



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:57 PM UTC

PDB ID : 6K5A / pdb_00006k5a
Title : Crystal structure of the E148D/R147A/F317A mutant in presence of 200 mM NaBr
Authors : Park, K.; Lim, H.H.
Deposited on : 2019-05-28
Resolution : 3.16 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:

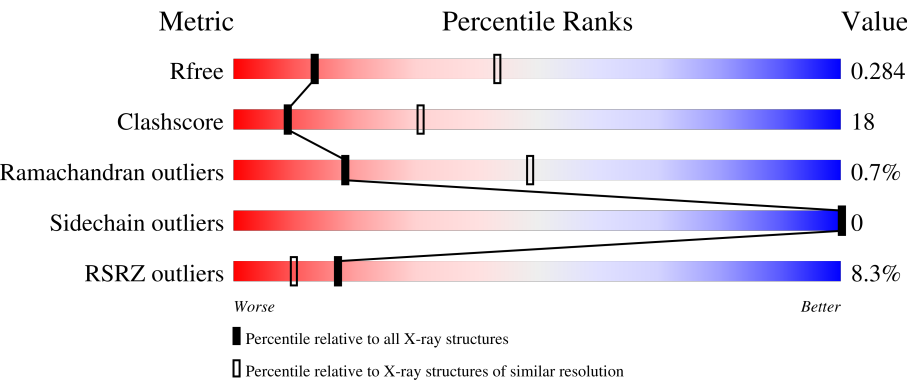
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	8% 60% 33% 7%
1	B	473	10% 53% 39% 7%
2	C	222	8% 74% 25%
2	E	222	9% 68% 31%
3	D	211	9% 60% 40%

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Mol	Chain	Length	Quality of chain
3	F	211	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BR	A	501	-	-	X	-
4	BR	B	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13175 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	440	Total	C	N	O	S	0	0	0
			3288	2162	552	554	20			
1	B	440	Total	C	N	O	S	0	0	0
			3288	2162	552	554	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	ARG	engineered mutation	UNP E9TIA0
A	148	ASP	GLU	engineered mutation	UNP E9TIA0
A	317	ALA	PHE	engineered mutation	UNP E9TIA0
B	147	ALA	ARG	engineered mutation	UNP E9TIA0
B	148	ASP	GLU	engineered mutation	UNP E9TIA0
B	317	ALA	PHE	engineered mutation	UNP E9TIA0

- Molecule 2 is a protein called 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			

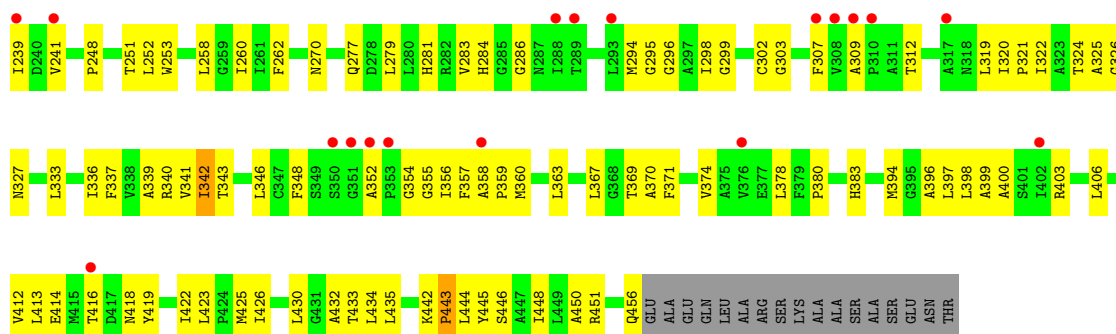
- Molecule 3 is a protein called Fab fragment, light chain.

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			

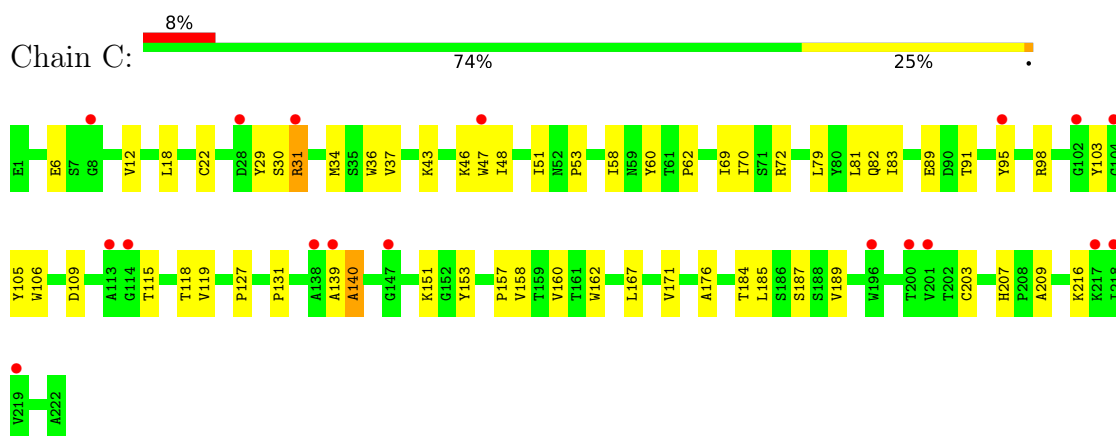
- Molecule 4 is BROMIDE ION (CCD ID: BR) (formula: Br) (labeled as "Ligand of Interest")

by depositor).

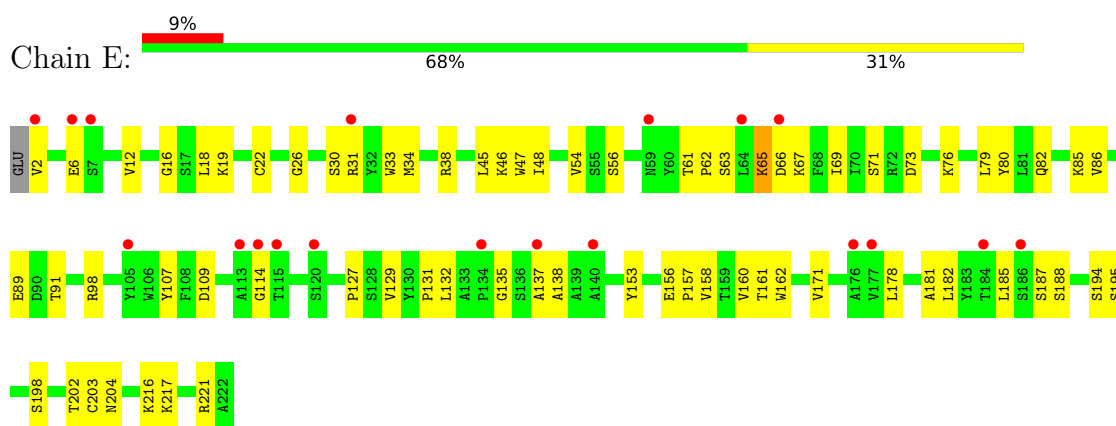
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Br 2	0	0
4	B	2	Total 2	Br 2	0	0



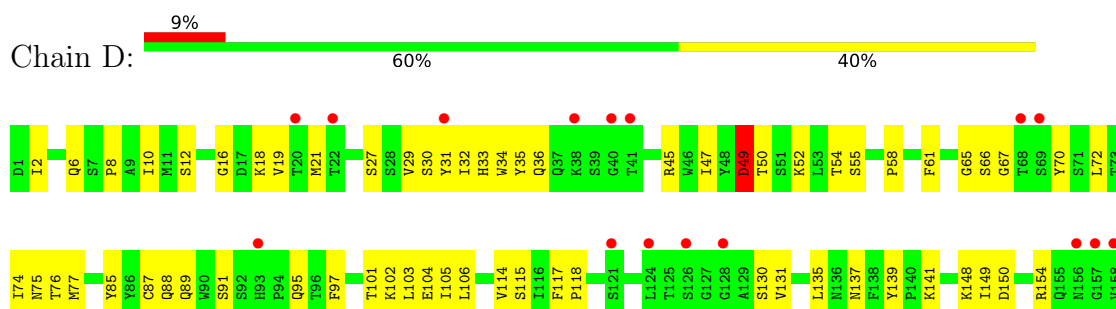
• Molecule 2: Fab fragment, heavy chain

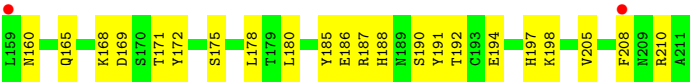


• Molecule 2: Fab fragment, heavy chain

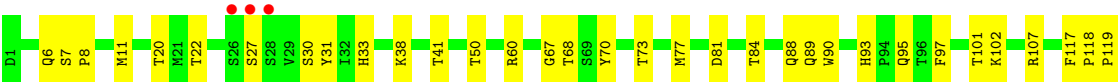
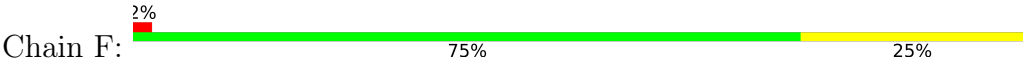


