



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:00 AM UTC

PDB ID : 6AD7 / pdb_00006ad7
Title : Crystal structure of the E148D mutant CLC-ec1 in 20 mM bromide
Authors : Lim, H.-H.; Park, K.
Deposited on : 2018-07-31
Resolution : 2.95 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

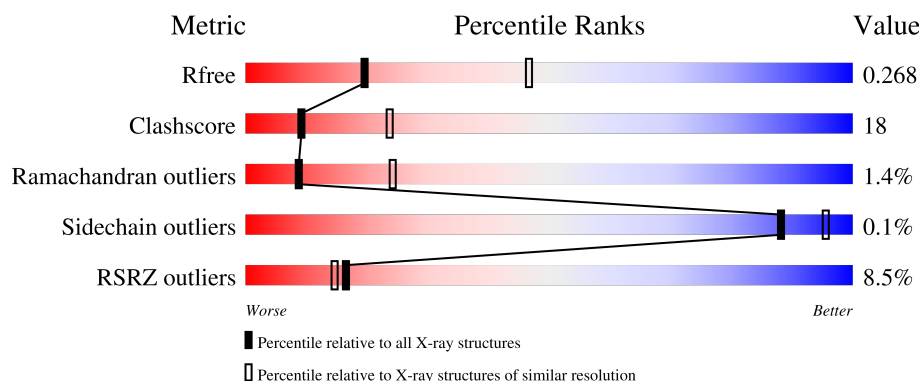
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	473	11% 62% 31% 6%
1	B	473	6% 60% 33% 7%
2	C	222	9% 69% 29% .
2	E	222	9% 76% 23% .
3	D	211	8% 63% 36% .

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Mol	Chain	Length	Quality of chain
3	F	211	6% 74% 24%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13243 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 H(+)/Cl(-) exchange transporter ClcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3332	2189	560	563	20			
1	B	442	Total	C	N	O	S	0	0	0
			3314	2179	557	558	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	ASP	GLU	engineered mutation	UNP P37019
B	148	ASP	GLU	engineered mutation	UNP P37019

- Molecule 2 is a protein called antibody Fab fragment heavy chain.

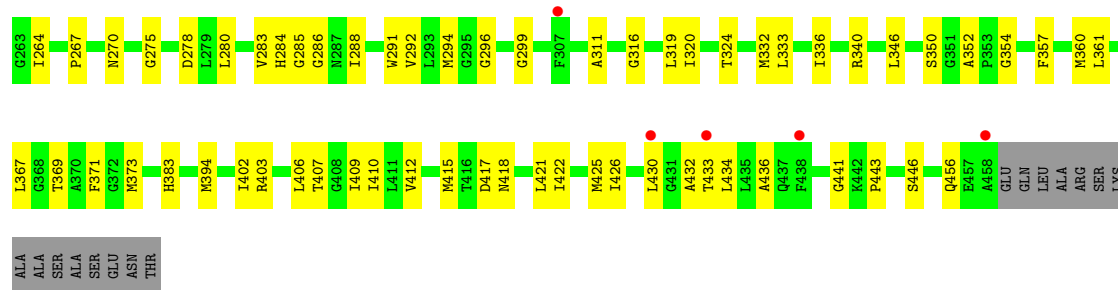
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total	C	N	O	S	0	0	0
			1681	1082	275	318	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called antibody Fab fragment light chain.

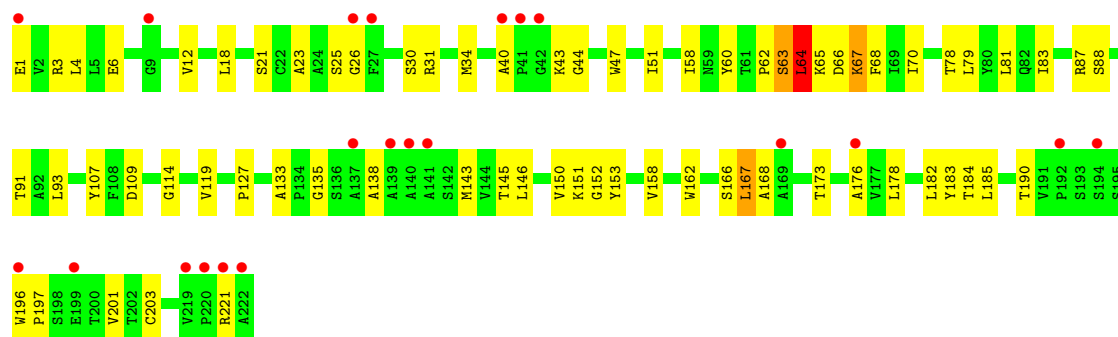
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

- Molecule 4 is BROMIDE ION (CCD ID: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

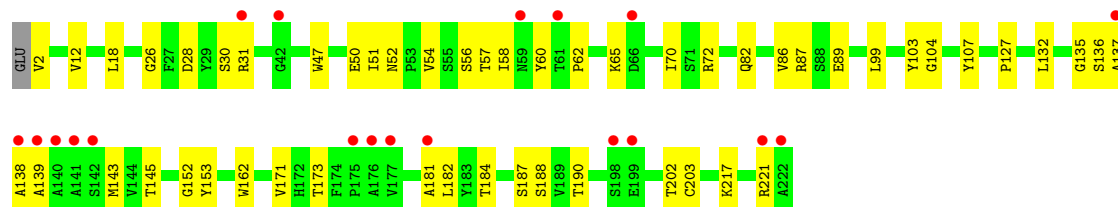
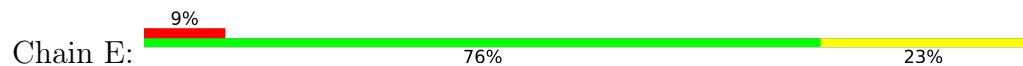
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Br 1	0	0
4	B	1	Total 1	Br 1	0	0



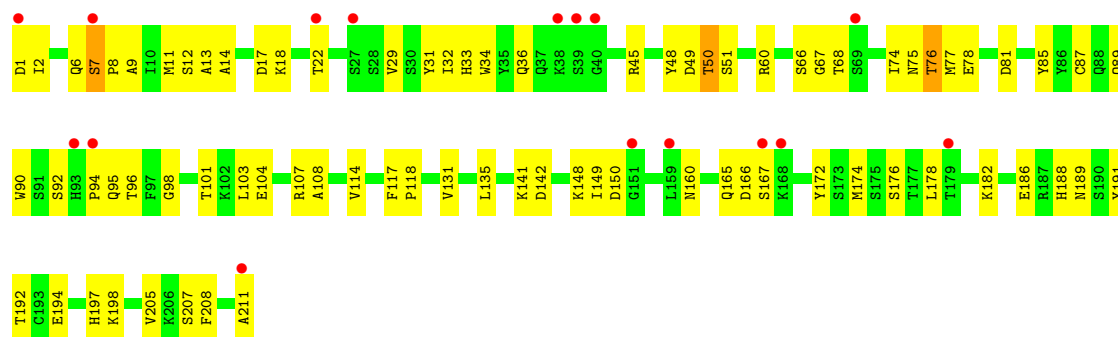
- Molecule 2: antibody Fab fragment heavy chain



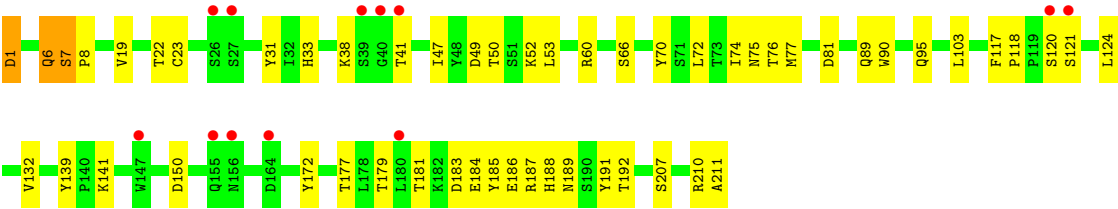
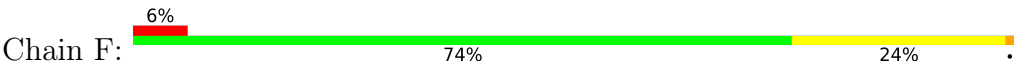
- Molecule 2: antibody Fab fragment heavy chain



