



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:43 PM UTC

PDB ID : 2ICE / pdb_00002ice
Title : CRIG bound to C3c
Authors : Wiesmann, C.
Deposited on : 2006-09-12
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

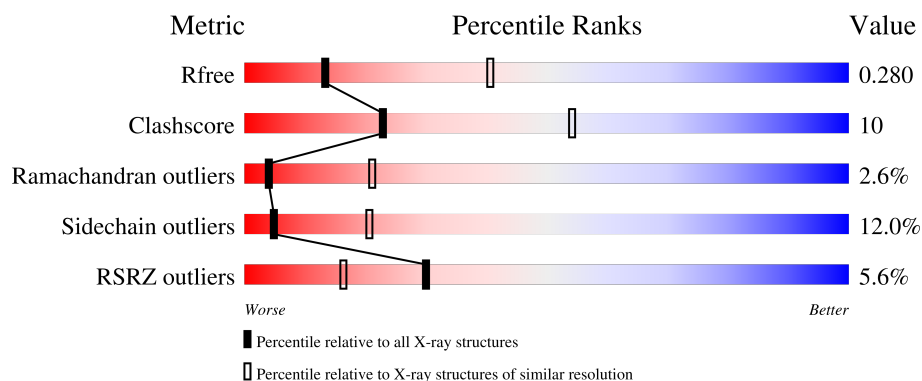
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	642	
1	D	642	
2	B	206	
2	E	206	
3	C	343	

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Mol	Chain	Length	Quality of chain
3	F	343	
4	S	119	
4	T	119	
5	G	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19619 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 Complement C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5008	3188	848	957	15			
1	D	630	Total	C	N	O	S	0	0	0
			4907	3127	828	937	15			

- Molecule 2 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1480	950	249	276	5			
2	E	183	Total	C	N	O	S	0	0	0
			1480	950	249	276	5			

- Molecule 3 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	296	Total	C	N	O	S	0	0	0
			2407	1517	395	475	20			
3	F	296	Total	C	N	O	S	0	0	0
			2407	1517	395	475	20			

- Molecule 4 is a protein called V-set and immunoglobulin domain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S	119	Total	C	N	O	S	0	0	0
			950	595	169	183	3			
4	T	119	Total	C	N	O	S	0	0	0
			950	595	169	183	3			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

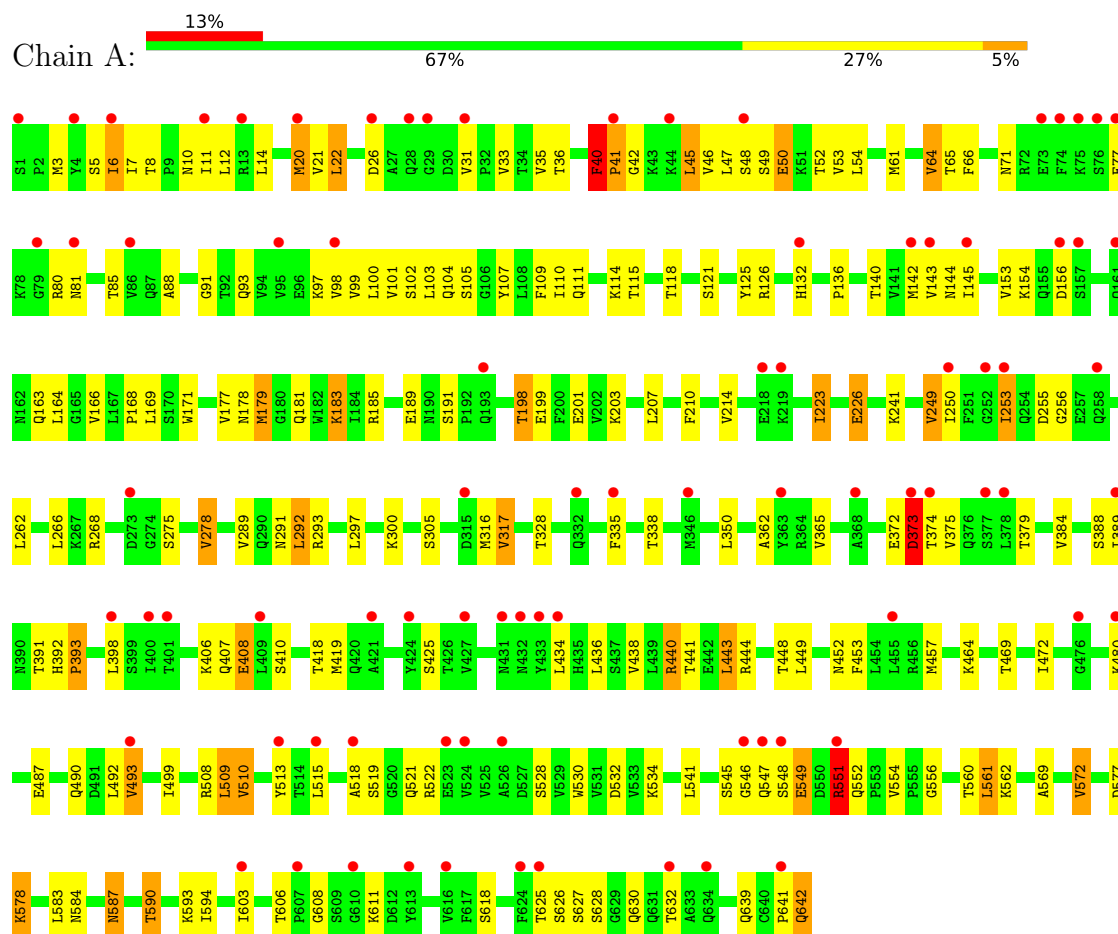
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		

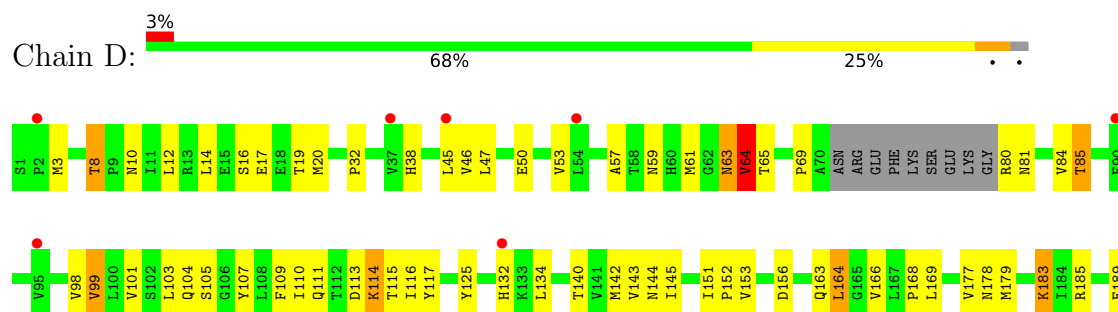
3 Residue-property plots

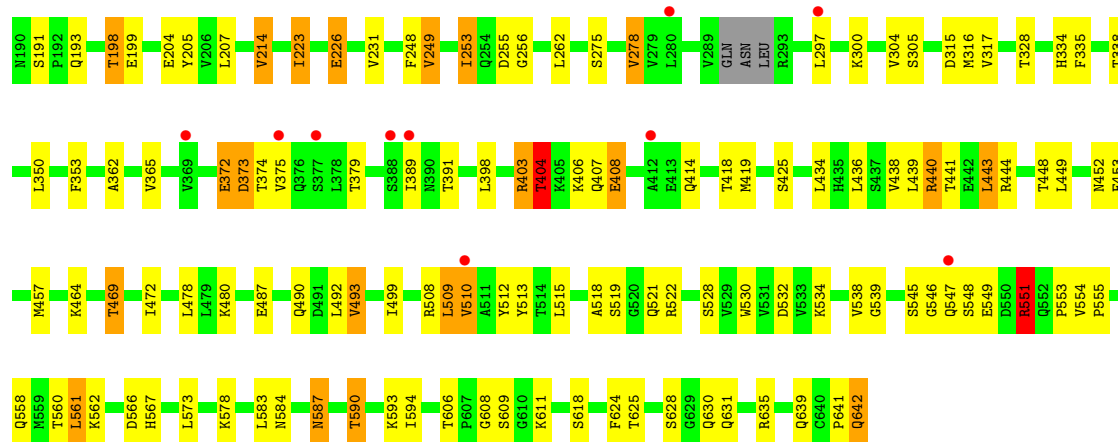
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Complement C3 beta chain