• Molecule 3: Fab fragment, light chain





● Molecule 3: 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	232.18Å 101.34Å 172.07Å 90.00° 132.10° 90.00°	Depositor
Resolution (Å)	39.69 – 3.16 39.69 – 3.16	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.69-3.16) 98.9 (39.69-3.16)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.222 , 0.276 0.235 , 0.284	Depositor DCC
R_{free} test set	2521 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	108.5	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13175	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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	0.44	0/3359	0.78	10/4561 (0.2%)
1	B	0.45	0/3359	0.79	5/4561 (0.1%)
2	C	0.50	0/1730	0.84	4/2367 (0.2%)
2	E	0.51	0/1721	0.78	3/2355 (0.1%)
3	D	0.50	0/1660	0.81	4/2257 (0.2%)
3	F	0.48	0/1660	0.73	0/2257
All	All	0.47	0/13489	0.79	26/18358 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
3	F	0	1
All	All	0	2

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	SER	N-CA-C	11.30	125.82	111.24
1	B	342	ILE	N-CA-C	10.82	121.48	110.23
2	C	140	ALA	N-CA-C	-9.51	96.03	110.30
2	E	65	LYS	N-CA-C	9.44	122.53	111.02
1	B	342	ILE	CB-CA-C	-7.99	101.48	111.70
2	C	140	ALA	CB-CA-C	7.85	120.97	110.06
2	E	65	LYS	CB-CA-C	-7.45	99.08	110.92
1	A	107	SER	CB-CA-C	-6.63	99.92	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	168	LYS	N-CA-C	6.61	118.37	111.03
1	A	204	MET	N-CA-C	6.33	118.18	111.28
1	B	283	VAL	N-CA-C	6.25	116.73	110.23
2	E	91	THR	N-CA-C	-6.05	100.95	109.96
1	A	417	ASP	CA-C-N	-5.93	114.85	122.79
1	A	417	ASP	C-N-CA	-5.93	114.85	122.79
1	A	426	ILE	CB-CA-C	-5.88	104.18	111.70
2	C	31	ARG	CB-CA-C	-5.81	101.77	111.23
3	D	66	SER	CB-CA-C	5.79	119.30	109.99
1	A	108	GLY	N-CA-C	-5.73	106.87	114.95
1	A	426	ILE	N-CA-C	5.68	116.14	110.23
1	A	356	ILE	CA-C-N	5.65	128.65	120.79
1	A	356	ILE	C-N-CA	5.65	128.65	120.79
1	B	283	VAL	CB-CA-C	-5.54	104.61	111.70
1	B	450	ALA	N-CA-C	5.50	117.73	111.02
3	D	49	ASP	CB-CA-C	-5.40	103.77	112.09
3	D	137	ASN	N-CA-C	5.38	122.25	110.80
2	C	48	ILE	CB-CA-C	-5.32	102.57	111.29

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	49	ASP	Mainchain
3	F	6	GLN	Peptide