- Molecule 3: antibody Fab fragment light chain



- Molecule 3: antibody Fab fragment light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	233.18Å 97.61Å 170.80Å 90.00° 131.79° 90.00°	Depositor
Resolution (Å)	49.04 – 2.95 49.04 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.04-2.95) 96.1 (49.04-2.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.223 , 0.269 0.222 , 0.268	Depositor DCC
R_{free} test set	2889 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13243	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: BR

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	0/3404	0.65	1/4620 (0.0%)
1	B	0.42	0/3386	0.65	2/4596 (0.0%)
2	C	0.50	0/1730	0.73	3/2367 (0.1%)
2	E	0.43	0/1721	0.68	0/2355
3	D	0.47	0/1660	0.74	0/2257
3	F	0.47	0/1660	0.74	2/2257 (0.1%)
All	All	0.44	0/13561	0.69	8/18452 (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
2	C	0	1
3	F	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	LEU	CA-C-N	-6.03	118.02	122.18
1	B	145	LEU	C-N-CA	-6.03	118.02	122.18
2	C	63	SER	CA-C-N	5.60	132.24	121.54
2	C	63	SER	C-N-CA	5.60	132.24	121.54
3	F	6	GLN	CA-C-N	5.50	135.23	121.80
3	F	6	GLN	C-N-CA	5.50	135.23	121.80
2	C	64	LEU	CA-CB-CG	5.25	134.69	116.30
1	A	220	ILE	CG1-CB-CG2	-5.22	95.03	110.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	66	ASP	Peptide
3	F	75	ASN	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	3332	0	3482	152	0
1	B	3314	0	3466	157	0
2	C	1681	0	1663	63	0
2	E	1672	0	1654	37	0
3	D	1621	0	1546	67	0
3	F	1621	0	1546	59	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
All	All	13243	0	13357	484	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (484) 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:A:150:PRO:O	1:A:154:ILE:HD12	1.41	1.19
1:A:430:LEU:HD22	1:B:223:ILE:CD1	1.79	1.12
1:A:430:LEU:HD22	1:B:223:ILE:HD11	1.34	1.09
1:A:119:GLN:HE21	1:B:18:ARG:HD3	1.15	1.08
1:B:17:ARG:HG2	1:B:20:GLN:HG2	1.33	1.06
1:A:150:PRO:C	1:A:154:ILE:HD12	1.82	1.05
1:A:119:GLN:NE2	1:B:18:ARG:HD3	1.72	1.05
2:C:60:TYR:HE2	2:C:70:ILE:HD12	1.22	1.01
2:C:60:TYR:CE2	2:C:70:ILE:CD1	2.44	0.99
3:D:95:GLN:OE1	3:D:95:GLN:N	1.99	0.95
1:A:223:ILE:HD11	1:B:430:LEU:HD13	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:THR:HG22	1:A:390:ALA:HB2	1.51	0.92
2:C:60:TYR:CE2	2:C:70:ILE:HD13	2.07	0.90
2:C:60:TYR:HE2	2:C:70:ILE:CD1	1.80	0.89
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.55	0.88
2:E:60:TYR:HE2	2:E:70:ILE:HD12	1.39	0.88
1:B:360:MET:HE1	1:B:402:ILE:CD1	2.04	0.86
3:F:7:SER:HB2	3:F:22:THR:H	1.38	0.86
1:B:360:MET:HE1	1:B:402:ILE:HD13	1.57	0.86
1:A:457:GLU:OE2	1:B:18:ARG:NH1	2.07	0.85
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.59	0.84
3:F:95:GLN:OE1	3:F:95:GLN:N	2.09	0.84
1:B:59:TRP:CZ2	1:B:63:GLN:NE2	2.46	0.82
2:E:60:TYR:CE2	2:E:70:ILE:HD12	2.14	0.82
3:F:77:MET:CE	3:F:103:LEU:HD21	2.09	0.82
1:A:101:ALA:HB3	1:A:130:VAL:HG11	1.62	0.81
2:C:91:THR:HG22	2:C:119:VAL:H	1.46	0.81
1:A:150:PRO:C	1:A:154:ILE:CD1	2.53	0.81
1:B:403:ARG:NH2	1:B:436:ALA:HB1	1.95	0.80
1:A:123:ARG:HH21	1:A:126:ARG:HH11	1.30	0.80
3:F:1:ASP:N	3:F:1:ASP:OD1	2.13	0.80
1:B:198:LEU:HD12	1:B:410:ILE:HD12	1.62	0.79
3:D:89:GLN:HE21	3:D:92:SER:H	1.27	0.79
1:B:176:THR:HG22	1:B:213:ILE:HA	1.64	0.79
1:A:219:PHE:CD2	1:B:430:LEU:HD11	2.18	0.78
3:F:7:SER:CB	3:F:22:THR:H	1.95	0.78
2:C:60:TYR:CE2	2:C:70:ILE:HD12	2.10	0.77
3:F:141:LYS:H	3:F:141:LYS:HD2	1.48	0.77
1:A:110:PRO:HG2	1:A:448:ILE:HD11	1.67	0.76
3:D:89:GLN:NE2	3:D:92:SER:H	1.84	0.76
1:B:316:GLY:O	1:B:319:LEU:HD23	1.86	0.75
3:F:77:MET:HE2	3:F:103:LEU:HD21	1.68	0.75
1:A:207:GLN:OE1	1:B:28:ARG:NH1	2.19	0.75
3:D:60:ARG:NH2	3:D:81:ASP:OD1	2.19	0.75
3:F:121:SER:HA	3:F:124:LEU:HD21	1.69	0.75
2:E:89:GLU:N	2:E:89:GLU:OE1	2.19	0.74
2:C:64:LEU:HD23	2:C:65:LYS:H	1.51	0.74
1:B:68:LEU:HD11	1:B:78:LEU:HB2	1.70	0.73
3:F:95:GLN:H	3:F:95:GLN:CD	1.95	0.73
3:F:141:LYS:HG3	3:F:172:TYR:CE1	2.24	0.73
3:D:6:GLN:HE21	3:D:98:GLY:HA3	1.54	0.73
3:D:95:GLN:H	3:D:95:GLN:CD	1.96	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:SER:HB3	3:D:22:THR:HB	1.70	0.72
3:D:141:LYS:HB3	3:D:172:TYR:CE2	2.25	0.72
2:E:135:GLY:O	2:E:137:ALA:N	2.21	0.72
1:A:430:LEU:HD22	1:B:223:ILE:HD12	1.72	0.72
1:A:219:PHE:CE2	1:B:430:LEU:HD11	2.24	0.72
1:B:332:MET:O	1:B:336:ILE:HG13	1.89	0.71
1:A:19:ARG:HA	1:A:22:ILE:HD12	1.71	0.71
1:A:430:LEU:CD2	1:B:223:ILE:CD1	2.64	0.71
1:A:426:ILE:HG23	1:B:219:PHE:CE2	2.26	0.71
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.71	0.71
1:A:206:PRO:HD2	1:A:211:THR:HG21	1.73	0.70
2:C:67:LYS:HG3	2:C:68:PHE:H	1.58	0.69
1:A:119:GLN:OE1	1:A:119:GLN:O	2.11	0.69
1:A:255:TYR:HB3	1:A:428:THR:HG23	1.75	0.68
3:F:77:MET:HE1	3:F:103:LEU:HD11	1.76	0.68
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.76	0.68
2:E:47:TRP:CD2	3:F:95:GLN:NE2	2.62	0.68
1:B:98:ARG:HH21	1:B:102:PRO:HB3	1.57	0.68
1:A:75:TYR:CE1	1:A:79:LEU:HD11	2.29	0.67
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.10	0.67
1:B:280:LEU:O	1:B:283:VAL:HG12	1.95	0.66
3:D:141:LYS:HA	3:D:172:TYR:HD2	1.59	0.66
3:D:189:ASN:HD21	3:D:211:ALA:H	1.41	0.66
1:A:148:ASP:O	1:A:152:VAL:HG12	1.95	0.66
1:B:57:VAL:O	1:B:61:GLN:HG3	1.96	0.66
2:E:202:THR:HG22	2:E:217:LYS:HA	1.77	0.66
1:A:234:HIS:O	1:A:235:GLU:HB2	1.95	0.66
1:A:369:THR:HG22	1:A:390:ALA:CB	2.26	0.66
2:E:47:TRP:CG	3:F:95:GLN:NE2	2.64	0.66
1:B:98:ARG:HB2	1:B:288:ILE:HD12	1.78	0.65
1:A:403:ARG:NH1	1:B:29:ASP:OD1	2.27	0.65
3:D:107:ARG:NH1	3:D:108:ALA:O	2.29	0.65
3:F:139:TYR:CZ	3:F:141:LYS:NZ	2.63	0.65
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.31	0.65
1:A:217:ALA:O	1:A:220:ILE:HG22	1.95	0.65
1:B:59:TRP:O	1:B:63:GLN:OE1	2.13	0.65
1:A:361:LEU:O	1:A:365:THR:HG23	1.97	0.65
1:A:423:LEU:HD13	1:B:230:ARG:HH21	1.62	0.64
3:F:19:VAL:HG21	3:F:77:MET:HE3	1.79	0.64
1:A:120:ARG:HG3	1:A:121:PRO:HD2	1.78	0.64