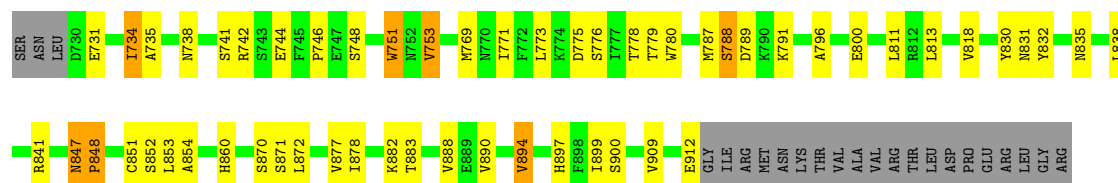


• Molecule 1: Complement C3 beta chain

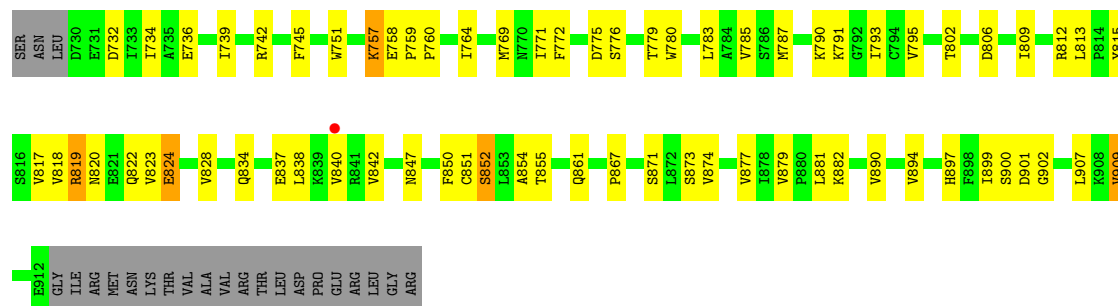




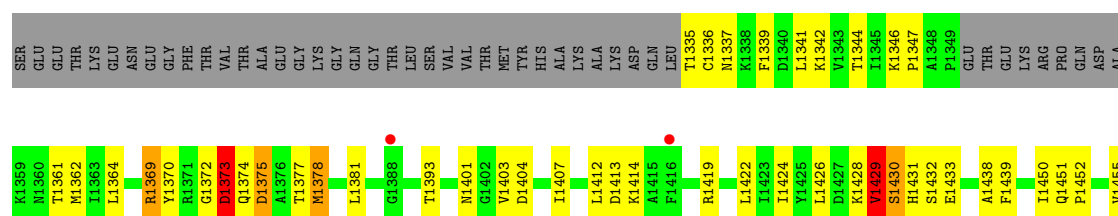
• Molecule 2: Complement C3 alpha chain

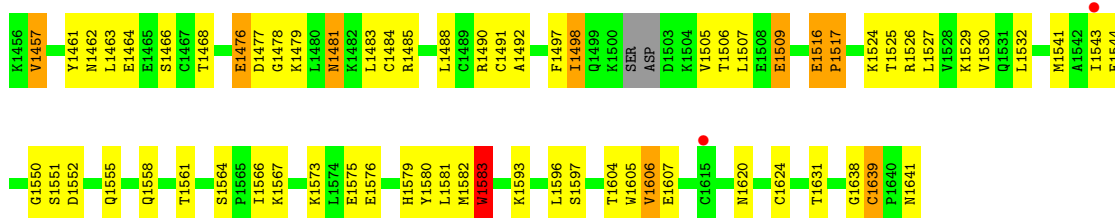


• Molecule 2: Complement C3 alpha chain

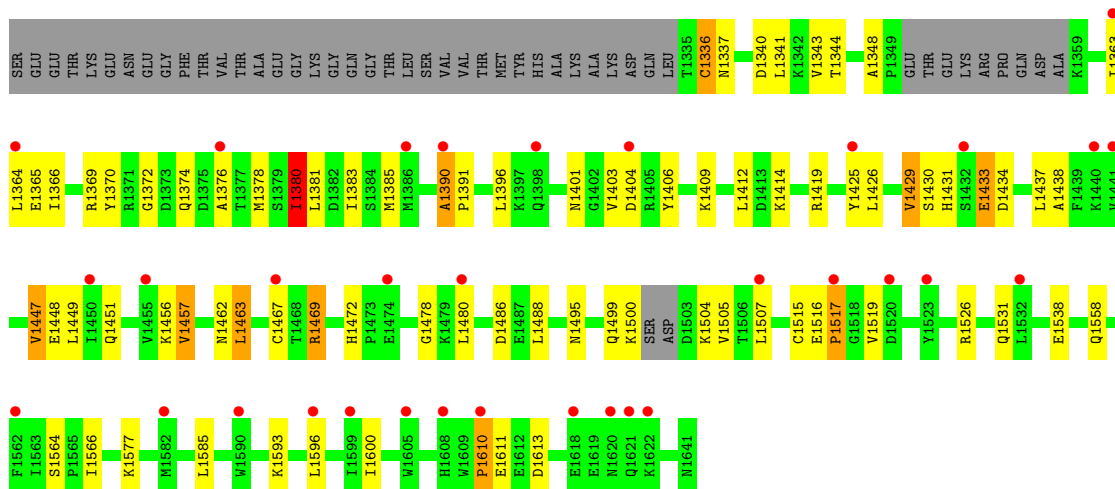


• Molecule 3: Complement C3 alpha chain

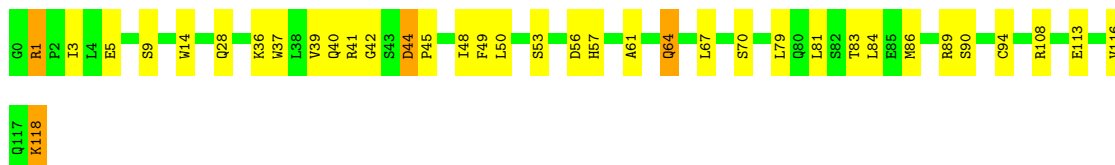




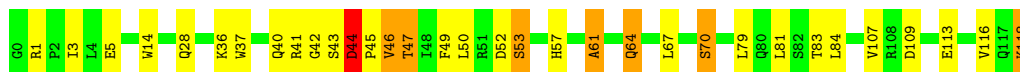
• Molecule 3: Complement C3 alpha chain



• Molecule 4: V-set and immunoglobulin domain-containing protein 4



• Molecule 4: V-set and immunoglobulin domain-containing protein 4



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	384.94Å 65.21Å 147.68Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.11	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.00-3.10) 94.9 (20.00-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.236 , 0.295 0.229 , 0.280	Depositor DCC
R_{free} test set	3112 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	19619	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: CA, NAG

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	0.69	0/5108	0.96	7/6939 (0.1%)
1	D	0.53	0/5004	0.82	4/6799 (0.1%)
2	B	0.71	0/1512	0.95	3/2055 (0.1%)
2	E	0.60	0/1512	0.87	1/2055 (0.0%)
3	C	0.63	4/2453 (0.2%)	0.88	3/3305 (0.1%)
3	F	0.53	0/2453	0.86	3/3305 (0.1%)
4	S	0.64	0/972	0.86	0/1323
4	T	0.53	0/972	1.03	6/1323 (0.5%)
All	All	0.61	4/19986 (0.0%)	0.89	27/27104 (0.1%)

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	A	0	3
1	D	0	3
2	B	0	1
3	C	0	1
4	S	0	1
4	T	0	2
All	All	0	11

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1607	GLU	CD-OE2	9.00	1.42	1.25
3	C	1620	ASN	CG-OD1	6.05	1.35	1.23
3	C	1607	GLU	CD-OE1	5.25	1.35	1.25
3	C	1430	SER	N-CA	5.16	1.49	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	PHE	CA-C-N	14.31	137.73	119.84
1	A	40	PHE	C-N-CA	14.31	137.73	119.84
4	T	47	THR	N-CA-C	-13.47	86.56	108.52
4	T	44	ASP	CA-C-N	9.70	131.97	119.84
4	T	44	ASP	C-N-CA	9.70	131.97	119.84
2	B	847	ASN	CA-C-N	8.19	130.08	119.84
2	B	847	ASN	C-N-CA	8.19	130.08	119.84
1	A	48	SER	N-CA-C	-7.18	104.55	113.38
4	T	46	VAL	N-CA-C	6.89	116.87	108.06
3	F	1390	ALA	CA-C-N	6.83	126.86	119.89
3	F	1390	ALA	C-N-CA	6.83	126.86	119.89
1	A	45	LEU	N-CA-C	6.58	119.00	108.41
1	A	21	VAL	N-CA-C	6.11	115.52	106.85
3	C	1430	SER	N-CA-C	5.97	113.68	108.78
3	F	1380	ILE	N-CA-C	5.81	116.49	108.12
1	A	587	ASN	N-CA-C	5.70	119.05	111.30
3	C	1373	ASP	N-CA-C	5.64	122.81	110.80
4	T	61	ALA	N-CA-C	5.43	118.70	111.75
1	A	572	VAL	N-CA-C	5.38	115.71	108.17
3	C	1430	SER	CB-CA-C	-5.35	109.36	117.07
4	T	46	VAL	CB-CA-C	-5.35	103.57	111.80
1	D	403	ARG	N-CA-C	-5.34	101.46	109.95
2	E	764	ILE	N-CA-C	5.19	115.43	108.17
1	D	404	THR	N-CA-C	5.16	121.79	110.80
1	D	256	GLY	N-CA-C	-5.14	106.48	113.37
1	D	587	ASN	N-CA-C	5.07	118.19	111.30
2	B	753	VAL	N-CA-C	5.01	115.69	108.48

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ASP	Peptide
1	A	372	GLU	Peptide
1	A	40	PHE	Peptide
2	B	751	TRP	Peptide
3	C	1373	ASP	Peptide
1	D	255	ASP	Peptide
1	D	372	GLU	Peptide
1	D	403	ARG	Peptide
4	S	44	ASP	Peptide

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Mol	Chain	Res	Type	Group
4	T	44	ASP	Peptide
4	T	46	VAL	Peptide

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	5008	0	5071	119	0
1	D	4907	0	4971	103	0
2	B	1480	0	1502	34	0
2	E	1480	0	1502	42	0
3	C	2407	0	2321	72	0
3	F	2407	0	2321	44	0
4	S	950	0	935	21	0
4	T	950	0	935	13	0
5	G	28	0	25	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
All	All	19619	0	19583	406	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 10.

