:A:657:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:VAL:HG13	1:C:531:ILE:HG12	1.89	0.53
1:A:444:SER:HB2	1:A:447:ASN:HD21	1.73	0.53
1:D:536:ASN:HD21	1:D:579:MET:H	1.57	0.53
1:C:669:ILE:HD12	1:C:670:ARG:HG2	1.90	0.53
1:A:627:LEU:HD21	1:A:653:ILE:HG21	1.90	0.53
1:C:536:ASN:HD22	1:C:536:ASN:N	2.06	0.52
1:B:458:LEU:HB3	1:B:529:LEU:HD23	1.92	0.52
1:B:585:LEU:O	1:B:589:GLN:HB2	2.09	0.52
1:A:672:ARG:HH11	1:A:672:ARG:HB2	1.75	0.52
1:B:445:THR:HG21	1:B:523:HIS:HD2	1.70	0.52
1:B:620:LEU:HD13	1:B:652:LEU:HD13	1.92	0.52
1:C:576:PHE:C	1:C:576:PHE:CD2	2.87	0.52
1:D:622:GLU:O	1:D:625:GLN:HG3	2.10	0.52
1:D:462:LEU:CD2	1:D:533:VAL:HG22	2.40	0.51
1:B:513:ALA:O	1:B:517:ILE:HG13	2.10	0.51
1:C:515:MET:HG2	1:C:516:ILE:N	2.23	0.51
1:C:667:HIS:O	1:C:668:ALA:C	2.53	0.51
1:A:490:TYR:O	1:A:605:LEU:HB2	2.11	0.51
1:B:590:PHE:O	1:B:591:ILE:C	2.52	0.51
1:C:661:TYR:O	1:C:664:ASP:HB2	2.11	0.51
1:B:458:LEU:HD21	1:B:479:ALA:HB1	1.91	0.50
1:C:583:LYS:O	1:C:587:VAL:HG23	2.11	0.50
1:D:518:SER:HB3	1:D:606:VAL:HG11	1.92	0.50
1:B:483:TYR:OH	1:B:484:ARG:NH1	2.41	0.50
1:D:430:ILE:HD12	1:D:430:ILE:N	2.19	0.50
1:B:541:ALA:HA	1:B:544:ARG:NH2	2.26	0.50
1:C:590:PHE:O	1:C:591:ILE:C	2.54	0.50
1:C:576:PHE:C	1:C:576:PHE:HD2	2.20	0.50
1:D:458:LEU:HG	1:D:526:LEU:HD13	1.93	0.50
1:D:620:LEU:C	1:D:622:GLU:N	2.69	0.50
1:B:465:ALA:HB1	1:B:473:SER:HB3	1.94	0.49
1:C:446:LEU:CG	1:C:604:GLU:HG2	2.41	0.49
1:D:448:THR:HG23	1:D:451:TYR:CD2	2.47	0.49
1:B:530:ARG:HD3	1:B:671:PHE:CD2	2.48	0.49
1:C:430:ILE:HG13	1:C:430:ILE:O	2.12	0.49
1:A:475:THR:O	1:A:494:HIS:HD2	1.96	0.49
1:C:543:VAL:HG22	1:C:575:PRO:HD2	1.93	0.49
1:B:560:ARG:HE	1:B:562:LEU:HD11	1.78	0.48
1:A:516:ILE:HG22	1:A:520:LEU:CD1	2.43	0.48
1:D:503:SER:O	1:D:504:SER:C	2.56	0.48
1:B:565:HIS:O	1:B:670:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:SER:O	1:B:447:ASN:HB2	2.12	0.48
1:D:523:HIS:HB3	1:D:525:TYR:CE1	2.49	0.48
1:B:475:THR:O	1:B:494:HIS:HA	2.13	0.48
1:B:577:TYR:CE1	1:B:579:MET:HA	2.48	0.48
1:C:621:LEU:C	1:C:623:GLN:H	2.22	0.48
1:D:461:TYR:CD2	1:D:462:LEU:N	2.82	0.48
1:B:582:ASP:O	1:B:583:LYS:C	2.57	0.48
1:B:562:LEU:HD12	1:B:562:LEU:N	2.28	0.48
1:D:534:GLU:OE2	1:D:579:MET:HG3	2.14	0.48
1:A:494:HIS:H	1:A:609:THR:CG2	2.22	0.48
1:C:617:ILE:H	1:C:617:ILE:CD1	2.18	0.47
1:A:456:LYS:C	1:A:526:LEU:HD23	2.39	0.47
1:A:504:SER:O	1:A:508:ILE:HG13	2.13	0.47
1:C:536:ASN:H	1:C:536:ASN:ND2	2.09	0.47
1:C:494:HIS:H	1:C:609:THR:HG21	1.79	0.47