1:A:200:ILE:HA	1:A:204:MET:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:141:LYS:HB3	3:D:172:TYR:CD2	2.33	0.63
1:A:211:THR:HB	1:A:213:ILE:HD12	1.81	0.63
1:A:110:PRO:CG	1:A:448:ILE:HD11	2.28	0.63
1:B:98:ARG:CB	1:B:288:ILE:HD12	2.28	0.63
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.34	0.63
3:D:14:ALA:O	3:D:17:ASP:HB3	1.98	0.63
3:D:160:ASN:OD1	3:D:176:SER:OG	2.11	0.63
1:A:434:LEU:HD11	1:B:220:ILE:HD11	1.80	0.63
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.33	0.63
1:B:125:TRP:CD1	1:B:126:ARG:HG2	2.34	0.62
2:E:143:MET:HE3	2:E:190:THR:HG22	1.81	0.62
1:B:88:VAL:HA	1:B:91:MET:HE2	1.80	0.62
3:F:132:VAL:HG12	3:F:177:THR:HG23	1.82	0.62
1:A:83:PHE:HD1	1:A:84:LEU:HD23	1.64	0.62
1:B:360:MET:HE1	1:B:402:ILE:HD11	1.79	0.62
3:F:7:SER:HB2	3:F:22:THR:N	2.13	0.62
1:A:62:ASN:OD1	1:A:63:GLN:N	2.32	0.62
2:E:137:ALA:O	2:E:139:ALA:N	2.32	0.62
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.33	0.62
1:A:126:ARG:O	1:A:130:VAL:HG12	1.99	0.62
1:B:17:ARG:O	1:B:19:ARG:N	2.33	0.62
1:A:430:LEU:CD2	1:B:223:ILE:HD12	2.27	0.61
1:B:71:THR:HG21	1:B:81:VAL:HG11	1.83	0.61
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.83	0.61
3:D:189:ASN:HD21	3:D:211:ALA:N	1.98	0.61
1:B:17:ARG:CG	1:B:20:GLN:HG2	2.20	0.61
1:B:422:ILE:HA	1:B:425:MET:HE3	1.82	0.61
2:E:60:TYR:CE2	2:E:70:ILE:CD1	2.84	0.61
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.83	0.60
2:C:67:LYS:HG3	2:C:68:PHE:N	2.16	0.60
3:D:36:GLN:HB2	3:D:85:TYR:CE2	2.36	0.60
1:A:143:MET:HB3	1:A:347:CYS:SG	2.41	0.60
1:A:201:ILE:HG21	1:B:201:ILE:HD13	1.82	0.60
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.36	0.60
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.81	0.60
3:F:47:ILE:CD1	3:F:53:LEU:CD2	2.79	0.60
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.34	0.60
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.84	0.60
3:D:141:LYS:HG3	3:D:142:ASP:OD2	2.02	0.60
2:E:51:ILE:HG13	2:E:58:ILE:HG12	1.84	0.60
2:C:151:LYS:HA	2:C:184:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:181:THR:HG23	3:F:184:GLU:H	1.67	0.60
1:B:229:TYR:O	1:B:233:ASN:HB2	2.02	0.59
3:F:124:LEU:HD23	3:F:124:LEU:H	1.66	0.59
1:B:98:ARG:HB2	1:B:288:ILE:CD1	2.32	0.59
1:B:107:SER:OG	1:B:109:ILE:HD12	2.03	0.59
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.38	0.59
2:C:109:ASP:OD1	3:D:45:ARG:NH1	2.36	0.59
3:F:139:TYR:OH	3:F:141:LYS:NZ	2.34	0.59
1:A:430:LEU:HD11	1:B:219:PHE:CE1	2.37	0.59
1:A:423:LEU:HB2	1:B:230:ARG:NH2	2.18	0.58
1:A:138:THR:OG1	1:A:143:MET:SD	2.59	0.58
2:C:87:ARG:O	2:C:119:VAL:HG11	2.02	0.58
3:D:77:MET:HG2	3:D:78:GLU:O	2.03	0.58
1:B:22:ILE:O	1:B:26:LEU:HD13	2.03	0.58
1:B:198:LEU:CD1	1:B:410:ILE:HD12	2.32	0.58
3:D:1:ASP:HB3	3:D:94:PRO:HD2	1.86	0.58
3:D:182:LYS:O	3:D:186:GLU:HG3	2.04	0.58
1:B:17:ARG:O	1:B:20:GLN:N	2.33	0.58
3:D:75:ASN:O	3:D:76:THR:HG22	2.04	0.58
1:B:176:THR:O	1:B:180:THR:HG23	2.04	0.57
2:C:3:ARG:HB2	2:C:25:SER:OG	2.05	0.57
3:F:89:GLN:O	3:F:95:GLN:HB2	2.04	0.57
1:B:68:LEU:HD12	1:B:71:THR:HG23	1.86	0.57
1:B:95:PHE:CE2	1:B:99:LYS:HD2	2.39	0.57
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.38	0.57
1:A:176:THR:O	1:A:180:THR:HG22	2.04	0.57
1:A:358:ALA:HA	1:A:361:LEU:HD12	1.87	0.57
1:B:320:ILE:O	1:B:324:THR:HG22	2.05	0.57
1:A:150:PRO:O	1:A:154:ILE:CD1	2.33	0.56
1:B:316:GLY:O	1:B:319:LEU:CD2	2.53	0.56
2:C:43:LYS:HG3	2:C:44:GLY:N	2.19	0.56
3:F:38:LYS:O	3:F:41:THR:HB	2.05	0.56
1:A:262:PHE:CZ	1:A:367:LEU:HD23	2.41	0.56
2:E:52:ASN:HD22	2:E:57:THR:HG22	1.68	0.56
3:D:166:ASP:OD1	3:D:167:SER:N	2.37	0.56
1:A:53:PHE:O	1:A:57:VAL:HG23	2.05	0.56
1:A:219:PHE:CE1	1:B:406:LEU:HD13	2.41	0.56
3:F:77:MET:HE1	3:F:103:LEU:HD21	1.86	0.56
1:A:205:ARG:HH22	1:B:205:ARG:HH12	1.53	0.56
1:B:256:LEU:O	1:B:260:ILE:HG23	2.06	0.56
1:A:219:PHE:HE2	1:B:426:ILE:HG23	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:HIS:O	1:B:286:GLY:N	2.35	0.56
1:A:430:LEU:HD11	1:B:219:PHE:CD1	2.41	0.56
1:A:36:LEU:HD13	1:B:434:LEU:HD21	1.86	0.56
1:A:110:PRO:CB	1:A:448:ILE:HD11	2.36	0.56
1:A:422:ILE:HA	1:A:425:MET:HE3	1.87	0.55
3:D:18:LYS:NZ	3:D:75:ASN:OD1	2.29	0.55
3:D:33:HIS:HD2	3:D:48:TYR:HB2	1.70	0.55
3:D:31:TYR:HA	3:D:50:THR:OG1	2.06	0.55
1:B:38:MET:O	1:B:42:VAL:HG23	2.07	0.55
2:C:60:TYR:CD2	2:C:70:ILE:CD1	2.88	0.55
2:C:64:LEU:CD2	2:C:65:LYS:H	2.19	0.55
1:A:91:MET:HG2	1:A:292:VAL:O	2.05	0.55
1:A:430:LEU:N	1:A:430:LEU:HD12	2.21	0.55
2:C:70:ILE:HD12	2:C:70:ILE:N	2.22	0.55
1:A:144:VAL:HG23	1:A:144:VAL:O	2.06	0.55
3:D:8:PRO:O	3:D:101:THR:HB	2.06	0.55
3:F:95:GLN:N	3:F:95:GLN:CD	2.61	0.55
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.75	0.55
2:E:87:ARG:HG3	2:E:89:GLU:OE1	2.06	0.55
2:E:173:THR:HG22	2:E:187:SER:OG	2.07	0.55
1:B:311:ALA:O	1:B:340:ARG:HD2	2.07	0.55
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.07	0.55
1:B:199:PHE:HA	1:B:407:THR:HG21	1.88	0.55
1:A:255:TYR:CD1	1:A:424:PRO:HB3	2.41	0.54
3:D:165:GLN:HB2	3:D:172:TYR:HE1	1.72	0.54
1:A:86:SER:OG	1:A:303:GLY:HA3	2.08	0.54
3:D:8:PRO:HD2	3:D:101:THR:HG21	1.89	0.54
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.43	0.54
2:E:18:LEU:O	2:E:82:GLN:HA	2.07	0.54
2:C:60:TYR:CD2	2:C:70:ILE:HD13	2.42	0.54
1:A:62:ASN:OD1	1:A:63:GLN:HG2	2.07	0.54
1:B:267:PRO:HB3	1:B:441:GLY:HA3	1.89	0.54
3:D:74:ILE:HG21	3:D:81:ASP:OD2	2.07	0.54
3:F:185:TYR:O	3:F:191:TYR:OH	2.26	0.54
1:A:77:LEU:O	1:A:81:VAL:HG23	2.07	0.54
1:B:172:GLU:O	1:B:176:THR:HG23	2.07	0.54
1:B:284:HIS:C	1:B:286:GLY:H	2.16	0.54
2:C:145:THR:HG22	2:C:190:THR:OG1	2.08	0.54
3:D:1:ASP:OD2	3:D:1:ASP:N	2.34	0.54
2:C:173:THR:HG23	2:C:185:LEU:HD13	1.89	0.54
1:A:109:ILE:HG13	1:A:152:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:40:ALA:HB3	2:C:43:LYS:HG2	1.90	0.53
1:A:98:ARG:HG2	1:A:98:ARG:HH11	1.72	0.53
1:B:68:LEU:HD11	1:B:78:LEU:CB	2.36	0.53
2:C:67:LYS:CG	2:C:68:PHE:H	2.18	0.53
1:A:92:PHE:O	1:A:96:LEU:HD23	2.09	0.53
1:B:165:ILE:HG22	1:B:166:PHE:CD2	2.44	0.53
3:F:184:GLU:HA	3:F:187:ARG:HD2	1.90	0.53
