



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:05 PM UTC

PDB ID : 8XRT / pdb_00008xrt
Title : The crystal structure of a GH3 enzyme CcBgl3B
Authors : Su, J.Y.
Deposited on : 2024-01-08
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

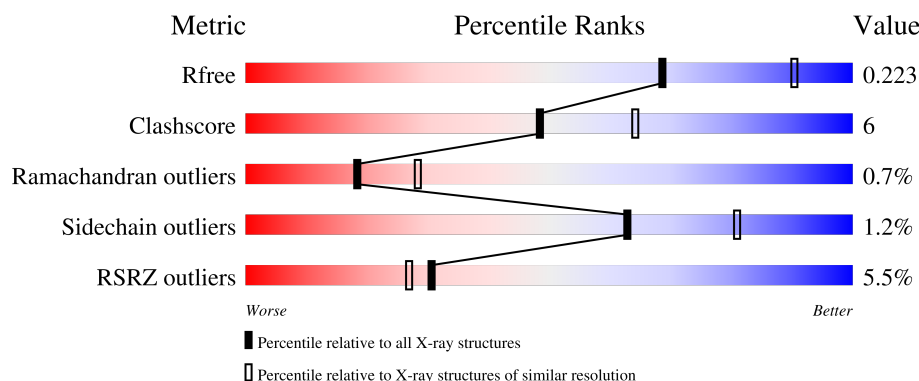
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	768	11% 75% 15% 8%
1	B	768	2% 87% 10% 2%
1	C	768	2% 86% 11% 1%
1	D	768	11% 75% 16% 8%
1	E	768	4% 86% 11% 1%

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Mol	Chain	Length	Quality of chain
1	F	768	% 89% 8% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 34706 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 GH3 enzyme CcBgl3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	750	Total	C	N	O	S	0	0	0
			5625	3539	999	1072	15			
1	F	751	Total	C	N	O	S	0	0	0
			5629	3544	999	1071	15			
1	A	709	Total	C	N	O	S	0	0	0
			5314	3337	946	1017	14			
1	B	750	Total	C	N	O	S	0	0	0
			5624	3541	998	1070	15			
1	C	747	Total	C	N	O	S	0	0	0
			5608	3530	995	1068	15			
1	D	703	Total	C	N	O	S	0	0	0
			5234	3283	931	1005	15			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

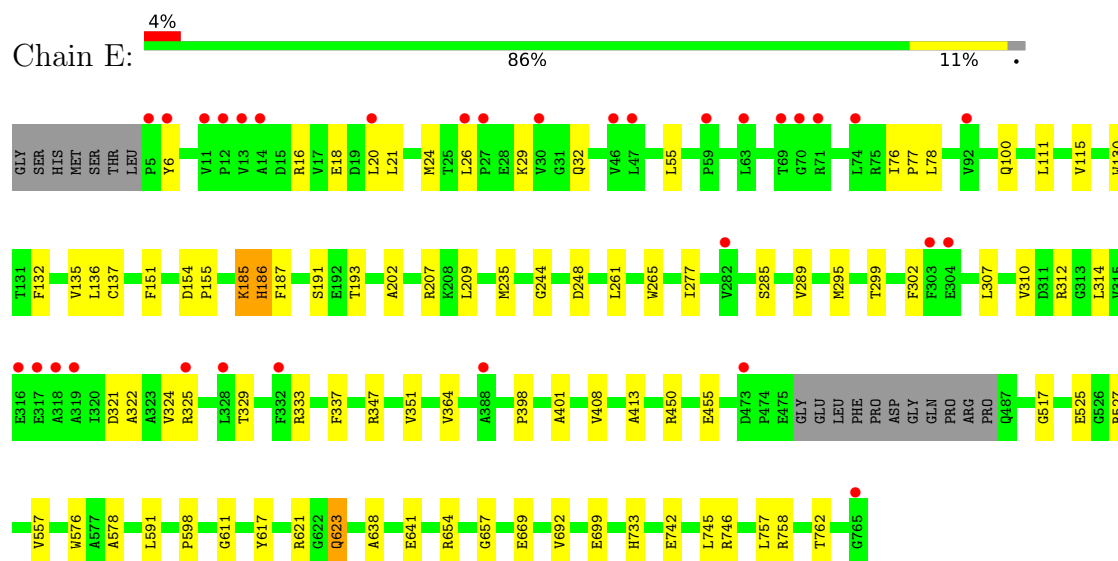
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	414	Total 414	O 414	0	0
3	F	472	Total 472	O 472	0	0
3	A	203	Total 203	O 203	0	0
3	B	236	Total 236	O 236	0	0
3	C	205	Total 205	O 205	0	0
3	D	136	Total 136	O 136	0	0

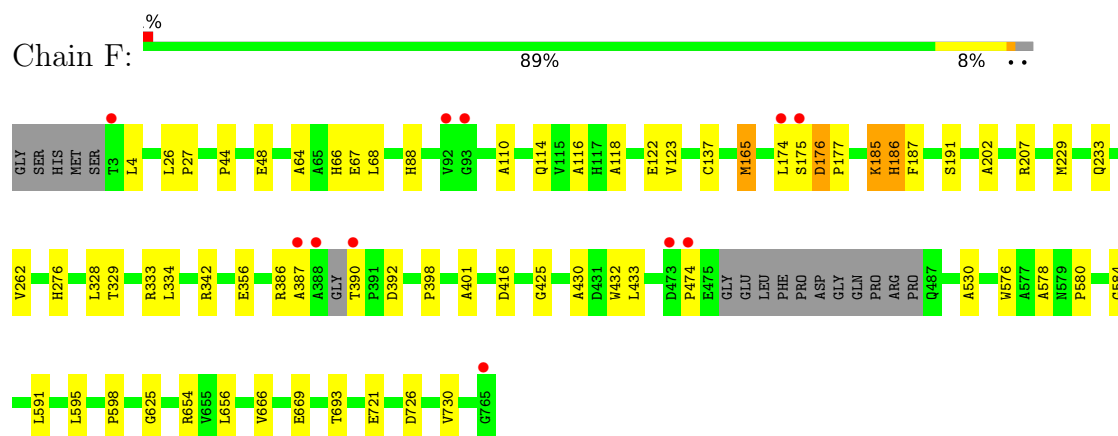
3 Residue-property plots [i](#)

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.

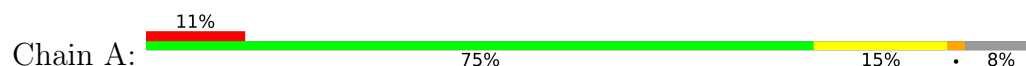
• Molecule 1: GH3 enzyme CcBgl3B

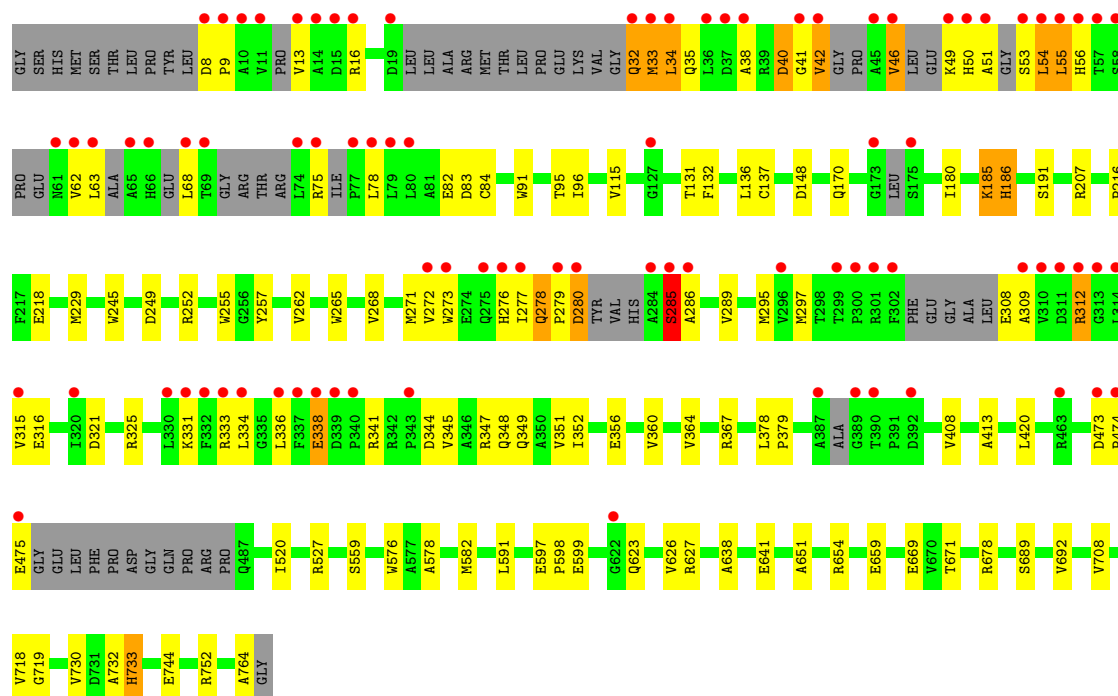


• Molecule 1: GH3 enzyme CcBgl3B

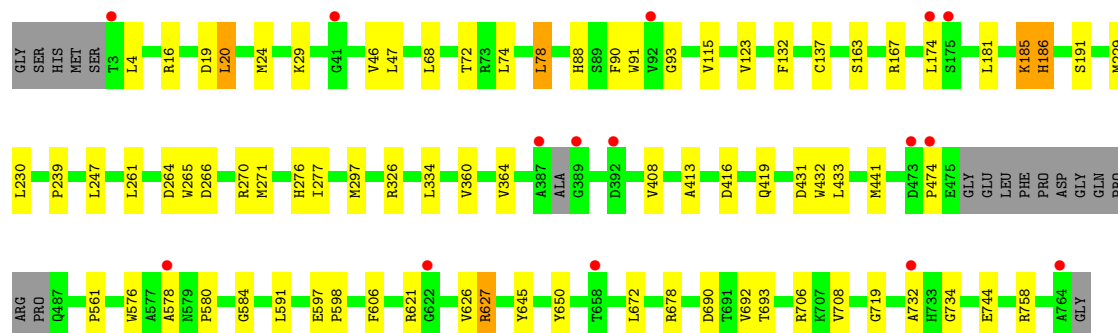
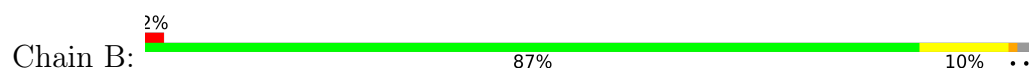


