



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:43 AM GMT

PDB ID : 2ICE
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

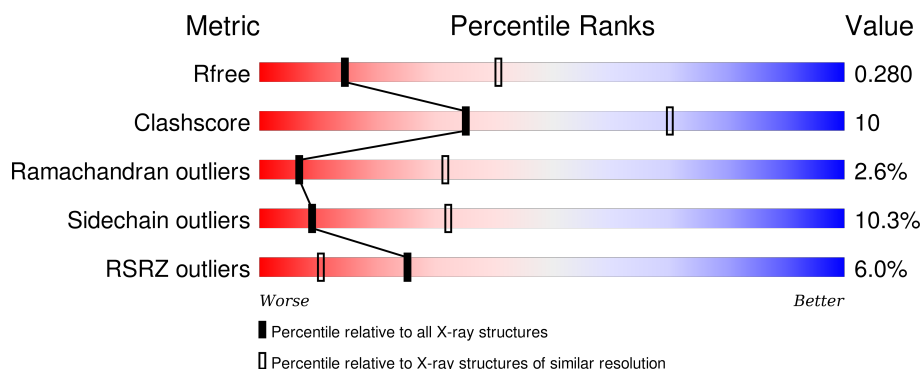
1 Overall quality at a glance

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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 $\leq 5\%$. 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	<div><div></div><div>27%</div><div></div><div>64%</div><div></div><div>19%</div><div></div><div>•</div><div>14%</div><div></div></div>
4	S	119	<div>%<div><div></div><div></div><div>72%</div><div></div><div>26%</div><div></div><div>•</div></div></div>
4	T	119	<div>2%<div><div></div><div></div><div>73%</div><div></div><div>24%</div><div></div><div>•</div></div></div>

2 Entry composition [i](#)

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 a polymer of unknown type called SUGAR (2-MER).

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

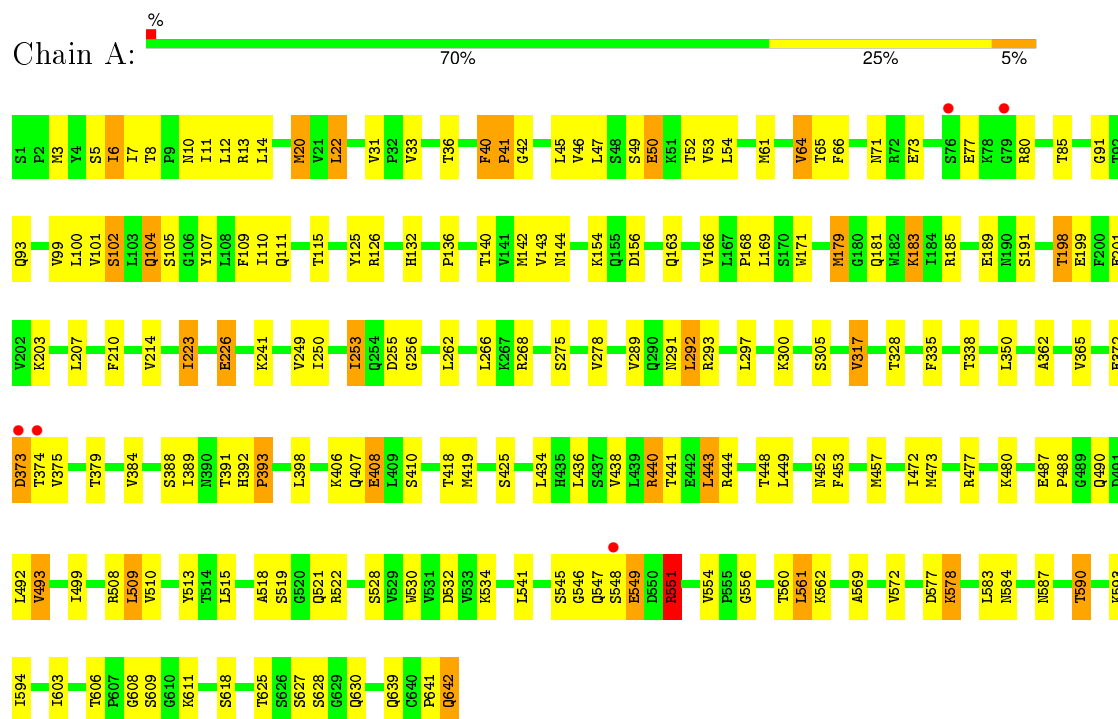
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