1:A:18:ARG:HH22	1:B:456:GLN:HG2	1.74	0.53
1:B:34:ALA:O	1:B:38:MET:HG2	2.09	0.53
1:A:318:ASN:O	1:A:321:PRO:HD2	2.08	0.53
1:B:59:TRP:CH2	1:B:63:GLN:NE2	2.77	0.53
3:F:186:GLU:HG2	3:F:210:ARG:NH1	2.23	0.53
1:B:91:MET:HG2	1:B:292:VAL:O	2.08	0.53
2:C:87:ARG:HG3	2:C:88:SER:N	2.24	0.53
1:B:158:ILE:O	1:B:162:VAL:HG23	2.09	0.53
1:B:180:THR:HG22	1:B:218:VAL:HG22	1.90	0.53
1:B:361:LEU:HD13	1:B:415:MET:HE1	1.90	0.53
1:A:75:TYR:CE1	1:A:79:LEU:CD1	2.92	0.52
2:C:93:LEU:HD11	2:C:114:GLY:HA3	1.91	0.52
3:D:118:PRO:HB3	3:D:208:PHE:CE1	2.44	0.52
1:A:84:LEU:O	1:A:88:VAL:HG23	2.09	0.52
1:B:417:ASP:C	1:B:418:ASN:HD22	2.18	0.52
1:A:119:GLN:O	1:A:120:ARG:HB2	2.09	0.52
1:A:219:PHE:O	1:A:223:ILE:HG13	2.10	0.52
1:A:161:MET:O	1:A:165:ILE:HG22	2.09	0.52
1:B:123:ARG:HH21	1:B:126:ARG:HD2	1.74	0.52
1:A:205:ARG:HH12	1:B:205:ARG:HH22	1.57	0.52
3:D:60:ARG:CZ	3:D:78:GLU:HG2	2.39	0.52
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.92	0.51
2:C:12:VAL:HG21	2:C:18:LEU:HD23	1.93	0.51
1:A:75:TYR:CZ	1:A:79:LEU:HD11	2.45	0.51
1:A:219:PHE:HE1	1:B:406:LEU:HD13	1.76	0.51
1:B:257:ILE:O	1:B:260:ILE:HG12	2.11	0.51
1:A:177:LEU:HA	1:A:180:THR:CG2	2.41	0.51
1:B:426:ILE:O	1:B:430:LEU:HD12	2.09	0.51
3:D:17:ASP:OD2	3:D:18:LYS:N	2.43	0.51
1:A:20:GLN:HG3	1:A:23:ARG:HH22	1.76	0.51
1:A:60:LEU:O	1:A:64:ARG:HG3	2.11	0.51
1:B:288:ILE:O	1:B:292:VAL:HG13	2.11	0.51
3:F:47:ILE:HG13	3:F:72:LEU:HD13	1.93	0.51
3:D:49:ASP:O	3:D:51:SER:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:77:MET:SD	3:D:103:LEU:HD21	2.51	0.50
2:C:91:THR:HG23	2:C:119:VAL:HG12	1.92	0.50
1:B:332:MET:HG3	1:B:336:ILE:HD11	1.92	0.50
3:D:12:SER:HA	3:D:104:GLU:O	2.10	0.50
3:F:189:ASN:HD21	3:F:211:ALA:HB3	1.77	0.50
3:F:47:ILE:HD13	3:F:53:LEU:CD2	2.42	0.50
1:A:365:THR:O	1:A:369:THR:HG23	2.12	0.50
1:B:205:ARG:HG3	1:B:207:GLN:HE21	1.76	0.50
1:B:319:LEU:HD23	1:B:319:LEU:H	1.76	0.50
2:E:135:GLY:HA2	2:E:221:ARG:HD2	1.94	0.50
1:A:328:PHE:O	1:A:373:MET:HE1	2.12	0.50
1:A:249:LEU:H	1:A:249:LEU:HD22	1.77	0.49
1:A:376:VAL:HG22	1:A:384:LEU:HB2	1.94	0.49
2:E:12:VAL:HG22	2:E:18:LEU:HD13	1.94	0.49
3:D:192:THR:HG22	3:D:207:SER:CB	2.42	0.49
1:A:138:THR:HG21	1:A:353:PRO:O	2.12	0.49
1:A:449:LEU:CD2	1:A:453:LEU:HG	2.42	0.49
1:B:68:LEU:CD1	1:B:71:THR:HG23	2.43	0.49
1:B:234:HIS:O	1:B:235:GLU:HB2	2.13	0.49
2:C:1:GLU:O	2:C:26:GLY:HA3	2.13	0.49
2:E:152:GLY:H	2:E:184:THR:HG22	1.78	0.49
1:B:78:LEU:HA	1:B:81:VAL:HG12	1.95	0.49
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.95	0.49
1:B:53:PHE:O	1:B:57:VAL:HG23	2.13	0.49
1:B:394:MET:HE2	1:B:412:VAL:HG22	1.95	0.49
3:F:186:GLU:HG2	3:F:210:ARG:HH11	1.77	0.49
1:A:410:ILE:O	1:A:414:GLU:HG3	2.12	0.48
1:A:411:LEU:HG	1:A:415:MET:HE2	1.95	0.48
3:F:49:ASP:O	3:F:50:THR:HB	2.13	0.48
1:B:118:ASP:CG	1:B:174:ARG:HH21	2.21	0.48
1:B:258:LEU:HD13	1:B:371:PHE:CG	2.48	0.48
3:D:149:ILE:HD11	3:D:178:LEU:HD21	1.95	0.48
2:C:196:TRP:CD1	2:C:197:PRO:HA	2.48	0.48
1:A:148:ASP:CG	1:A:357:PHE:HB2	2.38	0.48
1:A:258:LEU:HD23	1:A:428:THR:HG21	1.96	0.48
1:B:91:MET:HG3	1:B:296:GLY:HA3	1.94	0.48
1:B:202:GLU:OE1	1:B:407:THR:HG23	2.14	0.48
1:A:252:LEU:HD11	1:A:423:LEU:HD23	1.95	0.48
3:D:160:ASN:HB3	3:D:174:MET:HE2	1.96	0.48
1:B:74:ASN:HB3	1:B:77:LEU:CB	2.44	0.48
1:A:96:LEU:HB3	1:A:130:VAL:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:165:GLN:CB	3:D:172:TYR:HE1	2.26	0.48
1:A:205:ARG:HH22	1:B:205:ARG:NH1	2.12	0.48
3:D:150:ASP:OD1	3:D:188:HIS:HB3	2.14	0.48
1:B:75:TYR:O	1:B:78:LEU:HG	2.14	0.47
1:A:97:VAL:HA	1:A:130:VAL:HG21	1.96	0.47
1:A:205:ARG:HH12	1:B:205:ARG:NH2	2.11	0.47
1:A:219:PHE:HB3	1:B:430:LEU:CD2	2.44	0.47
1:B:90:ALA:HB2	1:B:299:GLY:HA3	1.96	0.47
1:B:234:HIS:O	1:B:235:GLU:CB	2.62	0.47
3:F:121:SER:HA	3:F:124:LEU:CD2	2.40	0.47
1:A:219:PHE:CE2	1:B:426:ILE:HG23	2.46	0.47
2:C:64:LEU:HD23	2:C:65:LYS:HB3	1.97	0.47
1:B:230:ARG:O	1:B:234:HIS:HD2	1.98	0.47
2:E:47:TRP:CG	3:F:95:GLN:HE21	2.32	0.47
2:E:132:LEU:HD13	3:F:132:VAL:HG21	1.95	0.47
2:C:166:SER:O	2:C:168:ALA:N	2.47	0.47
1:A:150:PRO:CA	1:A:154:ILE:HD12	2.43	0.47
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.49	0.47
2:E:181:ALA:O	2:E:182:LEU:HD12	2.15	0.47
1:A:219:PHE:CD2	1:B:430:LEU:CD1	2.96	0.47
1:A:18:ARG:NH2	1:B:456:GLN:HG2	2.30	0.47
1:A:234:HIS:O	1:A:235:GLU:CB	2.62	0.47
3:D:2:ILE:O	3:D:96:THR:HG21	2.15	0.47
1:A:116:LEU:HG	1:A:178:LEU:HD23	1.98	0.46
2:E:145:THR:HG22	3:F:117:PHE:HZ	1.80	0.46
1:A:101:ALA:CB	1:A:130:VAL:HG11	2.39	0.46
2:C:143:MET:HE3	2:C:190:THR:HG22	1.96	0.46
3:F:47:ILE:HD11	3:F:53:LEU:CD2	2.45	0.46
1:A:119:GLN:NE2	1:A:456:GLN:OE1	2.48	0.46
1:A:426:ILE:CG2	1:B:219:PHE:CE2	2.97	0.46
1:A:144:VAL:HG12	1:A:314:GLY:N	2.30	0.46
1:B:62:ASN:O	1:B:65:MET:HB2	2.14	0.46
2:C:6:GLU:N	2:C:6:GLU:OE1	2.49	0.46
2:E:54:VAL:HG23	2:E:56:SER:HB3	1.97	0.46
2:E:171:VAL:HA	2:E:188:SER:O	2.14	0.46
1:A:330:MET:HE2	1:A:370:ALA:HB1	1.98	0.46
2:E:28:ASP:O	2:E:30:SER:O	2.34	0.46
1:A:450:ALA:HB1	1:B:26:LEU:HD11	1.98	0.46
1:B:409:ILE:HD13	1:B:426:ILE:HG12	1.97	0.46
3:F:47:ILE:CD1	3:F:53:LEU:HD22	2.45	0.46
3:F:60:ARG:HG3	3:F:74:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:LEU:HD11	2:C:83:ILE:HD12	1.97	0.46
1:A:22:ILE:O	1:A:26:LEU:HD12	2.15	0.46
3:D:34:TRP:CZ3	3:D:87:CYS:HB3	2.50	0.46
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.98	0.46
3:F:183:ASP:HB3	3:F:187:ARG:NH1	2.30	0.46
1:A:104:ALA:O	1:A:131:LYS:NZ	2.35	0.45
3:D:191:TYR:HB2	3:D:208:PHE:CE2	2.52	0.45
1:A:263:GLY:HA3	1:A:435:LEU:HB2	1.97	0.45
1:A:123:ARG:NH2	1:A:126:ARG:HH11	2.06	0.45
1:A:403:ARG:NH2	1:A:441:GLY:O	2.49	0.45
1:A:430:LEU:N	1:A:430:LEU:CD1	2.79	0.45
1:A:449:LEU:HD23	1:A:453:LEU:HG	1.97	0.45
2:C:30:SER:O	2:C:31:ARG:HB2	2.16	0.45
1:A:255:TYR:O	1:A:428:THR:HG22	2.16	0.45
1:B:260:ILE:O	1:B:264:ILE:HG23	2.17	0.45
2:C:6:GLU:HA	2:C:21:SER:O	2.15	0.45
3:F:7:SER:CB	3:F:8:PRO:HD3	2.47	0.45
1:B:148:ASP:CG	1:B:357:PHE:HB2	2.42	0.45
1:A:447:ALA:O	1:A:451:ARG:HG3	2.17	0.45