• Molecule 1: GH3 enzyme CcBgl3B

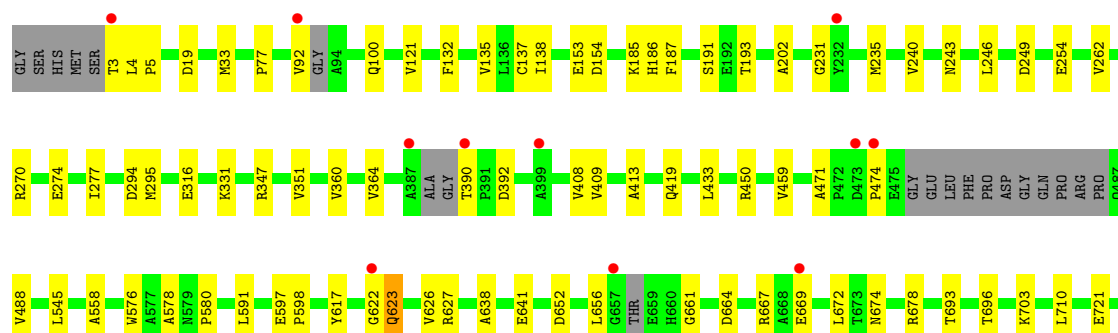
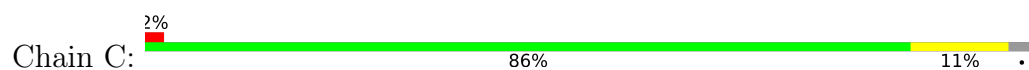




• Molecule 1: GH3 enzyme CcBgl3B

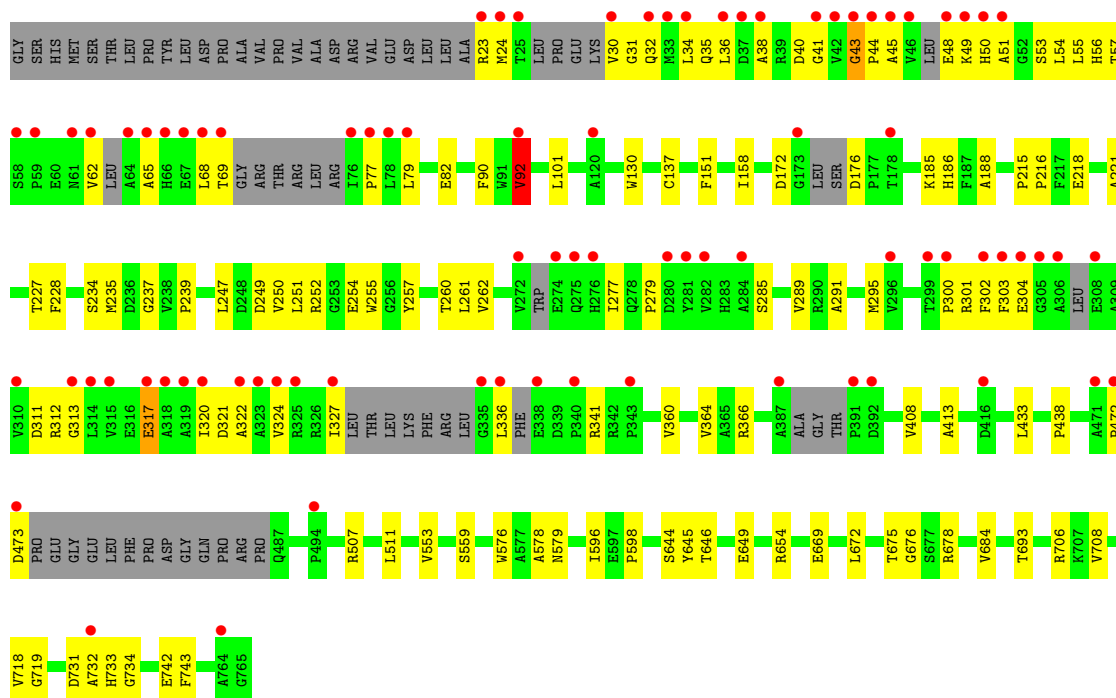
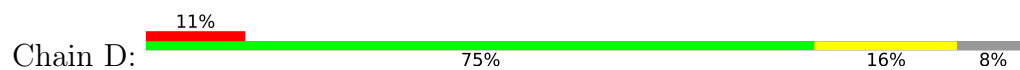


• Molecule 1: GH3 enzyme CcBgl3B





● Molecule 1: GH3 enzyme CcBgl3B



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.59Å 178.76Å 267.34Å 90.00° 100.76° 90.00°	Depositor
Resolution (Å)	19.93 – 2.40 19.93 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.93-2.40) 98.4 (19.93-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.41Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.189 , 0.225 0.192 , 0.223	Depositor DCC
R_{free} test set	2000 reflections (0.68%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34706	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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

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	0.42	0/5415	0.71	10/7385 (0.1%)
1	B	0.39	0/5746	0.66	5/7857 (0.1%)
1	C	0.36	0/5728	0.59	0/7831
1	D	0.37	0/5337	0.64	1/7284 (0.0%)
1	E	0.50	0/5749	0.73	7/7863 (0.1%)
1	F	0.52	0/5751	0.76	5/7864 (0.1%)
All	All	0.43	0/33726	0.68	28/46084 (0.1%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	ALA	CA-C-N	-7.54	110.18	120.28
1	A	286	ALA	C-N-CA	-7.54	110.18	120.28
1	A	333	ARG	N-CA-C	-7.50	103.09	111.71
1	E	623	GLN	N-CA-C	5.97	123.53	110.80
1	F	176	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	93	GLY	CA-C-N	-5.94	112.39	122.67
1	B	93	GLY	C-N-CA	-5.94	112.39	122.67
1	A	285	SER	N-CA-C	-5.87	104.84	112.23
1	F	625	GLY	CA-C-O	-5.75	118.31	122.45
1	F	185	LYS	N-CA-C	5.61	119.38	109.96
1	A	312	ARG	N-CA-C	-5.39	105.39	112.72
1	A	185	LYS	CA-C-N	5.37	131.80	121.54
1	A	185	LYS	C-N-CA	5.37	131.80	121.54
1	B	185	LYS	CA-C-N	5.36	131.77	121.54
1	B	185	LYS	C-N-CA	5.36	131.77	121.54
1	D	743	PHE	CA-CB-CG	5.34	119.14	113.80
1	E	302	PHE	CA-CB-CG	5.25	119.05	113.80
1	E	185	LYS	CA-C-N	5.24	130.06	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	185	LYS	C-N-CA	5.24	130.06	122.36
1	E	302	PHE	N-CA-C	-5.19	106.46	112.89
1	F	186	HIS	CB-CA-C	5.14	119.61	112.11
1	A	474	PRO	N-CA-C	-5.10	101.97	112.47
1	A	278	GLN	O-C-N	-5.09	116.81	121.34
1	F	187	PHE	CA-CB-CG	5.08	118.88	113.80
1	E	187	PHE	CA-CB-CG	5.05	118.85	113.80
1	B	627	ARG	CB-CG-CD	-5.03	99.74	111.30
1	E	186	HIS	CB-CA-C	5.02	118.25	111.82
1	A	62	VAL	N-CA-C	-5.01	105.50	110.62

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	5314	0	5202	79	0
1	B	5624	0	5533	61	0
1	C	5608	0	5519	59	0
1	D	5234	0	5101	77	0
1	E	5625	0	5534	59	0
1	F	5629	0	5538	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	203	0	0	4	0
3	B	236	0	0	5	0
3	C	205	0	0	5	0
3	D	136	0	0	1	0
3	E	414	0	0	4	0
3	F	472	0	0	4	0
All	All	34706	0	32427	360	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 6.