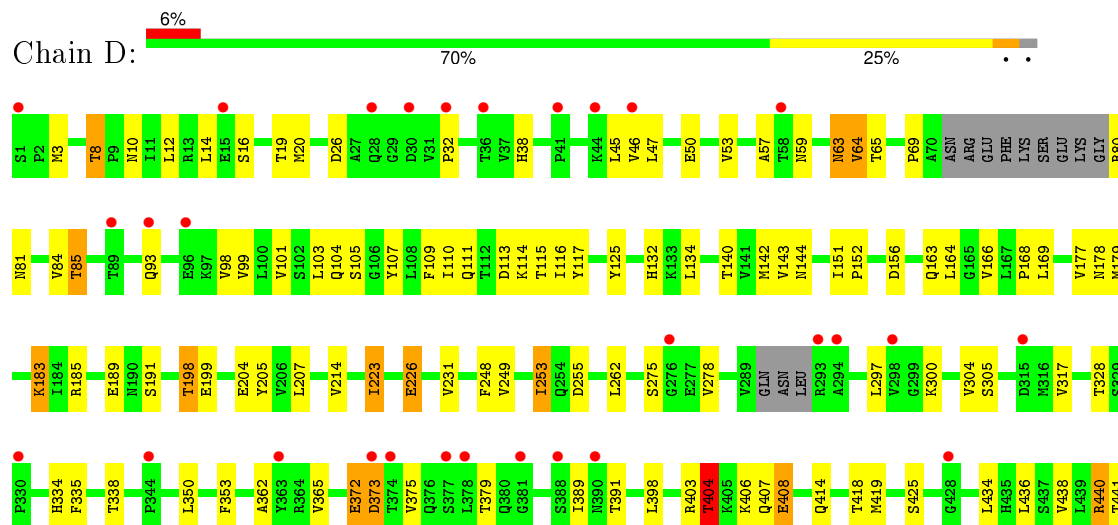
3 Residue-property plots

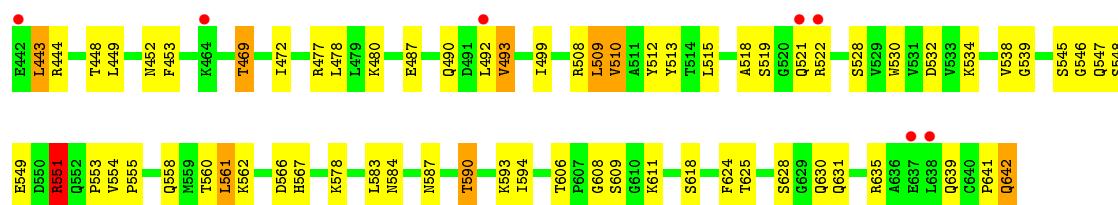
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Complement C3 beta chain