1:B:123:ARG:HE	1:B:126:ARG:NE	2.15	0.45
2:C:68:PHE:HB3	2:C:81:LEU:HD11	1.97	0.45
1:B:294:MET:HE2	1:B:294:MET:HB3	1.68	0.45
1:A:160:ARG:HD2	1:A:160:ARG:HA	1.63	0.44
2:C:166:SER:OG	2:C:167:LEU:N	2.50	0.44
3:D:141:LYS:CA	3:D:172:TYR:HD2	2.29	0.44
1:B:42:VAL:O	1:B:46:VAL:HG23	2.18	0.44
1:B:94:TYR:OH	1:B:352:ALA:HB2	2.17	0.44
1:B:78:LEU:HD12	1:B:79:LEU:HD23	1.98	0.44
2:C:23:ALA:HA	2:C:78:THR:HG22	1.99	0.44
2:C:176:ALA:HB2	2:C:185:LEU:HD23	1.99	0.44
3:D:107:ARG:HG3	3:D:108:ALA:O	2.18	0.44
1:B:211:THR:HG22	1:B:212:LEU:H	1.82	0.44
1:B:275:GLY:O	1:B:278:ASP:HB2	2.18	0.44
3:D:66:SER:O	3:D:68:THR:N	2.50	0.44
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.89	0.44
3:D:90:TRP:CZ2	3:D:95:GLN:NE2	2.86	0.44
3:D:148:LYS:HB2	3:D:192:THR:HG1	1.81	0.44
3:F:33:HIS:CE1	3:F:49:ASP:H	2.36	0.43
3:F:139:TYR:CE2	3:F:141:LYS:NZ	2.85	0.43
1:B:47:GLY:O	1:B:51:VAL:HG13	2.18	0.43
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:TYR:CD1	2:C:107:TYR:C	2.96	0.43
2:C:127:PRO:HB2	2:C:150:VAL:HG23	2.00	0.43
3:F:192:THR:OG1	3:F:207:SER:HB3	2.18	0.43
1:A:223:ILE:HG22	1:A:227:ILE:HD11	2.00	0.43
1:B:430:LEU:HA	1:B:433:THR:CG2	2.48	0.43
1:B:394:MET:HG2	1:B:412:VAL:HG22	2.00	0.43
2:C:146:LEU:HD12	2:C:201:VAL:HG11	2.01	0.43
3:F:120:SER:O	3:F:124:LEU:HD23	2.18	0.43
1:A:229:TYR:O	1:A:233:ASN:HB2	2.19	0.43
1:A:453:LEU:HB3	1:B:22:ILE:HD11	2.00	0.43
2:E:52:ASN:HB2	2:E:57:THR:CG2	2.48	0.43
1:A:107:SER:N	4:A:501:BR:BR	3.00	0.43
1:A:260:ILE:HG23	1:A:435:LEU:HG	2.00	0.43
1:B:180:THR:HG22	1:B:218:VAL:HA	2.01	0.43
1:B:259:GLY:O	1:B:432:ALA:HA	2.18	0.43
3:D:117:PHE:O	3:D:131:VAL:HG23	2.19	0.43
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.54	0.43
1:A:150:PRO:CA	1:A:154:ILE:CD1	2.97	0.43
2:C:91:THR:CG2	2:C:119:VAL:H	2.25	0.43
1:A:184:ALA:HB1	1:A:225:SER:HB2	2.00	0.43
2:C:12:VAL:O	2:C:119:VAL:HA	2.19	0.43
2:C:167:LEU:CD2	2:C:201:VAL:HG23	2.49	0.43
2:C:64:LEU:O	2:C:67:LYS:HD3	2.19	0.42
1:A:423:LEU:HB2	1:B:230:ARG:HH21	1.83	0.42
1:B:41:VAL:O	1:B:45:LEU:HG	2.18	0.42
1:A:177:LEU:HA	1:A:180:THR:HG22	2.01	0.42
1:B:169:LYS:HE2	1:B:169:LYS:HB2	1.82	0.42
2:C:153:TYR:CZ	2:C:158:VAL:CG2	3.01	0.42
1:A:18:ARG:HB3	1:B:119:GLN:OE1	2.19	0.42
1:A:130:VAL:O	1:A:134:GLY:N	2.45	0.42
1:A:426:ILE:HG22	1:B:223:ILE:HD11	2.02	0.42
3:F:177:THR:HG22	3:F:179:THR:HG22	2.02	0.42
2:C:51:ILE:HG13	2:C:58:ILE:HG12	2.00	0.42
3:D:29:VAL:HB	3:D:32:ILE:HD11	2.01	0.42
1:A:150:PRO:HD3	1:A:354:GLY:HA2	2.00	0.42
3:F:23:CYS:N	3:F:70:TYR:O	2.33	0.42
2:E:103:TYR:HD2	3:F:31:TYR:CE2	2.38	0.42
2:C:152:GLY:HA2	2:C:182:LEU:HB3	2.02	0.42
3:D:165:GLN:HA	3:D:172:TYR:CE1	2.55	0.42
1:B:231:ILE:HG22	1:B:232:PHE:CD1	2.55	0.42
3:D:8:PRO:HG2	3:D:11:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:49:ASP:HB2	3:F:52:LYS:HE3	2.01	0.42
1:A:109:ILE:HG23	1:A:204:MET:SD	2.60	0.42
3:D:192:THR:HG22	3:D:207:SER:HB3	2.02	0.42
1:A:143:MET:HB2	1:A:145:LEU:HD12	2.01	0.41
1:A:158:ILE:O	1:A:162:VAL:HG23	2.20	0.41
1:B:93:GLY:O	1:B:97:VAL:HG23	2.20	0.41
1:B:346:LEU:O	1:B:350:SER:HB3	2.20	0.41
1:B:267:PRO:HA	1:B:270:ASN:HB2	2.02	0.41
1:B:373:MET:HE2	1:B:373:MET:HB3	1.81	0.41
3:D:60:ARG:HH21	3:D:81:ASP:CG	2.28	0.41
1:B:160:ARG:HA	1:B:160:ARG:HD2	1.83	0.41
2:C:153:TYR:CZ	2:C:158:VAL:HG23	2.55	0.41
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.87	0.41
1:A:264:ILE:O	1:A:267:PRO:HD2	2.20	0.41
1:B:148:ASP:OD2	1:B:357:PHE:HB2	2.21	0.41
1:B:430:LEU:HA	1:B:433:THR:HG22	2.02	0.41
3:D:13:ALA:HB3	3:D:77:MET:HE1	2.02	0.41
2:E:2:VAL:HA	2:E:26:GLY:HA3	2.03	0.41
3:F:60:ARG:HD2	3:F:81:ASP:OD1	2.21	0.41
1:B:128:LEU:HD21	1:B:157:ASN:HB2	2.01	0.41
1:B:267:PRO:HB3	1:B:441:GLY:CA	2.50	0.41
1:B:383:HIS:NE2	2:E:50:GLU:OE2	2.47	0.41
2:C:70:ILE:HD12	2:C:70:ILE:H	1.84	0.41
1:A:421:LEU:O	1:A:425:MET:HG3	2.20	0.41
1:B:250:ASN:OD1	2:E:104:GLY:HA3	2.21	0.41
2:E:31:ARG:HG3	2:E:31:ARG:HH11	1.86	0.41
3:F:6:GLN:HE21	3:F:6:GLN:HB3	1.71	0.41
1:A:165:ILE:HD13	1:A:165:ILE:HG21	1.81	0.41
1:A:223:ILE:HG22	1:A:227:ILE:CD1	2.50	0.41
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.81	0.41
1:A:403:ARG:NH2	1:A:437:GLN:HA	2.36	0.41
1:B:98:ARG:NH1	1:B:291:TRP:CZ3	2.88	0.41
1:B:333:LEU:HD11	1:B:369:THR:HG22	2.01	0.41
3:D:89:GLN:NE2	3:D:92:SER:N	2.63	0.41
3:D:197:HIS:CG	3:D:198:LYS:H	2.39	0.41
3:F:77:MET:HE1	3:F:103:LEU:CD1	2.48	0.41
1:A:109:ILE:CG1	1:A:152:VAL:HG11	2.51	0.41
1:B:152:VAL:HG13	1:B:182:ALA:HB1	2.01	0.41
2:C:135:GLY:O	2:C:138:ALA:HB2	2.21	0.41
2:E:52:ASN:O	2:E:72:ARG:HD3	2.20	0.41
3:F:7:SER:HB3	3:F:8:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:HE	1:B:98:ARG:HA	1.85	0.41
2:C:133:ALA:HB3	2:C:221:ARG:HG3	2.03	0.41
1:B:421:LEU:O	1:B:425:MET:HG3	2.22	0.40
1:A:76:PRO:O	1:A:80:THR:HG23	2.21	0.40
1:A:270:ASN:OD1	1:A:401:SER:HB3	2.21	0.40
1:B:17:ARG:HH11	1:B:17:ARG:HD3	1.75	0.40
2:C:63:SER:O	2:C:64:LEU:O	2.39	0.40
2:C:127:PRO:HB3	2:C:153:TYR:HB3	2.03	0.40
2:C:196:TRP:CG	2:C:197:PRO:HA	2.56	0.40
2:E:99:LEU:HD23	2:E:99:LEU:HA	1.91	0.40
3:F:77:MET:HE3	3:F:77:MET:HB2	1.86	0.40
2:C:87:ARG:HG3	2:C:88:SER:H	1.86	0.40
3:D:18:LYS:HE3	3:D:18:LYS:HB2	1.92	0.40
3:D:60:ARG:NH2	3:D:78:GLU:HG2	2.36	0.40
1:A:238:LEU:HD13	1:A:238:LEU:HA	1.98	0.40
2:C:4:LEU:HD23	2:C:4:LEU:HA	1.85	0.40
2:E:12:VAL:HG11	2:E:86:VAL:HG21	2.04	0.40
1:B:138:THR:HG21	1:B:352:ALA:HB1	2.02	0.40
1:B:211:THR:HG22	1:B:212:LEU:N	2.37	0.40
2:C:88:SER:HA	2:C:119:VAL:HG13	2.04	0.40
3:D:192:THR:HG22	3:D:207:SER:HB2	2.02	0.40
3:F:150:ASP:OD2	3:F:188:HIS:HB3	2.21	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	442/473 (93%)	415 (94%)	24 (5%)	3 (1%)	18	40
1	B	440/473 (93%)	415 (94%)	20 (4%)	5 (1%)	11	29
2	C	220/222 (99%)	203 (92%)	13 (6%)	4 (2%)	6	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	219/222 (99%)	195 (89%)	20 (9%)	4 (2%)	6	19
3	D	209/211 (99%)	187 (90%)	17 (8%)	5 (2%)	4	13
3	F	209/211 (99%)	194 (93%)	12 (6%)	3 (1%)	9	24
All	All	1739/1812 (96%)	1609 (92%)	106 (6%)	24 (1%)	9	24

