Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 09:25 PM JST

PDB ID	:	6ADC
Title	:	Crystal structure of the E148A mutant CLC-ec1 in the presence of 50mM bromoacetate
Authors	:	Lim, H.-H.; Park, K.
Deposited on	:	2018-07-31
Resolution	:	3.06 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 (i) 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 (i)) were used in the production of this report:

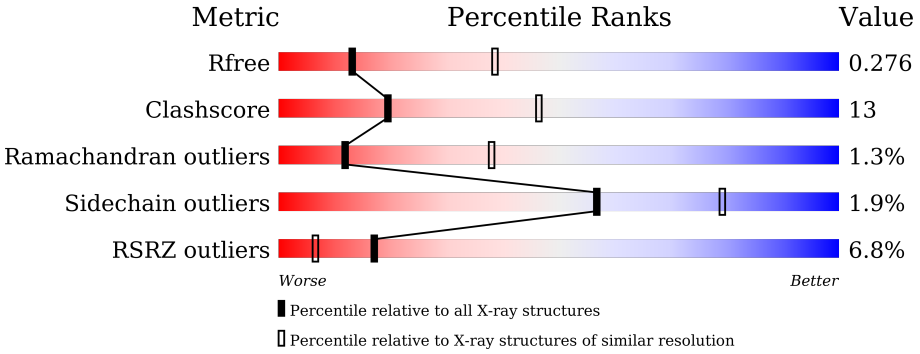
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.06 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}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 <=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	442	6% 72% 26% •
1	B	442	10% 72% 27% •
2	C	222	7% 75% 23% •
2	E	222	5% 73% 26% •
3	D	211	9% 64% 32% •
3	F	211	3% 74% 25%

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	BXA	A	501[A]	-	-	X	-
4	BXA	B	501[A]	-	-	X	-
4	BXA	B	501[B]	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13237 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
			Total	C	N	O	S			
1	A	442	3311	2178	557	556	20	0	0	0
1	B	442	3311	2178	557	556	20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

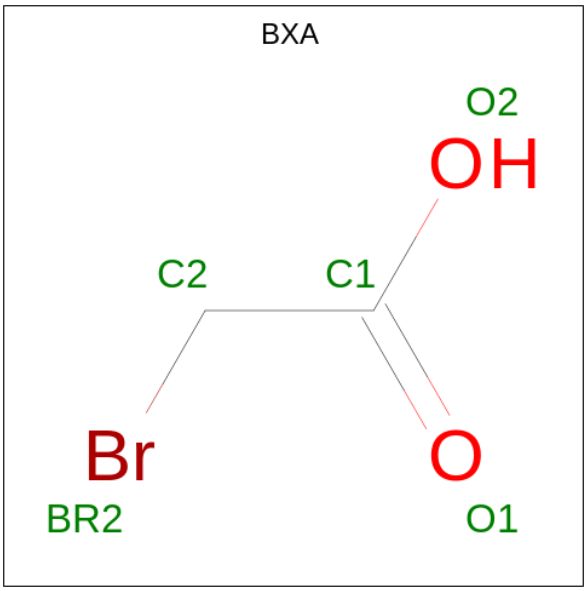
- Molecule 2 is a protein called antibody Fab fragment, heavy chain.

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

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

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

- Molecule 4 is bromoacetic acid (three-letter code: BXA) (formula: $C_2H_3BrO_2$).



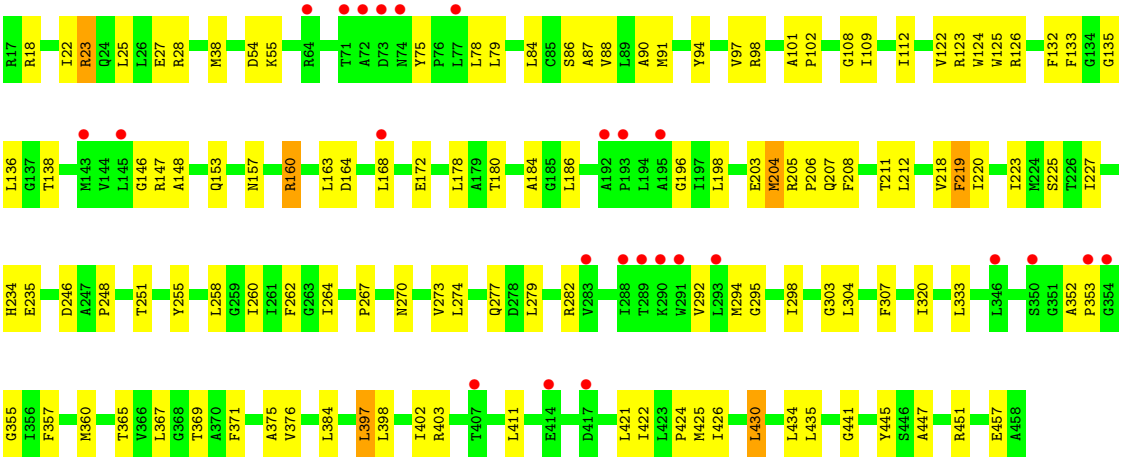
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	O		
4	A	1	10	2	4	4	0	1
			Total	Br	C	O		
4	B	1	10	2	4	4	0	1

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.