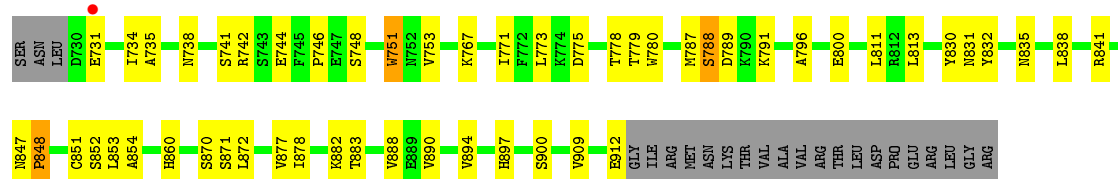


- Molecule 1: Complement C3 beta chain

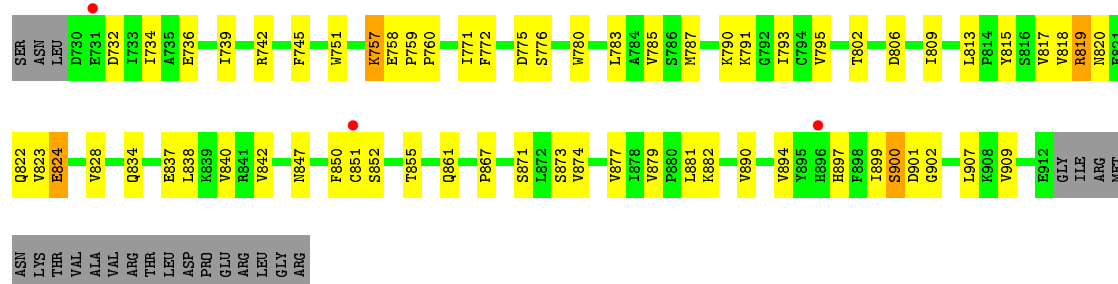




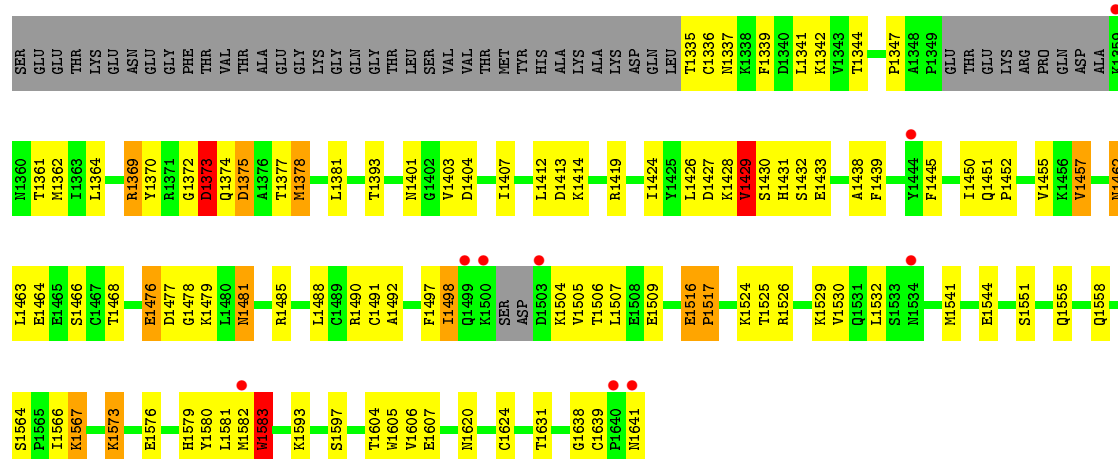
• Molecule 2: Complement C3 alpha chain



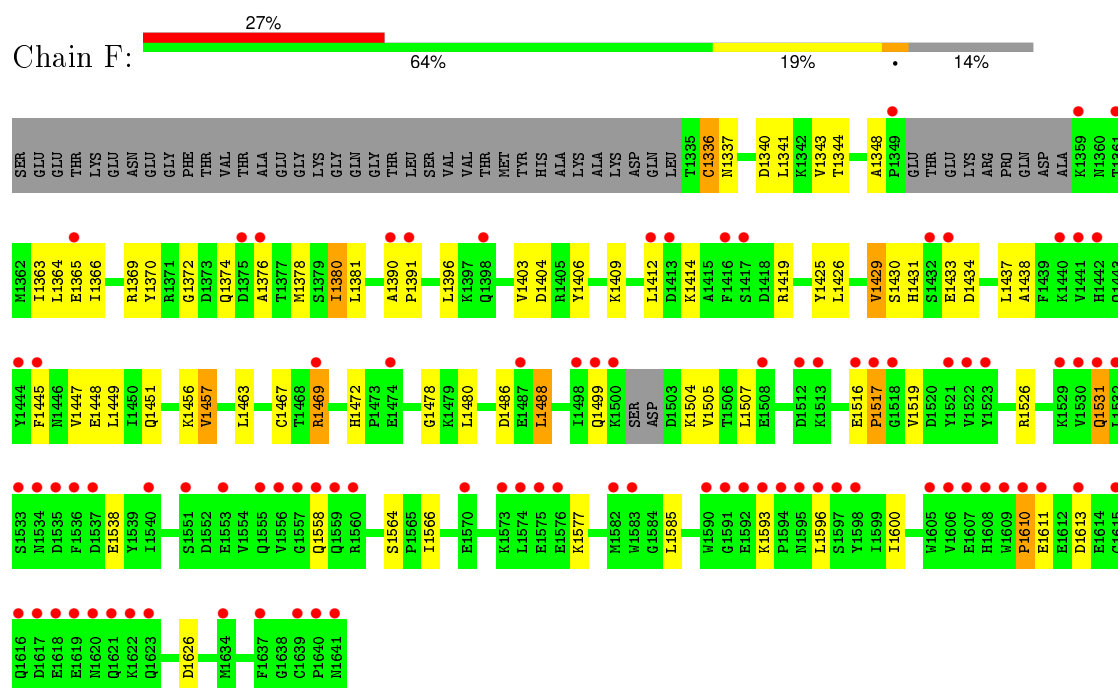
• Molecule 2: Complement C3 alpha chain



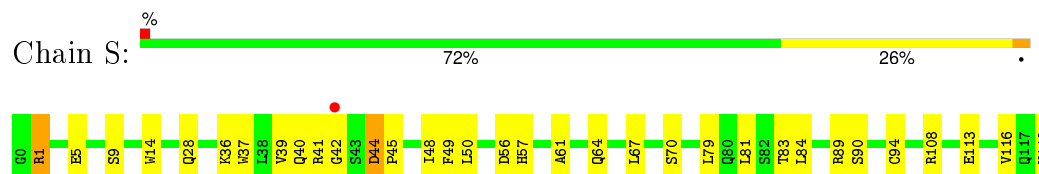
• Molecule 3: Complement C3 alpha chain



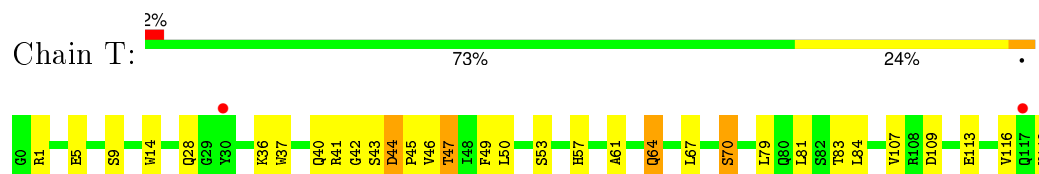
• Molecule 3: Complement C3 alpha chain



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



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



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 19.96 – 3.11	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.00-3.10) 95.3 (19.96-3.11)	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 (5.28%)	DCC
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 , 63.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 62022 reflections	Xtriage
F_o, F_c correlation	0.91	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, 0.375 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: 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	0.54	0/5108	0.67	0/6939
1	D	0.41	0/5004	0.59	0/6799
2	B	0.57	0/1512	0.66	0/2055
2	E	0.46	0/1512	0.59	0/2055
3	C	0.60	3/2453 (0.1%)	0.64	0/3305
3	F	0.38	0/2453	0.54	1/3305 (0.0%)
4	S	0.50	0/972	0.60	0/1323
4	T	0.41	0/972	0.64	1/1323 (0.1%)
All	All	0.49	3/19986 (0.0%)	0.62	2/27104 (0.0%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1607	GLU	CD-OE2	15.28	1.42	1.25
3	C	1607	GLU	CD-OE1	8.79	1.35	1.25
3	C	1620	ASN	CG-OD1	5.04	1.35	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	47	THR	N-CA-C	-9.05	86.56	111.00
3	F	1463	LEU	CA-CB-CG	5.08	126.97	115.30