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	18	ARG
1	B	235	GLU
2	C	64	LEU
2	C	67	LYS
2	E	136	SER
2	E	138	ALA
3	F	7	SER
1	A	234	HIS
1	A	235	GLU
3	D	67	GLY
3	D	76	THR
2	E	65	LYS
3	F	76	THR
1	A	29	ASP
2	C	167	LEU
3	D	50	THR
3	F	66	SER
1	B	144	VAL
3	D	9	ALA
2	E	62	PRO
1	B	285	GLY
3	D	7	SER
1	B	121	PRO
2	C	62	PRO

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	335/358 (94%)	335 (100%)	0	100	100
1	B	333/358 (93%)	332 (100%)	1 (0%)	86	92
2	C	182/182 (100%)	182 (100%)	0	100	100
2	E	181/182 (100%)	181 (100%)	0	100	100
3	D	185/185 (100%)	185 (100%)	0	100	100
3	F	185/185 (100%)	184 (100%)	1 (0%)	81	90
All	All	1401/1450 (97%)	1399 (100%)	2 (0%)	88	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	212	LEU
3	F	1	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	119	GLN
1	A	420	GLN
1	A	456	GLN
1	B	207	GLN
2	C	59	ASN
2	C	82	GLN
3	D	6	GLN
3	D	89	GLN
3	D	144	ASN
3	D	189	ASN
2	E	172	HIS
2	E	179	GLN
3	F	36	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 [i](#)