5.2 Too-close contacts [\(i\)](#)

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	3288	0	3445	141	0
1	B	3288	0	3445	194	0
2	C	1681	0	1663	43	0
2	E	1672	0	1654	46	0
3	D	1621	0	1546	74	0
3	F	1621	0	1546	43	0
4	A	2	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	7	0
All	All	13175	0	13299	489	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 (489) 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:356:ILE:N	4:B:501:BR:BR	2.40	1.09
1:B:445:TYR:OH	4:B:501:BR:BR	2.31	1.02
1:A:200:ILE:HA	1:A:204:MET:HB2	1.49	0.91
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.53	0.90
3:D:95:GLN:OE1	3:D:95:GLN:N	2.06	0.88
1:B:78:LEU:HD12	1:B:307:PHE:CE2	2.11	0.85
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.60	0.84
1:B:78:LEU:CD1	1:B:307:PHE:CZ	2.62	0.82
1:B:78:LEU:HD12	1:B:307:PHE:CZ	2.14	0.82
2:E:19:LYS:HE2	2:E:80:TYR:CD1	2.14	0.82
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.60	0.82
1:A:28:ARG:HH11	1:B:207:GLN:HG2	1.45	0.81
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.17	0.80
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.46	0.79
3:D:32:ILE:HD13	3:D:70:TYR:CE1	2.17	0.78
1:B:44:THR:HG23	1:B:228:MET:HE3	1.65	0.78
3:F:90:TRP:HD1	3:F:90:TRP:O	1.68	0.77
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.67	0.77
3:D:32:ILE:HD13	3:D:70:TYR:CD1	2.21	0.76
3:F:90:TRP:O	3:F:90:TRP:CD1	2.39	0.76
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.65	0.76
3:F:95:GLN:O	3:F:95:GLN:NE2	2.20	0.75
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.86	0.75
1:B:355:GLY:CA	4:B:501:BR:BR	2.89	0.75
1:B:78:LEU:HD11	1:B:307:PHE:CE1	2.21	0.74
1:A:180:THR:HG22	1:A:218:VAL:HA	1.69	0.74
1:B:53:PHE:HZ	1:B:139:LEU:HD23	1.52	0.74
1:A:205:ARG:HH12	1:B:205:ARG:HH12	1.35	0.74
1:B:32:PRO:HD2	1:B:35:ILE:HD12	1.70	0.73
3:D:6:GLN:NE2	3:D:85:TYR:O	2.21	0.73
3:F:7:SER:OG	3:F:8:PRO:HD3	1.88	0.73
2:C:185:LEU:C	2:C:185:LEU:HD12	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:LEU:HD13	1:B:425:MET:HE1	1.69	0.72
1:B:248:PRO:O	1:B:251:THR:HG22	1.89	0.72
1:B:53:PHE:HZ	1:B:139:LEU:CD2	2.03	0.72
1:B:90:ALA:HB2	1:B:299:GLY:HA3	1.72	0.72
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.24	0.72
1:A:198:LEU:HD11	1:B:198:LEU:HD21	1.72	0.71
1:A:430:LEU:HD21	1:B:219:PHE:HB3	1.72	0.71
1:A:379:PHE:HB3	1:A:382:TYR:CD2	2.27	0.69
3:D:76:THR:HG22	3:D:76:THR:O	1.91	0.69
1:A:456:GLN:O	1:B:18:ARG:NH1	2.25	0.69
3:F:192:THR:HB	3:F:207:SER:HB3	1.74	0.69
1:B:355:GLY:HA2	4:B:501:BR:BR	2.48	0.69
2:E:67:LYS:NZ	2:E:85:LYS:O	2.26	0.68
1:A:90:ALA:O	1:A:94:TYR:HD2	1.76	0.68
1:B:206:PRO:HD2	1:B:211:THR:HG21	1.74	0.68
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.75	0.68
1:B:144:VAL:HG21	1:B:343:THR:OG1	1.93	0.68
1:A:207:GLN:HG2	1:B:28:ARG:HH11	1.59	0.67
2:C:151:LYS:HA	2:C:184:THR:HG23	1.77	0.67
3:D:191:TYR:HB2	3:D:208:PHE:CE1	2.29	0.67
1:B:270:ASN:ND2	1:B:442:LYS:O	2.28	0.67
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.76	0.66
3:D:154:ARG:HH12	3:D:180:LEU:HD21	1.60	0.66
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.31	0.66
2:E:135:GLY:HA2	2:E:221:ARG:HD2	1.76	0.66
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.29	0.65
2:C:91:THR:HG23	2:C:118:THR:HA	1.77	0.65
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.32	0.65
1:B:64:ARG:O	1:B:68:LEU:HG	1.97	0.65
3:D:35:TYR:CD2	3:D:45:ARG:HA	2.32	0.65
1:A:239:ILE:HG23	1:A:321:PRO:HG3	1.79	0.64
1:B:53:PHE:CZ	1:B:139:LEU:HD23	2.33	0.64
1:B:90:ALA:HB3	1:B:296:GLY:HA2	1.80	0.64
2:E:38:ARG:HD3	2:E:48:ILE:HD11	1.80	0.63
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.80	0.63
1:B:78:LEU:HD11	1:B:307:PHE:CZ	2.33	0.63
3:D:77:MET:SD	3:D:103:LEU:HD21	2.39	0.63
1:B:239:ILE:HD13	1:B:320:ILE:HG21	1.81	0.62
1:A:376:VAL:HG22	1:A:384:LEU:HB2	1.80	0.62
1:A:414:GLU:OE1	1:B:419:TYR:OH	2.18	0.62
1:B:218:VAL:O	1:B:222:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:PHE:O	1:B:136:LEU:HG	1.99	0.62
1:B:258:LEU:HD13	1:B:371:PHE:CG	2.34	0.62
1:B:157:ASN:HD22	1:B:157:ASN:H	1.48	0.62
3:D:36:GLN:HB2	3:D:85:TYR:HE1	1.65	0.62
1:B:148:ASP:OD1	1:B:355:GLY:HA3	1.99	0.61
3:D:130:SER:HA	3:D:178:LEU:O	2.00	0.61
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.82	0.61
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.81	0.61
3:D:36:GLN:HB2	3:D:85:TYR:CE1	2.35	0.61
1:A:272:TRP:HE3	1:A:345:LEU:HD11	1.65	0.61
2:C:69:ILE:HB	2:C:82:GLN:HB2	1.82	0.61
1:B:374:VAL:O	1:B:378:LEU:HG	2.00	0.61
1:A:25:LEU:HD23	1:B:208:PHE:HE2	1.65	0.61
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.36	0.61
1:A:148:ASP:O	1:A:152:VAL:HG23	2.01	0.61
1:B:123:ARG:O	1:B:127:VAL:HG23	2.01	0.61
2:E:202:THR:HG22	2:E:217:LYS:HG3	1.82	0.61
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.82	0.60
1:A:29:ASP:OD2	1:A:216:LYS:NZ	2.33	0.60
1:B:42:VAL:O	1:B:46:VAL:HG23	2.00	0.60
2:E:129:VAL:O	2:E:216:LYS:HE3	2.01	0.60
3:D:35:TYR:HD2	3:D:45:ARG:HA	1.66	0.60
3:F:95:GLN:N	3:F:95:GLN:CD	2.59	0.60
1:B:124:TRP:NE1	1:B:164:ASP:OD2	2.29	0.60
1:A:223:ILE:HD12	1:B:430:LEU:HD22	1.83	0.60
3:F:135:LEU:HD13	3:F:174:MET:HE2	1.83	0.60
1:A:313:SER:OG	1:A:314:GLY:N	2.32	0.60
1:A:112:ILE:HD12	1:A:156:GLY:HA3	1.84	0.59
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.18	0.59
1:A:430:LEU:HD22	1:B:223:ILE:HD12	1.84	0.59
1:A:118:ASP:CG	1:A:174:ARG:HH21	2.11	0.59
1:A:430:LEU:HD11	1:B:219:PHE:CG	2.38	0.59
2:C:103:TYR:HD2	3:D:31:TYR:CZ	2.20	0.59
2:C:158:VAL:CG2	2:C:185:LEU:HD21	2.32	0.59
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.83	0.59
1:B:53:PHE:O	1:B:57:VAL:HG23	2.02	0.59
3:D:10:ILE:HG23	3:D:102:LYS:HB3	1.85	0.59
3:D:32:ILE:CD1	3:D:70:TYR:CE1	2.86	0.59
2:C:37:VAL:O	2:C:95:TYR:HB2	2.02	0.58
1:B:197:ILE:HD11	1:B:219:PHE:CD1	2.39	0.58
1:B:339:ALA:O	1:B:343:THR:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.84	0.58
1:B:180:THR:HG22	1:B:218:VAL:HA	1.86	0.58
3:F:60:ARG:NH2	3:F:81:ASP:OD1	2.36	0.58
3:D:95:GLN:H	3:D:95:GLN:CD	2.10	0.58
2:E:89:GLU:N	2:E:89:GLU:OE1	2.37	0.57
1:A:227:ILE:O	1:A:231:ILE:HG13	2.03	0.57
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.86	0.57
3:F:186:GLU:O	3:F:210:ARG:NH2	2.38	0.57
1:A:424:PRO:O	1:A:428:THR:OG1	2.20	0.57
1:A:35:ILE:HD11	1:A:173:ALA:HB2	1.87	0.56
1:B:38:MET:O	1:B:42:VAL:HG23	2.06	0.56
3:D:149:ILE:HG12	3:D:191:TYR:CD1	2.40	0.56
1:A:419:TYR:OH	1:B:414:GLU:OE1	2.18	0.56
2:C:153:TYR:OH	2:C:185:LEU:HD23	2.05	0.56
3:F:148:LYS:HA	3:F:152:SER:O	2.05	0.56
1:B:104:ALA:HB2	1:B:127:VAL:HG13	1.87	0.56
2:C:176:ALA:HA	2:C:185:LEU:HB3	1.86	0.56
3:F:146:LYS:HD3	3:F:148:LYS:HE3	1.88	0.56
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.88	0.56
1:A:383:HIS:HB2	2:C:106:TRP:CZ2	2.41	0.55
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.86	0.55
3:D:160:ASN:HA	3:D:175:SER:O	2.05	0.55
1:A:437:GLN:OE1	1:B:216:LYS:NZ	2.34	0.55
2:E:71:SER:HB3	2:E:80:TYR:HB2	1.89	0.55
1:A:90:ALA:HB2	1:A:299:GLY:HA3	1.88	0.55
1:B:416:THR:O	1:B:418:ASN:ND2	2.40	0.55
3:F:89:GLN:NE2	3:F:95:GLN:HA	2.22	0.55
3:D:31:TYR:HD1	3:D:49:ASP:CA	2.19	0.55
1:B:176:THR:O	1:B:180:THR:HG23	2.06	0.55
1:A:393:GLY:HA2	1:A:396:ALA:HB2	1.88	0.55
3:D:34:TRP:CH2	3:D:87:CYS:HB3	2.41	0.55
1:A:38:MET:HB3	1:A:177:LEU:HD11	1.89	0.55
1:B:262:PHE:CE1	1:B:367:LEU:HD23	2.42	0.55
3:D:105:ILE:N	3:D:165:GLN:HE22	2.05	0.54
1:B:184:ALA:HB1	1:B:225:SER:CB	2.37	0.54
1:A:219:PHE:CD2	1:B:430:LEU:HD11	2.42	0.54
1:A:42:VAL:O	1:A:46:VAL:HG23	2.08	0.54
3:F:169:ASP:OD1	3:F:171:THR:HG23	2.07	0.54
1:B:322:ILE:O	1:B:327:ASN:HB2	2.08	0.54
3:D:191:TYR:HB2	3:D:208:PHE:HE1	1.73	0.54
1:A:355:GLY:CA	4:A:501:BR:BR	3.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:135:GLY:O	2:E:137:ALA:N	2.32	0.54
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.42	0.54
1:B:309:ALA:HB3	1:B:312:THR:OG1	2.08	0.54
1:B:25:LEU:O	1:B:27:GLU:N	2.41	0.54
1:A:430:LEU:HD23	1:B:220:ILE:HG12	1.89	0.54
2:C:185:LEU:HD12	2:C:185:LEU:O	2.07	0.53
1:B:230:ARG:O	1:B:234:HIS:HB3	2.08	0.53
1:B:430:LEU:HA	1:B:433:THR:HG22	1.91	0.53
1:B:68:LEU:HD21	1:B:82:ALA:HB2	1.89	0.53
2:E:61:THR:O	2:E:63:SER:N	2.42	0.53
1:B:60:LEU:O	1:B:64:ARG:HG3	2.09	0.53
1:B:68:LEU:HD13	1:B:307:PHE:CD1	2.43	0.53
1:B:258:LEU:HD13	1:B:371:PHE:CD2	2.43	0.53
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.43	0.53
2:C:30:SER:OG	2:C:31:ARG:N	2.40	0.53
3:F:89:GLN:O	3:F:95:GLN:HB2	2.09	0.53
3:D:58:PRO:HG2	3:D:61:PHE:CD1	2.44	0.53
1:B:154:ILE:O	1:B:158:ILE:HG13	2.08	0.53
1:B:239:ILE:HG23	1:B:321:PRO:HG3	1.91	0.53
1:A:449:LEU:O	1:A:453:LEU:HG	2.09	0.53
1:B:200:ILE:O	1:B:205:ARG:HG2	2.09	0.53
1:A:18:ARG:NH1	1:B:456:GLN:O	2.42	0.52
1:A:250:ASN:ND2	1:A:382:TYR:HE1	2.08	0.52
3:D:31:TYR:HD1	3:D:49:ASP:C	2.17	0.52
3:D:30:SER:H	3:D:91:SER:CB	2.22	0.52
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.90	0.52
1:B:357:PHE:HE1	1:B:398:LEU:HD13	1.74	0.52
3:F:165:GLN:HG3	3:F:172:TYR:CZ	2.45	0.52
3:F:167:SER:O	3:F:168:LYS:HD3	2.10	0.52
1:A:394:MET:CE	1:A:415:MET:HE3	2.40	0.52
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.32	0.52
2:E:19:LYS:HE2	2:E:80:TYR:CE1	2.44	0.52
1:B:107:SER:OG	1:B:348:PHE:CZ	2.57	0.52
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.42	0.52
2:E:178:LEU:HD11	2:E:181:ALA:HA	1.91	0.52
3:D:118:PRO:HB3	3:D:208:PHE:CE2	2.45	0.52
1:B:253:TRP:H	1:B:253:TRP:CD1	2.28	0.52
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.26	0.51
1:A:220:ILE:HG12	1:B:430:LEU:HD23	1.92	0.51
1:B:68:LEU:HD22	1:B:78:LEU:HD11	1.93	0.51
3:F:27:SER:O	3:F:68:THR:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:THR:HG22	1:A:218:VAL:CA	2.40	0.51
1:A:205:ARG:NH1	1:B:205:ARG:HH12	2.03	0.51
3:D:154:ARG:NH1	3:D:180:LEU:HD21	2.25	0.51
1:A:216:LYS:HD3	1:B:434:LEU:CD2	2.41	0.51
1:B:23:ARG:HA	1:B:26:LEU:HD12	1.93	0.51
1:B:356:ILE:HG22	4:B:501:BR:BR	2.66	0.51
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.46	0.51
1:B:128:LEU:HB2	1:B:129:PRO:HD3	1.92	0.51
2:E:16:GLY:O	2:E:86:VAL:HG23	2.11	0.51
1:A:28:ARG:NH1	1:B:207:GLN:HG2	2.19	0.51
1:A:279:LEU:HA	1:A:282:ARG:HH11	1.76	0.51
3:D:150:ASP:OD2	3:D:188:HIS:HB3	2.11	0.51
1:A:223:ILE:CD1	1:B:430:LEU:HD22	2.40	0.50
1:B:144:VAL:O	1:B:145:LEU:HG	2.12	0.50
1:B:184:ALA:O	1:B:225:SER:OG	2.27	0.50
2:C:139:ALA:O	2:C:140:ALA:C	2.53	0.50
3:F:148:LYS:HB2	3:F:192:THR:HG23	1.93	0.50
1:A:208:PHE:HE1	1:B:25:LEU:HD23	1.77	0.50
1:B:78:LEU:HA	1:B:81:VAL:HG22	1.94	0.50
1:B:182:ALA:HB1	1:B:204:MET:HE1	1.94	0.50
3:D:150:ASP:HA	3:D:190:SER:HB3	1.93	0.50
2:E:65:LYS:O	2:E:66:ASP:OD1	2.29	0.50
1:A:284:HIS:C	1:A:286:GLY:H	2.20	0.49
1:A:430:LEU:HA	1:A:433:THR:HG22	1.94	0.49
1:B:160:ARG:NE	1:B:163:LEU:HD23	2.27	0.49
2:C:60:TYR:HE1	2:C:70:ILE:HG13	1.77	0.49
3:F:7:SER:OG	3:F:22:THR:HB	2.11	0.49
3:D:34:TRP:N	3:D:47:ILE:O	2.44	0.49
3:D:88:GLN:HB2	3:D:97:PHE:CD2	2.48	0.49
3:D:131:VAL:N	3:D:178:LEU:O	2.42	0.49
3:F:118:PRO:HB3	3:F:208:PHE:CE2	2.47	0.49
1:B:90:ALA:CB	1:B:299:GLY:HA3	2.39	0.49
2:E:2:VAL:HA	2:E:26:GLY:HA3	1.94	0.49
2:E:185:LEU:C	2:E:185:LEU:HD12	2.37	0.49
3:F:8:PRO:O	3:F:101:THR:HG23	2.12	0.49
1:B:41:VAL:O	1:B:45:LEU:HG	2.13	0.49
1:B:284:HIS:C	1:B:286:GLY:H	2.19	0.49
2:E:156:GLU:OE1	2:E:157:PRO:HA	2.13	0.49
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.95	0.49
1:A:219:PHE:CG	1:B:430:LEU:HD11	2.47	0.49
1:A:346:LEU:O	1:A:350:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:MET:HG3	1:B:296:GLY:HA3	1.95	0.49
1:A:90:ALA:O	1:A:94:TYR:CD2	2.62	0.48
1:A:154:ILE:O	1:A:158:ILE:HG13	2.12	0.48
1:A:253:TRP:O	1:A:257:ILE:HG13	2.13	0.48
2:C:171:VAL:HG22	2:C:189:VAL:HG23	1.95	0.48
3:D:197:HIS:CD2	3:D:198:LYS:H	2.31	0.48
2:E:161:THR:OG1	2:E:204:ASN:HB2	2.12	0.48
