Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:50 AM GMT

PDB ID	:	3N4Q
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

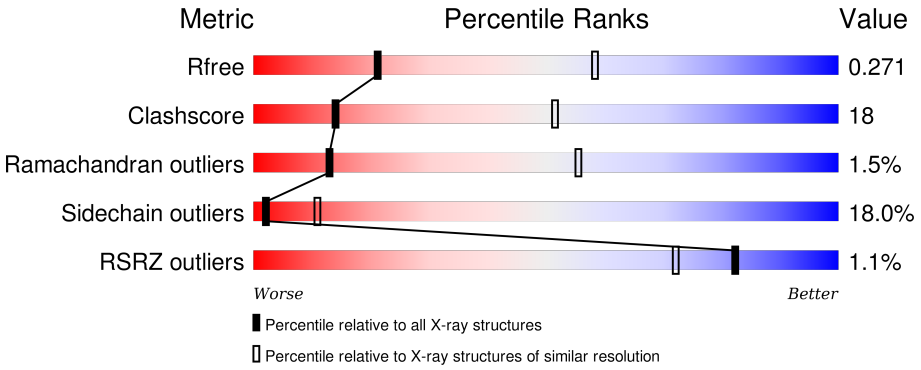
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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% 47% 24% 6% 23%
1	B	279	45% 29% 5% 21%
1	C	279	% 45% 25% 7% 22%
1	D	279	% 45% 25% 7% 23%

2 Entry composition (i)

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 (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

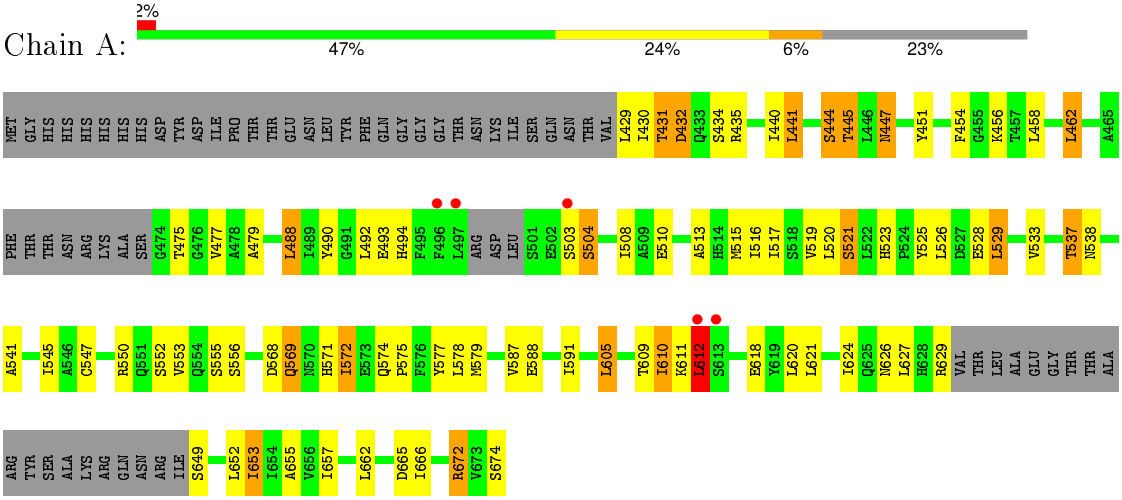
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	11	Total O 11 11	0	0
4	B	17	Total O 17 17	0	0
4	C	15	Total O 15 15	0	0
4	D	13	Total O 13 13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