All (360) 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:137:CYS:SG	3:B:1087:HOH:O	2.25	0.93
1:F:137:CYS:SG	3:F:1247:HOH:O	2.32	0.87
1:B:181:LEU:HD21	1:B:334:LEU:HD21	1.62	0.80
1:A:46:VAL:HG23	1:A:50:HIS:HA	1.67	0.74
1:E:26:LEU:HD21	1:E:310:VAL:HG21	1.70	0.74
1:C:100:GLN:HE22	1:C:135:VAL:H	1.35	0.73
1:A:367:ARG:NH1	1:A:599:GLU:OE2	2.23	0.72
1:C:652:ASP:N	3:C:902:HOH:O	2.22	0.71
1:D:598:PRO:HG2	1:D:644:SER:HA	1.73	0.71
1:F:116:ALA:HB2	1:F:165:MET:HG3	1.73	0.70
1:B:266:ASP:HB3	1:B:270:ARG:HH21	1.54	0.70
1:D:35:GLN:HG3	1:D:53:SER:HB3	1.74	0.69
1:C:728:THR:HG22	1:C:738:VAL:HG22	1.73	0.69
1:B:265:TRP:O	1:B:270:ARG:NH2	2.27	0.67
1:E:654:ARG:NH1	1:E:669:GLU:OE1	2.27	0.67
1:A:55:LEU:HD11	1:A:265:TRP:HZ3	1.60	0.67
1:E:209:LEU:HD22	1:E:235:MET:HE1	1.77	0.67
1:D:34:LEU:HD22	1:D:36:LEU:HG	1.78	0.67
1:C:576:TRP:CZ2	1:C:578:ALA:HB2	2.31	0.65
1:F:656:LEU:HD11	1:F:669:GLU:HG3	1.77	0.65
1:C:576:TRP:CE2	1:C:578:ALA:HB2	2.33	0.64
1:B:626:VAL:HG23	1:B:627:ARG:HG3	1.77	0.64
1:E:591:LEU:HD11	1:E:598:PRO:HG3	1.79	0.64
1:B:229:MET:HE2	1:B:297:MET:HE1	1.80	0.64
1:D:218:GLU:OE1	1:D:255:TRP:NE1	2.30	0.64
1:D:250:VAL:HA	1:D:254:GLU:HG3	1.81	0.63
1:D:32:GLN:HG2	1:D:324:VAL:HG13	1.80	0.63
1:A:360:VAL:O	1:A:364:VAL:HG23	1.99	0.63
1:B:270:ARG:NE	3:B:901:HOH:O	2.31	0.62
1:C:3:THR:O	1:C:3:THR:OG1	2.13	0.62
1:B:185:LYS:NZ	3:B:910:HOH:O	2.31	0.62
1:F:591:LEU:HD11	1:F:598:PRO:HG3	1.81	0.62
1:D:732:ALA:O	1:D:734:GLY:N	2.33	0.62
1:A:576:TRP:CE2	1:A:578:ALA:HB2	2.34	0.62
1:B:88:HIS:CD2	1:B:123:VAL:HG22	2.35	0.61
1:A:54:LEU:HB2	1:A:78:LEU:HD13	1.83	0.61
1:C:627:ARG:NH1	3:C:906:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:667:ARG:NH1	1:C:721:GLU:OE2	2.34	0.61
1:E:20:LEU:HD21	1:E:76:ILE:HG12	1.83	0.60
1:B:561:PRO:HB3	1:B:606:PHE:CD1	2.36	0.60
1:C:137:CYS:HB3	1:C:191:SER:HB3	1.83	0.60
1:C:360:VAL:O	1:C:364:VAL:HG23	2.01	0.60
1:A:591:LEU:HD11	1:A:598:PRO:HG3	1.82	0.60
1:F:425:GLY:HA2	1:F:433:LEU:HD23	1.84	0.60
1:A:96:ILE:H	1:A:582:MET:HE2	1.65	0.60
1:D:654:ARG:NH2	1:D:669:GLU:OE1	2.35	0.60
1:B:431:ASP:OD1	1:B:432:TRP:HE3	1.85	0.60
1:D:69:THR:HG21	1:D:77:PRO:HA	1.84	0.60
1:A:137:CYS:HB3	1:A:191:SER:HB3	1.83	0.60
1:B:672:LEU:HD12	1:B:708:VAL:HG11	1.85	0.59
1:E:277:ILE:HA	1:F:693:THR:O	2.03	0.59
1:A:651:ALA:HB3	1:A:671:THR:HB	1.85	0.59
1:C:316:GLU:CD	1:C:316:GLU:H	2.10	0.59
1:B:266:ASP:HB3	1:B:270:ARG:NH2	2.18	0.58
1:D:77:PRO:HG2	1:D:336:LEU:HB3	1.85	0.58
1:B:360:VAL:O	1:B:364:VAL:HG23	2.04	0.58
1:A:277:ILE:HA	1:B:693:THR:O	2.04	0.58
1:C:661:GLY:O	1:C:724:VAL:HG11	2.03	0.58
1:D:172:ASP:HB2	1:D:176:ASP:HB2	1.84	0.58
1:D:732:ALA:C	1:D:734:GLY:H	2.11	0.58
1:A:54:LEU:HB2	1:A:78:LEU:CD1	2.34	0.57
1:C:597:GLU:OE1	1:C:678:ARG:NH1	2.36	0.57
1:A:32:GLN:O	1:A:33:MET:C	2.48	0.57
1:C:202:ALA:HB3	1:C:235:MET:HG2	1.84	0.57
1:A:285:SER:O	1:A:289:VAL:HG23	2.05	0.57
1:D:234:SER:HA	1:D:239:PRO:HA	1.87	0.56
1:A:9:PRO:HA	1:A:16:ARG:HH12	1.70	0.56
1:C:185:LYS:NZ	3:C:911:HOH:O	2.38	0.56
1:A:752:ARG:NH1	3:A:905:HOH:O	2.37	0.56
1:C:240:VAL:HA	1:C:243:ASN:HB2	1.88	0.56
1:E:329:THR:O	1:E:333:ARG:HG3	2.05	0.56
1:E:398:PRO:HG2	1:E:401:ALA:HB3	1.86	0.56
1:C:185:LYS:HD3	1:C:186:HIS:CE1	2.40	0.56
1:C:474:PRO:HD3	1:C:488:VAL:HG11	1.87	0.56
1:D:32:GLN:HG3	1:D:327:ILE:HD13	1.87	0.56
1:C:471:ALA:O	1:C:488:VAL:HG12	2.05	0.56
1:D:65:ALA:HA	1:D:68:LEU:HD12	1.87	0.55
1:A:207:ARG:NH2	3:A:909:HOH:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:HD11	1:B:68:LEU:HD22	1.89	0.55
1:A:252:ARG:NH1	1:A:257:TYR:O	2.40	0.55
1:F:342:ARG:NE	3:F:902:HOH:O	2.23	0.55
1:A:278:GLN:C	1:A:280:ASP:H	2.14	0.55
1:B:88:HIS:CD2	1:B:123:VAL:HA	2.42	0.55
1:D:34:LEU:CD2	1:D:36:LEU:HG	2.37	0.55
1:E:111:LEU:HG	1:E:364:VAL:HG22	1.89	0.55
1:A:344:ASP:O	1:A:348:GLN:HG3	2.07	0.54
1:C:672:LEU:HB3	1:C:710:LEU:HD11	1.89	0.54
1:C:626:VAL:HG23	1:C:627:ARG:HG3	1.90	0.54
1:D:57:THR:HG21	1:D:62:VAL:HG22	1.89	0.54
1:C:193:THR:HG22	1:C:202:ALA:HB2	1.89	0.54
1:D:285:SER:O	1:D:289:VAL:HG23	2.08	0.54
1:D:227:THR:HG22	1:D:260:THR:HB	1.89	0.54
1:C:703:LYS:NZ	3:C:914:HOH:O	2.41	0.54
1:A:46:VAL:HA	1:A:50:HIS:H	1.73	0.54
1:B:431:ASP:OD1	1:B:431:ASP:N	2.38	0.54
1:C:262:VAL:HG23	1:C:295:MET:HB2	1.90	0.54
1:D:247:LEU:HD12	1:D:291:ALA:HB1	1.90	0.54
1:E:621:ARG:HD2	1:E:699:GLU:HG2	1.89	0.53
1:E:185:LYS:HD3	1:E:186:HIS:CE1	2.43	0.53
1:A:276:HIS:O	1:B:692:VAL:HG13	2.09	0.53
1:A:345:VAL:O	1:A:349:GLN:HG3	2.09	0.53
1:C:154:ASP:OD1	1:C:617:TYR:OH	2.22	0.53
1:B:326:ARG:HD3	3:B:923:HOH:O	2.09	0.53
1:B:591:LEU:HD11	1:B:598:PRO:HG3	1.91	0.53
1:C:5:PRO:HG2	1:C:19:ASP:CG	2.33	0.53
1:B:326:ARG:NH2	3:B:917:HOH:O	2.41	0.53
1:C:746:ARG:NH2	1:C:753:GLU:OE1	2.41	0.53
1:A:315:VAL:HG22	1:A:316:GLU:H	1.73	0.53
1:E:347:ARG:HH21	1:E:351:VAL:HG11	1.75	0.52
1:C:753:GLU:OE2	1:C:758:ARG:NH1	2.42	0.52
1:A:527:ARG:NH2	3:A:914:HOH:O	2.42	0.52
1:A:654:ARG:NH1	1:A:669:GLU:OE2	2.42	0.52
1:D:576:TRP:CE2	1:D:578:ALA:HB2	2.45	0.52
1:F:576:TRP:CZ2	1:F:578:ALA:HB2	2.45	0.52
1:A:689:SER:HB3	1:A:744:GLU:HB3	1.90	0.52
1:C:638:ALA:N	1:C:641:GLU:OE1	2.32	0.51
1:C:696:THR:OG1	1:D:237:GLY:HA2	2.10	0.51
1:D:137:CYS:SG	1:D:186:HIS:HB2	2.51	0.51
1:D:251:LEU:HD21	1:D:261:LEU:HD21	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:VAL:HA	1:D:327:ILE:CG2	2.41	0.51
1:E:299:THR:N	3:E:908:HOH:O	2.37	0.51
1:A:692:VAL:HG22	1:B:276:HIS:HB3	1.93	0.51
1:B:706:ARG:NH1	1:B:719:GLY:O	2.44	0.51
1:C:408:VAL:HG12	1:C:413:ALA:HB1	1.92	0.51
1:E:137:CYS:SG	1:E:186:HIS:HB2	2.50	0.51
1:F:26:LEU:HB3	1:F:27:PRO:HD3	1.92	0.51
1:E:137:CYS:HB3	1:E:191:SER:HB3	1.93	0.51
1:C:277:ILE:HA	1:D:693:THR:O	2.11	0.51
1:C:693:THR:O	1:D:277:ILE:HA	2.10	0.51
1:A:53:SER:HA	1:A:78:LEU:HB3	1.92	0.51
1:B:47:LEU:CD1	1:B:68:LEU:HD22	2.40	0.51
1:B:576:TRP:CE2	1:B:578:ALA:HB2	2.46	0.51
1:C:100:GLN:NE2	3:C:905:HOH:O	2.30	0.51
1:F:66:HIS:HB3	1:F:342:ARG:NH2	2.25	0.50
1:A:277:ILE:HG13	1:A:278:GLN:HG2	1.91	0.50
1:B:431:ASP:OD1	1:B:432:TRP:CE3	2.64	0.50
1:D:45:ALA:HA	1:D:49:LYS:HB2	1.93	0.50
1:A:347:ARG:NH1	1:A:351:VAL:HG21	2.26	0.50
1:A:218:GLU:HB2	1:A:255:TRP:CZ2	2.47	0.50
1:E:100:GLN:HE22	1:E:135:VAL:HB	1.76	0.50
1:A:245:TRP:O	1:A:249:ASP:HB2	2.12	0.50
1:E:154:ASP:OD1	1:E:617:TYR:OH	2.22	0.50
1:D:188:ALA:O	1:D:235:MET:HE1	2.12	0.50
1:E:527:ARG:NH1	3:E:910:HOH:O	2.41	0.50
1:A:115:VAL:CG2	1:A:364:VAL:HG21	2.41	0.50
1:C:33:MET:HG2	1:C:294:ASP:O	2.11	0.49
1:D:38:ALA:C	1:D:40:ASP:H	2.20	0.49
1:B:239:PRO:CG	1:B:277:ILE:HD12	2.42	0.49
1:A:268:VAL:HA	1:A:271:MET:HE2	1.93	0.49
1:B:19:ASP:O	1:B:20:LEU:CB	2.60	0.49
1:B:239:PRO:HG3	1:B:277:ILE:HD12	1.93	0.49
1:C:135:VAL:HG22	1:C:185:LYS:HD2	1.93	0.49
1:D:511:LEU:HD11	1:D:553:VAL:HG23	1.94	0.49
1:C:249:ASP:O	1:C:254:GLU:HG3	2.11	0.49
1:E:18:GLU:HG3	1:E:21:LEU:HD12	1.94	0.49
1:A:84:CYS:HB2	1:A:131:THR:OG1	2.13	0.49
1:C:187:PHE:CE2	1:C:246:LEU:HG	2.47	0.49
1:B:239:PRO:HG3	1:B:277:ILE:CD1	2.42	0.49
1:F:726:ASP:OD2	3:F:901:HOH:O	2.20	0.48
1:A:659:GLU:OE2	1:A:764:ALA:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:ASP:HB3	1:E:325:ARG:HH21	1.78	0.48
1:A:638:ALA:O	1:A:641:GLU:HG2	2.13	0.48
1:B:47:LEU:HD11	1:B:68:LEU:HB3	1.95	0.48
1:D:34:LEU:HD23	1:D:35:GLN:N	2.28	0.48
1:B:132:PHE:HB3	1:B:185:LYS:HE3	1.95	0.48
1:F:576:TRP:CE2	1:F:578:ALA:HB2	2.48	0.48
1:C:390:THR:C	1:C:392:ASP:H	2.21	0.48
1:E:55:LEU:HD11	1:E:265:TRP:CZ3	2.49	0.48
1:B:115:VAL:CG2	1:B:364:VAL:HG21	2.43	0.48
1:D:708:VAL:HG21	1:D:718:VAL:HG21	1.96	0.48
1:E:576:TRP:CE2	1:E:578:ALA:HB2	2.48	0.48
1:F:88:HIS:CD2	1:F:123:VAL:HA	2.49	0.48
1:A:82:GLU:OE1	1:A:83:ASP:N	2.39	0.48
1:A:35:GLN:HG2	1:A:53:SER:HB3	1.96	0.48
1:A:35:GLN:HG2	1:A:53:SER:CB	2.44	0.48
1:B:408:VAL:HG12	1:B:413:ALA:HB1	1.95	0.48
1:F:44:PRO:HA	1:F:48:GLU:HG3	1.96	0.48
1:E:18:GLU:HA	1:E:21:LEU:HB2	1.95	0.48
1:A:669:GLU:HG2	1:A:719:GLY:HA2	1.96	0.48
1:D:249:ASP:O	1:D:254:GLU:HG3	2.14	0.47
1:D:324:VAL:HA	1:D:327:ILE:HG22	1.96	0.47
1:E:692:VAL:HG12	1:F:276:HIS:HB3	1.96	0.47
1:B:419:GLN:HG3	1:B:580:PRO:HD2	1.97	0.47