1:A:356:ILE:N	4:A:501:BR:BR	2.93	0.48
3:D:149:ILE:HG12	3:D:191:TYR:CE1	2.47	0.48
1:B:142:GLY:O	1:B:302:CYS:HB3	2.13	0.48
3:D:29:VAL:O	3:D:70:TYR:OH	2.25	0.48
1:B:107:SER:HG	1:B:348:PHE:HE1	1.54	0.48
1:B:260:ILE:HG12	1:B:435:LEU:HG	1.96	0.48
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.96	0.48
2:E:135:GLY:C	2:E:137:ALA:H	2.20	0.48
1:A:19:ARG:HA	1:A:22:ILE:HD12	1.96	0.48
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.95	0.48
1:B:179:ALA:O	1:B:182:ALA:N	2.47	0.48
1:B:355:GLY:C	4:B:501:BR:BR	3.10	0.48
3:D:106:LEU:HG	3:D:139:TYR:OH	2.14	0.48
3:D:186:GLU:HA	3:D:210:ARG:NH2	2.28	0.48
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.95	0.48
1:A:146:GLY:C	1:A:148:ASP:H	2.22	0.48
1:B:94:TYR:CE1	1:B:295:GLY:HA3	2.49	0.47
1:B:337:PHE:O	1:B:341:VAL:HG23	2.13	0.47
2:C:37:VAL:HG22	2:C:47:TRP:HA	1.94	0.47
1:A:91:MET:HG2	1:A:292:VAL:O	2.14	0.47
1:A:205:ARG:HH12	1:B:205:ARG:NH1	2.08	0.47
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.96	0.47
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.96	0.47
1:A:184:ALA:HB1	1:A:225:SER:CB	2.45	0.47
1:A:430:LEU:HD22	1:B:223:ILE:CD1	2.44	0.47
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.49	0.47
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.49	0.47
1:A:148:ASP:OD1	1:A:149:GLY:N	2.47	0.47
1:A:158:ILE:O	1:A:162:VAL:HG13	2.15	0.47
1:B:143:MET:HE3	1:B:298:ILE:HG22	1.96	0.47
1:A:112:ILE:HG13	1:A:153:GLN:HA	1.97	0.47
1:A:208:PHE:CE1	1:B:25:LEU:HD23	2.49	0.47
1:B:94:TYR:CZ	1:B:295:GLY:HA3	2.49	0.47
1:B:336:ILE:O	1:B:340:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:PHE:HE1	1:B:398:LEU:CD1	2.27	0.47
2:C:30:SER:O	2:C:31:ARG:HB2	2.15	0.47
3:D:30:SER:H	3:D:91:SER:HB3	1.79	0.47
2:E:34:MET:HB2	2:E:79:LEU:HD13	1.97	0.47
1:B:160:ARG:HD2	1:B:160:ARG:HA	1.55	0.47
1:B:444:LEU:O	1:B:448:ILE:HG13	2.15	0.47
1:A:28:ARG:HH21	1:B:443:PRO:HB3	1.79	0.47
1:A:103:GLU:HB2	1:A:111:GLU:CD	2.40	0.46
3:D:54:THR:HG22	3:D:55:SER:H	1.80	0.46
3:D:74:ILE:HD12	3:D:77:MET:HG3	1.97	0.46
1:A:379:PHE:CB	1:A:382:TYR:HD2	2.29	0.46
1:A:426:ILE:HG23	1:B:219:PHE:CE1	2.51	0.46
1:B:294:MET:HE2	1:B:294:MET:HB3	1.86	0.46
2:E:182:LEU:HD23	2:E:182:LEU:HA	1.78	0.46
1:A:403:ARG:NH1	1:A:441:GLY:O	2.43	0.46
3:D:185:TYR:CE1	3:D:191:TYR:CE2	3.04	0.46
1:A:160:ARG:HD2	1:A:160:ARG:HA	1.60	0.46
1:B:59:TRP:CZ3	1:B:60:LEU:HD23	2.50	0.46
2:C:18:LEU:HD11	2:C:83:ILE:HD12	1.97	0.46
1:A:427:ILE:HD11	1:B:227:ILE:HD11	1.97	0.46
1:B:360:MET:HG2	1:B:397:LEU:HD13	1.98	0.46
3:D:169:ASP:OD1	3:D:171:THR:OG1	2.32	0.46
2:E:45:LEU:O	2:E:46:LYS:HG2	2.16	0.46
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.46	0.46
1:A:86:SER:OG	1:A:303:GLY:HA3	2.15	0.46
1:A:430:LEU:HD11	1:B:219:PHE:CD1	2.51	0.46
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.50	0.46
1:B:122:VAL:HG11	1:B:160:ARG:HB2	1.98	0.46
3:D:18:LYS:NZ	3:D:75:ASN:OD1	2.48	0.46
2:E:73:ASP:OD2	2:E:76:LYS:HB2	2.16	0.46
1:B:107:SER:HG	1:B:348:PHE:HZ	1.54	0.45
3:F:134:PHE:C	3:F:135:LEU:HD12	2.41	0.45
1:A:434:LEU:HD11	1:B:220:ILE:HD11	1.99	0.45
2:C:36:TRP:NE1	2:C:81:LEU:HB2	2.31	0.45
3:D:49:ASP:HB2	3:D:52:LYS:HD3	1.98	0.45
1:A:241:VAL:HG21	1:A:324:THR:HG21	1.99	0.45
1:A:195:ALA:N	1:A:414:GLU:OE2	2.47	0.45
1:B:355:GLY:HA3	4:B:501:BR:BR	2.71	0.45
1:A:125:TRP:HD1	1:A:126:ARG:HG3	1.80	0.45
1:A:270:ASN:ND2	1:A:442:LYS:O	2.49	0.45
1:A:355:GLY:HA3	4:A:501:BR:BR	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:PHE:CE2	1:B:396:ALA:HB3	2.52	0.45
3:D:74:ILE:CD1	3:D:77:MET:HG3	2.47	0.45
2:E:6:GLU:CD	2:E:114:GLY:H	2.25	0.45
2:E:194:SER:O	2:E:198:SER:HB3	2.16	0.45
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.52	0.45
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.98	0.45
1:B:277:GLN:OE1	1:B:451:ARG:NH2	2.50	0.45
1:A:206:PRO:HD2	1:A:211:THR:HG21	1.98	0.45
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.99	0.45
3:F:20:THR:HG23	3:F:73:THR:OG1	2.16	0.45
1:B:357:PHE:CE1	1:B:398:LEU:CD1	3.00	0.45
1:A:410:ILE:O	1:A:414:GLU:HG3	2.16	0.45
1:B:58:ALA:O	1:B:61:GLN:N	2.50	0.45
1:B:90:ALA:CB	1:B:296:GLY:HA2	2.47	0.45
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.98	0.45
1:A:131:LYS:O	1:A:135:GLY:N	2.40	0.45
1:A:182:ALA:HB1	1:A:204:MET:HE2	1.99	0.45
2:E:221:ARG:NH2	3:F:118:PRO:HD2	2.31	0.45
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.46	0.44
1:B:309:ALA:CB	1:B:312:THR:OG1	2.64	0.44
1:A:139:LEU:HD22	1:A:145:LEU:HB2	1.99	0.44
1:B:25:LEU:O	1:B:26:LEU:C	2.60	0.44
1:B:86:SER:OG	1:B:303:GLY:HA3	2.17	0.44
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.98	0.44
3:D:33:HIS:HA	3:D:47:ILE:O	2.17	0.44
3:F:31:TYR:HA	3:F:50:THR:OG1	2.18	0.44
1:A:379:PHE:HB3	1:A:382:TYR:HD2	1.76	0.44
1:B:106:GLY:O	1:B:131:LYS:NZ	2.50	0.44
1:B:383:HIS:HB3	2:E:33:TRP:CZ2	2.52	0.44
2:C:89:GLU:O	2:C:89:GLU:HG2	2.18	0.44
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.99	0.44
1:A:28:ARG:HH21	1:B:443:PRO:CB	2.31	0.44
1:A:180:THR:HG22	1:A:218:VAL:HG22	1.99	0.44
1:A:180:THR:CG2	1:A:218:VAL:HA	2.44	0.44
1:B:252:LEU:HD11	1:B:423:LEU:HD23	1.98	0.44
3:D:19:VAL:HG21	3:D:77:MET:SD	2.58	0.44
1:B:68:LEU:HD22	1:B:78:LEU:CD1	2.48	0.44
1:B:123:ARG:HH21	1:B:126:ARG:HD3	1.83	0.44
1:B:319:LEU:H	1:B:319:LEU:HG	1.61	0.44
1:B:333:LEU:HD11	1:B:369:THR:HG22	2.00	0.44
1:B:380:PRO:HG2	3:F:93:HIS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:187:ARG:HB2	3:D:188:HIS:CE1	2.52	0.44
1:B:356:ILE:HG12	1:B:356:ILE:O	2.18	0.44
2:E:69:ILE:HB	2:E:82:GLN:HG3	1.99	0.44
1:A:90:ALA:HB3	1:A:296:GLY:HA2	2.00	0.44
1:A:94:TYR:OH	1:A:352:ALA:HB2	2.18	0.44
3:D:76:THR:O	3:D:76:THR:CG2	2.61	0.44
1:A:407:THR:O	1:A:411:LEU:N	2.44	0.44
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.53	0.44
3:D:34:TRP:CG	3:D:72:LEU:HD12	2.53	0.44
2:E:47:TRP:CE3	3:F:95:GLN:NE2	2.84	0.44
1:B:337:PHE:CE1	1:B:363:LEU:HD22	2.53	0.44
2:C:37:VAL:HG13	2:C:46:LYS:O	2.18	0.44
2:C:103:TYR:HD2	3:D:31:TYR:HH	1.63	0.44
2:E:6:GLU:N	2:E:6:GLU:OE1	2.51	0.44
1:A:86:SER:HB2	1:A:300:GLY:HA2	1.99	0.43
1:B:241:VAL:HG21	1:B:324:THR:HG21	1.99	0.43
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.99	0.43
1:A:198:LEU:HG	1:A:410:ILE:HD12	1.99	0.43
1:A:391:ILE:HD13	1:A:391:ILE:HA	1.77	0.43
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.52	0.43
1:B:357:PHE:CE1	1:B:398:LEU:HD13	2.54	0.43
2:C:29:TYR:HE1	2:C:72:ARG:HD3	1.83	0.43
1:A:94:TYR:OH	1:A:350:SER:OG	2.16	0.43
1:A:127:VAL:HB	1:A:157:ASN:HD22	1.83	0.43
1:B:68:LEU:HD13	1:B:307:PHE:CE1	2.53	0.43
3:D:58:PRO:HG2	3:D:61:PHE:CE1	2.53	0.43
1:A:119:GLN:O	1:A:120:ARG:HD2	2.19	0.43
1:A:101:ALA:HB3	1:A:130:VAL:HG11	1.99	0.43
1:B:59:TRP:HZ3	1:B:60:LEU:HD23	1.84	0.43
1:B:187:ALA:O	1:B:191:ASN:N	2.49	0.43
1:B:279:LEU:O	1:B:279:LEU:HD23	2.18	0.43
3:F:38:LYS:O	3:F:41:THR:HB	2.18	0.43
1:A:420:GLN:HG2	1:A:421:LEU:HD23	2.01	0.43
1:B:62:ASN:O	1:B:66:GLY:N	2.49	0.43
1:B:87:ALA:O	1:B:91:MET:HG3	2.19	0.43
1:B:356:ILE:C	1:B:359:PRO:HD2	2.44	0.43
1:A:174:ARG:O	1:A:178:LEU:HB2	2.19	0.43
1:A:194:LEU:HD21	1:B:422:ILE:HD11	2.00	0.43
2:E:30:SER:O	2:E:31:ARG:HB2	2.19	0.43
3:F:107:ARG:HG3	3:F:139:TYR:CD2	2.54	0.43
3:D:77:MET:HE2	3:D:77:MET:HB3	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:115:SER:HB3	3:D:117:PHE:CE1	2.54	0.43
3:F:90:TRP:CE3	3:F:95:GLN:HG3	2.54	0.43
1:A:87:ALA:HA	1:A:296:GLY:HA2	2.01	0.42
1:A:397:LEU:HA	1:A:397:LEU:HD23	1.78	0.42
1:B:91:MET:CG	1:B:296:GLY:HA3	2.49	0.42
1:B:108:GLY:HA3	1:B:153:GLN:OE1	2.19	0.42
3:F:119:PRO:HD3	3:F:131:VAL:HG22	2.00	0.42
1:B:107:SER:OG	1:B:348:PHE:CE1	2.62	0.42
1:B:423:LEU:HD12	1:B:423:LEU:HA	1.75	0.42
2:E:135:GLY:C	2:E:137:ALA:N	2.78	0.42
2:E:153:TYR:CE2	2:E:158:VAL:HG13	2.55	0.42
1:B:128:LEU:O	1:B:132:PHE:HB2	2.19	0.42
3:D:8:PRO:O	3:D:101:THR:HG23	2.19	0.42
3:D:30:SER:O	3:D:91:SER:HB3	2.20	0.42
3:D:34:TRP:CD2	3:D:72:LEU:HD12	2.53	0.42
1:A:32:PRO:O	1:A:35:ILE:N	2.49	0.42
1:A:367:LEU:HD12	1:A:367:LEU:HA	1.73	0.42
1:A:401:SER:O	1:A:444:LEU:HB2	2.19	0.42
2:E:202:THR:HB	2:E:216:LYS:O	2.19	0.42
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.27	0.42
1:B:206:PRO:CD	1:B:211:THR:HG21	2.44	0.42
2:C:167:LEU:HD23	2:C:189:VAL:HG21	2.00	0.42
3:D:194:GLU:CG	3:D:205:VAL:HG12	2.39	0.42
1:B:184:ALA:HB1	1:B:225:SER:HB3	2.00	0.42
3:D:21:MET:SD	3:D:85:TYR:HB2	2.60	0.42
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.34	0.42
1:B:125:TRP:HD1	1:B:126:ARG:HG3	1.78	0.42
1:B:342:ILE:O	1:B:346:LEU:HD13	2.20	0.42
2:C:105:TYR:CD1	3:D:91:SER:HA	2.55	0.42
2:E:131:PRO:O	2:E:132:LEU:HD23	2.20	0.42
3:F:60:ARG:HD2	3:F:81:ASP:OD2	2.20	0.42
1:A:145:LEU:HD21	1:A:347:CYS:HB3	2.01	0.42
1:B:182:ALA:CB	1:B:204:MET:HE1	2.49	0.42
1:B:284:HIS:C	1:B:286:GLY:N	2.78	0.41
2:E:54:VAL:HG23	2:E:56:SER:HB3	2.00	0.41
1:A:403:ARG:NH2	1:B:29:ASP:O	2.53	0.41
1:B:117:GLU:HA	1:B:209:ARG:HH12	1.84	0.41
1:B:394:MET:HE2	1:B:412:VAL:HG22	2.02	0.41
2:C:43:LYS:HB3	2:C:43:LYS:HE2	1.84	0.41
2:C:58:ILE:HD13	2:C:70:ILE:O	2.20	0.41
2:E:47:TRP:CD2	3:F:95:GLN:NE2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:VAL:O	1:A:345:LEU:HG	2.21	0.41
1:B:150:PRO:CG	1:B:354:GLY:HA2	2.50	0.41
1:B:320:ILE:HB	1:B:321:PRO:HD3	2.01	0.41
2:C:12:VAL:CG2	2:C:119:VAL:HG22	2.50	0.41
2:E:171:VAL:HA	2:E:188:SER:O	2.19	0.41
3:F:11:MET:HE3	3:F:11:MET:HB2	1.86	0.41
3:D:89:GLN:O	3:D:95:GLN:HB2	2.20	0.41
1:A:376:VAL:HG22	1:A:384:LEU:CB	2.46	0.41
1:A:451:ARG:O	1:A:455:LYS:HG3	2.20	0.41
1:A:372:GLY:HA2	1:A:375:ALA:HB3	2.03	0.41
1:B:84:LEU:HA	1:B:87:ALA:HB3	2.03	0.41
1:B:123:ARG:NE	1:B:126:ARG:HD2	2.26	0.41
2:E:160:VAL:HG11	2:E:187:SER:CB	2.51	0.41
1:A:29:ASP:CG	1:A:216:LYS:HZ2	2.26	0.41
1:A:143:MET:HE2	1:A:347:CYS:SG	2.61	0.41
1:A:219:PHE:HZ	1:B:406:LEU:HD13	1.86	0.41
1:B:133:PHE:HA	1:B:136:LEU:HD12	2.03	0.41
1:B:188:ALA:HB2	1:B:225:SER:OG	2.21	0.41
2:C:160:VAL:HG11	2:C:187:SER:HB2	2.02	0.41
2:C:176:ALA:HB2	2:C:185:LEU:HD23	2.03	0.41
3:D:31:TYR:HA	3:D:50:THR:OG1	2.21	0.41
3:F:84:THR:HA	3:F:102:LYS:HA	2.03	0.41
1:A:355:GLY:HA2	4:A:501:BR:BR	2.76	0.41
1:B:358:ALA:HB3	1:B:359:PRO:HD3	2.02	0.41
3:D:12:SER:HB2	3:D:106:LEU:HD12	2.03	0.41
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.96	0.41
1:B:25:LEU:C	1:B:27:GLU:N	2.78	0.41
2:C:6:GLU:HG2	2:C:115:THR:HG23	2.03	0.41
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.89	0.41
1:A:348:PHE:CD2	1:A:356:ILE:HD12	2.56	0.40
1:B:399:ALA:O	1:B:403:ARG:HA	2.22	0.40
2:C:53:PRO:HA	2:C:72:ARG:CZ	2.51	0.40
1:B:153:GLN:O	1:B:157:ASN:ND2	2.49	0.40
1:B:370:ALA:O	1:B:374:VAL:HG23	2.21	0.40
3:D:2:ILE:HD12	3:D:27:SER:HB2	2.02	0.40
2:E:131:PRO:C	2:E:132:LEU:HD23	2.46	0.40
1:A:122:VAL:HG11	1:A:160:ARG:HB2	2.03	0.40
1:B:443:PRO:HB2	1:B:446:SER:HB2	2.02	0.40
2:C:131:PRO:HD3	2:C:216:LYS:HG2	2.03	0.40
3:F:30:SER:HA	3:F:70:TYR:OH	2.21	0.40
3:F:77:MET:HE2	3:F:77:MET:HB3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ILE:HD12	1:A:422:ILE:HA	1.89	0.40
1:B:324:THR:C	1:B:326:GLY:H	2.30	0.40
1:A:224:MET:O	1:A:228:MET:HG2	2.22	0.40
1:A:423:LEU:HD13	1:B:230:ARG:CZ	2.52	0.40
3:D:12:SER:HA	3:D:104:GLU:O	2.21	0.40
2:E:12:VAL:HG11	2:E:18:LEU:HD22	2.03	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	438/473 (93%)	398 (91%)	39 (9%)	1 (0%)	43	71
1	B	438/473 (93%)	400 (91%)	34 (8%)	4 (1%)	14	43
2	C	220/222 (99%)	194 (88%)	24 (11%)	2 (1%)	14	43
2	E	219/222 (99%)	197 (90%)	19 (9%)	3 (1%)	9	34
3	D	209/211 (99%)	191 (91%)	17 (8%)	1 (0%)	24	55
3	F	209/211 (99%)	197 (94%)	11 (5%)	1 (0%)	24	55
All	All	1733/1812 (96%)	1577 (91%)	144 (8%)	12 (1%)	18	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	26	LEU
1	B	325	ALA
2	E	62	PRO
1	A	285	GLY
2	C	157	PRO
2	E	138	ALA