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
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	116	0
1	D	4907	0	4971	97	0
2	B	1480	0	1502	32	0
2	E	1480	0	1502	38	0
3	C	2407	0	2321	66	0
3	F	2407	0	2321	42	0
4	S	950	0	935	20	0
4	T	950	0	935	12	0
5	A	28	0	25	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
All	All	19619	0	19583	384	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 (384) 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
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
2:B:851:CYS:HG	3:C:1491:CYS:HG	1.26	0.81
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
1:A:3:MET:HE3	1:A:522:ARG:HG2	1.68	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:A:268:ARG:HB2	3:C:1378:MET:HE3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
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
2:B:882:LYS:O	2:B:909:VAL:HG11	2.00	0.61
3:C:1375:ASP:CG	3:C:1430:SER:HB2	2.21	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
1:A:6:ILE:HG12	1:A:20:MET:HE3	1.83	0.60
3:C:1582:MET:HA	3:C:1605:TRP:O	2.02	0.60
3:C:1369:ARG:HG2	3:C:1430:SER:C	2.21	0.60
1:A:546:GLY:CA	1:A:562:LYS:HB2	2.31	0.60
1:D:606:THR:HG22	1:D:608:GLY:H	1.67	0.60
4:S:67:LEU:HG	4:S:79:LEU:HD11	1.84	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:C:1525:THR:OG1	3:C:1541:MET:HE2	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:D:487:GLU:H	1:D:490:GLN:HE21	1.53	0.57
3:C:1336:CYS:HB3	3:C:1339:PHE:O	2.05	0.57
3:F:1611:GLU:HG3	3:F:1613:ASP:H	1.70	0.57
1:D:248:PHE:CZ	3:F:1380:ILE:HD11	2.40	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:547:GLN:HG3	1:A:560:THR:HB	1.86	0.56
1:A:472:ILE:HG12	1:A:509:LEU:HD22	1.88	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:T:40:GLN:OE1	4:T:44:ASP:HA	2.07	0.55
4:S:84:LEU:HD23	4:S:116:VAL:HG22	1.88	0.55
1:A:578:LYS:HE3	2:B:800:GLU:OE2	2.06	0.55
3:C:1516:GLU:HB2	3:C:1517:PRO:HD2	1.87	0.54
2:B:860:HIS:HE1	3:C:1451:GLN:HE22	1.54	0.54
1:A:472:ILE:HD12	1:A:480:LYS:HB3	1.89	0.54
3:C:1462:ASN:HD22	3:C:1462:ASN:C	2.11	0.54
2:B:860:HIS:CE1	3:C:1451:GLN:NE2	2.75	0.54
4:S:40:GLN:OE1	4:S:44:ASP:HA	2.08	0.54
3:C:1347:PRO:HA	3:C:1362:MET:HG2	1.90	0.54
2:B:860:HIS:HE1	3:C:1451:GLN:NE2	2.05	0.54
1:A:183:LYS:HG2	1:A:185:ARG:HH12	1.72	0.54
3:F:1488:LEU:H	3:F:1488:LEU:HD23	1.74	0.53
1:A:551:ARG:HA	1:A:551:ARG:CZ	2.38	0.53
1:A:11:ILE:HD12	1:A:603:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:1369:ARG:HE	3:F:1430:SER:H	1.57	0.53
3:C:1414:LYS:HB3	3:C:1419:ARG:HE	1.74	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:F:1526:ARG:HH21	3:F:1577:LYS:HG2	1.73	0.52
2:E:817:VAL:HG23	2:E:909:VAL:HG13	1.90	0.52
3:C:1481:ASN:OD1	3:C:1567:LYS:HG2	2.09	0.52
3:C:1498:ILE:HD12	3:C:1605:TRP:HB2	1.91	0.52
1:D:642:GLN:HA	1:D:642:GLN:OE1	2.08	0.52
1:A:291:ASN:O	1:A:293:ARG:N	2.33	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:CZ	1:D:551:ARG:HA	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:D:546:GLY:HA2	1:D:562:LYS:HB2	1.91	0.52
1:D:472:ILE:HG12	1:D:509:LEU:HD22	1.92	0.52
1:A:168:PRO:O	1:A:169:LEU:HD23	2.10	0.52
1:D:434:LEU:HB2	1:D:513:TYR:HE2	1.75	0.52
1:D:338:THR:HG21	1:D:350:LEU:HD23	1.92	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:HH11	1:D:551:ARG:HA	1.75	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
3:C:1375:ASP:N	3:C:1375:ASP:OD1	2.44	0.51
1:A:241:LYS:HG3	2:B:832:TYR:CE2	2.46	0.51
2:B:877:VAL:HG21	3:C:1452:PRO:HG2	1.93	0.51
1:A:249:VAL:HG21	1:A:278:VAL:HG11	1.93	0.50
1:D:510:VAL:HG13	1:D:528:SER:HB3	1.93	0.50
1:A:440:ARG:HA	1:A:440:ARG:HE	1.76	0.50
1:A:210:PHE:CZ	1:A:317:VAL:HG13	2.46	0.50
1:D:223:ILE:HD11	1:D:328:THR:HG22	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:C:1403:VAL:O	3:C:1404:ASP:CB	2.60	0.49
3:C:1377:THR:O	3:C:1378:MET:C	2.51	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:407:GLN:O	1:D:408:GLU:CB	2.61	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
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.94	0.49