1:D:665:ASP:C	1:D:667:HIS:H	2.23	0.47
1:C:442:ARG:CZ	1:C:617:ILE:HD11	2.45	0.47
1:C:488:LEU:HD21	1:C:602:SER:HB3	1.95	0.47
1:C:624:ILE:O	1:C:626:ASN:N	2.47	0.47
1:A:587:VAL:HG22	1:A:657:ILE:HG21	1.96	0.46
1:B:568:ASP:HB2	1:B:574:GLN:HG3	1.96	0.46
1:B:510:GLU:OE2	1:B:510:GLU:HA	2.15	0.46
1:B:565:HIS:CD2	1:B:672:ARG:HB3	2.51	0.46
1:C:536:ASN:N	1:C:536:ASN:ND2	2.63	0.46
1:C:620:LEU:O	1:C:624:ILE:HG13	2.16	0.46
1:D:459:TYR:O	1:D:479:ALA:HA	2.16	0.45
1:A:430:ILE:CD1	1:A:624:ILE:HG22	2.46	0.45
1:A:458:LEU:HD11	1:A:479:ALA:HB1	1.98	0.45
1:C:662:LEU:C	1:C:664:ASP:N	2.73	0.45
1:A:451:TYR:HA	1:A:454:PHE:HD1	1.75	0.45
1:A:494:HIS:HE2	1:A:651:ASP:HB2	1.81	0.45
1:D:461:TYR:CD1	1:D:658:MET:HB3	2.51	0.45
1:D:570:ASN:OD1	1:D:570:ASN:N	2.48	0.45
1:B:589:GLN:CD	1:B:593:ARG:HH21	2.25	0.45
1:C:582:ASP:HA	1:C:585:LEU:HD12	1.99	0.45
1:A:456:LYS:O	1:A:526:LEU:HA	2.17	0.45
1:B:621:LEU:O	1:B:625:GLN:HB2	2.16	0.45
1:D:620:LEU:C	1:D:622:GLU:H	2.24	0.45
1:B:432:ASP:OD1	1:B:432:ASP:N	2.45	0.45
1:A:430:ILE:HD13	1:A:624:ILE:HG22	1.98	0.45
1:A:475:THR:O	1:A:494:HIS:CD2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:PHE:O	1:B:565:HIS:HD2	2.00	0.45
1:B:624:ILE:C	1:B:626:ASN:N	2.74	0.44
1:A:605:LEU:HD12	1:A:605:LEU:C	2.43	0.44
1:A:517:ILE:O	1:A:521:SER:HB3	2.16	0.44
1:A:538:ASN:OD1	1:A:538:ASN:C	2.61	0.44
1:B:564:TYR:CE1	1:B:670:ARG:HB2	2.52	0.44
1:B:627:LEU:O	1:B:628:HIS:ND1	2.51	0.44
1:A:510:GLU:HA	1:A:510:GLU:OE2	2.16	0.44
1:A:515:MET:HE3	1:A:516:ILE:HG13	1.99	0.44
1:C:494:HIS:NE2	1:C:651:ASP:HB2	2.32	0.44
1:C:568:ASP:OD1	1:C:569:GLN:N	2.51	0.44
1:D:440:ILE:H	1:D:440:ILE:HG13	1.66	0.44
1:D:620:LEU:O	1:D:622:GLU:N	2.50	0.44
1:D:474:GLY:O	1:D:651:ASP:CG	2.61	0.44
1:B:629:ARG:O	1:B:630:VAL:HB	2.18	0.44
1:A:445:THR:HG22	1:A:454:PHE:HE2	1.83	0.43
1:A:462:LEU:HD23	1:A:462:LEU:H	1.83	0.43
1:C:513:ALA:O	1:C:517:ILE:HG13	2.18	0.43
1:D:568:ASP:O	1:D:569:GLN:C	2.61	0.43
1:B:590:PHE:O	1:B:594:PHE:N	2.44	0.43
1:C:669:ILE:H	1:C:669:ILE:HG13	1.54	0.43
1:D:443:TYR:H	1:D:602:SER:HA	1.83	0.43
1:A:493:GLU:CA	1:A:609:THR:HG21	2.47	0.43
1:B:517:ILE:HD13	1:B:556:SER:OG	2.18	0.43
1:B:566:THR:HA	1:B:670:ARG:HH22	1.84	0.43
1:C:518:SER:O	1:C:522:LEU:HD12	2.19	0.43
1:C:565:HIS:HB3	1:C:573:GLU:CB	2.48	0.43
1:C:585:LEU:H	1:C:585:LEU:HG	1.55	0.43
1:A:517:ILE:HA	1:A:520:LEU:HD12	2.00	0.43
1:B:515:MET:O	1:B:519:VAL:HG23	2.18	0.43
1:B:444:SER:HB3	1:B:447:ASN:HD22	1.84	0.43