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Mol	Chain	Res	Type
1	B	443	PRO
2	C	62	PRO
3	D	67	GLY
2	E	195	SER
3	F	67	GLY
1	B	144	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/356 (93%)	330 (100%)	0	100	100
1	B	330/356 (93%)	330 (100%)	0	100	100
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%)	185 (100%)	0	100	100
All	All	1393/1446 (96%)	1393 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	HIS
1	B	157	ASN
2	C	74	ASN
2	C	82	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 4 ligands modelled in this entry, 4 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	440/473 (93%)	0.53	38 (8%)	16 9	81, 111, 139, 157	0
1	B	440/473 (93%)	0.75	48 (10%)	10 6	90, 117, 149, 173	0
2	C	222/222 (100%)	0.49	18 (8%)	18 10	75, 104, 140, 171	0
2	E	221/222 (99%)	0.40	19 (8%)	16 9	79, 102, 134, 166	0
3	D	211/211 (100%)	0.70	18 (8%)	16 9	92, 115, 134, 151	0
3	F	211/211 (100%)	0.14	4 (1%)	66 45	76, 96, 149, 160	0
All	All	1745/1812 (96%)	0.54	145 (8%)	17 10	75, 110, 143, 173	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	ASP	7.5
1	B	72	ALA	6.8
3	D	157	GLY	6.3
3	D	156	ASN	6.2
1	B	307	PHE	6.0
1	B	183	ALA	5.6
1	B	95	PHE	5.4
2	C	113	ALA	5.2
1	A	447	ALA	4.9
1	A	374	VAL	4.6
1	B	308	VAL	4.6
3	D	40	GLY	4.6
1	B	159	GLY	4.6
2	E	113	ALA	4.4
3	D	20	THR	4.4
3	D	93	HIS	4.3
1	A	378	LEU	4.3
2	C	8	GLY	4.3
1	B	96	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	258	LEU	4.2
1	B	104	ALA	4.2
2	E	114	GLY	4.2
1	A	198	LEU	4.2
1	A	212	LEU	4.1
1	B	198	LEU	4.0
2	C	200	THR	4.0
1	A	448	ILE	4.0
1	B	239	ILE	3.9
3	D	124	LEU	3.9
3	D	69	SER	3.8
2	C	196	TRP	3.8
1	B	289	THR	3.8
1	A	321	PRO	3.8
2	E	184	THR	3.8
1	B	69	VAL	3.7
1	B	196	GLY	3.7
1	A	452	THR	3.7
1	B	309	ALA	3.6
1	A	166	PHE	3.6
1	A	84	LEU	3.5
3	D	159	LEU	3.5
1	B	70	HIS	3.5
1	B	241	VAL	3.5
3	D	158	VAL	3.4
1	B	177	LEU	3.4
3	D	22	THR	3.4
2	C	31	ARG	3.4
3	F	28	SER	3.4
1	B	293	LEU	3.4
2	C	217	LYS	3.4
3	D	128	GLY	3.3
1	B	161	MET	3.3
1	A	249	LEU	3.3
1	A	184	ALA	3.3
1	B	133	PHE	3.2
1	B	186	LEU	3.2
2	C	102	GLY	3.1
1	B	201	ILE	3.1
2	C	47	TRP	3.1
1	A	182	ALA	3.1
3	D	208	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	171	ASP	3.0
3	D	38	LYS	3.0
1	B	179	ALA	3.0
2	C	219	VAL	3.0
1	B	178	LEU	2.9
1	B	352	ALA	2.9
2	E	177	VAL	2.9
2	E	137	ALA	2.9
2	E	59	ASN	2.8
2	C	139	ALA	2.8
2	C	201	VAL	2.8
1	B	180	THR	2.8
1	A	379	PHE	2.8
1	A	237	ALA	2.8
1	A	450	ALA	2.8
2	E	7	SER	2.8
1	A	261	ILE	2.7
2	C	28	ASP	2.7
1	A	373	MET	2.7
3	D	126	SER	2.7
2	E	115	THR	2.6
1	B	200	ILE	2.6
1	B	235	GLU	2.6
2	E	2	VAL	2.6
3	F	26	SER	2.6
2	C	104	GLY	2.6
1	A	67	ALA	2.6
1	B	376	VAL	2.6
1	A	320	ILE	2.5
1	B	199	PHE	2.5
1	A	168	LEU	2.5
1	B	288	ILE	2.5
1	A	165	ILE	2.5
3	D	121	SER	2.5
3	D	41	THR	2.5
3	F	27	SER	2.4
1	B	416	THR	2.4
2	C	114	GLY	2.4
2	E	140	ALA	2.4
1	B	350	SER	2.4
1	B	34	ALA	2.4
1	B	195	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	207	GLN	2.4
1	A	367	LEU	2.4
1	B	351	GLY	2.4
2	C	218	ILE	2.4
1	A	269	PHE	2.3
1	A	222	VAL	2.3
1	A	380	PRO	2.3
2	C	95	TYR	2.3
2	E	186	SER	2.3
1	A	235	GLU	2.3
3	F	176	SER	2.3
1	B	25	LEU	2.3
2	E	134	PRO	2.3
2	E	120	SER	2.3
1	B	94	TYR	2.3
2	C	138	ALA	2.2
1	A	395	GLY	2.2
1	B	310	PRO	2.2
1	B	353	PRO	2.2
2	C	147	GLY	2.2
1	B	402	ILE	2.2
1	A	292	VAL	2.1
2	E	31	ARG	2.1
2	E	66	ASP	2.1
1	B	143	MET	2.1
1	B	160	ARG	2.1
1	A	178	LEU	2.1
1	A	209	ARG	2.1
1	A	179	ALA	2.1
1	B	317	ALA	2.1
2	E	105	TYR	2.1
3	D	31	TYR	2.1
3	D	68	THR	2.1
1	A	442	LYS	2.0
2	E	64	LEU	2.0
1	B	75	TYR	2.0
1	B	358	ALA	2.0
1	A	443	PRO	2.0
2	E	6	GLU	2.0
1	A	376	VAL	2.0
2	E	176	ALA	2.0
1	B	61	GLN	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](#)