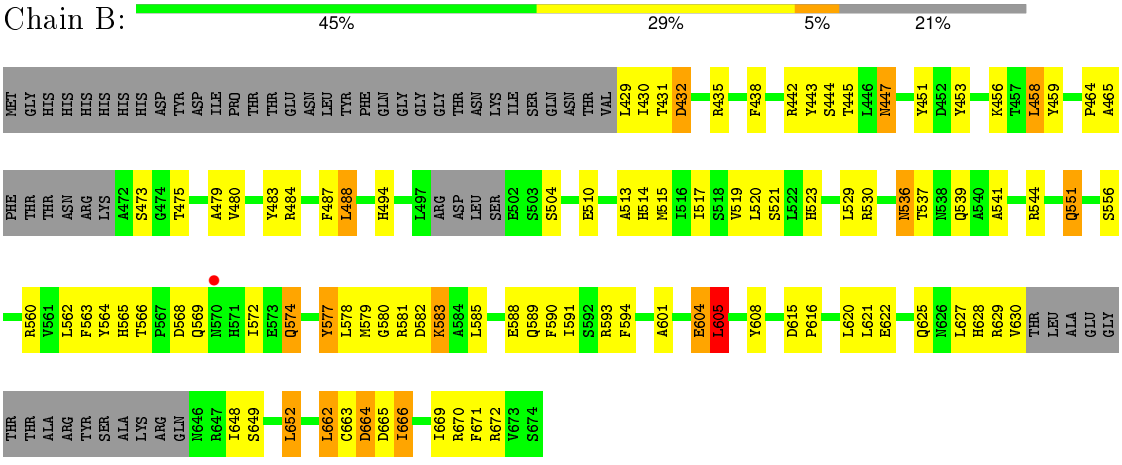
- Molecule 1: TERMINASE SUBUNIT UL89 PROTEIN

Chain A:



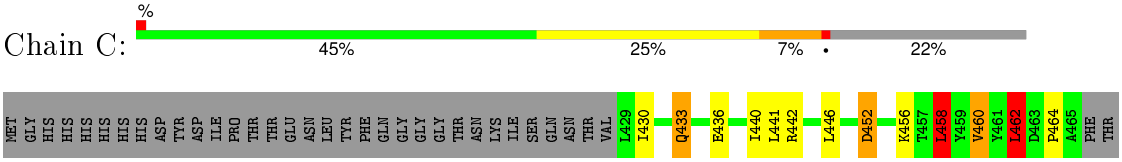
- Molecule 1: TERMINASE SUBUNIT UL89 PROTEIN

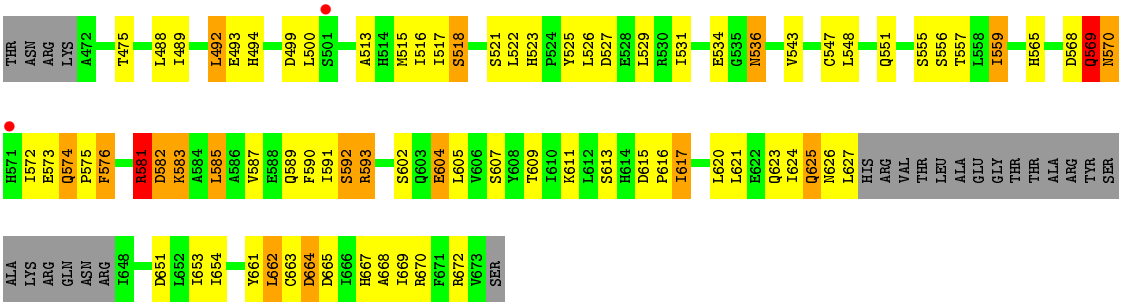
Chain B:



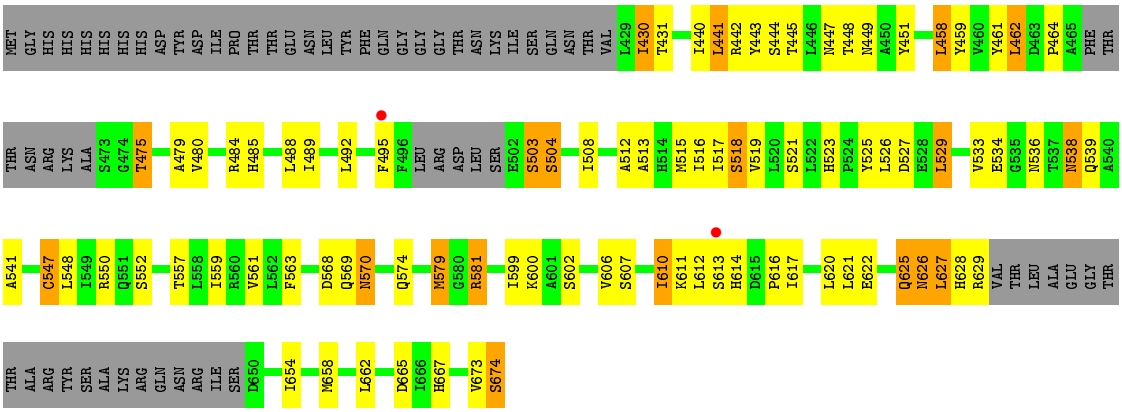
- Molecule 1: TERMINASE SUBUNIT UL89 PROTEIN