All (406) 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)
3:C:1370:TYR:O	3:C:1431:HIS:HB2	1.54	1.06
1:A:365:VAL:H	1:A:379:THR:HG22	1.22	1.02
1:D:365:VAL:H	1:D:379:THR:HG22	1.24	1.01
3:C:1516:GLU:HB3	3:C:1517:PRO:CD	1.98	0.93
4:S:44:ASP:HB2	4:S:45:PRO:HD3	1.51	0.91
1:A:268:ARG:HB2	3:C:1378:MET:HE3	1.55	0.89
3:C:1369:ARG:NH2	3:C:1430:SER:HB3	1.88	0.88
1:A:6:ILE:HD12	1:A:7:ILE:N	1.89	0.87
3:C:1516:GLU:HB3	3:C:1517:PRO:HD2	1.55	0.85
3:C:1516:GLU:CB	3:C:1517:PRO:HD2	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HD22	1:A:33:VAL:HG11	1.60	0.80
1:A:551:ARG:HA	1:A:551:ARG:NH1	1.98	0.78
3:F:1457:VAL:HG23	3:F:1467:CYS:HB2	1.67	0.77
1:D:551:ARG:NH1	1:D:551:ARG:HA	2.00	0.77
3:C:1516:GLU:CB	3:C:1517:PRO:CD	2.63	0.76
3:F:1341:LEU:HB3	3:F:1469:ARG:HD3	1.66	0.75
1:D:561:LEU:HD22	2:E:771:ILE:HD13	1.68	0.74
1:A:40:PHE:CD2	1:A:41:PRO:HD2	2.23	0.74
1:A:590:THR:HG22	1:A:593:LYS:H	1.53	0.73
3:F:1414:LYS:HD3	3:F:1419:ARG:HD3	1.70	0.73
3:C:1403:VAL:O	3:C:1404:ASP:HB2	1.89	0.71
3:C:1370:TYR:N	3:C:1430:SER:O	2.16	0.71
1:D:10:ASN:HB3	1:D:635:ARG:HD3	1.72	0.70
2:B:734:ILE:HD12	2:B:900:SER:HB3	1.73	0.70
1:D:248:PHE:HZ	3:F:1380:ILE:HD11	1.58	0.69
4:S:61:ALA:HA	4:S:64:GLN:HE21	1.58	0.69
3:C:1369:ARG:NH1	3:C:1430:SER:H	1.91	0.68
3:C:1555:GLN:H	3:C:1558:GLN:HE21	1.39	0.68
1:A:606:THR:HG22	1:A:608:GLY:H	1.58	0.68
1:A:628:SER:HB2	1:A:630:GLN:OE1	1.94	0.68
1:A:268:ARG:HB2	3:C:1378:MET:CE	2.24	0.67
1:A:253:ILE:HD11	1:A:262:LEU:HD21	1.76	0.67
1:D:249:VAL:CG2	1:D:278:VAL:HG21	2.25	0.67
1:D:163:GLN:HG3	1:D:166:VAL:O	1.95	0.66
1:A:549:GLU:HG3	4:S:56:ASP:O	1.95	0.66
1:D:249:VAL:HG21	1:D:278:VAL:HG21	1.78	0.66
1:A:487:GLU:H	1:A:490:GLN:HE21	1.44	0.66
1:A:249:VAL:HG21	1:A:278:VAL:HG21	1.78	0.66
1:A:407:GLN:O	1:A:408:GLU:HB2	1.96	0.66
3:C:1375:ASP:CG	3:C:1430:SER:HB2	2.21	0.66
1:A:6:ILE:HD12	1:A:7:ILE:H	1.60	0.65
1:A:556:GLY:HA2	2:B:773:LEU:O	1.97	0.65
4:T:61:ALA:HA	4:T:64:GLN:HE21	1.60	0.65
1:A:487:GLU:H	1:A:490:GLN:NE2	1.95	0.65
3:C:1369:ARG:HG2	3:C:1430:SER:C	2.21	0.64
1:A:40:PHE:CD2	1:A:41:PRO:CD	2.80	0.64
1:A:249:VAL:CG2	1:A:278:VAL:HG21	2.28	0.64
2:B:851:CYS:HG	3:C:1491:CYS:HG	1.43	0.64
2:E:824:GLU:HB2	2:E:877:VAL:HG12	1.80	0.64
1:D:641:PRO:O	1:D:642:GLN:HB2	1.98	0.64
1:D:628:SER:HB2	1:D:630:GLN:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:842:VAL:HG11	2:E:874:VAL:HG21	1.81	0.63
1:D:590:THR:HG22	1:D:593:LYS:H	1.64	0.62
3:C:1369:ARG:HB3	3:C:1431:HIS:HA	1.81	0.62
2:E:847:ASN:HB3	2:E:850:PHE:HB2	1.81	0.62
1:D:407:GLN:O	1:D:408:GLU:HB2	1.99	0.62
1:A:31:VAL:HG13	1:A:54:LEU:HB2	1.81	0.62
1:D:573:LEU:HD13	2:E:769:MET:HE1	1.82	0.62
2:B:882:LYS:O	2:B:909:VAL:HG11	2.00	0.61
1:D:115:THR:HB	1:D:584:ASN:OD1	2.01	0.60
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.84	0.60
1:A:642:GLN:OE1	1:A:642:GLN:HA	2.02	0.60
3:C:1525:THR:OG1	3:C:1541:MET:HE2	2.02	0.60
3:C:1582:MET:HA	3:C:1605:TRP:O	2.02	0.60
1:A:546:GLY:CA	1:A:562:LYS:HB2	2.31	0.60
4:S:67:LEU:HG	4:S:79:LEU:HD11	1.84	0.60
1:D:606:THR:HG22	1:D:608:GLY:H	1.67	0.60
3:C:1369:ARG:HG3	3:C:1429:VAL:HG23	1.83	0.59
2:E:877:VAL:HG23	3:F:1480:LEU:HD11	1.84	0.59
3:F:1343:VAL:HG12	3:F:1366:ILE:HG12	1.85	0.59
3:F:1369:ARG:HB3	3:F:1430:SER:O	2.03	0.59
3:C:1462:ASN:C	3:C:1462:ASN:HD22	2.11	0.59
3:F:1593:LYS:HE2	3:F:1596:LEU:HD11	1.83	0.59
3:C:1369:ARG:CZ	3:C:1430:SER:HB3	2.33	0.59
2:E:897:HIS:HB3	2:E:899:ILE:HG12	1.84	0.59
1:A:530:TRP:CH2	1:A:532:ASP:HB2	2.38	0.58
4:T:67:LEU:HG	4:T:79:LEU:HD11	1.84	0.58
1:A:641:PRO:O	1:A:642:GLN:HB2	2.03	0.58
4:S:1:ARG:HH11	4:S:108:ARG:HH21	1.50	0.58
1:D:546:GLY:CA	1:D:562:LYS:HB2	2.33	0.58
3:C:1525:THR:O	3:C:1579:HIS:HA	2.04	0.58
1:A:163:GLN:HG3	1:A:166:VAL:O	2.03	0.58
1:D:487:GLU:H	1:D:490:GLN:NE2	2.02	0.58
1:A:47:LEU:HD22	1:A:66:PHE:HB2	1.85	0.57
1:A:457:MET:HE3	1:A:513:TYR:CE1	2.40	0.57
4:T:44:ASP:HB2	4:T:45:PRO:HD3	1.86	0.57
1:D:253:ILE:HD11	1:D:262:LEU:HD21	1.85	0.57
4:T:84:LEU:HD23	4:T:116:VAL:HG22	1.87	0.57
1:A:40:PHE:CG	1:A:41:PRO:CD	2.88	0.57
3:C:1336:CYS:HB3	3:C:1339:PHE:O	2.05	0.57
1:D:487:GLU:H	1:D:490:GLN:HE21	1.53	0.57
3:F:1611:GLU:HG3	3:F:1613:ASP:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:PHE:CZ	3:F:1380:ILE:HD11	2.40	0.57
1:A:316:MET:HE2	3:C:1463:LEU:HB2	1.87	0.57
2:E:840:VAL:HG22	2:E:894:VAL:HG12	1.87	0.57
3:F:1344:THR:HB	3:F:1365:GLU:HB3	1.87	0.57
3:C:1369:ARG:HG2	3:C:1430:SER:O	2.05	0.56
1:A:183:LYS:HG2	1:A:185:ARG:NH1	2.20	0.56
1:A:472:ILE:HG12	1:A:509:LEU:HD22	1.88	0.56
1:A:547:GLN:HG3	1:A:560:THR:HB	1.86	0.56
4:S:37:TRP:HB2	4:S:49:PHE:HB3	1.88	0.56
1:D:472:ILE:HD12	1:D:480:LYS:HB3	1.87	0.56
1:A:93:GLN:HE21	1:A:627:SER:HB2	1.72	0.55
4:T:37:TRP:HB2	4:T:49:PHE:HB3	1.87	0.55
3:C:1381:LEU:HD12	3:C:1426:LEU:HD21	1.88	0.55
1:D:547:GLN:HG3	1:D:560:THR:HB	1.87	0.55
4:S:84:LEU:HD23	4:S:116:VAL:HG22	1.88	0.55
4:T:40:GLN:OE1	4:T:44:ASP:HA	2.07	0.55
1:A:578:LYS:HE3	2:B:800:GLU:OE2	2.06	0.55
2:B:860:HIS:HE1	3:C:1451:GLN:HE22	1.54	0.54
3:C:1516:GLU:HB2	3:C:1517:PRO:HD2	1.87	0.54
1:A:472:ILE:HD12	1:A:480:LYS:HB3	1.89	0.54
2:B:860:HIS:CE1	3:C:1451:GLN:NE2	2.75	0.54
3:C:1347:PRO:HA	3:C:1362:MET:HG2	1.90	0.54
4:S:40:GLN:OE1	4:S:44:ASP:HA	2.08	0.54
2:B:860:HIS:HE1	3:C:1451:GLN:NE2	2.05	0.54
3:C:1377:THR:O	3:C:1378:MET:C	2.51	0.54
3:C:1582:MET:HE3	3:C:1606:VAL:HG23	1.90	0.54
1:A:183:LYS:HG2	1:A:185:ARG:HH12	1.72	0.54
3:F:1488:LEU:HD23	3:F:1488:LEU:H	1.74	0.53
1:A:11:ILE:HD12	1:A:603:ILE:HG22	1.90	0.53
1:A:110:ILE:HB	1:A:198:THR:OG1	2.09	0.53
1:A:115:THR:HB	1:A:584:ASN:OD1	2.09	0.53
1:A:551:ARG:HA	1:A:551:ARG:CZ	2.38	0.53
2:E:819:ARG:HG3	2:E:820:ASN:CG	2.33	0.53
1:D:316:MET:HE2	3:F:1463:LEU:HB2	1.91	0.53
3:C:1414:LYS:HB3	3:C:1419:ARG:HE	1.74	0.53
3:F:1369:ARG:HE	3:F:1430:SER:H	1.57	0.53
1:A:362:ALA:O	1:A:379:THR:HG21	2.09	0.53
1:D:362:ALA:O	1:D:379:THR:HG21	2.09	0.53
3:C:1481:ASN:OD1	3:C:1567:LYS:HG2	2.09	0.52
2:E:817:VAL:HG23	2:E:909:VAL:HG13	1.90	0.52
3:F:1526:ARG:HH21	3:F:1577:LYS:HG2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1498:ILE:HD12	3:C:1605:TRP:HB2	1.91	0.52
1:A:291:ASN:O	1:A:293:ARG:N	2.33	0.52
2:B:744:GLU:C	2:B:746:PRO:HD3	2.34	0.52
1:D:642:GLN:OE1	1:D:642:GLN:HA	2.08	0.52
1:A:22:LEU:HD13	1:A:52:THR:HG21	1.92	0.52
1:A:551:ARG:HA	1:A:551:ARG:HH11	1.74	0.52
1:D:551:ARG:HA	1:D:551:ARG:CZ	2.39	0.52
1:D:567:HIS:CG	2:E:760:PRO:HG3	2.45	0.52
4:S:1:ARG:HH11	4:S:108:ARG:NH2	2.08	0.52
1:D:19:THR:HB	1:D:478:LEU:HB2	1.92	0.52
1:A:168:PRO:O	1:A:169:LEU:HD23	2.10	0.52
1:D:338:THR:HG21	1:D:350:LEU:HD23	1.92	0.52
1:D:434:LEU:HB2	1:D:513:TYR:HE2	1.75	0.52
1:D:472:ILE:HG12	1:D:509:LEU:HD22	1.92	0.52
1:D:546:GLY:HA2	1:D:562:LYS:HB2	1.91	0.52
1:A:407:GLN:O	1:A:408:GLU:CB	2.58	0.52
1:D:113:ASP:HB3	2:E:751:TRP:CZ3	2.45	0.52
1:D:551:ARG:HA	1:D:551:ARG:HH11	1.75	0.51
1:A:519:SER:C	1:A:521:GLN:H	2.19	0.51
1:A:546:GLY:HA2	1:A:562:LYS:HB2	1.92	0.51
2:B:735:ALA:HB3	2:B:738:ASN:HD22	1.75	0.51
3:C:1583:TRP:HB2	3:C:1605:TRP:H	1.76	0.51
2:B:831:ASN:ND2	2:B:838:LEU:HG	2.26	0.51
1:A:241:LYS:HG3	2:B:832:TYR:CE2	2.46	0.51
3:C:1375:ASP:OD1	3:C:1375:ASP:N	2.44	0.51
2:B:877:VAL:HG21	3:C:1452:PRO:HG2	1.93	0.51
1:A:210:PHE:CZ	1:A:317:VAL:HG13	2.46	0.50
1:A:249:VAL:HG21	1:A:278:VAL:HG11	1.93	0.50
1:A:440:ARG:HA	1:A:440:ARG:HE	1.76	0.50
1:D:510:VAL:HG13	1:D:528:SER:HB3	1.93	0.50
1:D:223:ILE:HD11	1:D:328:THR:HG22	1.94	0.50
3:C:1476:GLU:C	3:C:1478:GLY:H	2.19	0.50
3:F:1391:PRO:HB2	3:F:1396:LEU:HD11	1.93	0.50
1:D:453:PHE:HB2	1:D:493:VAL:HG23	1.94	0.50
1:D:555:PRO:HB3	2:E:775:ASP:HA	1.93	0.50
3:C:1407:ILE:HD11	3:C:1424:ILE:HG12	1.93	0.50
1:D:16:SER:HB3	1:D:132:HIS:HE1	1.77	0.50
1:D:63:ASN:O	1:D:64:VAL:HG22	2.12	0.50
1:D:519:SER:C	1:D:521:GLN:H	2.19	0.50
3:C:1457:VAL:O	3:C:1466:SER:HB2	2.12	0.49
1:D:335:PHE:CD2	1:D:419:MET:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:MET:HE3	1:D:513:TYR:CE1	2.46	0.49
1:D:143:VAL:C	1:D:144:ASN:HD22	2.20	0.49
3:C:1403:VAL:O	3:C:1404:ASP:CB	2.60	0.49
3:C:1497:PHE:O	3:C:1498:ILE:C	2.56	0.49
1:D:8:THR:HG23	1:D:20:MET:SD	2.53	0.49
1:D:444:ARG:HD3	4:T:107:VAL:HB	1.93	0.49
2:E:894:VAL:CG2	2:E:897:HIS:HB2	2.42	0.49
3:C:1581:LEU:HG	3:C:1583:TRP:HZ3	1.77	0.49
1:D:558:GLN:HG3	2:E:772:PHE:CD1	2.48	0.49
1:D:12:LEU:HG	1:D:99:VAL:HG11	1.94	0.49
1:D:391:THR:HG22	1:D:398:LEU:HD11	1.95	0.49
1:D:407:GLN:O	1:D:408:GLU:CB	2.61	0.49
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.94	0.49
3:C:1638:GLY:O	3:C:1639:CYS:C	2.55	0.48
4:S:14:TRP:CD1	4:S:86:MET:HE2	2.49	0.48
1:A:546:GLY:HA3	1:A:562:LYS:HB2	1.95	0.48
1:D:249:VAL:HG21	1:D:278:VAL:HG11	1.94	0.48
4:T:61:ALA:HA	4:T:64:GLN:NE2	2.27	0.48
1:A:457:MET:HE3	1:A:513:TYR:HE1	1.79	0.48
2:E:894:VAL:HG21	2:E:897:HIS:HB2	1.96	0.48
3:F:1456:LYS:HA	3:F:1467:CYS:O	2.13	0.48
3:C:1476:GLU:O	3:C:1477:ASP:HB2	2.13	0.48
1:D:84:VAL:HG22	1:D:101:VAL:HG22	1.95	0.48
1:A:338:THR:HG21	1:A:350:LEU:HD23	1.95	0.48
1:D:297:LEU:HA	1:D:300:LYS:HD2	1.95	0.48
1:D:538:VAL:HG12	2:E:791:LYS:HD3	1.94	0.48
4:S:89:ARG:O	4:S:90:SER:HB2	2.13	0.48
1:A:143:VAL:C	1:A:144:ASN:HD22	2.22	0.48
2:E:809:ILE:HD13	2:E:890:VAL:HG23	1.95	0.48
1:D:624:PHE:O	1:D:631:GLN:HA	2.14	0.47
2:E:837:GLU:HB3	2:E:867:PRO:HA	1.97	0.47
1:A:100:LEU:HD12	1:A:101:VAL:H	1.79	0.47
1:A:20:MET:HE1	1:A:88:ALA:HB2	1.96	0.47
1:A:335:PHE:CD2	1:A:419:MET:HB3	2.49	0.47