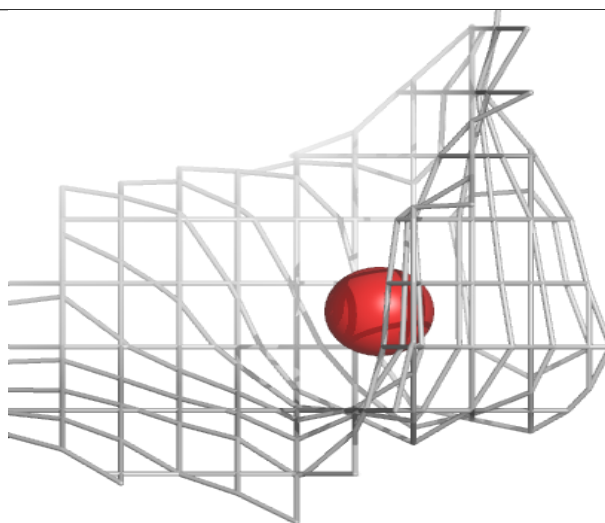
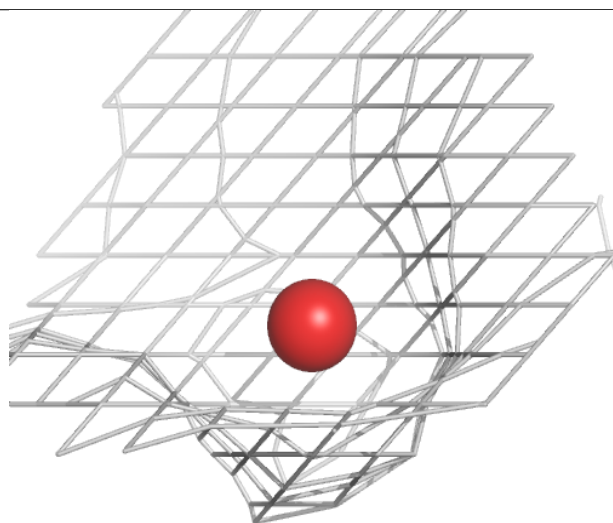
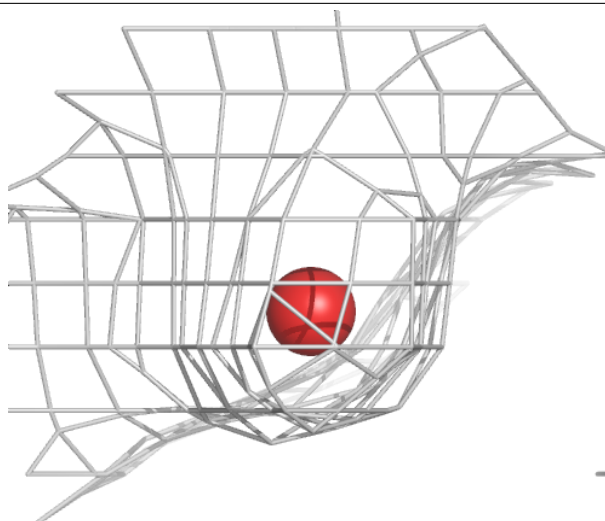
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.84	0.14	196,196,196,196	0
4	BR	B	502	1/1	0.85	0.16	150,150,150,150	0
4	BR	B	501	1/1	0.88	0.19	203,203,203,203	0
4	BR	A	502	1/1	0.90	0.19	160,160,160,160	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.