1:C:185:LYS:HG2	1:C:186:HIS:CD2	2.49	0.47
1:A:40:ASP:OD1	1:A:41:GLY:N	2.48	0.47
1:A:347:ARG:O	1:A:351:VAL:HG22	2.14	0.47
1:B:645:TYR:HB3	1:B:678:ARG:HD2	1.96	0.47
1:C:664:ASP:O	1:C:724:VAL:HG12	2.15	0.47
1:F:329:THR:O	1:F:333:ARG:HG3	2.14	0.47
1:D:320:ILE:O	1:D:324:VAL:HG23	2.14	0.47
1:D:300:PRO:C	1:D:302:PHE:H	2.22	0.47
1:E:576:TRP:CZ2	1:E:578:ALA:HB2	2.49	0.47
1:C:622:GLY:O	1:C:623:GLN:HB3	2.15	0.47
1:A:185:LYS:HE3	1:A:186:HIS:CE1	2.49	0.47
1:A:272:VAL:HG13	1:A:273:TRP:N	2.30	0.46
1:A:626:VAL:HG23	1:A:627:ARG:HG3	1.98	0.46
1:D:221:ALA:HB2	1:D:228:PHE:CZ	2.50	0.46
1:E:77:PRO:HD2	1:E:337:PHE:CZ	2.50	0.46
1:A:265:TRP:CE3	1:A:297:MET:HE3	2.50	0.46
1:B:46:VAL:HG22	1:B:78:LEU:HD21	1.96	0.46
1:C:558:ALA:O	1:C:578:ALA:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:HD12	1:B:47:LEU:N	2.30	0.46
1:D:185:LYS:HD2	1:D:186:HIS:NE2	2.31	0.46
1:D:576:TRP:CZ2	1:D:578:ALA:HB2	2.51	0.46
1:E:193:THR:HG22	1:E:202:ALA:HB2	1.97	0.46
1:D:731:ASP:HB2	3:D:931:HOH:O	2.14	0.46
1:A:148:ASP:HB3	1:A:559:SER:HB2	1.98	0.46
1:A:669:GLU:HA	1:A:718:VAL:O	2.16	0.46
1:A:185:LYS:HG2	1:A:186:HIS:CD2	2.51	0.46
1:B:580:PRO:HG2	1:B:584:GLY:HA3	1.98	0.46
1:C:409:VAL:HG21	1:C:545:LEU:HD11	1.97	0.46
1:E:136:LEU:HD12	1:E:136:LEU:N	2.31	0.46
1:B:230:LEU:CD1	1:B:261:LEU:HD11	2.46	0.46
1:C:656:LEU:HD11	1:C:669:GLU:OE1	2.16	0.46
1:C:674:ASN:HB2	1:C:710:LEU:HB3	1.98	0.45
1:D:53:SER:OG	1:D:79:LEU:O	2.32	0.45
1:D:646:THR:OG1	1:D:676:GLY:HA3	2.16	0.45
1:B:576:TRP:CZ2	1:B:578:ALA:HB2	2.50	0.45
1:D:645:TYR:HB3	1:D:678:ARG:HD2	1.98	0.45
1:E:24:MET:HE2	1:E:29:LYS:HA	1.99	0.45
1:F:207:ARG:HG3	1:F:730:VAL:HG12	1.98	0.45
1:B:441:MET:HE2	1:B:441:MET:HB3	1.84	0.45
1:E:525:GLU:O	1:E:527:ARG:NH2	2.50	0.45
1:D:732:ALA:C	1:D:734:GLY:N	2.75	0.45
1:E:408:VAL:HG12	1:E:413:ALA:HB1	1.99	0.45
1:D:304:GLU:OE1	1:D:304:GLU:N	2.41	0.45
1:B:744:GLU:OE2	1:B:758:ARG:HD3	2.16	0.45
1:C:77:PRO:O	1:C:331:LYS:NZ	2.44	0.45
1:D:215:PRO:HB2	1:D:216:PRO:HD3	1.98	0.45
1:E:26:LEU:HA	1:E:29:LYS:HD2	1.98	0.45
1:E:100:GLN:HG3	1:E:151:PHE:CE1	2.52	0.45
1:E:115:VAL:CG2	1:E:364:VAL:HG21	2.47	0.45
1:F:386:ARG:HG3	1:F:595:LEU:HD22	1.98	0.45
1:A:378:LEU:HA	1:A:379:PRO:C	2.42	0.45
1:E:746:ARG:HA	1:E:757:LEU:O	2.17	0.45
1:A:278:GLN:C	1:A:280:ASP:N	2.75	0.45
1:E:322:ALA:O	1:E:325:ARG:HG2	2.16	0.44
1:F:580:PRO:HG2	1:F:584:GLY:HA3	1.98	0.44
1:D:559:SER:HA	1:D:579:ASN:OD1	2.17	0.44
1:B:265:TRP:HD1	1:B:270:ARG:HH22	1.65	0.44
1:D:247:LEU:O	1:D:251:LEU:HB3	2.17	0.44
1:D:252:ARG:NH2	1:D:257:TYR:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HA	1:A:50:HIS:N	2.33	0.44
1:B:90:PHE:O	1:B:433:LEU:HD11	2.17	0.44
1:B:621:ARG:NH2	1:B:690:ASP:O	2.50	0.44
1:C:121:VAL:HG13	1:C:347:ARG:HH12	1.82	0.44
1:C:132:PHE:O	1:C:185:LYS:HE3	2.17	0.44
1:C:450:ARG:NH1	1:C:459:VAL:O	2.45	0.44
1:D:317:GLU:O	1:D:320:ILE:HB	2.18	0.44
1:E:244:GLY:O	1:E:248:ASP:HB2	2.18	0.44
1:D:706:ARG:NH1	1:D:719:GLY:O	2.50	0.44
1:F:229:MET:HG3	1:F:262:VAL:HG13	1.99	0.44
1:F:666:VAL:O	1:F:721:GLU:HA	2.18	0.44
1:A:170:GLN:HG2	1:A:180:ILE:O	2.18	0.44
1:A:207:ARG:NH1	1:A:730:VAL:O	2.42	0.44
1:A:321:ASP:O	1:A:325:ARG:HG3	2.18	0.44
1:A:344:ASP:HB3	1:A:347:ARG:HB3	1.99	0.44
1:C:419:GLN:HG3	1:C:580:PRO:HD2	2.00	0.44
1:B:16:ARG:O	1:B:19:ASP:O	2.35	0.44
1:A:32:GLN:HA	1:A:51:ALA:HA	2.00	0.43
1:C:270:ARG:HD2	1:C:274:GLU:OE1	2.17	0.43
1:C:231:GLY:O	1:C:240:VAL:CG1	2.65	0.43
1:B:230:LEU:O	1:B:264:ASP:HB2	2.17	0.43
1:A:408:VAL:HG12	1:A:413:ALA:HB1	2.00	0.43
1:A:420:LEU:HD21	1:A:582:MET:HG2	1.99	0.43
1:F:176:ASP:HA	1:F:177:PRO:HD3	1.89	0.43
1:A:651:ALA:HB2	3:A:907:HOH:O	2.19	0.43
1:D:312:ARG:N	1:D:312:ARG:HD2	2.34	0.43
1:F:137:CYS:HB3	1:F:191:SER:HB3	2.00	0.43
1:A:708:VAL:HG21	1:A:718:VAL:HG21	2.00	0.43
1:E:154:ASP:HA	1:E:155:PRO:HD3	1.89	0.43
1:B:163:SER:OG	1:B:167:ARG:NH1	2.51	0.43
1:D:321:ASP:O	1:D:322:ALA:C	2.59	0.43
1:B:732:ALA:C	1:B:734:GLY:H	2.27	0.43
1:D:55:LEU:HD13	1:D:56:HIS:CD2	2.54	0.43
1:D:408:VAL:HG12	1:D:413:ALA:HB1	2.01	0.43
1:A:38:ALA:HB1	1:A:42:VAL:HG13	2.01	0.43
1:B:24:MET:HE2	1:B:29:LYS:HA	2.00	0.43
1:E:322:ALA:HA	1:E:325:ARG:CZ	2.48	0.42
1:D:38:ALA:HB2	1:D:54:LEU:HD13	2.01	0.42
1:D:472:PRO:O	1:D:473:ASP:C	2.61	0.42
1:E:26:LEU:HG	1:E:307:LEU:CD2	2.49	0.42
1:A:56:HIS:HA	1:A:82:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:PRO:HG3	1:B:692:VAL:HG11	2.01	0.42
1:A:576:TRP:CZ2	1:A:578:ALA:HB2	2.54	0.42
1:D:311:ASP:OD2	1:D:312:ARG:NH1	2.52	0.42
1:E:6:TYR:HA	1:E:16:ARG:HG2	2.01	0.42
1:E:285:SER:O	1:E:289:VAL:HG23	2.20	0.42
1:B:597:GLU:OE1	1:B:678:ARG:HD3	2.19	0.42
1:D:360:VAL:O	1:D:364:VAL:HG23	2.18	0.42
1:F:88:HIS:CD2	1:F:123:VAL:HG22	2.54	0.42
1:D:101:LEU:HD12	1:D:101:LEU:HA	1.87	0.42
1:E:611:GLY:HA3	1:F:530:ALA:O	2.19	0.42
1:E:742:GLU:OE2	1:E:762:THR:OG1	2.37	0.42
1:E:100:GLN:NE2	1:E:135:VAL:HB	2.34	0.42
1:E:312:ARG:HG3	1:E:314:LEU:HG	2.01	0.42
1:F:64:ALA:O	1:F:68:LEU:HG	2.20	0.42
1:A:262:VAL:HA	1:A:295:MET:HB2	2.01	0.42
1:C:591:LEU:HD11	1:C:598:PRO:HG3	2.02	0.42
1:A:229:MET:HA	1:A:262:VAL:O	2.19	0.42
1:D:41:GLY:C	1:D:43:GLY:H	2.28	0.42
1:E:32:GLN:HB3	1:E:324:VAL:HG22	2.02	0.42
1:E:100:GLN:CG	1:E:151:PHE:CE1	3.03	0.42
1:F:654:ARG:NH1	3:F:905:HOH:O	2.26	0.42
1:B:626:VAL:HG23	1:B:627:ARG:CG	2.46	0.42
1:D:151:PHE:HB2	1:D:158:ILE:HG12	2.00	0.42
1:E:745:LEU:O	1:E:758:ARG:HA	2.20	0.42
1:F:110:ALA:O	1:F:114:GLN:HG3	2.20	0.42
1:A:732:ALA:O	1:A:733:HIS:HB2	2.20	0.42
1:A:91:TRP:NE1	1:A:352:ILE:HD13	2.35	0.41
1:D:92:VAL:O	1:D:438:PRO:HD3	2.20	0.41
1:D:649:GLU:HG3	1:D:675:THR:HG21	2.02	0.41
1:E:130:TRP:CZ3	1:E:295:MET:HE2	2.55	0.41
1:A:278:GLN:O	1:A:280:ASP:N	2.54	0.41
1:A:338:GLU:H	1:A:338:GLU:HG3	1.61	0.41
1:C:746:ARG:HA	1:C:757:LEU:O	2.19	0.41
1:D:235:MET:HE3	1:D:235:MET:HB2	1.66	0.41
1:F:425:GLY:HA2	1:F:433:LEU:CD2	2.50	0.41
1:B:137:CYS:HB3	1:B:191:SER:HB3	2.02	0.41
1:D:366:ARG:HG2	1:D:596:ILE:HD13	2.03	0.41
1:A:95:THR:HA	1:A:582:MET:CE	2.51	0.41
1:C:138:ILE:HD11	1:C:153:GLU:O	2.21	0.41
1:D:31:GLY:O	1:D:51:ALA:HA	2.21	0.41
1:E:132:PHE:HB3	1:E:185:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:ARG:NH2	3:E:941:HOH:O	2.53	0.41
1:E:295:MET:HE3	1:E:295:MET:HB3	1.91	0.41
1:E:450:ARG:HG2	1:E:450:ARG:HH11	1.85	0.41
1:E:455:GLU:HG2	3:E:1081:HOH:O	2.21	0.41
1:E:638:ALA:O	1:E:641:GLU:HG2	2.21	0.41
1:F:430:ALA:HB1	1:F:432:TRP:CE2	2.56	0.41
1:A:32:GLN:O	1:A:34:LEU:HB2	2.20	0.41
1:B:271:MET:HG2	1:B:277:ILE:HD11	2.02	0.41
1:D:44:PRO:HB2	1:D:48:GLU:HB3	2.02	0.41
1:D:130:TRP:CZ2	1:D:227:THR:HG21	2.55	0.41
1:D:311:ASP:C	1:D:313:GLY:H	2.28	0.41
1:D:669:GLU:HA	1:D:718:VAL:O	2.21	0.41
1:E:517:GLY:HA3	1:E:557:VAL:O	2.21	0.41
1:C:638:ALA:O	1:C:641:GLU:HG2	2.20	0.41
1:E:261:LEU:HD23	1:E:261:LEU:HA	1.92	0.40
1:F:202:ALA:HB2	1:F:233:GLN:HG3	2.03	0.40
1:A:132:PHE:CG	1:A:229:MET:HE1	2.56	0.40
1:D:30:VAL:HG12	1:D:303:PHE:CD1	2.56	0.40
1:D:90:PHE:O	1:D:433:LEU:HD11	2.21	0.40
1:D:672:LEU:HD11	1:D:684:VAL:CG2	2.51	0.40
1:A:136:LEU:HD23	1:A:216:PRO:HB2	2.01	0.40
1:C:137:CYS:SG	1:C:186:HIS:HB2	2.61	0.40
1:F:398:PRO:HG2	1:F:401:ALA:HB3	2.03	0.40
1:A:597:GLU:OE1	1:A:678:ARG:NH1	2.54	0.40
1:B:137:CYS:SG	1:B:186:HIS:HB2	2.61	0.40
1:B:247:LEU:HD22	1:B:261:LEU:HD21	2.02	0.40
1:C:347:ARG:NH1	1:C:351:VAL:HG11	2.36	0.40
1:E:78:LEU:HD23	1:E:78:LEU:HA	1.84	0.40
1:F:118:ALA:O	1:F:122:GLU:HG3	2.22	0.40
1:F:387:ALA:HB3	1:F:390:THR:CG2	2.52	0.40
1:B:72:THR:O	1:B:74:LEU:N	2.53	0.40
1:B:88:HIS:ND1	1:B:91:TRP:HB2	2.36	0.40
1:F:185:LYS:HG2	1:F:186:HIS:CE1	2.56	0.40
1:A:520:ILE:HD12	1:A:520:ILE:HA	1.97	0.40
1:D:56:HIS:HA	1:D:82:GLU:OE2	2.21	0.40
1:D:262:VAL:HA	1:D:295:MET:O	2.22	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	677/768 (88%)	631 (93%)	38 (6%)	8 (1%)	10	16
1	B	744/768 (97%)	702 (94%)	36 (5%)	6 (1%)	16	25
1	C	737/768 (96%)	706 (96%)	29 (4%)	2 (0%)	36	50
1	D	679/768 (88%)	629 (93%)	43 (6%)	7 (1%)	12	20
1	E	746/768 (97%)	702 (94%)	41 (6%)	3 (0%)	30	43
1	F	745/768 (97%)	715 (96%)	26 (4%)	4 (0%)	24	37
All	All	4328/4608 (94%)	4085 (94%)	213 (5%)	30 (1%)	18	28