2:E:819:ARG:HG3	2:E:820:ASN:CG	2.33	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:546:GLY:HA3	1:A:562:LYS:HB2	1.95	0.48
3:F:1456:LYS:HA	3:F:1467:CYS:O	2.13	0.48
2:E:894:VAL:HG21	2:E:897:HIS:HB2	1.96	0.48
1:D:84:VAL:HG22	1:D:101:VAL:HG22	1.95	0.48
3:C:1476:GLU:O	3:C:1477:ASP:HB2	2.13	0.48
1:A:338:THR:HG21	1:A:350:LEU:HD23	1.95	0.48
1:D:538:VAL:HG12	2:E:791:LYS:HD3	1.94	0.48
1:D:297:LEU:HA	1:D:300:LYS:HD2	1.95	0.48
4:S:89:ARG:O	4:S:90:SER:HB2	2.13	0.48
2:E:809:ILE:HD13	2:E:890:VAL:HG23	1.95	0.48
2:E:837:GLU:HB3	2:E:867:PRO:HA	1.97	0.47
1:D:624:PHE:O	1:D:631:GLN:HA	2.14	0.47
1:A:100:LEU:HD12	1:A:101:VAL:H	1.79	0.47
2:B:744:GLU:C	2:B:746:PRO:HD3	2.34	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:335:PHE:CD2	1:A:419:MET:HB3	2.49	0.47
1:D:183:LYS:HG3	1:D:199:GLU:HG2	1.97	0.47
1:A:561:LEU:HD22	2:B:771:ILE:HD13	1.95	0.47
3:C:1462:ASN:HD22	3:C:1463:LEU:N	2.12	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
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
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
3:C:1530:VAL:HG12	3:C:1532:LEU:HD12	1.96	0.47
1:A:453:PHE:HB2	1:A:493:VAL:HG23	1.97	0.47
3:C:1369:ARG:HD3	3:C:1433:GLU:O	2.14	0.47
2:E:851:CYS:HB3	2:E:879:VAL:HB	1.96	0.47
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.50	0.47
1:D:110:ILE:HB	1:D:198:THR:OG1	2.15	0.47
3:F:1429:VAL:HG13	3:F:1429:VAL:O	2.15	0.47
1:A:6:ILE:HG12	1:A:20:MET:CE	2.45	0.47
1:D:443:LEU:CD2	1:D:499:ILE:HG13	2.44	0.47
2:E:742:ARG:HB3	2:E:775:ASP:HB3	1.96	0.46
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
1:A:519:SER:C	1:A:521:GLN:H	2.19	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: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:A:154:LYS:HD2	1:A:171:TRP:CD1	2.50	0.46
1:D:249:VAL:HA	1:D:305:SER:O	2.15	0.46
3:F:1406:TYR:HD2	3:F:1425:TYR:CD1	2.34	0.46
3:F:1364:LEU:O	3:F:1438:ALA:HA	2.16	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: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
1:D:164:LEU:O	2:E:787:MET:HG2	2.16	0.46
1:A:181:GLN:HE22	1:A:201:GLU:HG3	1.80	0.46
3:F:1369:ARG:HA	3:F:1429:VAL:HG23	1.96	0.46
2:E:882:LYS:O	2:E:909:VAL:HB	2.16	0.46
3:C:1526:ARG:NH1	3:C:1544:GLU:OE2	2.49	0.46
3:C:1525:THR:CB	3:C:1541:MET:HE2	2.45	0.45
1:A:541:LEU:HD23	2:B:796:ALA:HB2	1.98	0.45
2:E:838:LEU:HD13	2:E:894:VAL:HG11	1.98	0.45
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.98	0.45
2:B:830:TYR:CD1	2:B:871:SER:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1364:LEU:O	3:C:1438:ALA:HA	2.16	0.45
4:T:50:LEU:HB3	4:T:57:HIS:HB2	1.98	0.45
1:D:168:PRO:O	1:D:169:LEU:HD23	2.16	0.45
1:D:3:MET:HB2	1:D:522:ARG:NH2	2.32	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
3:C:1476:GLU:C	3:C:1478:GLY:H	2.19	0.45
1:D:519:SER:C	1:D:521:GLN:H	2.19	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
2:B:734:ILE:HG13	2:B:734:ILE:H	1.57	0.45
1:A:249:VAL:HA	1:A:305:SER:O	2.17	0.45
4:S:61:ALA:HA	4:S:64:GLN:NE2	2.30	0.45
3:C:1497:PHE:O	3:C:1498:ILE:C	2.56	0.45
1:D:143:VAL:C	1:D:144:ASN:HD22	2.20	0.45
2:B:811:LEU:HG	2:B:813:LEU:CD1	2.47	0.45
4:S:44:ASP:HB2	4:S:45:PRO:CD	2.35	0.44
1:A:569:ALA:HB2	2:B:788:SER:HB2	1.98	0.44
3:F:1403:VAL:O	3:F:1404:ASP:HB2	2.17	0.44
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.99	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
1:D:248:PHE:HE1	3:F:1378:MET:HG2	1.82	0.44
1:D:134:LEU:HB3	2:E:793:ILE:HG22	1.99	0.44
1:D:334:HIS:HB2	1:D:353:PHE:HB3	2.00	0.44
3:C:1638:GLY:O	3:C:1639:CYS:C	2.55	0.44
1:D:436:LEU:HA	1:D:452:ASN:O	2.18	0.44
1:D:561:LEU:CD2	2:E:771:ILE:HD13	2.43	0.44
1:D:19:THR:HA	1:D:65:THR:HG22	2.00	0.44
1:D:226:GLU:HG3	1:D:226:GLU:H	1.51	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:S:39:VAL:HG12	4:S:48:ILE:HG23	2.00	0.44
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
1:A:143:VAL:C	1:A:144:ASN:HD22	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:546:GLY:HA3	1:D:562:LYS:HB2	1.99	0.43
1:A:80:ARG:HA	1:A:80:ARG:HD3	1.82	0.43