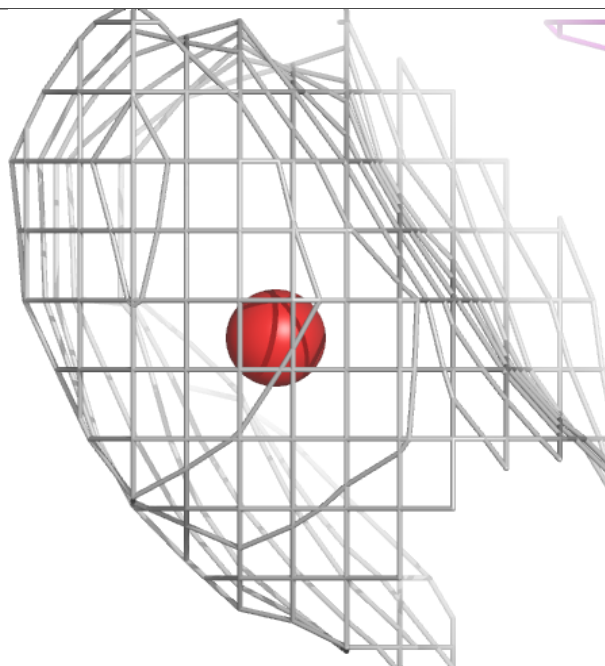
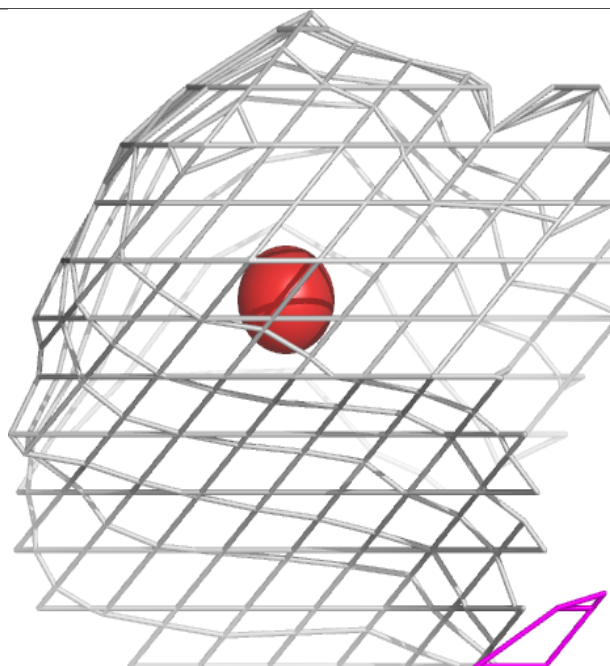
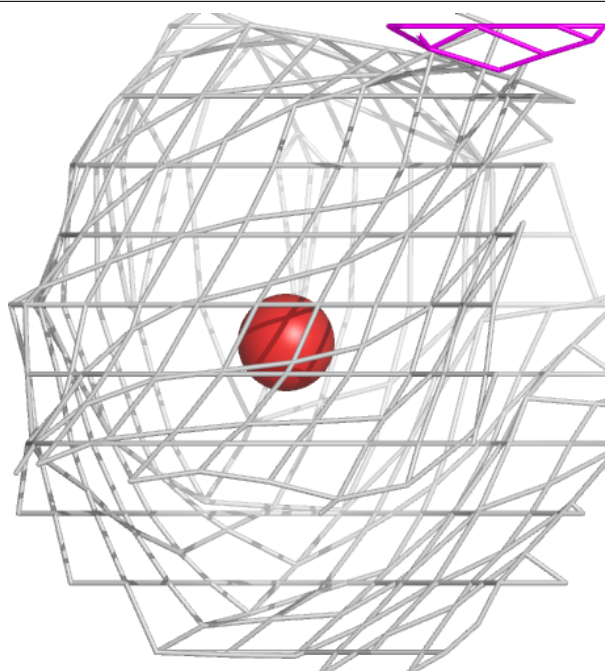
Electron density around BR A 501:

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



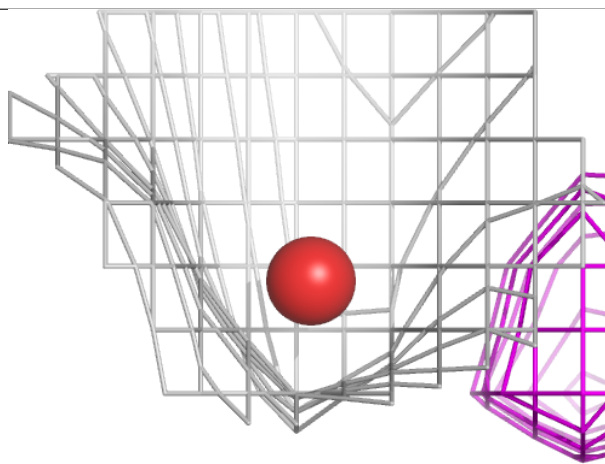
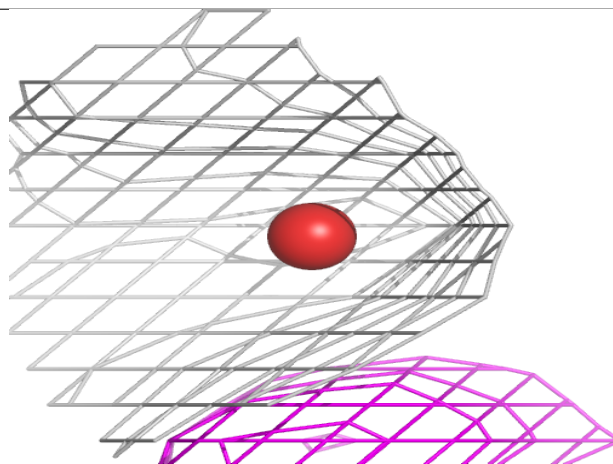
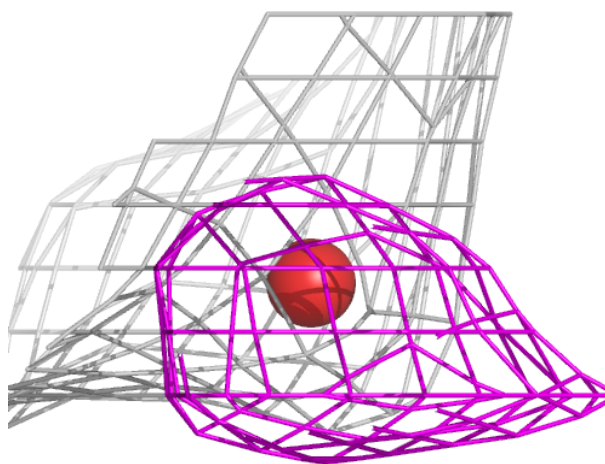
Electron density around BR B 502:

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



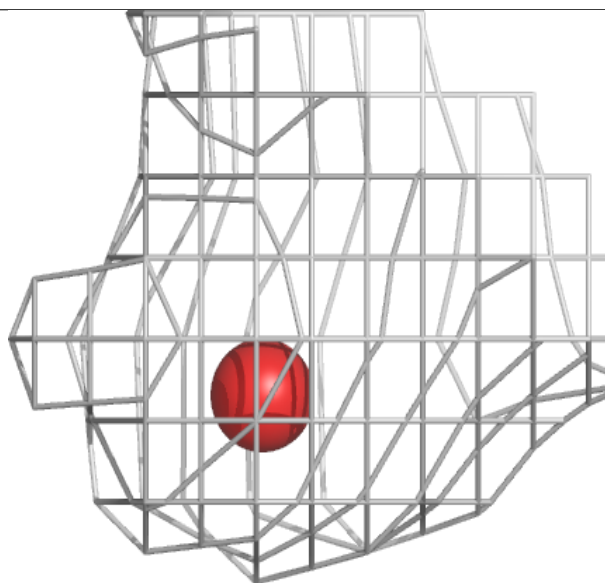
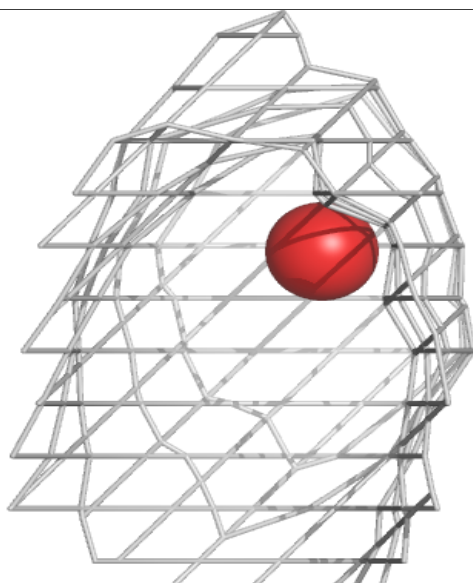
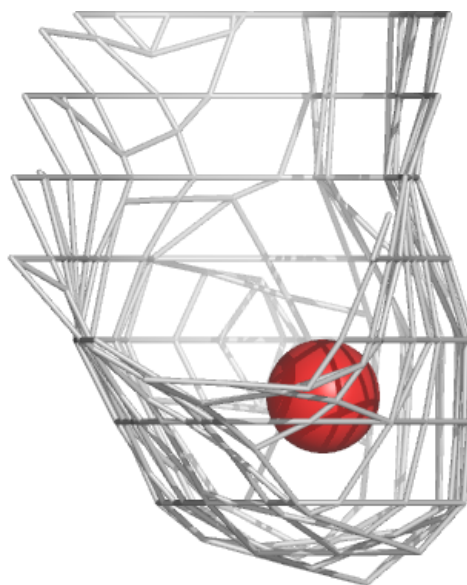
Electron density around BR B 501:

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



Electron density around BR A 502:

$2mF_o-DF_c$ (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.