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	623	GLN
1	E	733	HIS
1	F	416	ASP
1	A	309	ALA
1	B	20	LEU
1	B	416	ASP
1	F	4	LEU
1	F	175	SER
1	A	341	ARG
1	B	4	LEU
1	D	43	GLY
1	F	392	ASP
1	A	40	ASP
1	A	186	HIS
1	A	334	LEU
1	B	174	LEU
1	D	341	ARG
1	D	733	HIS
1	A	33	MET
1	B	186	HIS

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Mol	Chain	Res	Type
1	C	4	LEU
1	C	623	GLN
1	D	50	HIS
1	A	623	GLN
1	A	733	HIS
1	B	474	PRO
1	D	92	VAL
1	D	279	PRO
1	D	301	ARG
1	E	657	GLY

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	543/589 (92%)	521 (96%)	22 (4%)	27	46
1	B	573/589 (97%)	571 (100%)	2 (0%)	86	93
1	C	573/589 (97%)	571 (100%)	2 (0%)	86	93
1	D	530/589 (90%)	524 (99%)	6 (1%)	65	82
1	E	574/589 (98%)	574 (100%)	0	100	100
1	F	573/589 (97%)	566 (99%)	7 (1%)	63	81
All	All	3366/3534 (95%)	3327 (99%)	39 (1%)	63	81

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	67	GLU
1	F	165	MET
1	F	174	LEU
1	F	328	LEU
1	F	334	LEU
1	F	356	GLU
1	F	474	PRO
1	A	8	ASP

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Mol	Chain	Res	Type
1	A	13	VAL
1	A	32	GLN
1	A	34	LEU
1	A	42	VAL
1	A	46	VAL
1	A	49	LYS
1	A	54	LEU
1	A	55	LEU
1	A	63	LEU
1	A	68	LEU
1	A	75	ARG
1	A	280	ASP
1	A	285	SER
1	A	308	GLU
1	A	312	ARG
1	A	331	LYS
1	A	336	LEU
1	A	338	GLU
1	A	356	GLU
1	A	473	ASP
1	A	475	GLU
1	B	78	LEU
1	B	650	TYR
1	C	92	VAL
1	C	433	LEU
1	D	23	ARG
1	D	24	MET
1	D	92	VAL
1	D	317	GLU
1	D	507	ARG
1	D	742	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	100	GLN
1	E	349	GLN
1	E	417	HIS
1	F	276	HIS
1	F	623	GLN
1	F	633	GLN
1	A	32	GLN