4:S:37:TRP:CH2	4:S:94:CYS:HB2	2.54	0.43
3:F:1406:TYR:HB3	3:F:1425:TYR:HB2	2.00	0.43
2:E:785:VAL:HG22	2:E:795:VAL:HG22	1.99	0.43
1:D:440:ARG:HA	1:D:440:ARG:HE	1.84	0.43
4:T:36:LYS:HG3	4:T:50:LEU:CD1	2.49	0.43
1:A:101:VAL:HG12	1:A:102:SER:N	2.34	0.43
1:A:163:GLN:NE2	1:A:163:GLN:HA	2.33	0.43
1:D:404:THR:HG22	1:D:414:GLN:OE1	2.19	0.43
1:A:12:LEU:HG	1:A:99:VAL:CG1	2.49	0.43
1:A:384:VAL:HB	1:A:440:ARG:NH1	2.34	0.42
1:D:114:LYS:HB2	1:D:117:TYR:CZ	2.54	0.42
1:A:510:VAL:HG13	1:A:528:SER:HB3	1.99	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
1:D:116:ILE:HG12	1:D:205:TYR:CE2	2.54	0.42
1:D:80:ARG:O	1:D:81:ASN:HB2	2.20	0.42
3:F:1409:LYS:HA	3:F:1412:LEU:HD13	2.01	0.42
2:E:734:ILE:HD12	2:E:900:SER:HB3	2.00	0.42
1:A:183:LYS:HB3	1:A:185:ARG:HH11	1.84	0.42
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.49	0.42
1:A:111:GLN:O	1:A:125:TYR:HA	2.19	0.42
3:C:1430:SER:OG	3:C:1431:HIS:N	2.52	0.42
1:A:443:LEU:CD2	1:A:499:ILE:HG13	2.49	0.42
4:S:1:ARG:H	4:S:1:ARG:CZ	2.32	0.42
1:A:183:LYS:HG3	1:A:199:GLU:HG2	2.02	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:F:1390:ALA:HA	3:F:1391:PRO:HD3	1.81	0.42
4:S:36:LYS:HG3	4:S:50:LEU:CD1	2.49	0.42
3:C:1530:VAL:HG23	3:C:1576:GLU:HG2	2.02	0.42
3:C:1431:HIS:O	3:C:1432:SER:C	2.58	0.42
1:A:210:PHE:CZ	1:A:317:VAL:CG1	3.02	0.42
1:A:140:THR:HG22	1:A:189:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:1610:PRO:HB2	3:F:1611:GLU:H	1.69	0.41
1:D:214:VAL:O	1:D:214:VAL:HG23	2.20	0.41
1:A:457:MET:HE3	1:A:513:TYR:HE1	1.85	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:440:ARG:NE	1:A:440:ARG:HA	2.35	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
2:E:757:LYS:HG3	2:E:757:LYS:H	1.77	0.41
3:C:1524:LYS:HA	3:C:1580:TYR:O	2.20	0.41
1:A:268:ARG:HB2	3:C:1378:MET:HE2	2.01	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
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:101:VAL:CG1	1:A:102:SER:N	2.82	0.41
1:A:297:LEU:HA	1:A:300:LYS:HD2	2.02	0.41
1:A:107:TYR:CE2	1:A:132:HIS:HA	2.55	0.41
1:A:289:VAL:HG12	1:A:291:ASN:H	1.86	0.41
2:E:822:GLN:HA	2:E:879:VAL:HG22	2.01	0.41
1:D:539:GLY:HA3	1:D:566:ASP:OD2	2.20	0.41
1:D:204:GLU:HG2	2:E:815:TYR:CE2	2.56	0.41
3:F:1341:LEU:HD22	3:F:1457:VAL:HG22	2.02	0.41
4:S:89:ARG:NH1	4:S:116:VAL:H	2.19	0.41
1:A:14:LEU:HA	1:A:14:LEU:HD23	1.83	0.41
1:A:6:ILE:C	1:A:6:ILE:HD12	2.38	0.41
3:F:1433:GLU:HB3	3:F:1434:ASP:H	1.68	0.41
1:A:473:MET:HE1	1:A:603:ILE:HD11	2.02	0.41
1:D:534:LYS:NZ	4:T:109:ASP:OD2	2.53	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
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
2:E:877:VAL:HG22	3:F:1451:GLN:HE21	1.86	0.40
2:B:852:SER:O	2:B:854:ALA:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASP:OD1	1:A:373:ASP:N	2.53	0.40
1:D:372:GLU:HA	1:D:373:ASP:HB2	2.03	0.40
2:E:901:ASP:OD2	2:E:902:GLY:N	2.44	0.40
2:B:778:THR:OG1	2:B:779:THR:N	2.54	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
1:D:362:ALA:O	1:D:379:THR:CG2	2.69	0.40
3:F:1376:ALA:HB3	3:F:1429:VAL:O	2.22	0.40
1:D:444:ARG:NH2	1:D:534:LYS:HE2	2.37	0.40
3:C:1372:GLY:O	3:C:1374:GLN:N	2.47	0.40
1:A:457:MET:HE3	1:A:513:TYR:CE1	2.56	0.40
2:E:776:SER:HB2	2:E:780:TRP:CZ2	2.56	0.40
1:A:577:ASP:HB2	2:B:780:TRP:CZ3	2.57	0.40
1:A:179:MET:HG3	1:A:203:LYS:HA	2.04	0.40
1:A:136:PRO:HG3	2:B:787:MET:HG3	2.03	0.40
1:D:469:THR:HB	1:D:512:TYR:CE2	2.57	0.40
3:C:1364:LEU:HD23	3:C:1439:PHE:CZ	2.56	0.40
3:C:1639:CYS:C	3:C:1641:ASN:H	2.24	0.40
2:E:736:GLU:HA	2:E:739:ILE:HD12	2.04	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%)	7	32
1	D	624/642 (97%)	581 (93%)	27 (4%)	16 (3%)	7	32
2	B	181/206 (88%)	170 (94%)	9 (5%)	2 (1%)	17	55
2	E	181/206 (88%)	160 (88%)	20 (11%)	1 (1%)	30	68
3	C	290/343 (84%)	235 (81%)	42 (14%)	13 (4%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	290/343 (84%)	244 (84%)	35 (12%)	11 (4%)	4	22
4	S	117/119 (98%)	103 (88%)	13 (11%)	1 (1%)	21	61
4	T	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	7	32
All	All	2440/2620 (93%)	2194 (90%)	183 (8%)	63 (3%)	7	32