2:B:894:VAL:CG2	2:B:897:HIS:HB2	2.44	0.47
4:S:50:LEU:HB3	4:S:57:HIS:HB2	1.96	0.47
1:D:140:THR:HG22	1:D:189:GLU:HB2	1.95	0.47
1:A:20:MET:HE2	1:A:35:VAL:HG21	1.97	0.47
1:A:561:LEU:HD22	2:B:771:ILE:HD13	1.95	0.47
1:D:183:LYS:HG3	1:D:199:GLU:HG2	1.97	0.47
1:A:11:ILE:HD12	1:A:603:ILE:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ARG:NH2	1:A:534:LYS:HE2	2.28	0.47
3:C:1462:ASN:HD22	3:C:1463:LEU:N	2.12	0.47
4:S:14:TRP:CE3	4:S:118:LYS:HG3	2.49	0.47
3:C:1516:GLU:HB3	3:C:1517:PRO:HD3	1.89	0.47
1:A:453:PHE:HB2	1:A:493:VAL:HG23	1.97	0.47
3:C:1530:VAL:HG12	3:C:1532:LEU:HD12	1.96	0.47
3:F:1370:TYR:HB2	3:F:1429:VAL:O	2.14	0.47
3:F:1472:HIS:H	3:F:1478:GLY:H	1.62	0.47
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.50	0.47
3:C:1369:ARG:HD3	3:C:1433:GLU:O	2.14	0.47
1:D:110:ILE:HB	1:D:198:THR:OG1	2.15	0.47
2:E:851:CYS:HB3	2:E:879:VAL:HB	1.96	0.47
1:A:6:ILE:HG12	1:A:20:MET:CE	2.45	0.47
3:F:1429:VAL:O	3:F:1429:VAL:HG13	2.15	0.47
3:C:1431:HIS:O	3:C:1432:SER:C	2.58	0.47
1:D:443:LEU:CD2	1:D:499:ILE:HG13	2.44	0.47
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.97	0.46
1:D:530:TRP:CH2	1:D:532:ASP:HB2	2.51	0.46
2:E:742:ARG:HB3	2:E:775:ASP:HB3	1.96	0.46
1:A:391:THR:HG22	1:A:398:LEU:HD11	1.98	0.46
1:A:22:LEU:HD11	1:A:64:VAL:HB	1.98	0.46
1:A:154:LYS:HD2	1:A:171:TRP:CD1	2.50	0.46
1:D:111:GLN:O	1:D:125:TYR:HA	2.16	0.46
3:F:1531:GLN:HB2	3:F:1538:GLU:HB2	1.98	0.46
1:D:249:VAL:HA	1:D:305:SER:O	2.15	0.46
3:F:1364:LEU:O	3:F:1438:ALA:HA	2.16	0.46
3:F:1406:TYR:HD2	3:F:1425:TYR:CD1	2.34	0.46
3:F:1457:VAL:CG2	3:F:1467:CYS:HB2	2.43	0.46
1:A:226:GLU:H	1:A:226:GLU:HG3	1.45	0.46
1:A:47:LEU:CD2	1:A:66:PHE:HB2	2.46	0.46
1:A:97:LYS:NZ	1:A:632:THR:O	2.45	0.46
1:A:181:GLN:HE22	1:A:201:GLU:HG3	1.80	0.46
1:D:164:LEU:O	2:E:787:MET:HG2	2.16	0.46
1:D:443:LEU:HD21	1:D:499:ILE:HG13	1.98	0.46
3:F:1406:TYR:HD2	3:F:1425:TYR:HD1	1.64	0.46
3:C:1526:ARG:NH1	3:C:1544:GLU:OE2	2.49	0.46
2:E:882:LYS:O	2:E:909:VAL:HB	2.16	0.46
3:F:1369:ARG:HA	3:F:1429:VAL:HG23	1.96	0.46
1:A:6:ILE:HD12	1:A:6:ILE:C	2.38	0.45
1:A:541:LEU:HD23	2:B:796:ALA:HB2	1.98	0.45
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:830:TYR:CD1	2:B:871:SER:HB3	2.51	0.45
3:C:1364:LEU:O	3:C:1438:ALA:HA	2.16	0.45
2:E:838:LEU:HD13	2:E:894:VAL:HG11	1.98	0.45
1:D:3:MET:HB2	1:D:522:ARG:NH2	2.32	0.45
1:D:168:PRO:O	1:D:169:LEU:HD23	2.16	0.45
4:T:50:LEU:HB3	4:T:57:HIS:HB2	1.98	0.45
2:E:759:PRO:HA	2:E:760:PRO:HD3	1.72	0.45
3:F:1369:ARG:HD2	3:F:1434:ASP:HA	1.98	0.45
1:A:50:GLU:HB3	1:A:64:VAL:HG22	1.99	0.45
1:D:231:VAL:HG21	1:D:304:VAL:HG21	1.99	0.45
3:F:1564:SER:HB3	3:F:1600:ILE:HD12	1.98	0.45
1:A:249:VAL:HA	1:A:305:SER:O	2.17	0.45
2:B:734:ILE:H	2:B:734:ILE:HG13	1.57	0.45
3:C:1639:CYS:C	3:C:1641:ASN:H	2.24	0.45
4:S:61:ALA:HA	4:S:64:GLN:NE2	2.30	0.45
2:B:811:LEU:HG	2:B:813:LEU:CD1	2.47	0.45
1:A:569:ALA:HB2	2:B:788:SER:HB2	1.98	0.44
4:S:44:ASP:HB2	4:S:45:PRO:CD	2.35	0.44
1:D:315:ASP:CG	2:E:812:ARG:HH21	2.25	0.44
1:A:3:MET:HE3	1:A:522:ARG:HG2	1.98	0.44
2:B:831:ASN:OD1	2:B:831:ASN:C	2.60	0.44
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.99	0.44
1:D:457:MET:HE3	1:D:513:TYR:HE1	1.82	0.44
3:F:1403:VAL:O	3:F:1404:ASP:HB2	2.17	0.44
3:C:1455:VAL:O	3:C:1468:THR:HA	2.18	0.44
3:C:1462:ASN:HD21	3:C:1464:GLU:HB2	1.81	0.44
1:D:183:LYS:HB3	1:D:185:ARG:HH11	1.82	0.44
1:A:223:ILE:HD11	1:A:328:THR:HG22	1.99	0.44
3:C:1550:GLY:C	3:C:1552:ASP:H	2.26	0.44
1:D:134:LEU:HB3	2:E:793:ILE:HG22	1.99	0.44
1:D:248:PHE:HE1	3:F:1378:MET:HG2	1.82	0.44
1:D:334:HIS:HB2	1:D:353:PHE:HB3	2.00	0.44
1:D:436:LEU:HA	1:D:452:ASN:O	2.18	0.44
3:C:1428:LYS:C	3:C:1429:VAL:HG12	2.43	0.44
1:D:19:THR:HA	1:D:65:THR:HG22	2.00	0.44
1:D:226:GLU:H	1:D:226:GLU:HG3	1.51	0.44
1:D:561:LEU:CD2	2:E:771:ILE:HD13	2.43	0.44
4:S:39:VAL:HG12	4:S:48:ILE:HG23	2.00	0.44
1:D:10:ASN:HB3	1:D:635:ARG:CD	2.45	0.44
1:D:248:PHE:CE1	3:F:1378:MET:HG2	2.53	0.44
4:T:52:ASP:O	4:T:53:SER:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:CA	1:A:50:GLU:OE1	2.66	0.43
1:D:553:PRO:HD2	2:E:802:THR:O	2.18	0.43
1:A:472:ILE:HA	1:A:508:ARG:O	2.18	0.43
3:C:1509:GLU:H	3:C:1509:GLU:HG2	1.61	0.43
3:C:1525:THR:HB	3:C:1541:MET:HE3	2.00	0.43
1:D:472:ILE:HA	1:D:508:ARG:O	2.18	0.43
2:E:813:LEU:HD23	2:E:907:LEU:HB3	2.00	0.43
2:E:901:ASP:CG	2:E:902:GLY:H	2.24	0.43
3:F:1348:ALA:HB2	3:F:1363:ILE:HG12	1.99	0.43
1:D:443:LEU:HD11	1:D:449:LEU:HD22	2.00	0.43
3:F:1516:GLU:HB3	3:F:1517:PRO:HD2	2.01	0.43
1:A:3:MET:HE2	1:A:626:SER:OG	2.19	0.43
1:A:80:ARG:HD3	1:A:80:ARG:HA	1.82	0.43
1:D:546:GLY:HA3	1:D:562:LYS:HB2	1.99	0.43
4:S:37:TRP:CH2	4:S:94:CYS:HB2	2.54	0.43
1:D:440:ARG:HE	1:D:440:ARG:HA	1.84	0.43
2:E:785:VAL:HG22	2:E:795:VAL:HG22	1.99	0.43
3:F:1406:TYR:HB3	3:F:1425:TYR:HB2	2.00	0.43
4:T:36:LYS:HG3	4:T:50:LEU:CD1	2.49	0.43
1:A:12:LEU:HG	1:A:99:VAL:CG1	2.49	0.43
1:A:163:GLN:HA	1:A:163:GLN:NE2	2.33	0.43
1:D:404:THR:HG22	1:D:414:GLN:OE1	2.19	0.43
1:A:20:MET:HE2	1:A:35:VAL:CG2	2.49	0.42
1:A:384:VAL:HB	1:A:440:ARG:NH1	2.34	0.42
1:A:510:VAL:HG13	1:A:528:SER:HB3	1.99	0.42
3:C:1369:ARG:HD3	3:C:1433:GLU:C	2.43	0.42
1:D:114:LYS:HB2	1:D:117:TYR:CZ	2.54	0.42
2:E:852:SER:C	2:E:854:ALA:H	2.27	0.42
1:A:40:PHE:CD2	1:A:41:PRO:HD3	2.54	0.42
3:C:1341:LEU:HD21	3:C:1455:VAL:HG12	2.01	0.42
3:C:1527:LEU:HD23	3:C:1575:GLU:C	2.45	0.42
1:D:80:ARG:O	1:D:81:ASN:HB2	2.20	0.42
1:D:116:ILE:HG12	1:D:205:TYR:CE2	2.54	0.42
2:E:734:ILE:HD12	2:E:900:SER:HB3	2.00	0.42
3:F:1409:LYS:HA	3:F:1412:LEU:HD13	2.01	0.42
1:A:111:GLN:O	1:A:125:TYR:HA	2.19	0.42
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.49	0.42
1:A:183:LYS:HB3	1:A:185:ARG:HH11	1.84	0.42
1:A:443:LEU:CD2	1:A:499:ILE:HG13	2.49	0.42
3:C:1430:SER:OG	3:C:1431:HIS:N	2.52	0.42
1:A:183:LYS:HG3	1:A:199:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:1:ARG:CZ	4:S:1:ARG:H	2.32	0.42
1:D:109:PHE:CZ	1:D:594:ILE:HG23	2.55	0.42
1:A:20:MET:HB3	1:A:66:PHE:HE2	1.84	0.42
1:A:40:PHE:CE2	1:A:41:PRO:HD3	2.55	0.42
3:C:1530:VAL:HG23	3:C:1576:GLU:HG2	2.02	0.42
4:S:36:LYS:HG3	4:S:50:LEU:CD1	2.49	0.42
3:F:1390:ALA:HA	3:F:1391:PRO:HD3	1.81	0.42
1:A:140:THR:HG22	1:A:189:GLU:HB2	2.02	0.42
1:A:210:PHE:CZ	1:A:317:VAL:CG1	3.02	0.42
3:C:1481:ASN:O	3:C:1492:ALA:HB3	2.20	0.42
1:D:558:GLN:HG3	2:E:772:PHE:CE1	2.55	0.42
2:B:813:LEU:HD21	2:B:888:VAL:HB	2.02	0.41
3:C:1461:TYR:CD1	3:C:1461:TYR:C	2.98	0.41
1:D:193:GLN:CD	1:D:193:GLN:H	2.28	0.41
1:D:214:VAL:HG23	1:D:214:VAL:O	2.20	0.41
3:F:1610:PRO:HB2	3:F:1611:GLU:H	1.69	0.41
1:D:85:THR:HG23	1:D:98:VAL:HG13	2.02	0.41
3:F:1447:VAL:HG22	3:F:1448:GLU:H	1.85	0.41
1:A:109:PHE:CZ	1:A:594:ILE:HG23	2.54	0.41
1:A:436:LEU:HA	1:A:452:ASN:O	2.19	0.41
1:A:440:ARG:HA	1:A:440:ARG:NE	2.35	0.41
3:C:1524:LYS:HA	3:C:1580:TYR:O	2.20	0.41
2:E:757:LYS:H	2:E:757:LYS:HG3	1.77	0.41
1:A:392:HIS:HA	1:A:393:PRO:HD3	1.86	0.41
1:A:6:ILE:HG12	1:A:20:MET:SD	2.61	0.41
1:A:101:VAL:CG1	1:A:102:SER:N	2.82	0.41
1:A:107:TYR:CE2	1:A:132:HIS:HA	2.55	0.41
1:A:118:THR:O	1:A:121:SER:OG	2.37	0.41
1:A:297:LEU:HA	1:A:300:LYS:HD2	2.02	0.41
2:B:831:ASN:HD21	2:B:838:LEU:HG	1.83	0.41
1:D:107:TYR:CE2	1:D:132:HIS:HA	2.55	0.41
1:A:289:VAL:HG12	1:A:291:ASN:H	1.86	0.41
1:D:204:GLU:HG2	2:E:815:TYR:CE2	2.56	0.41
1:D:539:GLY:HA3	1:D:566:ASP:OD2	2.20	0.41
2:E:822:GLN:HA	2:E:879:VAL:HG22	2.01	0.41
1:A:14:LEU:HD23	1:A:14:LEU:HA	1.83	0.41
4:S:89:ARG:NH1	4:S:116:VAL:H	2.19	0.41
3:F:1341:LEU:HD22	3:F:1457:VAL:HG22	2.02	0.41
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.86	0.41
1:D:151:ILE:HA	1:D:152:PRO:HD2	1.91	0.41
1:D:534:LYS:NZ	4:T:109:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1433:GLU:HB3	3:F:1434:ASP:H	1.68	0.41
4:T:14:TRP:CE3	4:T:118:LYS:HG3	2.55	0.41
1:A:250:ILE:HD12	1:A:266:LEU:HB2	2.03	0.41
2:B:847:ASN:HA	2:B:848:PRO:HD2	1.69	0.41
3:C:1401:ASN:HD22	3:C:1401:ASN:HA	1.67	0.41
3:F:1381:LEU:HD12	3:F:1426:LEU:HD21	2.03	0.41
1:A:373:ASP:OD1	1:A:373:ASP:N	2.53	0.40
2:B:778:THR:OG1	2:B:779:THR:N	2.54	0.40
2:B:852:SER:O	2:B:854:ALA:N	2.54	0.40
1:D:372:GLU:HA	1:D:373:ASP:HB2	2.03	0.40
2:E:877:VAL:HG22	3:F:1451:GLN:HE21	1.86	0.40
2:E:901:ASP:OD2	2:E:902:GLY:N	2.44	0.40
2:B:775:ASP:O	2:B:776:SER:C	2.64	0.40
4:S:89:ARG:HH11	4:S:116:VAL:H	1.69	0.40
1:D:32:PRO:HA	1:D:53:VAL:HA	2.03	0.40
3:C:1372:GLY:O	3:C:1374:GLN:N	2.47	0.40
1:D:362:ALA:O	1:D:379:THR:CG2	2.69	0.40
1:D:444:ARG:NH2	1:D:534:LYS:HE2	2.37	0.40
3:F:1376:ALA:HB3	3:F:1429:VAL:O	2.22	0.40
1:A:136:PRO:HG3	2:B:787:MET:HG3	2.03	0.40
1:A:179:MET:HG3	1:A:203:LYS:HA	2.04	0.40
1:A:577:ASP:HB2	2:B:780:TRP:CZ3	2.57	0.40
1:D:469:THR:HB	1:D:512:TYR:CE2	2.57	0.40
2:E:776:SER:HB2	2:E:780:TRP:CZ2	2.56	0.40
3:C:1364:LEU:HD23	3:C:1439:PHE:CZ	2.56	0.40
2:E:736:GLU:HA	2:E:739:ILE:HD12	2.04	0.40
3:F:1365:GLU:C	3:F:1366:ILE:HG13	2.46	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	640/642 (100%)	601 (94%)	23 (4%)	16 (2%)	4	21
1	D	624/642 (97%)	581 (93%)	27 (4%)	16 (3%)	4	21
2	B	181/206 (88%)	170 (94%)	9 (5%)	2 (1%)	11	39
2	E	181/206 (88%)	160 (88%)	20 (11%)	1 (1%)	21	52
3	C	290/343 (84%)	235 (81%)	42 (14%)	13 (4%)	2	12
3	F	290/343 (84%)	244 (84%)	35 (12%)	11 (4%)	2	15
4	S	117/119 (98%)	103 (88%)	13 (11%)	1 (1%)	14	44
4	T	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	4	21
All	All	2440/2620 (93%)	2194 (90%)	183 (8%)	63 (3%)	4	21