Chain C:





- Molecule 1: TERMINASE SUBUNIT UL89 PROTEIN



4 Data and refinement statistics (i)

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 – 3.19	Depositor EDS
% Data completeness (in resolution range)	89.6 (44.05-3.20) 89.6 (44.05-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.90 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.207 , 0.283 0.200 , 0.271	Depositor DCC
R_{free} test set	1108 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	75.1	Xtriage
Anisotropy	0.820	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 68.6	EDS
Estimated twinning fraction	0.046 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 21659 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.61	0/1770	0.75	1/2399 (0.0%)
1	B	0.58	1/1809 (0.1%)	0.74	2/2452 (0.1%)
1	C	0.58	0/1789	0.74	3/2427 (0.1%)
1	D	0.55	0/1756	0.69	0/2380
All	All	0.58	1/7124 (0.0%)	0.73	6/9658 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	622	GLU	CG-CD	5.10	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	488	LEU	CA-CB-CG	7.49	132.52	115.30
1	C	458	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	605	LEU	CA-CB-CG	5.69	128.38	115.30
1	C	569	GLN	N-CA-C	-5.46	96.27	111.00
1	B	578	LEU	CA-CB-CG	5.35	127.60	115.30
1	C	462	LEU	CA-CB-CG	5.28	127.43	115.30

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	64	0
1	B	1775	0	1751	67	0
1	C	1755	0	1732	70	0
1	D	1722	0	1691	59	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	1	0
4	D	13	0	0	0	0
All	All	7056	0	6881	254	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 18.