There are no oligosaccharides in this entry.

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 [i](#)

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	444/473 (93%)	0.69	52 (11%) 9 8	48, 72, 105, 144	0
1	B	442/473 (93%)	0.51	29 (6%) 24 21	49, 71, 114, 149	0
2	C	222/222 (100%)	0.51	21 (9%) 14 12	35, 64, 112, 155	0
2	E	221/222 (99%)	0.50	19 (8%) 16 14	41, 65, 105, 150	0
3	D	211/211 (100%)	0.69	16 (7%) 20 18	46, 74, 98, 114	0
3	F	211/211 (100%)	0.24	12 (5%) 29 24	39, 57, 108, 132	0
All	All	1751/1812 (96%)	0.54	149 (8%) 16 15	35, 69, 109, 155	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	ASP	6.3
1	A	168	LEU	6.2
1	A	99	LYS	5.8
2	E	222	ALA	5.6
3	D	211	ALA	5.2
1	A	166	PHE	5.2
2	E	138	ALA	5.0
1	B	59	TRP	4.9
2	C	139	ALA	4.9
3	D	1	ASP	4.6
2	C	26	GLY	4.5
1	A	234	HIS	4.4
1	A	377	GLU	4.3
2	C	141	ALA	4.2
3	F	39	SER	4.2
1	A	184	ALA	4.1
1	A	170	GLY	4.1
1	A	100	TYR	4.0
1	A	180	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	34	ALA	4.0
1	A	218	VAL	4.0
2	C	41	PRO	4.0
2	E	142	SER	3.9
1	A	165	ILE	3.9
1	A	236	VAL	3.9
1	A	222	VAL	3.8
1	A	447	ALA	3.7
2	C	140	ALA	3.7
1	A	119	GLN	3.5
1	A	235	GLU	3.5
3	D	40	GLY	3.4
3	D	39	SER	3.4
2	C	194	SER	3.4
1	B	55	LYS	3.4
2	C	1	GLU	3.4
1	A	458	ALA	3.4
1	B	235	GLU	3.3
2	C	137	ALA	3.3
2	E	137	ALA	3.3
2	E	140	ALA	3.2
2	E	176	ALA	3.2
3	F	41	THR	3.2
2	C	169	ALA	3.2
3	D	159	LEU	3.1
1	A	212	LEU	3.1
2	E	177	VAL	3.1
1	B	219	PHE	3.0
1	A	233	ASN	3.0
2	C	42	GLY	3.0
3	F	26	SER	3.0
1	A	215	ILE	2.9
3	F	27	SER	2.9
1	A	288	ILE	2.9
1	A	444	LEU	2.9
2	C	221	ARG	2.9
2	C	222	ALA	2.9
3	D	93	HIS	2.9
1	A	126	ARG	2.9
1	A	223	ILE	2.9
2	E	139	ALA	2.8
2	E	198	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	220	ILE	2.8
3	D	22	THR	2.8
1	B	35	ILE	2.8
1	B	430	LEU	2.8
2	E	61	THR	2.8
3	F	180	LEU	2.8
1	B	70	HIS	2.8
1	A	221	GLY	2.8
1	B	66	GLY	2.8
1	A	445	TYR	2.7
1	B	72	ALA	2.7
2	E	181	ALA	2.7
1	A	21	LEU	2.7
1	A	95	PHE	2.7
2	C	40	ALA	2.7
1	A	216	LYS	2.7
2	C	196	TRP	2.7
2	E	199	GLU	2.7
1	B	33	LEU	2.6
1	B	168	LEU	2.6
3	F	164	ASP	2.6
1	A	23	ARG	2.6
1	B	210	TYR	2.6
2	C	9	GLY	2.6
1	A	62	ASN	2.5
3	F	120	SER	2.5
2	C	219	VAL	2.5
2	C	220	PRO	2.5
1	B	433	THR	2.5
2	E	59	ASN	2.5
1	A	207	GLN	2.5
3	D	69	SER	2.4
2	C	199	GLU	2.4
1	A	34	ALA	2.4
1	B	75	TYR	2.4
1	B	200	ILE	2.4
1	A	283	VAL	2.4
2	E	31	ARG	2.4
1	B	438	PHE	2.4
3	D	27	SER	2.4
1	B	307	PHE	2.3
1	A	209	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	42	GLY	2.3
3	D	167	SER	2.3
1	B	234	HIS	2.3
1	A	200	ILE	2.3
1	A	243	LYS	2.3
1	B	212	LEU	2.3
3	F	155	GLN	2.2
2	C	192	PRO	2.2
3	D	179	THR	2.2
3	D	7	SER	2.2
1	B	183	ALA	2.2
1	B	458	ALA	2.2
1	A	448	ILE	2.2
1	A	240	ASP	2.2
1	A	182	ALA	2.2
3	D	168	LYS	2.2
1	A	380	PRO	2.2
1	A	242	GLY	2.2
1	B	177	LEU	2.2
1	B	22	ILE	2.2
1	B	69	VAL	2.2
2	E	175	PRO	2.2
1	B	79	LEU	2.2
3	F	156	ASN	2.1
3	D	38	LYS	2.1
3	F	40	GLY	2.1
3	F	147	TRP	2.1
1	A	237	ALA	2.1
2	C	27	PHE	2.1
1	A	197	ILE	2.1
1	A	70	HIS	2.1
2	E	66	ASP	2.1
3	D	151	GLY	2.1
2	C	176	ALA	2.1
1	A	225	SER	2.1
3	F	121	SER	2.1
1	B	63	GLN	2.1
1	B	207	GLN	2.1
1	A	172	GLU	2.1
1	A	460	GLN	2.0
1	B	95	PHE	2.0
1	A	71	THR	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	94	PRO	2.0
1	A	167	ARG	2.0
2	E	221	ARG	2.0
2	E	141	ALA	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](#)