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Mol	Chain	Res	Type
1	A	186	HIS
1	A	623	GLN
1	A	633	GLN
1	B	50	HIS
1	B	276	HIS
1	B	349	GLN
1	B	461	HIS
1	B	623	GLN
1	B	633	GLN
1	C	100	GLN
1	C	114	GLN
1	C	186	HIS
1	C	461	HIS
1	C	633	GLN
1	C	733	HIS
1	D	623	GLN
1	D	633	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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	709/768 (92%)	0.33	87 (12%) 8 6	37, 52, 122, 155	0
1	B	750/768 (97%)	-0.16	15 (2%) 65 60	37, 51, 73, 105	0
1	C	747/768 (97%)	-0.11	13 (1%) 69 65	30, 53, 76, 110	0
1	D	703/768 (91%)	0.48	83 (11%) 9 6	30, 60, 131, 154	0
1	E	750/768 (97%)	-0.20	32 (4%) 40 36	28, 40, 87, 102	0
1	F	751/768 (97%)	-0.50	11 (1%) 72 68	27, 38, 57, 110	0
All	All	4410/4608 (95%)	-0.03	241 (5%) 30 27	27, 50, 95, 155	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	VAL	8.4
1	A	51	ALA	7.2
1	A	13	VAL	6.8
1	D	64	ALA	6.7
1	A	11	VAL	6.6
1	A	46	VAL	6.5
1	D	25	THR	6.3
1	D	30	VAL	6.3
1	A	310	VAL	6.2
1	D	306	ALA	6.0
1	A	36	LEU	5.9
1	A	173	GLY	5.9
1	C	764	ALA	5.7
1	A	332	PHE	5.7
1	D	305	GLY	5.5
1	A	302	PHE	5.4
1	D	173	GLY	5.4
1	D	44	PRO	5.2
1	A	74	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	5.2
1	A	68	LEU	5.2
1	D	310	VAL	5.2
1	A	280	ASP	5.1
1	A	337	PHE	5.0
1	A	65	ALA	5.0
1	D	327	ILE	4.9
1	A	63	LEU	4.9
1	A	309	ALA	4.8
1	F	474	PRO	4.7
1	D	69	THR	4.7
1	A	62	VAL	4.7
1	D	62	VAL	4.7
1	F	765	GLY	4.7
1	D	320	ILE	4.6
1	F	174	LEU	4.6
1	D	303	PHE	4.6
1	A	474	PRO	4.6
1	B	474	PRO	4.6
1	A	284	ALA	4.6
1	D	324	VAL	4.4
1	C	657	GLY	4.4
1	D	42	VAL	4.3
1	D	92	VAL	4.3
1	A	10	ALA	4.3
1	D	24	MET	4.3
1	C	387	ALA	4.3
1	A	19	ASP	4.2
1	D	78	LEU	4.2
1	D	392	ASP	4.2
1	A	57	THR	4.1
1	B	92	VAL	4.1
1	D	336	LEU	4.1
1	A	77	PRO	4.1
1	A	78	LEU	4.1
1	A	336	LEU	4.1
1	A	9	PRO	4.0
1	C	92	VAL	4.0
1	A	300	PRO	4.0
1	D	59	PRO	4.0
1	A	38	ALA	4.0
1	A	54	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	68	LEU	4.0
1	E	11	VAL	4.0
1	A	387	ALA	3.9
1	D	58	SER	3.9
1	D	61	ASN	3.9
1	A	286	ALA	3.9
1	A	58	SER	3.9
1	D	335	GLY	3.8
1	D	76	ILE	3.8
1	A	299	THR	3.7
1	A	50	HIS	3.7
1	A	334	LEU	3.7
1	D	282	VAL	3.7
1	D	322	ALA	3.7
1	E	316	GLU	3.6
1	A	80	LEU	3.6
1	E	5	PRO	3.6
1	A	389	GLY	3.6
1	D	23	ARG	3.6
1	D	46	VAL	3.6
1	D	45	ALA	3.6
1	E	63	LEU	3.6
1	D	272	VAL	3.6
1	A	14	ALA	3.5
1	A	279	PRO	3.5
1	A	49	LYS	3.4
1	C	3	THR	3.4
1	E	388	ALA	3.4
1	D	391	PRO	3.4
1	D	43	GLY	3.4
1	A	45	ALA	3.3
1	A	33	MET	3.3
1	A	8	ASP	3.3
1	D	281	TYR	3.3
1	A	53	SER	3.2
1	D	471	ALA	3.2
1	A	61	ASN	3.2
1	D	77	PRO	3.2
1	D	50	HIS	3.2
1	B	764	ALA	3.2
1	A	66	HIS	3.2
1	D	314	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	387	ALA	3.1
1	A	32	GLN	3.1
1	B	392	ASP	3.1
1	E	30	VAL	3.1
1	D	49	LYS	3.1
1	D	51	ALA	3.1
1	B	473	ASP	3.1
1	A	175	SER	3.1
1	B	41	GLY	3.1
1	F	92	VAL	3.1
1	D	387	ALA	3.0
1	D	274	GLU	3.0
1	A	314	LEU	3.0
1	A	272	VAL	3.0
1	D	323	ALA	3.0
1	E	317	GLU	3.0
1	D	48	GLU	3.0
1	D	65	ALA	3.0
1	D	473	ASP	3.0
1	D	302	PHE	3.0
1	A	338	GLU	2.9
1	E	765	GLY	2.9
1	A	34	LEU	2.9
1	A	285	SER	2.9
1	E	27	PRO	2.9
1	E	13	VAL	2.8
1	E	20	LEU	2.8
1	A	16	ARG	2.8
1	D	338	GLU	2.8
1	D	41	GLY	2.8
1	D	299	THR	2.8
1	A	127	GLY	2.7
1	A	275	GLN	2.7
1	A	475	GLU	2.7
1	D	472	PRO	2.7
1	E	92	VAL	2.7
1	F	473	ASP	2.7
1	E	303	PHE	2.7
1	D	313	GLY	2.7
1	A	277	ILE	2.7
1	A	273	TRP	2.7
1	A	312	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	658	THR	2.7
1	E	14	ALA	2.7
1	A	343	PRO	2.6
1	A	55	LEU	2.6
1	D	34	LEU	2.6
1	E	473	ASP	2.6
1	A	75	ARG	2.6
1	A	330	LEU	2.6
1	A	41	GLY	2.6
1	E	71	ARG	2.6
1	D	317	GLU	2.6
1	D	319	ALA	2.6
1	D	764	ALA	2.6
1	E	70	GLY	2.6
1	A	37	ASP	2.6
1	A	311	ASP	2.6
1	D	37	ASP	2.6
1	E	74	LEU	2.6
1	A	301	ARG	2.5
1	D	325	ARG	2.5
1	C	474	PRO	2.5
1	A	320	ILE	2.5
1	B	175	SER	2.5
1	E	325	ARG	2.5
1	C	232	TYR	2.5
1	D	33	MET	2.5
1	D	36	LEU	2.5
1	D	32	GLN	2.5
1	E	319	ALA	2.5
1	A	463	ARG	2.5
1	D	340	PRO	2.5
1	A	313	GLY	2.5
1	B	174	LEU	2.5
1	F	388	ALA	2.5
1	B	3	THR	2.5
1	D	318	ALA	2.5
1	F	93	GLY	2.4
1	B	622	GLY	2.4
1	A	79	LEU	2.4
1	A	56	HIS	2.4
1	D	315	VAL	2.4
1	A	339	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	390	THR	2.4
1	A	390	THR	2.4
1	A	622	GLY	2.4
1	E	328	LEU	2.4
1	A	392	ASP	2.4
1	D	276	HIS	2.4
1	F	387	ALA	2.4
1	E	304	GLU	2.4
1	A	340	PRO	2.3
1	D	275	GLN	2.3
1	D	178	THR	2.3
1	E	6	TYR	2.3
1	C	399	ALA	2.3
1	D	300	PRO	2.3
1	E	12	PRO	2.3
1	E	318	ALA	2.3
1	C	622	GLY	2.3
1	E	26	LEU	2.3
1	D	416	ASP	2.3
1	D	343	PRO	2.2
1	D	66	HIS	2.2
1	A	331	LYS	2.2
1	A	15	ASP	2.2
1	C	669	GLU	2.2
1	E	59	PRO	2.2
1	A	315	VAL	2.2
1	D	38	ALA	2.2
1	D	732	ALA	2.2
1	E	332	PHE	2.2
1	F	175	SER	2.2
1	D	67	GLU	2.2
1	D	494	PRO	2.2
1	E	282	VAL	2.1
1	D	308	GLU	2.1
1	A	473	ASP	2.1
1	E	46	VAL	2.1
1	A	276	HIS	2.1
1	B	578	ALA	2.1
1	F	3	THR	2.1
1	D	79	LEU	2.1
1	A	296	VAL	2.1
1	D	296	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	120	ALA	2.1
1	A	333	ARG	2.1
1	D	304	GLU	2.1
1	D	280	ASP	2.1
1	B	732	ALA	2.1
1	D	284	ALA	2.1
1	C	390	THR	2.1
1	E	47	LEU	2.0
1	C	732	ALA	2.0
1	B	389	GLY	2.0
1	E	69	THR	2.0
1	C	473	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