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PRO
1	A	373	ASP
1	A	551	ARG
3	C	1373	ASP
3	C	1516	GLU
3	C	1517	PRO
1	D	59	ASN
1	D	373	ASP
1	D	404	THR
1	D	551	ARG
3	F	1337	ASN
3	F	1505	VAL
3	F	1517	PRO
1	A	42	GLY
1	A	104	GLN
1	A	256	GLY
1	A	408	GLU
1	A	545	SER
1	A	548	SER
1	A	549	GLU
2	B	853	LEU
3	C	1337	ASN
3	C	1450	ILE
3	C	1476	GLU
3	C	1481	ASN
3	C	1583	TRP
4	S	42	GLY

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Mol	Chain	Res	Type
1	D	63	ASN
1	D	64	VAL
1	D	104	GLN
1	D	408	GLU
1	D	548	SER
1	D	549	GLU
3	F	1336	CYS
3	F	1429	VAL
3	F	1449	LEU
4	T	42	GLY
1	A	292	LEU
1	A	518	ALA
2	B	848	PRO
3	C	1573	LYS
1	D	375	VAL
1	D	518	ALA
1	D	545	SER
2	E	834	GLN
3	F	1610	PRO
1	A	375	VAL
3	C	1429	VAL
3	C	1551	SER
1	D	57	ALA
1	D	69	PRO
3	F	1372	GLY
3	F	1431	HIS
3	F	1499	GLN
1	A	410	SER
1	D	50	GLU
3	F	1519	VAL
4	T	70	SER
1	A	91	GLY
4	T	43	SER
1	A	393	PRO
3	C	1498	ILE
3	C	1505	VAL