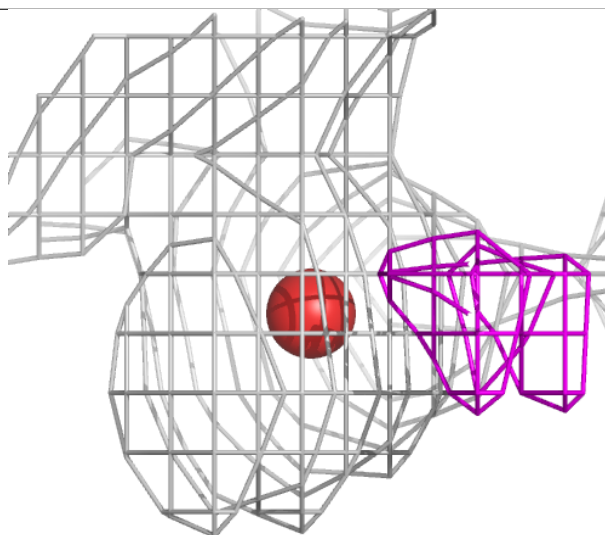
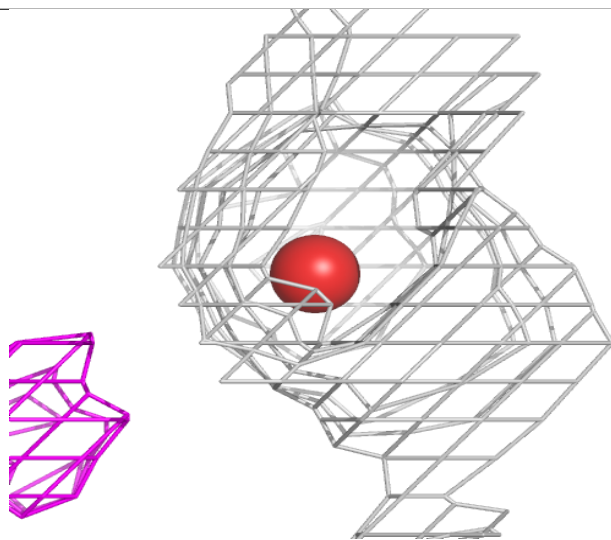
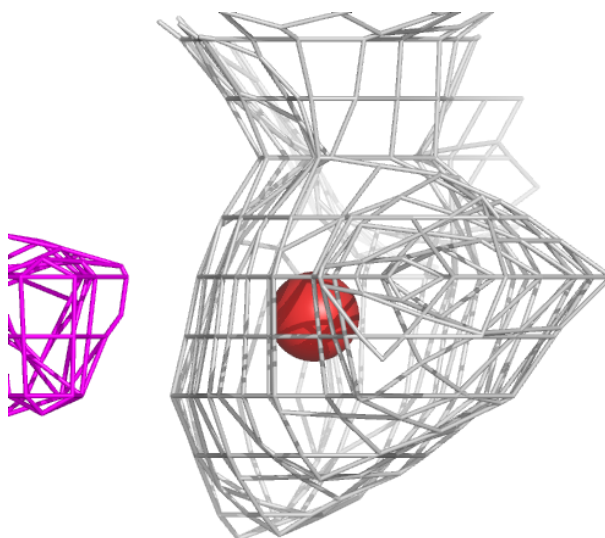
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BR	A	501	1/1	0.90	0.17	130,130,130,130	0
4	BR	B	501	1/1	0.93	0.13	117,117,117,117	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.

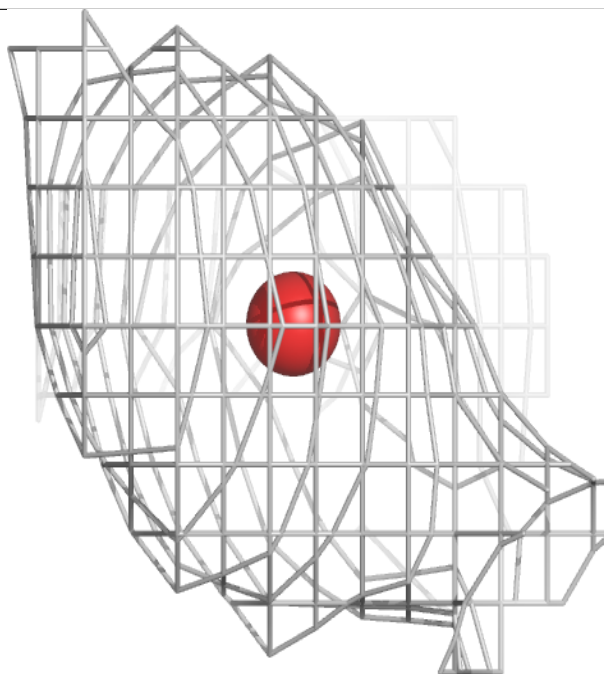
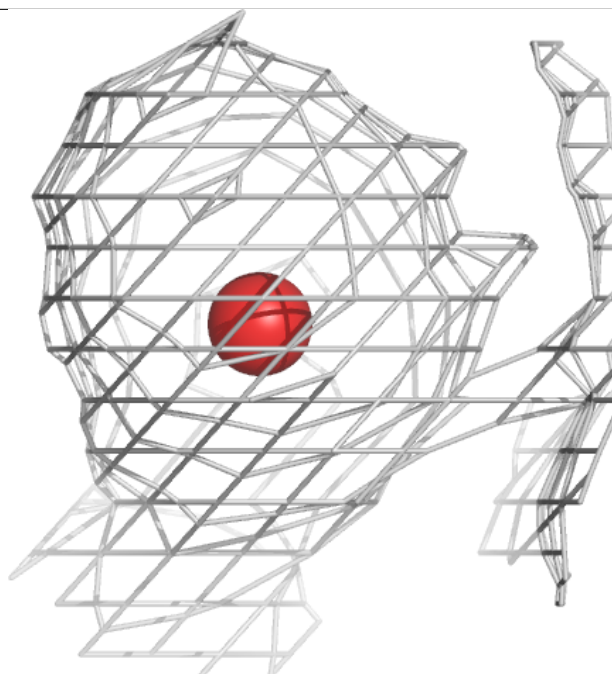
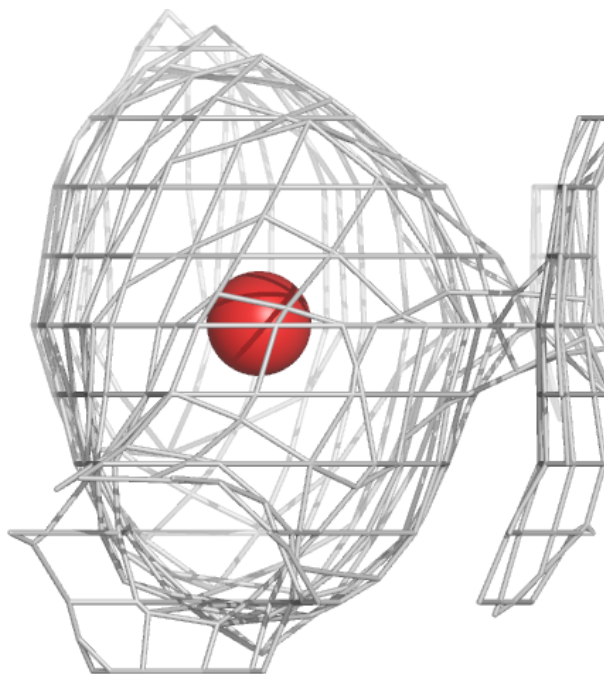
Electron density around BR A 501:

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



Electron density around BR B 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.