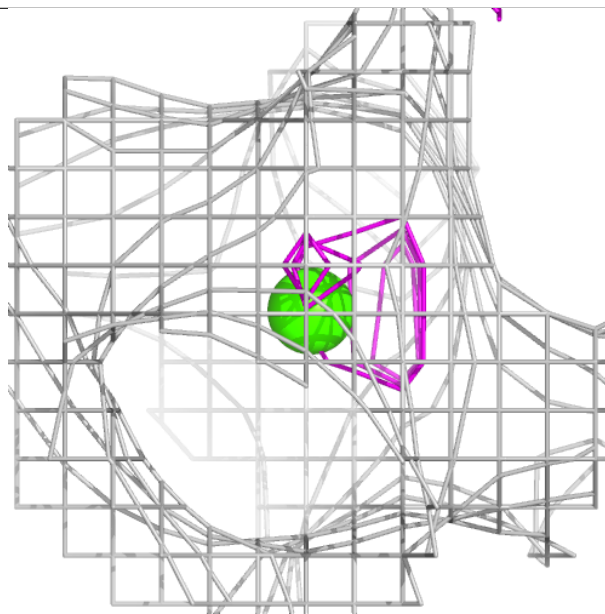
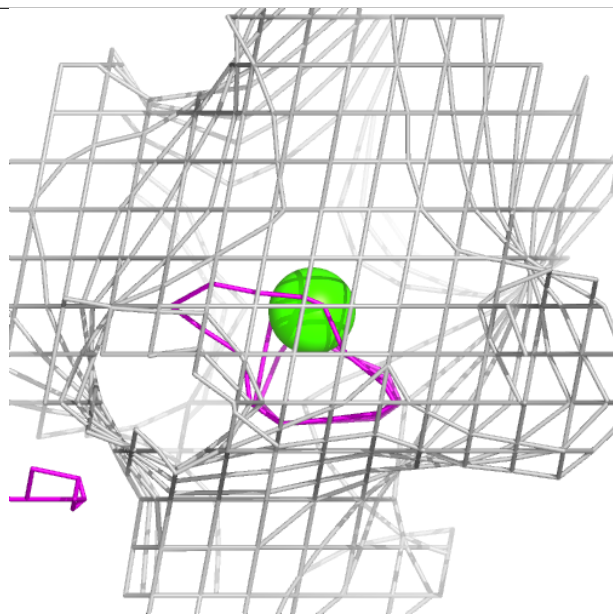
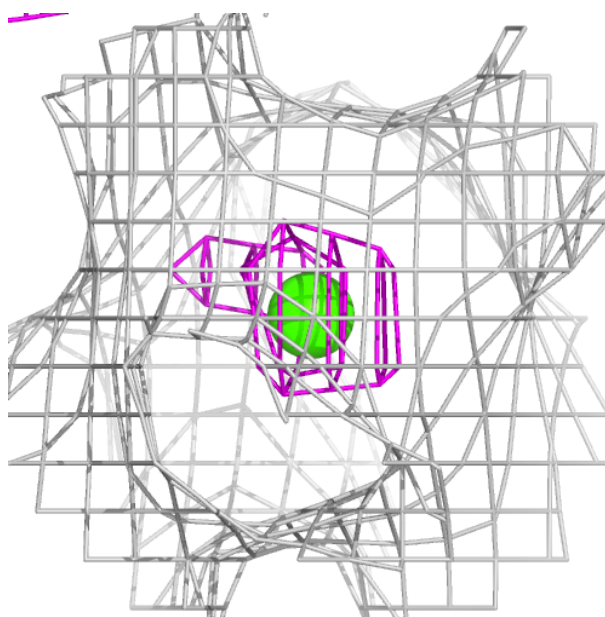
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	801	1/1	0.96	0.11	71,71,71,71	0
2	CA	C	801	1/1	0.96	0.05	84,84,84,84	0
2	CA	E	801	1/1	0.99	0.05	53,53,53,53	0
2	CA	B	801	1/1	0.99	0.03	74,74,74,74	0
2	CA	F	801	1/1	0.99	0.03	55,55,55,55	0
2	CA	D	801	1/1	0.99	0.04	71,71,71,71	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

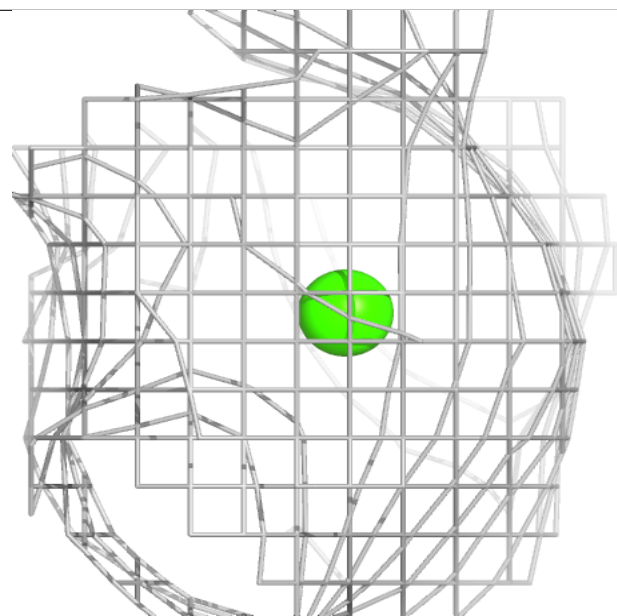
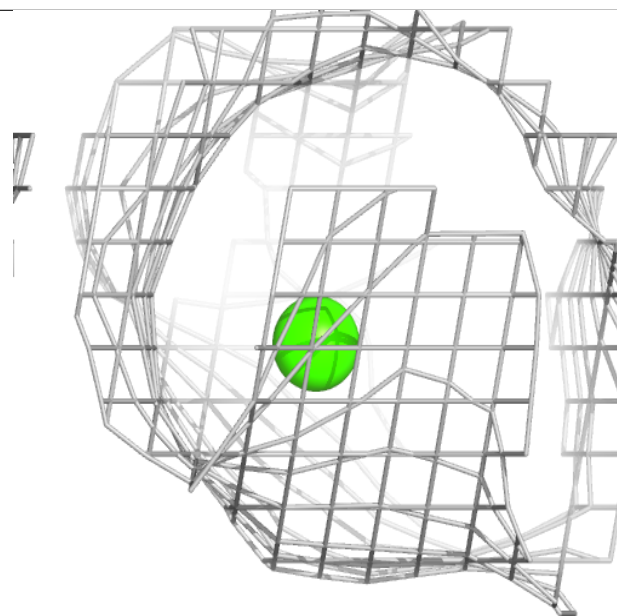
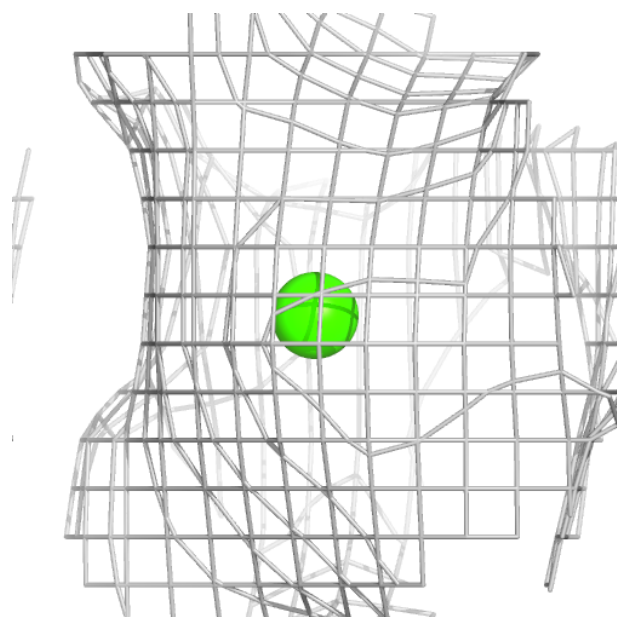
Electron density around CA A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



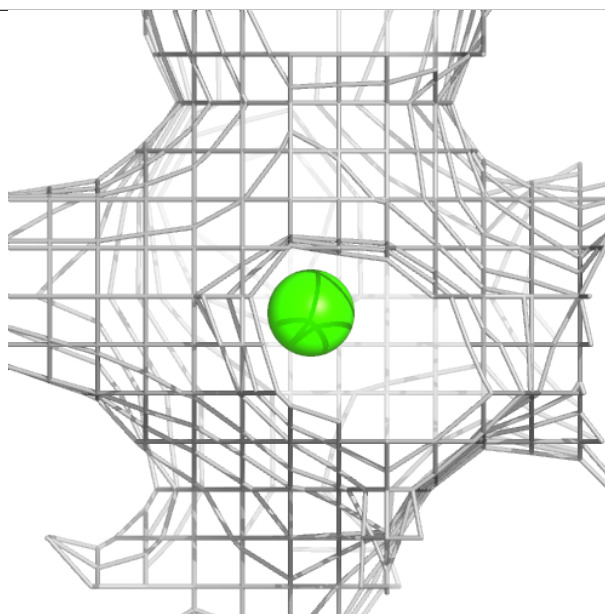
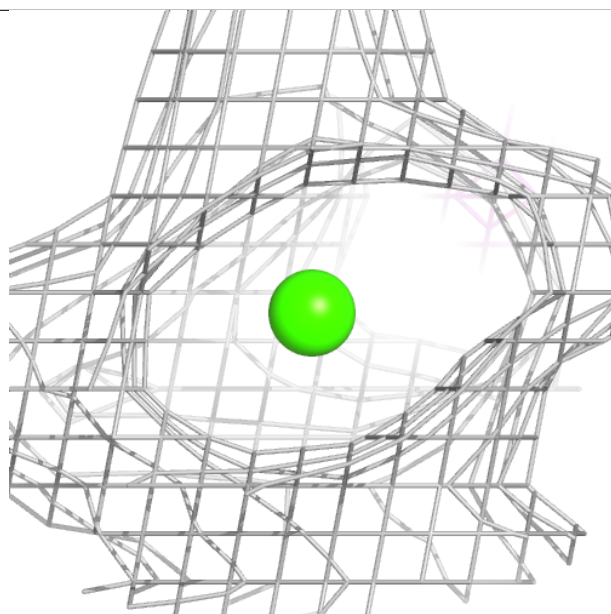
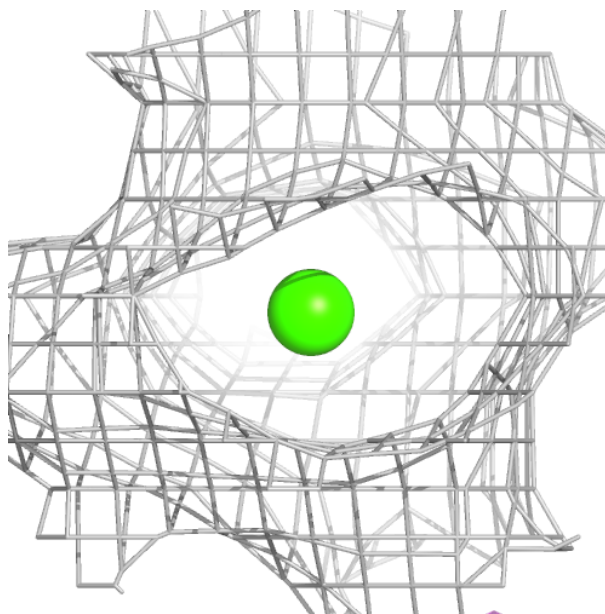
Electron density around CA C 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