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
1	D	63	ASN
1	D	64	VAL
1	D	104	GLN
1	D	408	GLU
1	D	548	SER
1	D	549	GLU

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Mol	Chain	Res	Type
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 ⓘ

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%)	499 (88%)	67 (12%)	6 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	555/566 (98%)	500 (90%)	55 (10%)	10	34
2	B	171/191 (90%)	157 (92%)	14 (8%)	14	47
2	E	171/191 (90%)	152 (89%)	19 (11%)	8	29
3	C	270/309 (87%)	234 (87%)	36 (13%)	5	20
3	F	270/309 (87%)	253 (94%)	17 (6%)	22	58
4	S	109/109 (100%)	100 (92%)	9 (8%)	14	46
4	T	109/109 (100%)	97 (89%)	12 (11%)	8	30
All	All	2221/2350 (94%)	1992 (90%)	229 (10%)	9	32

All (229) 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	13	ARG
1	A	20	MET
1	A	22	LEU
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	73	GLU
1	A	77	GLU
1	A	85	THR
1	A	102	SER
1	A	104	GLN
1	A	105	SER
1	A	142	MET
1	A	156	ASP
1	A	179	MET
1	A	183	LYS
1	A	191	SER

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Mol	Chain	Res	Type
1	A	198	THR
1	A	207	LEU
1	A	214	VAL
1	A	223	ILE
1	A	226	GLU
1	A	253	ILE
1	A	275	SER
1	A	292	LEU
1	A	317	VAL
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	477	ARG
1	A	488	PRO
1	A	492	LEU
1	A	493	VAL
1	A	509	LEU
1	A	515	LEU
1	A	551	ARG
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	609	SER
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	741	SER
2	B	748	SER

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Mol	Chain	Res	Type
2	B	767	LYS
2	B	788	SER
2	B	789	ASP
2	B	791	LYS
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	912	GLU
3	C	1335	THR
3	C	1342	LYS
3	C	1344	THR
3	C	1361	THR
3	C	1369	ARG
3	C	1373	ASP
3	C	1375	ASP
3	C	1378	MET
3	C	1393	THR
3	C	1412	LEU
3	C	1413	ASP
3	C	1427	ASP
3	C	1428	LYS
3	C	1429	VAL
3	C	1445	PHE
3	C	1457	VAL
3	C	1462	ASN
3	C	1479	LYS
3	C	1485	ARG
3	C	1488	LEU
3	C	1490	ARG
3	C	1504	LYS
3	C	1506	THR
3	C	1507	LEU
3	C	1529	LYS
3	C	1564	SER
3	C	1566	ILE
3	C	1567	LYS
3	C	1573	LYS
3	C	1583	TRP
3	C	1593	LYS

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Mol	Chain	Res	Type
3	C	1597	SER
3	C	1604	THR
3	C	1606	VAL
3	C	1624	CYS
3	C	1631	THR
4	S	1	ARG
4	S	5	GLU
4	S	9	SER
4	S	28	GLN
4	S	41	ARG
4	S	70	SER
4	S	81	LEU
4	S	83	THR
4	S	113	GLU
1	D	8	THR
1	D	14	LEU
1	D	26	ASP
1	D	38	HIS
1	D	45	LEU
1	D	46	VAL
1	D	47	LEU
1	D	85	THR
1	D	93	GLN
1	D	103	LEU
1	D	105	SER
1	D	142	MET
1	D	156	ASP
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	223	ILE
1	D	226	GLU
1	D	253	ILE
1	D	275	SER
1	D	317	VAL
1	D	389	ILE
1	D	404	THR
1	D	406	LYS

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Mol	Chain	Res	Type
1	D	418	THR
1	D	425	SER
1	D	438	VAL
1	D	440	ARG
1	D	441	THR
1	D	443	LEU
1	D	448	THR
1	D	469	THR
1	D	477	ARG
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	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

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Mol	Chain	Res	Type
2	E	871	SER
2	E	873	SER
2	E	881	LEU
2	E	900	SER
3	F	1336	CYS
3	F	1340	ASP
3	F	1374	GLN
3	F	1380	ILE
3	F	1437	LEU
3	F	1445	PHE
3	F	1457	VAL
3	F	1469	ARG
3	F	1486	ASP
3	F	1488	LEU
3	F	1504	LYS
3	F	1507	LEU
3	F	1531	GLN
3	F	1558	GLN
3	F	1566	ILE
3	F	1585	LEU
3	F	1626	ASP
4	T	1	ARG
4	T	5	GLU
4	T	9	SER
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	81	ASN
1	A	93	GLN
1	A	144	ASN
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	162	ASN
1	A	163	GLN
1	A	181	GLN
1	A	225	ASN
1	A	490	GLN
2	B	738	ASN
2	B	820	ASN
2	B	836	GLN
2	B	860	HIS
2	B	896	HIS
2	B	897	HIS
3	C	1401	ASN
3	C	1451	GLN
3	C	1462	ASN
3	C	1472	HIS
3	C	1558	GLN
3	C	1621	GLN
4	S	28	GLN
4	S	64	GLN
4	S	104	ASN
4	S	105	GLN
1	D	28	GLN
1	D	144	ASN
1	D	163	GLN
1	D	225	ASN
1	D	490	GLN
1	D	552	GLN
2	E	738	ASN
3	F	1337	ASN
3	F	1443	GLN
3	F	1451	GLN
3	F	1462	ASN
4	T	59	GLN
4	T	64	GLN
4	T	104	ASN
4	T	105	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 carbohydrates 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	A	643	1,5	14,14,15	0.46	0	15,19,21	2.31	2 (13%)
5	NAG	A	644	5	14,14,15	0.51	0	15,19,21	0.81	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	A	643	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	644	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	643	NAG	C3-C4-C5	2.44	114.44	110.20
5	A	643	NAG	C1-O5-C5	8.11	122.54	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