1:A:441:LEU:HG	1:B:443:TYR:CE2	2.53	0.43
1:D:441:LEU:HD23	1:D:441:LEU:HA	1.84	0.43
1:D:515:MET:O	1:D:519:VAL:HG23	2.18	0.43
1:B:624:ILE:C	1:B:626:ASN:H	2.26	0.43
1:C:590:PHE:C	1:C:590:PHE:CD2	2.96	0.43
1:A:462:LEU:N	1:A:462:LEU:CD2	2.81	0.43
1:B:551:GLN:HE21	1:B:551:GLN:HB3	1.65	0.43
1:C:582:ASP:OD1	1:C:585:LEU:HD12	2.19	0.43
1:D:654:ILE:O	1:D:658:MET:HG2	2.19	0.43
1:C:650:ASP:OD1	1:C:650:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:TYR:HE2	1:B:662:LEU:HD11	1.84	0.42
1:C:624:ILE:O	1:C:627:LEU:HG	2.19	0.42
1:A:431:THR:O	1:A:435:ARG:HG3	2.20	0.42
1:D:444:SER:HB3	1:D:447:ASN:HD22	1.84	0.42
1:D:538:ASN:ND2	1:D:541:ALA:H	2.15	0.42
1:A:445:THR:HG22	1:A:454:PHE:CE2	2.55	0.42
1:D:504:SER:O	1:D:508:ILE:HG13	2.19	0.42
1:D:557:THR:HG23	1:D:559:ILE:HG22	2.02	0.42
1:A:431:THR:HB	1:A:434:SER:H	1.85	0.42
1:D:489:ILE:HG13	1:D:600:LYS:O	2.20	0.42
1:A:513:ALA:O	1:A:517:ILE:HG13	2.20	0.41
1:B:442:ARG:HG2	1:B:601:ALA:HB3	2.02	0.41
1:D:629:ARG:HA	1:D:629:ARG:NE	2.33	0.41
1:A:574:GLN:HA	1:A:575:PRO:HD3	1.75	0.41
1:C:493:GLU:OE1	1:C:609:THR:HB	2.20	0.41
1:D:492:LEU:O	1:D:607:SER:CB	2.66	0.41
1:A:577:TYR:HE2	1:A:579:MET:HB2	1.85	0.41
1:C:589:GLN:HE22	1:C:661:TYR:HD1	1.68	0.41
1:C:624:ILE:C	1:C:626:ASN:N	2.78	0.41
1:D:462:LEU:CD2	1:D:533:VAL:HA	2.50	0.41
1:A:652:LEU:O	1:A:655:ALA:HB3	2.21	0.41
1:B:438:PHE:HD2	1:B:621:LEU:HD21	1.85	0.41
1:B:514:HIS:CD2	1:B:608:TYR:CD1	3.09	0.41
1:C:458:LEU:HB2	1:C:526:LEU:HD22	2.02	0.41
1:B:560:ARG:HE	1:B:560:ARG:HB3	1.74	0.41
1:B:666:ILE:H	1:B:666:ILE:HG13	1.59	0.41
1:C:441:LEU:HD21	1:D:443:TYR:CE2	2.56	0.41
1:C:523:HIS:HB2	1:C:526:LEU:HD12	2.03	0.41
1:A:610:ILE:HD13	1:A:610:ILE:HA	1.87	0.41
1:B:503:SER:O	1:B:504:SER:C	2.63	0.41
1:C:433:GLN:HG3	1:D:484:ARG:HH12	1.85	0.41
1:D:529:LEU:HB2	1:D:561:VAL:HG12	2.02	0.41
1:D:673:VAL:HG12	1:D:674:SER:H	1.86	0.41
1:A:541:ALA:O	1:A:545:ILE:HG13	2.21	0.41
1:A:553:VAL:O	1:A:556:SER:N	2.50	0.41
1:B:629:ARG:O	1:B:630:VAL:CB	2.69	0.41
1:C:456:LYS:HG2	1:C:525:TYR:O	2.21	0.41
1:C:436:GLU:O	1:C:440:ILE:HG13	2.21	0.40
1:D:538:ASN:HB3	1:D:541:ALA:HB3	2.03	0.40
1:D:627:LEU:HD13	1:D:628:HIS:H	1.86	0.40
1:B:451:TYR:O	1:B:453:TYR:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:PHE:O	1:B:565:HIS:CD2	2.74	0.40
1:B:577:TYR:CD1	1:B:577:TYR:C	2.99	0.40
1:A:441:LEU:HD23	1:A:441:LEU:HA	1.95	0.40
1:C:556:SER:O	1:C:557:THR:HB	2.21	0.40
1:A:493:GLU:OE1	1:A:609:THR:HG22	2.21	0.40