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	566/566 (100%)	489 (86%)	77 (14%)	3	16
1	D	555/566 (98%)	489 (88%)	66 (12%)	5	21
2	B	171/191 (90%)	153 (90%)	18 (10%)	6	26
2	E	171/191 (90%)	151 (88%)	20 (12%)	5	22
3	C	270/309 (87%)	233 (86%)	37 (14%)	3	15
3	F	270/309 (87%)	247 (92%)	23 (8%)	10	35
4	S	109/109 (100%)	96 (88%)	13 (12%)	5	21
4	T	109/109 (100%)	96 (88%)	13 (12%)	5	21
All	All	2221/2350 (94%)	1954 (88%)	267 (12%)	5	21

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	6	ILE
1	A	8	THR
1	A	10	ASN
1	A	20	MET
1	A	22	LEU
1	A	26	ASP
1	A	36	THR
1	A	45	LEU
1	A	46	VAL
1	A	49	SER
1	A	50	GLU
1	A	53	VAL
1	A	61	MET
1	A	64	VAL
1	A	65	THR
1	A	71	ASN
1	A	77	GLU
1	A	81	ASN
1	A	85	THR
1	A	98	VAL
1	A	103	LEU
1	A	105	SER
1	A	114	LYS

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Mol	Chain	Res	Type
1	A	142	MET
1	A	145	ILE
1	A	153	VAL
1	A	156	ASP
1	A	164	LEU
1	A	177	VAL
1	A	178	ASN
1	A	179	MET
1	A	183	LYS
1	A	191	SER
1	A	198	THR
1	A	207	LEU
1	A	214	VAL
1	A	223	ILE
1	A	226	GLU
1	A	249	VAL
1	A	253	ILE
1	A	275	SER
1	A	278	VAL
1	A	292	LEU
1	A	317	VAL
1	A	373	ASP
1	A	374	THR
1	A	388	SER
1	A	389	ILE
1	A	406	LYS
1	A	418	THR
1	A	425	SER
1	A	438	VAL
1	A	440	ARG
1	A	441	THR
1	A	443	LEU
1	A	448	THR
1	A	464	LYS
1	A	469	THR
1	A	492	LEU
1	A	493	VAL
1	A	509	LEU
1	A	510	VAL
1	A	515	LEU
1	A	551	ARG
1	A	552	GLN

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Mol	Chain	Res	Type
1	A	554	VAL
1	A	561	LEU
1	A	578	LYS
1	A	583	LEU
1	A	587	ASN
1	A	590	THR
1	A	611	LYS
1	A	618	SER
1	A	625	THR
1	A	639	GLN
1	A	642	GLN
2	B	731	GLU
2	B	734	ILE
2	B	741	SER
2	B	748	SER
2	B	769	MET
2	B	788	SER
2	B	789	ASP
2	B	791	LYS
2	B	818	VAL
2	B	835	ASN
2	B	841	ARG
2	B	870	SER
2	B	872	LEU
2	B	883	THR
2	B	890	VAL
2	B	894	VAL
2	B	899	ILE
2	B	912	GLU
3	C	1335	THR
3	C	1342	LYS
3	C	1344	THR
3	C	1346	LYS
3	C	1361	THR
3	C	1369	ARG
3	C	1375	ASP
3	C	1378	MET
3	C	1393	THR
3	C	1412	LEU
3	C	1413	ASP
3	C	1422	LEU
3	C	1429	VAL