All (254) 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:A:456:LYS:HD3	1:A:525:TYR:O	1.73	0.90
1:B:568:ASP:CG	1:B:569:GLN:H	1.77	0.87
1:D:430:ILE:H	1:D:430:ILE:HD12	1.40	0.85
1:C:617:ILE:HD13	1:C:617:ILE:H	1.39	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HH11	1:C:581:ARG:H	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:B:568:ASP:CG	1:B:569:GLN:N	2.49	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: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:N	1:A:432:ASP:OD1	2.32	0.62
1:C:581:ARG:NH1	1:C:581:ARG:H	1.97	0.62
1:D:563:PHE:HD1	1:D:674:SER:HG	1.47	0.61
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
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:B:589:GLN:HG2	1:B:593:ARG:HE	1.66	0.59
1:C:589:GLN:O	1:C:593:ARG:HG3	2.01	0.59
1:A:440:ILE:HG22	1:B:447:ASN:HB3	1.83	0.59
1:C:617:ILE:O	1:C:621:LEU:HD12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LEU:HB3	1:A:477:VAL:HG22	1.85	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:HD23	1:A:462:LEU:N	2.20	0.57
1:D:610:ILE:HG22	1:D:610:ILE:O	2.05	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:622:GLU:O	1:D:626:ASN:ND2	2.38	0.56
1:C:662:LEU:C	1:C:664:ASP:H	2.08	0.55
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: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: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:B:604:GLU:CD	1:B:604:GLU:H	2.11	0.53
1:C:460:VAL:HG13	1:C:531:ILE:HG12	1.89	0.53
1:A:653:ILE:O	1:A:657:ILE:HG13	2.08	0.53
1:A:515:MET:HE3	1:A:516:ILE:HG13	1.88	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:N	1:C:536:ASN:HD22	2.06	0.52
1:B:458:LEU:HB3	1:B:529:LEU:HD23	1.92	0.52
1:C:494:HIS:C	1:C:609:THR:HG21	2.30	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:605:LEU:C	1:B:605:LEU:HD12	2.30	0.52
1:B:620:LEU:HD13	1:B:652:LEU:HD13	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:490:TYR:O	1:A:605:LEU:HB2	2.11	0.51
1:D:568:ASP:CG	1:D:569:GLN:H	2.14	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:C:573:GLU:C	1:C:574:GLN:HE21	2.14	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:N	1:D:430:ILE:HD12	2.19	0.50
1:B:541:ALA:HA	1:B:544:ARG:NH2	2.26	0.50
1:C:624:ILE:C	1:C:626:ASN:H	2.14	0.50
1:D:458:LEU:HG	1:D:526:LEU:HD13	1.93	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:615:ASP:O	1:B:616:PRO:C	2.50	0.49
1:B:530:ARG:HD3	1:B:671:PHE:CD2	2.48	0.49
1:C:430:ILE:O	1:C:430:ILE:HG13	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:B:565:HIS:O	1:B:670:ARG:NH2	2.46	0.48
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:577:TYR:CE1	1:B:579:MET:HA	2.48	0.48
1:D:461:TYR:CD2	1:D:462:LEU:N	2.82	0.48
1:B:475:THR:O	1:B:494:HIS:HA	2.13	0.48
1:B:562:LEU:N	1:B:562:LEU:HD12	2.28	0.48
1:D:534:GLU:OE2	1:D:579:MET:HG3	2.14	0.48
1:C:494:HIS:HE2	1:C:651:ASP:HB2	1.78	0.48
1:A:494:HIS:H	1:A:609:THR:CG2	2.22	0.48
1:C:617:ILE:CD1	1:C:617:ILE:H	2.18	0.47
1:C:536:ASN:H	1:C:536:ASN:ND2	2.09	0.47
1:A:504:SER:O	1:A:508:ILE:HG13	2.13	0.47
1:C:494:HIS:H	1:C:609:THR:HG21	1.79	0.47
1:C:576:PHE:CD2	1:C:576:PHE:C	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:510:GLU:OE2	1:A:510:GLU:HA	2.16	0.46
1:C:667:HIS:O	1:C:668:ALA:C	2.53	0.46
1:B:568:ASP:HB2	1:B:574:GLN:HG3	1.96	0.46
1:B:565:HIS:CD2	1:B:672:ARG:HB3	2.51	0.46
1:B:510:GLU:OE2	1:B:510:GLU:HA	2.15	0.46
1:B:590:PHE:O	1:B:591:ILE:C	2.52	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:A:451:TYR:HA	1:A:454:PHE:HD1	1.75	0.45
1:D:461:TYR:CD1	1:D:658:MET:HB3	2.51	0.45
1:D:570:ASN:N	1:D:570:ASN:OD1	2.48	0.45
1:C:590:PHE:O	1:C:591:ILE:C	2.54	0.45
1:C:576:PHE:C	1:C:576:PHE:HD2	2.20	0.45
1:C:582:ASP:HA	1:C:585:LEU:HD12	1.99	0.45