1:B:445:THR:HG21	1:B:523:HIS:NE2	2.33	0.40
1:B:588:GLU:HG2	1:C:592:SER:HA	2.03	0.40
1:C:624:ILE:HG12	1:C:653:ILE:HD13	2.03	0.40
1:A:528:GLU:HG2	1:A:529:LEU:N	2.33	0.40
1:B:656:VAL:O	1:B:657:ILE:C	2.65	0.40
1:C:452:ASP:OD1	1:C:452:ASP:N	2.54	0.40
1:D:590:PHE:CD2	1:D:590:PHE:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	208/279 (75%)	188 (90%)	15 (7%)	5 (2%)	4	28
1	B	213/279 (76%)	182 (85%)	29 (14%)	2 (1%)	14	47
1	C	213/279 (76%)	179 (84%)	30 (14%)	4 (2%)	6	33
1	D	206/279 (74%)	178 (86%)	26 (13%)	2 (1%)	12	45
All	All	840/1116 (75%)	727 (86%)	100 (12%)	13 (2%)	8	37

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	612	LEU
1	C	569	GLN
1	D	504	SER

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Mol	Chain	Res	Type
1	A	537	THR
1	A	569	GLN
1	C	581	ARG
1	A	571	HIS
1	A	626	ASN
1	B	464	PRO
1	C	625	GLN
1	C	582	ASP
1	B	580	GLY
1	D	610	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/242 (78%)	151 (80%)	37 (20%)	1	8
1	B	192/242 (79%)	154 (80%)	38 (20%)	1	8
1	C	190/242 (78%)	153 (80%)	37 (20%)	1	8
1	D	186/242 (77%)	154 (83%)	32 (17%)	2	10
All	All	756/968 (78%)	612 (81%)	144 (19%)	1	9

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	429	LEU
1	A	431	THR
1	A	432	ASP
1	A	436	GLU
1	A	441	LEU
1	A	444	SER
1	A	445	THR
1	A	447	ASN
1	A	462	LEU
1	A	480	VAL
1	A	488	LEU

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Mol	Chain	Res	Type
1	A	489	ILE
1	A	503	SER
1	A	504	SER
1	A	517	ILE
1	A	521	SER
1	A	529	LEU
1	A	537	THR
1	A	538	ASN
1	A	547	CYS
1	A	552	SER
1	A	555	SER
1	A	569	GLN
1	A	572	ILE
1	A	578	LEU
1	A	583	LYS
1	A	605	LEU
1	A	610	ILE
1	A	612	LEU
1	A	618	GLU
1	A	620	LEU
1	A	621	LEU
1	A	653	ILE
1	A	662	LEU
1	A	665	ASP
1	A	666	ILE
1	A	672	ARG
1	B	429	LEU
1	B	430	ILE
1	B	431	THR
1	B	432	ASP
1	B	437	GLU
1	B	445	THR
1	B	446	LEU
1	B	447	ASN
1	B	456	LYS
1	B	458	LEU
1	B	460	VAL
1	B	480	VAL
1	B	488	LEU
1	B	504	SER
1	B	520	LEU
1	B	521	SER

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Mol	Chain	Res	Type
1	B	536	ASN
1	B	537	THR
1	B	539	GLN
1	B	551	GLN
1	B	572	ILE
1	B	574	GLN
1	B	578	LEU
1	B	585	LEU
1	B	603	GLN
1	B	604	GLU
1	B	605	LEU
1	B	610	ILE
1	B	612	LEU
1	B	618	GLU
1	B	648	ILE
1	B	649	SER
1	B	652	LEU
1	B	662	LEU
1	B	663	CYS
1	B	664	ASP
1	B	666	ILE
1	B	669	ILE
1	C	429	LEU
1	C	433	GLN
1	C	452	ASP
1	C	458	LEU
1	C	460	VAL
1	C	462	LEU
1	C	492	LEU
1	C	499	ASP
1	C	500	LEU
1	C	518	SER
1	C	521	SER