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Mol	Chain	Res	Type
3	C	1457	VAL
3	C	1479	LYS
3	C	1483	LEU
3	C	1484	CYS
3	C	1485	ARG
3	C	1488	LEU
3	C	1490	ARG
3	C	1506	THR
3	C	1507	LEU
3	C	1509	GLU
3	C	1529	LYS
3	C	1543	ILE
3	C	1561	THR
3	C	1564	SER
3	C	1566	ILE
3	C	1583	TRP
3	C	1593	LYS
3	C	1596	LEU
3	C	1597	SER
3	C	1604	THR
3	C	1606	VAL
3	C	1624	CYS
3	C	1631	THR
3	C	1639	CYS
4	S	1	ARG
4	S	3	ILE
4	S	5	GLU
4	S	9	SER
4	S	28	GLN
4	S	41	ARG
4	S	53	SER
4	S	64	GLN
4	S	70	SER
4	S	81	LEU
4	S	83	THR
4	S	113	GLU
4	S	118	LYS
1	D	8	THR
1	D	14	LEU
1	D	17	GLU
1	D	38	HIS
1	D	45	LEU

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Mol	Chain	Res	Type
1	D	46	VAL
1	D	47	LEU
1	D	61	MET
1	D	64	VAL
1	D	85	THR
1	D	99	VAL
1	D	103	LEU
1	D	105	SER
1	D	114	LYS
1	D	142	MET
1	D	145	ILE
1	D	153	VAL
1	D	156	ASP
1	D	164	LEU
1	D	177	VAL
1	D	178	ASN
1	D	179	MET
1	D	183	LYS
1	D	191	SER
1	D	198	THR
1	D	207	LEU
1	D	214	VAL
1	D	223	ILE
1	D	226	GLU
1	D	249	VAL
1	D	253	ILE
1	D	275	SER
1	D	278	VAL
1	D	317	VAL
1	D	374	THR
1	D	389	ILE
1	D	404	THR
1	D	406	LYS
1	D	418	THR
1	D	425	SER
1	D	438	VAL
1	D	439	LEU
1	D	440	ARG
1	D	441	THR
1	D	443	LEU
1	D	448	THR
1	D	464	LYS

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Mol	Chain	Res	Type
1	D	469	THR
1	D	492	LEU
1	D	493	VAL
1	D	509	LEU
1	D	510	VAL
1	D	515	LEU
1	D	551	ARG
1	D	554	VAL
1	D	561	LEU
1	D	578	LYS
1	D	583	LEU
1	D	587	ASN
1	D	590	THR
1	D	609	SER
1	D	611	LYS
1	D	618	SER
1	D	625	THR
1	D	639	GLN
1	D	642	GLN
2	E	732	ASP
2	E	745	PHE
2	E	757	LYS
2	E	758	GLU
2	E	779	THR
2	E	783	LEU
2	E	790	LYS
2	E	806	ASP
2	E	818	VAL
2	E	819	ARG
2	E	823	VAL
2	E	824	GLU
2	E	828	VAL
2	E	852	SER
2	E	855	THR
2	E	861	GLN
2	E	871	SER
2	E	873	SER
2	E	881	LEU
2	E	909	VAL
3	F	1336	CYS
3	F	1340	ASP
3	F	1374	GLN

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Mol	Chain	Res	Type
3	F	1380	ILE
3	F	1383	ILE
3	F	1385	MET
3	F	1401	ASN
3	F	1433	GLU
3	F	1437	LEU
3	F	1447	VAL
3	F	1457	VAL
3	F	1462	ASN
3	F	1463	LEU
3	F	1469	ARG
3	F	1486	ASP
3	F	1495	ASN
3	F	1500	LYS
3	F	1504	LYS
3	F	1507	LEU
3	F	1515	CYS
3	F	1558	GLN
3	F	1566	ILE
3	F	1585	LEU
4	T	1	ARG
4	T	3	ILE
4	T	5	GLU
4	T	28	GLN
4	T	41	ARG
4	T	47	THR
4	T	53	SER
4	T	64	GLN
4	T	70	SER
4	T	81	LEU
4	T	83	THR
4	T	113	GLU
4	T	118	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	25	HIS
1	A	38	HIS
1	A	81	ASN
1	A	93	GLN

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Mol	Chain	Res	Type
1	A	144	ASN
1	A	161	GLN
1	A	163	GLN
1	A	225	ASN
1	A	420	GLN
1	A	450	ASN
1	A	484	GLN
1	A	490	GLN
2	B	738	ASN
2	B	820	ASN
2	B	860	HIS
2	B	896	HIS
2	B	897	HIS
3	C	1360	ASN
3	C	1398	GLN
3	C	1401	ASN
3	C	1451	GLN
3	C	1462	ASN
3	C	1472	HIS
3	C	1558	GLN
3	C	1595	ASN
3	C	1621	GLN
4	S	28	GLN
4	S	64	GLN
4	S	104	ASN
1	D	28	GLN
1	D	59	ASN
1	D	60	HIS
1	D	144	ASN
1	D	163	GLN
1	D	225	ASN
1	D	254	GLN
1	D	311	HIS
1	D	420	GLN
1	D	484	GLN
1	D	490	GLN
1	D	552	GLN
2	E	738	ASN
2	E	805	GLN
2	E	834	GLN
2	E	860	HIS
2	E	861	GLN

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Mol	Chain	Res	Type
3	F	1337	ASN
3	F	1451	GLN
4	T	28	GLN
4	T	40	GLN
4	T	59	GLN
4	T	64	GLN
4	T	104	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 ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	G	1	1,5	14,14,15	0.47	0	17,19,21	2.26	3 (17%)
5	NAG	G	2	5	14,14,15	0.53	0	17,19,21	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	G	1	NAG	C1-O5-C5	7.73	122.54	112.19
5	G	1	NAG	O5-C5-C4	3.16	118.53	110.83
5	G	1	NAG	C3-C4-C5	2.32	114.44	110.23

There are no chirality outliers.

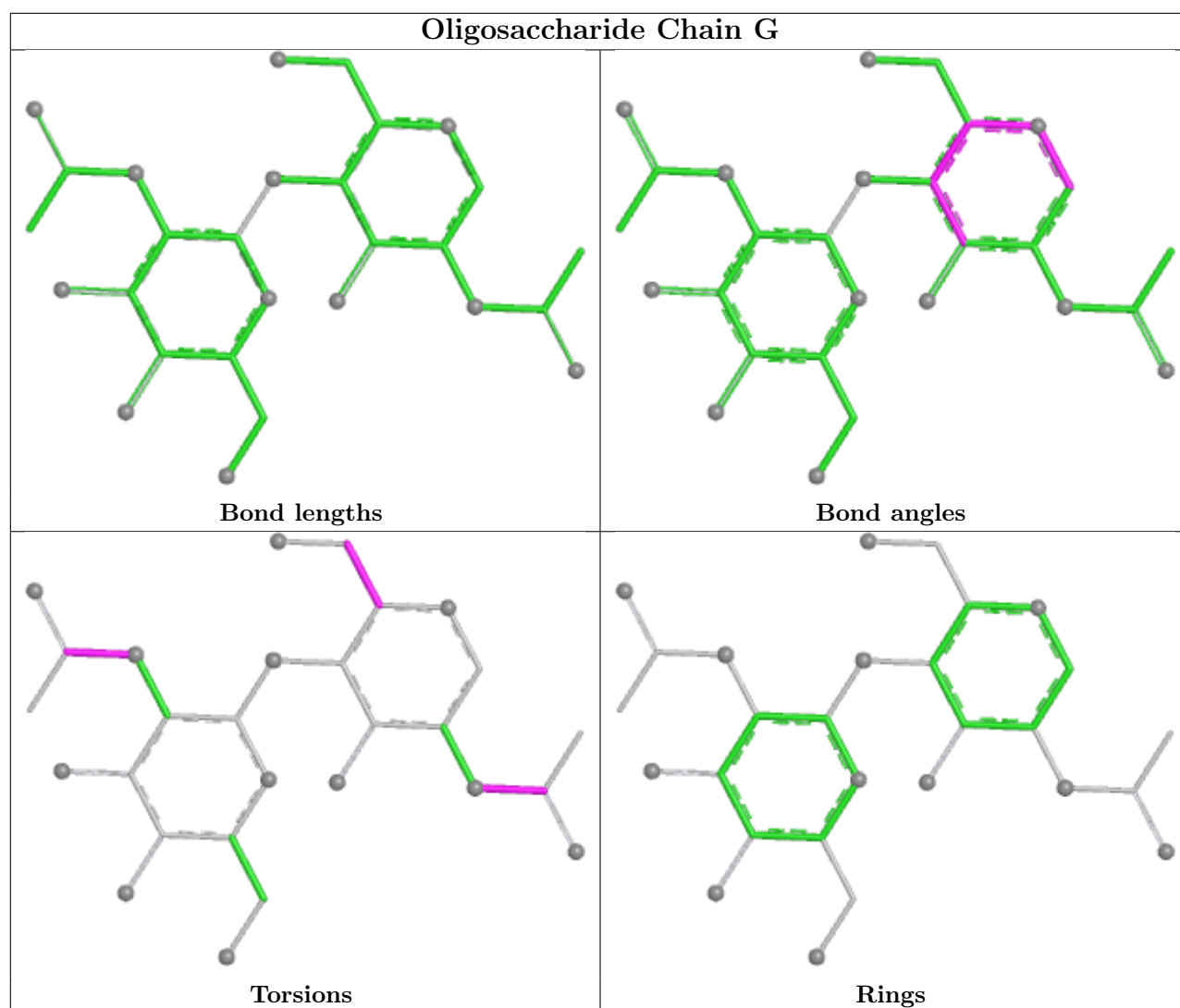
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C8-C7-N2-C2
5	G	1	NAG	C4-C5-C6-O6
5	G	2	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 ⓘ