1:D:620:LEU:C	1:D:622:GLU:N	2.69	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:B:432:ASP:N	1:B:432:ASP:OD1	2.45	0.45
1:B:563:PHE:O	1:B:565:HIS:HD2	2.00	0.45
1:A:475:THR:O	1:A:494:HIS:CD2	2.70	0.45
1:A:430:ILE:HD13	1:A:624:ILE:HG22	1.98	0.45
1:D:515:MET:HE3	1:D:516:ILE:HG13	1.99	0.44
1:B:564:TYR:CE1	1:B:670:ARG:HB2	2.52	0.44
1:A:517:ILE:O	1:A:521:SER:HB3	2.16	0.44
1:B:627:LEU:O	1:B:628:HIS:ND1	2.51	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:620:LEU:O	1:D:622:GLU:N	2.50	0.44
1:D:440:ILE:HG13	1:D:440:ILE:H	1.66	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:503:SER:O	1:D:504:SER:C	2.56	0.43
1:C:669:ILE:HG13	1:C:669:ILE:H	1.54	0.43
1:B:590:PHE:O	1:B:594:PHE:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:TYR:H	1:D:602:SER:HA	1.83	0.43
1:B:566:THR:HA	1:B:670:ARG:HH22	1.84	0.43
1:C:621:LEU:C	1:C:623:GLN:H	2.22	0.43
1:A:493:GLU:CA	1:A:609:THR:HG21	2.47	0.43
1:C:565:HIS:HB3	1:C:573:GLU:CB	2.48	0.43
1:B:517:ILE:HD13	1:B:556:SER:OG	2.18	0.43
1:C:518:SER:O	1:C:522:LEU:HD12	2.19	0.43
1:C:585:LEU:H	1:C:585:LEU:HG	1.55	0.43
1:B:582:ASP:O	1:B:583:LYS:C	2.57	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:D:515:MET:O	1:D:519:VAL:HG23	2.18	0.43
1:A:441:LEU:HG	1:B:443:TYR:CE2	2.53	0.43
1:D:441:LEU:HA	1:D:441:LEU:HD23	1.84	0.43
1:D:581:ARG:HH11	1:D:581:ARG:HB2	1.83	0.43
1:A:462:LEU:CD2	1:A:462:LEU:N	2.81	0.43
1:B:551:GLN:HB3	1:B:551:GLN:HE21	1.65	0.43
1:D:654:ILE:O	1:D:658:MET:HG2	2.19	0.43
1:C:582:ASP:OD1	1:C:585:LEU:HD12	2.19	0.43
1:A:456:LYS:C	1:A:526:LEU:HD23	2.39	0.42
1:D:665:ASP:C	1:D:667:HIS:H	2.23	0.42
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:D:538:ASN:ND2	1:D:541:ALA:H	2.15	0.42
1:D:444:SER:HB3	1:D:447:ASN:HD22	1.84	0.42
1:A:431:THR:O	1:A:435:ARG:HG3	2.20	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:D:489:ILE:HG13	1:D:600:LYS:O	2.20	0.42
1:D:581:ARG:HH11	1:D:581:ARG:CG	2.33	0.42
1:A:431:THR:HB	1:A:434:SER:H	1.85	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:NE	1:D:629:ARG:HA	2.33	0.41
1:C:493:GLU:OE1	1:C:609:THR:HB	2.20	0.41
1:A:574:GLN:HA	1:A:575:PRO:HD3	1.75	0.41
1:D:492:LEU:O	1:D:607:SER:CB	2.66	0.41
1:C:589:GLN:HE22	1:C:661:TYR:HD1	1.68	0.41
1:A:577:TYR:HE2	1:A:579:MET:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:LEU:CD2	1:D:533:VAL:HA	2.50	0.41
1:D:620:LEU:C	1:D:622:GLU:H	2.24	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:HB3	1:B:560:ARG:HE	1.74	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:B:666:ILE:H	1:B:666:ILE:HG13	1.59	0.41
1:D:673:VAL:HG12	1:D:674:SER:H	1.86	0.41
1:C:662:LEU:C	1:C:664:ASP:N	2.73	0.41
1:D:529:LEU:HB2	1:D:561:VAL:HG12	2.02	0.41
1:C:433:GLN:HG3	1:D:484:ARG:HH12	1.85	0.41
1:A:610:ILE:HD13	1:A:610:ILE:HA	1.87	0.41
1:C:556:SER:O	1:C:557:THR:HB	2.21	0.41
1:A:541:ALA:O	1:A:545:ILE:HG13	2.21	0.41
1:B:629:ARG:O	1:B:630:VAL:CB	2.69	0.41
1:A:553:VAL:O	1:A:556:SER:N	2.50	0.41
1:C:456:LYS:HG2	1:C:525:TYR:O	2.21	0.41
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:C:436:GLU:O	1:C:440:ILE:HG13	2.21	0.40
1:B:563:PHE:O	1:B:565:HIS:CD2	2.74	0.40
1:B:589:GLN:CD	1:B:593:ARG:HH21	2.25	0.40
1:B:451:TYR:O	1:B:453:TYR:N	2.54	0.40
1:A:441:LEU:HA	1:A:441:LEU:HD23	1.95	0.40
1:B:445:THR:HG21	1:B:523:HIS:NE2	2.33	0.40
1:A:493:GLU:OE1	1:A:609:THR:HG22	2.21	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:C:452:ASP:N	1:C:452:ASP:OD1	2.54	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%)	7 43
1	B	213/279 (76%)	182 (85%)	29 (14%)	2 (1%)	21 67
1	C	213/279 (76%)	179 (84%)	30 (14%)	4 (2%)	10 50
1	D	206/279 (74%)	178 (86%)	26 (13%)	2 (1%)	19 65
All	All	840/1116 (75%)	727 (86%)	100 (12%)	13 (2%)	13 55