1	C	522	LEU
1	C	529	LEU
1	C	536	ASN
1	C	547	CYS
1	C	548	LEU
1	C	551	GLN
1	C	555	SER
1	C	559	ILE
1	C	573	GLU

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Mol	Chain	Res	Type
1	C	574	GLN
1	C	576	PHE
1	C	581	ARG
1	C	583	LYS
1	C	585	LEU
1	C	592	SER
1	C	593	ARG
1	C	604	GLU
1	C	605	LEU
1	C	613	SER
1	C	617	ILE
1	C	625	GLN
1	C	648	ILE
1	C	662	LEU
1	C	663	CYS
1	C	664	ASP
1	C	669	ILE
1	D	430	ILE
1	D	431	THR
1	D	441	LEU
1	D	445	THR
1	D	458	LEU
1	D	462	LEU
1	D	475	THR
1	D	488	LEU
1	D	489	ILE
1	D	495	PHE
1	D	503	SER
1	D	518	SER
1	D	521	SER
1	D	529	LEU
1	D	539	GLN
1	D	547	CYS
1	D	548	LEU
1	D	552	SER
1	D	570	ASN
1	D	574	GLN
1	D	579	MET
1	D	581	ARG
1	D	599	ILE
1	D	600	LYS
1	D	613	SER

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Mol	Chain	Res	Type
1	D	614	HIS
1	D	621	LEU
1	D	625	GLN
1	D	626	ASN
1	D	627	LEU
1	D	662	LEU
1	D	674	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	ASN
1	A	449	ASN
1	A	486	GLN
1	A	569	GLN
1	A	589	GLN
1	B	486	GLN
1	B	514	HIS
1	B	538	ASN
1	B	539	GLN
1	B	551	GLN
1	B	565	HIS
1	B	574	GLN
1	B	603	GLN
1	B	623	GLN
1	C	433	GLN
1	C	536	ASN
1	C	554	GLN
1	C	569	GLN
1	C	570	ASN
1	C	574	GLN
1	C	589	GLN
1	C	625	GLN
1	D	447	ASN
1	D	514	HIS
1	D	523	HIS
1	D	536	ASN
1	D	538	ASN
1	D	539	GLN
1	D	551	GLN
1	D	589	GLN
1	D	628	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	216/279 (77%)	-0.33	2 (0%) 81 64	46, 77, 119, 164	6 (2%)
1	B	221/279 (79%)	-0.41	0 100 100	43, 76, 110, 154	2 (0%)
1	C	219/279 (78%)	-0.41	2 (0%) 81 64	54, 80, 128, 180	4 (1%)
1	D	214/279 (76%)	-0.12	6 (2%) 55 35	35, 84, 120, 148	12 (5%)
All	All	870/1116 (77%)	-0.32	10 (1%) 78 61	35, 79, 122, 180	24 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	611	LYS	5.2
1	D	581	ARG	5.2
1	A	622	GLU	3.6
1	C	436	GLU	3.2
1	D	537	THR	2.8
1	D	433	GLN	2.7
1	D	579	MET	2.6
1	C	666	ILE	2.5
1	A	581	ARG	2.5
1	D	495	PHE	2.1

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	MN	B	3	1/1	0.91	0.08	55,55,55,55	0
3	MG	B	2	1/1	0.91	0.11	40,40,40,40	0
2	MN	C	5	1/1	0.95	0.06	58,58,58,58	0
2	MN	A	2	1/1	0.95	0.04	55,55,55,55	0
3	MG	C	4	1/1	0.96	0.07	65,65,65,65	0
2	MN	B	4	1/1	0.97	0.04	52,52,52,52	0
2	MN	D	8	1/1	0.97	0.09	64,64,64,64	0
3	MG	D	3	1/1	0.97	0.04	38,38,38,38	0
2	MN	A	1	1/1	0.98	0.03	58,58,58,58	0
2	MN	C	6	1/1	0.98	0.05	58,58,58,58	0
3	MG	A	675	1/1	0.99	0.04	29,29,29,29	0
2	MN	D	7	1/1	0.99	0.03	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.