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

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%)	-0.42	5 (0%) 87 75	17, 47, 84, 126	0
1	D	630/642 (98%)	0.24	36 (5%) 27 11	17, 50, 123, 142	0
2	B	183/206 (88%)	-0.59	1 (0%) 91 83	13, 37, 64, 82	0
2	E	183/206 (88%)	-0.28	3 (1%) 74 55	12, 49, 91, 95	0
3	C	296/343 (86%)	-0.14	9 (3%) 54 29	19, 60, 94, 116	0
3	F	296/343 (86%)	1.53	91 (30%) 1 0	42, 133, 199, 223	0
4	S	119/119 (100%)	-0.48	1 (0%) 87 75	22, 46, 68, 94	0
4	T	119/119 (100%)	-0.22	2 (1%) 73 52	22, 46, 68, 94	0
All	All	2468/2620 (94%)	0.02	148 (5%) 25 10	12, 51, 161, 223	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1610	PRO	12.8
3	F	1608	HIS	9.3
1	D	1	SER	7.2
3	F	1607	GLU	6.8
1	D	374	THR	6.8
3	F	1517	PRO	6.6
3	F	1534	ASN	6.5
3	F	1500	LYS	6.5
3	F	1432	SER	6.4
3	F	1557	GLY	6.3
3	F	1622	LYS	6.1
3	F	1559	GLN	6.1
3	F	1621	GLN	5.9
3	F	1639	CYS	5.9
3	F	1433	GLU	5.8
3	F	1640	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	373	ASP	5.2
1	D	378	LEU	5.2
3	C	1641	ASN	5.1
3	F	1616	GLN	4.9
3	F	1619	GLU	4.8
3	F	1623	GLN	4.7
1	D	41	PRO	4.7
1	D	428	GLY	4.7
3	F	1558	GLN	4.6
3	F	1618	GLU	4.6
3	F	1617	ASP	4.5
3	F	1590	TRP	4.5
3	F	1375	ASP	4.4
3	F	1412	LEU	4.4
3	F	1597	SER	4.4
3	F	1573	LYS	4.3
3	F	1499	GLN	4.3
3	F	1531	GLN	4.3
3	F	1359	LYS	4.3
3	F	1615	CYS	4.2
3	F	1574	LEU	4.1
3	F	1605	TRP	4.1
3	F	1641	ASN	4.1
3	F	1441	VAL	4.1
3	F	1530	VAL	4.0
1	D	377	SER	3.9
3	F	1611	GLU	3.9
3	F	1592	GLU	3.9
1	D	44	LYS	3.8
3	F	1620	ASN	3.6
3	C	1359	LYS	3.6
1	D	521	GLN	3.5
3	F	1533	SER	3.5
3	F	1555	GLN	3.5
1	D	638	LEU	3.5
3	F	1576	GLU	3.5
2	E	896	HIS	3.5
1	D	58	THR	3.5
1	D	298	VAL	3.4
3	F	1532	LEU	3.4
3	F	1613	ASP	3.4
3	F	1529	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
3	F	1575	GLU	3.4
3	F	1416	PHE	3.4
1	D	28	GLN	3.3
1	D	46	VAL	3.3
3	F	1535	ASP	3.3
3	F	1634	MET	3.2
1	D	30	ASP	3.2
1	D	32	PRO	3.2
3	F	1398	GLN	3.2
3	F	1508	GLU	3.2
3	F	1442	HIS	3.2
3	F	1606	VAL	3.2
3	F	1390	ALA	3.1
1	D	492	LEU	3.1
1	D	344	PRO	3.1
3	C	1503	ASP	3.1
1	A	374	THR	3.1
3	F	1595	ASN	3.0
3	F	1518	GLY	3.0
1	D	96	GLU	3.0
3	F	1349	PRO	3.0
1	A	373	ASP	3.0
1	D	442	GLU	3.0
3	F	1537	ASP	2.9
1	D	293	ARG	2.9
3	F	1513	LYS	2.9
3	F	1593	LYS	2.9
1	D	93	GLN	2.8
3	F	1376	ALA	2.8
3	F	1444	TYR	2.8
1	D	464	LYS	2.7
1	A	79	GLY	2.7
3	F	1582	MET	2.7
1	D	89	THR	2.7
3	F	1551	SER	2.7
3	C	1640	PRO	2.7
1	A	548	SER	2.7
3	F	1474	GLU	2.7
4	T	30	TYR	2.6
3	F	1560	ARG	2.6
3	F	1512	ASP	2.6
1	D	294	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	1522	VAL	2.6
3	F	1440	LYS	2.6
3	F	1536	PHE	2.5
3	F	1523	TYR	2.5
3	F	1598	TYR	2.5
1	D	330	PRO	2.5
3	F	1417	SER	2.5
3	C	1444	TYR	2.5
3	F	1516	GLU	2.5
1	D	522	ARG	2.5
3	F	1556	VAL	2.5
1	D	381	GLY	2.5
3	F	1570	GLU	2.4
1	D	15	GLU	2.4
2	B	731	GLU	2.4
2	E	731	GLU	2.4
2	E	851	CYS	2.4
1	D	390	ASN	2.3
3	F	1591	GLY	2.3
3	F	1540	ILE	2.3
3	F	1553	GLU	2.3
3	F	1361	THR	2.3
1	D	388	SER	2.3
3	F	1594	PRO	2.3
4	T	117	GLN	2.3
3	F	1637	PHE	2.3
3	F	1365	GLU	2.2
3	F	1498	ILE	2.2
1	D	637	GLU	2.2
1	A	76	SER	2.2
1	D	363	TYR	2.2
3	F	1413	ASP	2.2
1	D	315	ASP	2.2
3	F	1609	TRP	2.2
3	F	1596	LEU	2.2
3	C	1534	ASN	2.2
3	C	1499	GLN	2.1
3	F	1445	PHE	2.1
3	F	1521	TYR	2.1
3	F	1469	ARG	2.1
3	C	1582	MET	2.1
3	F	1391	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	1500	LYS	2.1
3	F	1583	TRP	2.1
3	F	1487	GLU	2.1
1	D	276	GLY	2.1
4	S	42	GLY	2.0
1	D	36	THR	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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	643	14/15	0.95	0.16	-0.50	51,58,71,76	0
5	NAG	A	644	14/15	0.90	0.40	-	82,87,88,89	0

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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	CA	D	643	1/1	0.96	0.04	-2.26	64,64,64,64	0
6	CA	A	645	1/1	0.94	0.06	-2.62	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.