All (13) Ramachandran outliers are listed below:

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

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%)	154 (82%)	34 (18%)	2 11
1	B	192/242 (79%)	160 (83%)	32 (17%)	3 13
1	C	190/242 (78%)	154 (81%)	36 (19%)	2 10
1	D	186/242 (77%)	152 (82%)	34 (18%)	2 10
All	All	756/968 (78%)	620 (82%)	136 (18%)	2 11

All (136) 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	441	LEU
1	A	444	SER
1	A	445	THR
1	A	447	ASN
1	A	462	LEU
1	A	488	LEU
1	A	503	SER
1	A	504	SER
1	A	521	SER
1	A	529	LEU
1	A	537	THR
1	A	547	CYS
1	A	552	SER
1	A	555	SER
1	A	568	ASP
1	A	569	GLN
1	A	572	ILE
1	A	578	LEU
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	629	ARG
1	A	649	SER
1	A	653	ILE
1	A	662	LEU
1	A	665	ASP
1	A	666	ILE

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Mol	Chain	Res	Type
1	A	672	ARG
1	B	429	LEU
1	B	430	ILE
1	B	431	THR
1	B	432	ASP
1	B	447	ASN
1	B	456	LYS
1	B	458	LEU
1	B	480	VAL
1	B	488	LEU
1	B	504	SER
1	B	520	LEU
1	B	521	SER
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	577	TYR
1	B	581	ARG
1	B	583	LYS
1	B	604	GLU
1	B	605	LEU
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	665	ASP
1	B	666	ILE
1	B	669	ILE
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

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Mol	Chain	Res	Type
1	C	521	SER
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	569	GLN
1	C	570	ASN
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	662	LEU
1	C	663	CYS
1	C	664	ASP
1	C	665	ASP
1	C	672	ARG
1	D	430	ILE
1	D	431	THR
1	D	441	LEU
1	D	445	THR
1	D	449	ASN
1	D	458	LEU
1	D	462	LEU
1	D	475	THR
1	D	485	HIS
1	D	488	LEU
1	D	495	PHE
1	D	503	SER
1	D	518	SER
1	D	521	SER
1	D	527	ASP

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Mol	Chain	Res	Type
1	D	529	LEU
1	D	538	ASN
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	613	SER
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

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

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

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Mol	Chain	Res	Type
1	D	551	GLN
1	D	574	GLN
1	D	626	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

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

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, 95^{th} 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%)	-0.32	5 (2%)	64	49	48, 77, 119, 164	6 (2%)
1	B	221/279 (79%)	-0.40	1 (0%)	91	87	53, 76, 110, 154	2 (0%)
1	C	219/279 (78%)	-0.32	2 (0%)	85	78	54, 82, 128, 180	4 (1%)
1	D	214/279 (76%)	-0.22	2 (0%)	85	78	57, 86, 122, 148	12 (5%)
All	All	870/1116 (77%)	-0.32	10 (1%)	82	72	48, 80, 123, 180	24 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	612	LEU	3.3
1	D	613	SER	3.1
1	D	495	PHE	3.0
1	A	497	LEU	3.0
1	A	503	SER	2.8
1	C	571	HIS	2.4
1	A	613	SER	2.2
1	C	501	SER	2.2
1	A	496	PHE	2.0
1	B	570	ASN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	MN	D	7	1/1	0.97	0.09	-2.27	60,60,60,60	0
3	MG	B	2	1/1	0.88	0.10	-2.59	40,40,40,40	0
2	MN	D	8	1/1	0.98	0.18	-	64,64,64,64	0
2	MN	C	6	1/1	0.98	0.06	-	58,58,58,58	0
2	MN	A	2	1/1	0.96	0.14	-	55,55,55,55	0
2	MN	B	3	1/1	0.98	0.05	-	55,55,55,55	0
3	MG	D	3	1/1	0.92	0.05	-	38,38,38,38	0
3	MG	A	675	1/1	0.95	0.08	-	29,29,29,29	0
2	MN	B	4	1/1	0.96	0.07	-	52,52,52,52	0
2	MN	A	1	1/1	0.96	0.12	-	58,58,58,58	0
3	MG	C	4	1/1	0.93	0.17	-	65,65,65,65	0
2	MN	C	5	1/1	0.96	0.07	-	58,58,58,58	0

6.5 Other polymers

There are no such residues in this entry.