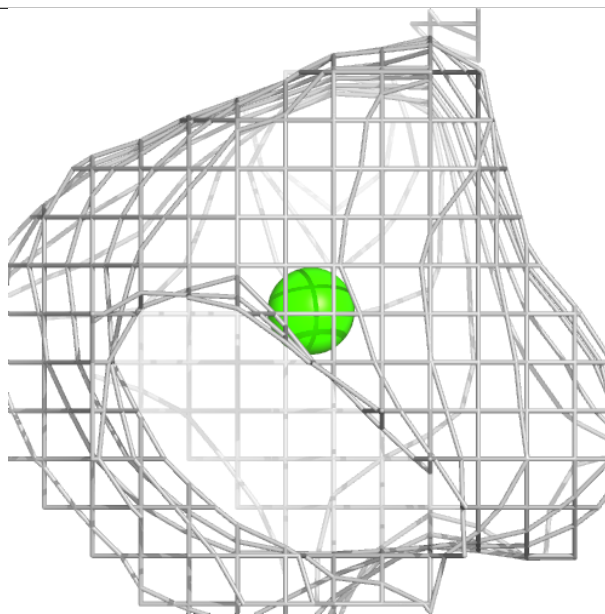
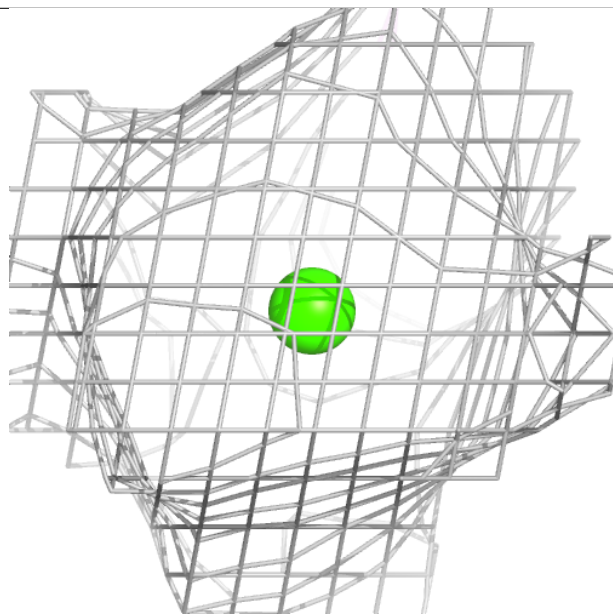
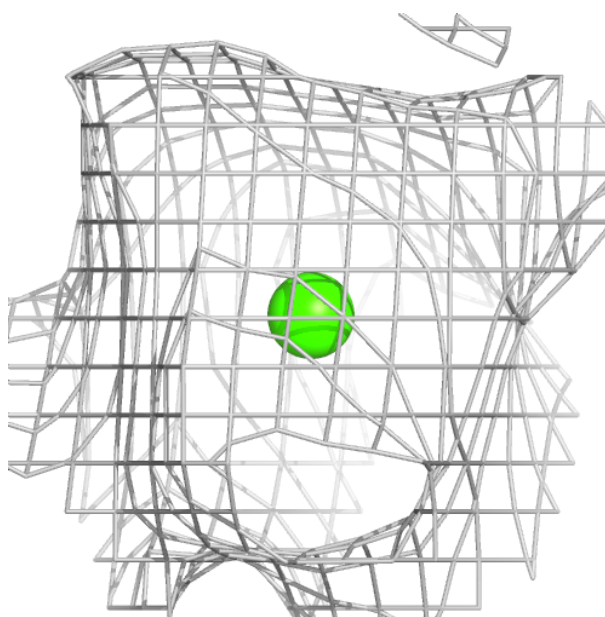
Electron density around CA E 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



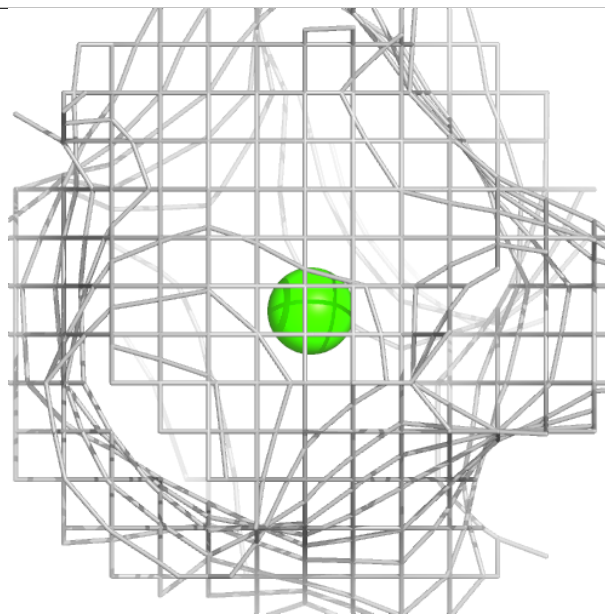
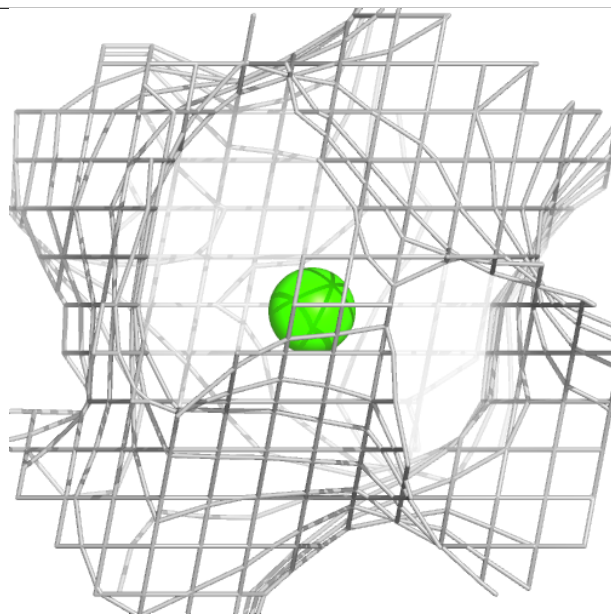
Electron density around CA B 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



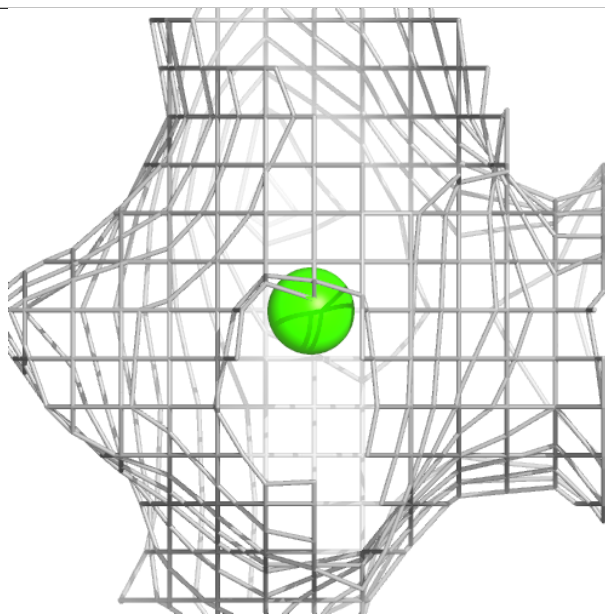
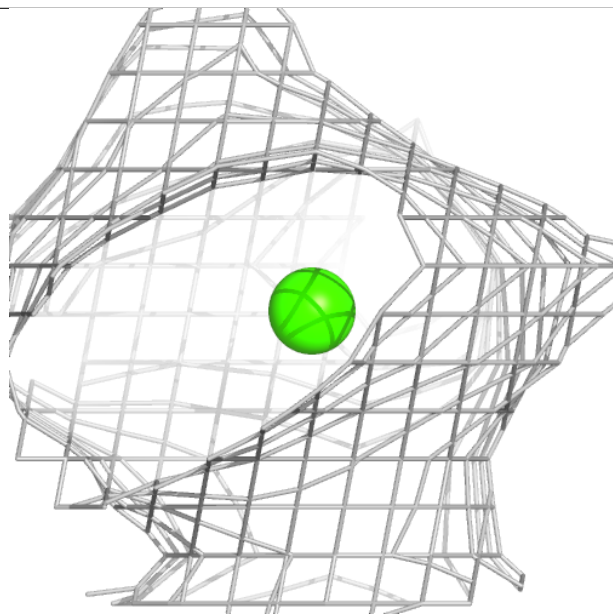
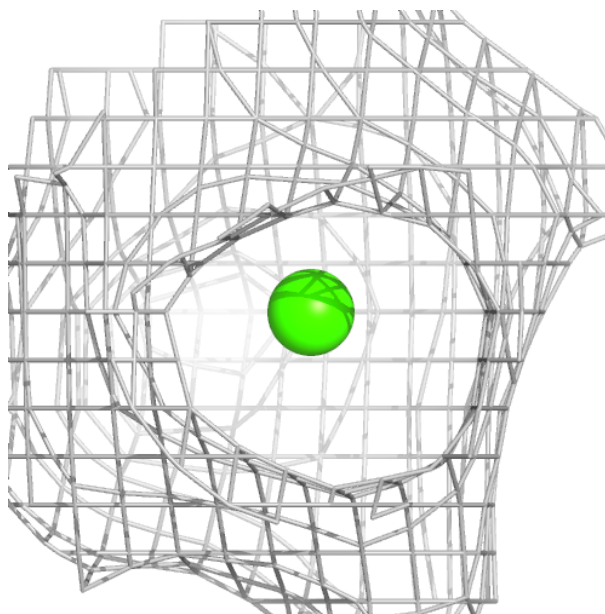
Electron density around CA F 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA D 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.