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	642/642 (100%)	1.03	84 (13%) 7 4	17, 47, 84, 126	0
1	D	630/642 (98%)	0.48	17 (2%) 56 35	17, 50, 123, 142	0
2	B	183/206 (88%)	-0.27	0 100 100	13, 37, 64, 82	0
2	E	183/206 (88%)	0.16	1 (0%) 87 73	12, 49, 91, 95	0
3	C	296/343 (86%)	0.16	4 (1%) 73 53	19, 60, 94, 116	0
3	F	296/343 (86%)	0.98	33 (11%) 10 5	42, 133, 199, 223	0
4	S	119/119 (100%)	0.02	0 100 100	22, 46, 68, 94	0
4	T	119/119 (100%)	0.06	0 100 100	22, 46, 68, 94	0
All	All	2468/2620 (94%)	0.52	139 (5%) 30 16	12, 51, 161, 223	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	548	SER	7.3
3	F	1582	MET	6.5
1	A	76	SER	5.3
1	A	79	GLY	4.4
3	F	1532	LEU	4.0
1	A	546	GLY	3.9
1	A	48	SER	3.7
3	F	1390	ALA	3.5
1	A	524	VAL	3.5
1	A	424	TYR	3.4
3	F	1376	ALA	3.4
1	A	373	ASP	3.4
1	A	610	GLY	3.4
1	A	73	GLU	3.3
1	A	434	LEU	3.2
1	A	31	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	28	GLN	3.2
1	A	551	ARG	3.2
3	F	1622	LYS	3.1
1	A	547	GLN	3.1
1	A	77	GLU	3.1
1	A	95	VAL	3.1
1	A	75	LYS	3.0
1	D	54	LEU	3.0
1	A	258	GLN	3.0
1	A	332	GLN	3.0
1	A	493	VAL	3.0
1	A	603	ILE	2.9
1	A	433	TYR	2.9
1	D	90	PHE	2.9
3	F	1605	TRP	2.9
1	A	398	LEU	2.9
1	D	388	SER	2.8
3	F	1610	PRO	2.8
1	A	374	THR	2.8
3	F	1404	ASP	2.7
1	A	389	ILE	2.7
1	D	297	LEU	2.7
1	A	634	GLN	2.7
1	A	378	LEU	2.6
1	A	253	ILE	2.6
1	A	431	ASN	2.6
3	C	1388	GLY	2.6
1	D	547	GLN	2.6
1	A	250	ILE	2.6
3	C	1615	CYS	2.6
1	A	193	GLN	2.6
3	F	1621	GLN	2.6
1	A	156	ASP	2.5
1	D	369	VAL	2.5
1	A	526	ALA	2.5
1	A	132	HIS	2.5
1	A	632	THR	2.5
3	F	1425	TYR	2.5
1	A	6	ILE	2.5
1	A	145	ILE	2.5
1	A	315	ASP	2.5
1	A	641	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	840	VAL	2.5
1	A	1	SER	2.4
3	F	1363	ILE	2.4
3	F	1599	ILE	2.4
1	A	81	ASN	2.4
1	A	4	TYR	2.4
3	F	1441	VAL	2.4
1	A	20	MET	2.4
1	A	161	GLN	2.4
1	A	74	PHE	2.4
1	A	157	SER	2.4
1	A	346	MET	2.3
3	F	1590	TRP	2.3
1	D	2	PRO	2.3
1	D	412	ALA	2.3
1	D	280	LEU	2.3
3	C	1416	PHE	2.3
1	A	143	VAL	2.3
1	A	616	VAL	2.3
1	A	41	PRO	2.3
1	A	518	ALA	2.3
3	F	1608	HIS	2.3
1	A	44	LYS	2.3
1	A	219	LYS	2.3
1	A	11	ILE	2.3
1	D	389	ILE	2.3
3	C	1543	ILE	2.3
3	F	1507	LEU	2.3
1	A	273	ASP	2.3
1	A	427	VAL	2.3
1	D	37	VAL	2.3
3	F	1474	GLU	2.2
1	A	368	ALA	2.2
1	A	363	TYR	2.2
3	F	1432	SER	2.2
3	F	1523	TYR	2.2
1	A	98	VAL	2.2
1	D	510	VAL	2.2
1	A	607	PRO	2.2
1	A	624	PHE	2.2
1	A	401	THR	2.2
1	A	26	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	252	GLY	2.2
1	A	13	ARG	2.2
1	A	142	MET	2.2
1	D	45	LEU	2.2
3	F	1440	LYS	2.2
1	A	377	SER	2.2
1	D	377	SER	2.2
3	F	1450	ILE	2.2
1	A	476	GLY	2.1
1	A	335	PHE	2.1
3	F	1520	ASP	2.1
1	D	132	HIS	2.1
1	A	409	LEU	2.1
1	A	421	ALA	2.1
1	A	218	GLU	2.1
3	F	1517	PRO	2.1
1	A	86	VAL	2.1
1	A	480	LYS	2.1
1	A	513	TYR	2.1
1	A	625	THR	2.1
3	F	1386	MET	2.1
1	A	29	GLY	2.1
3	F	1455	VAL	2.1
1	A	432	ASN	2.1
1	A	515	LEU	2.1
3	F	1467	CYS	2.1
1	A	455	LEU	2.0
1	A	613	TYR	2.0
3	F	1398	GLN	2.0
3	F	1562	PHE	2.0
1	A	523	GLU	2.0
1	A	400	ILE	2.0
3	F	1620	ASN	2.0
1	D	95	VAL	2.0
1	D	375	VAL	2.0
3	F	1618	GLU	2.0
3	F	1364	LEU	2.0
3	F	1480	LEU	2.0
3	F	1596	LEU	2.0

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

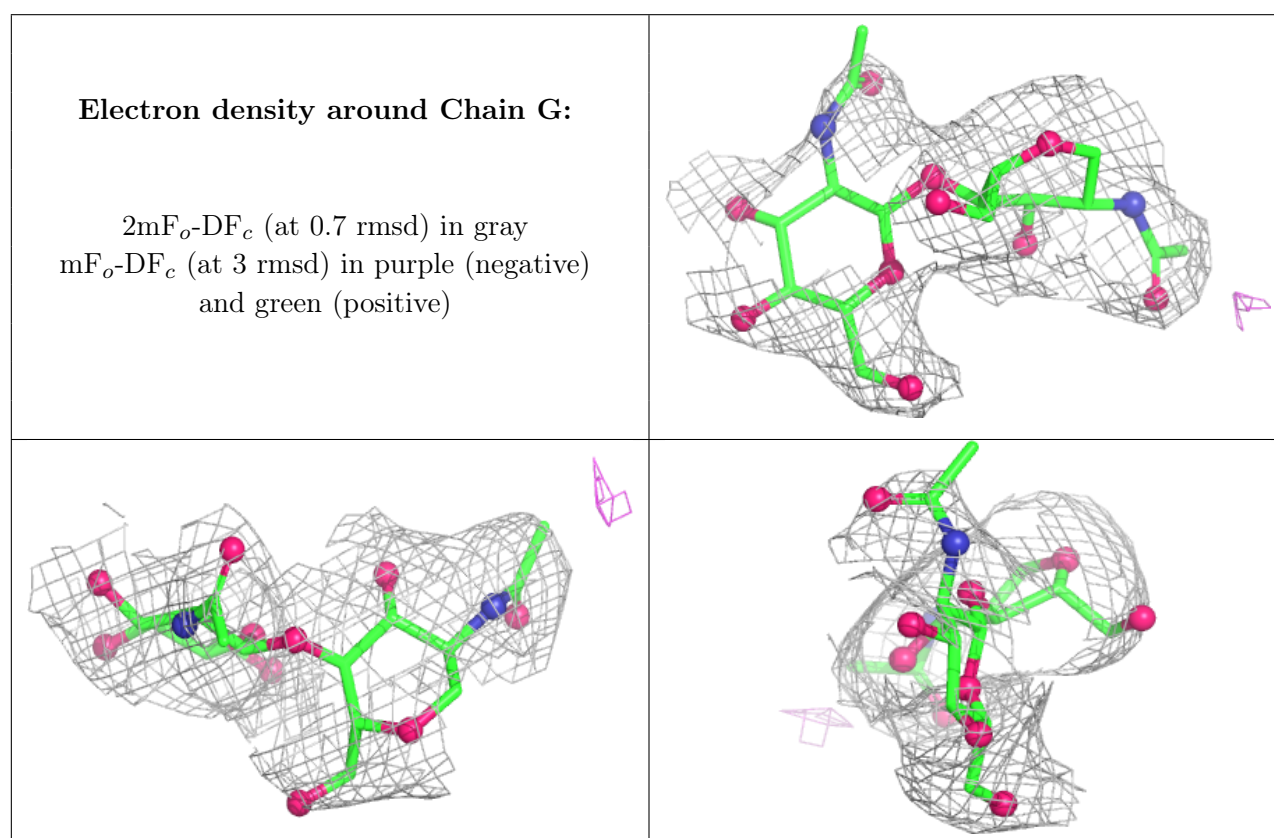
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	G	1	14/15	-	-	51,58,71,76	0
5	NAG	G	2	14/15	-	-	82,87,88,89	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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($\text{\AA}^2$)	Q<0.9
6	CA	D	643	1/1	0.93	0.08	64,64,64,64	0
6	CA	A	645	1/1	0.96	0.08	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.