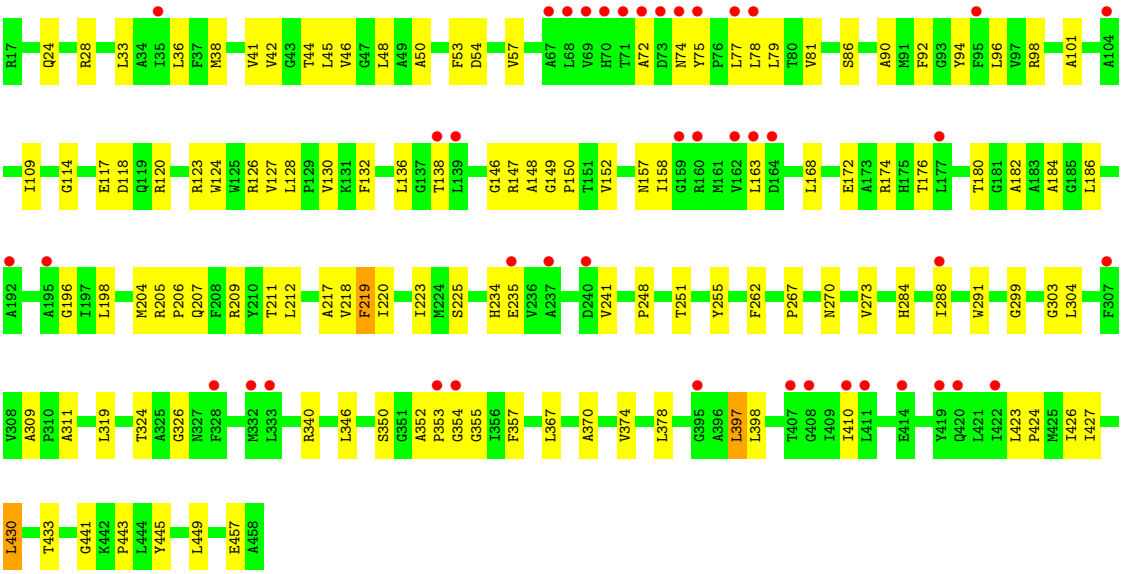
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain A:



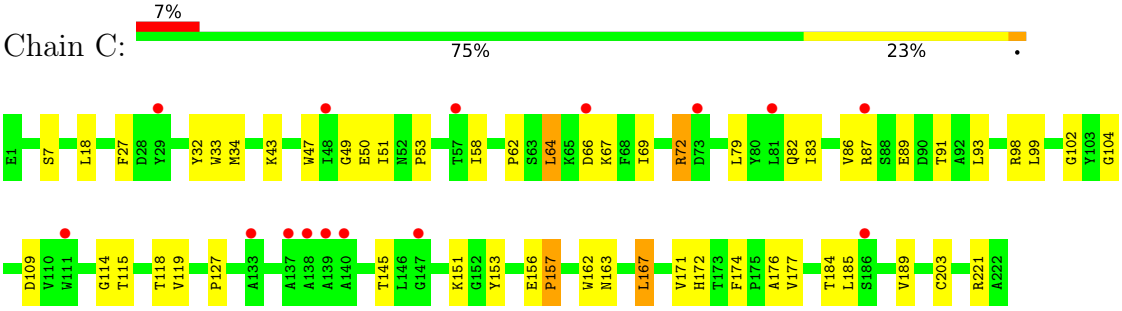
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain B:



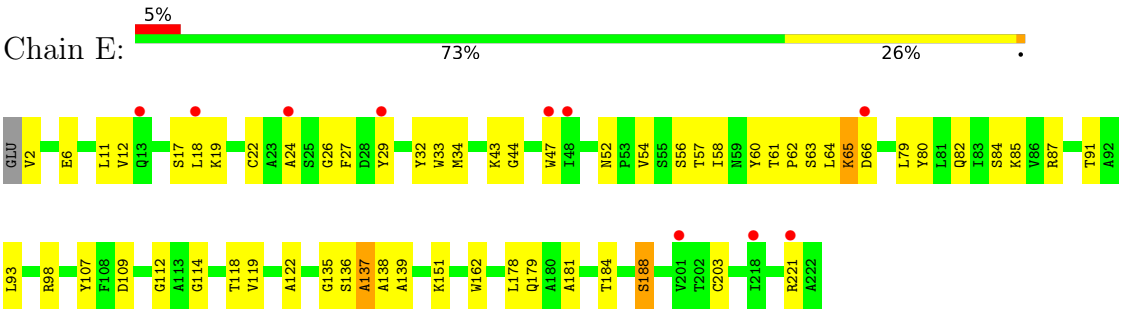
• Molecule 2: antibody Fab fragment, heavy chain

Chain C:



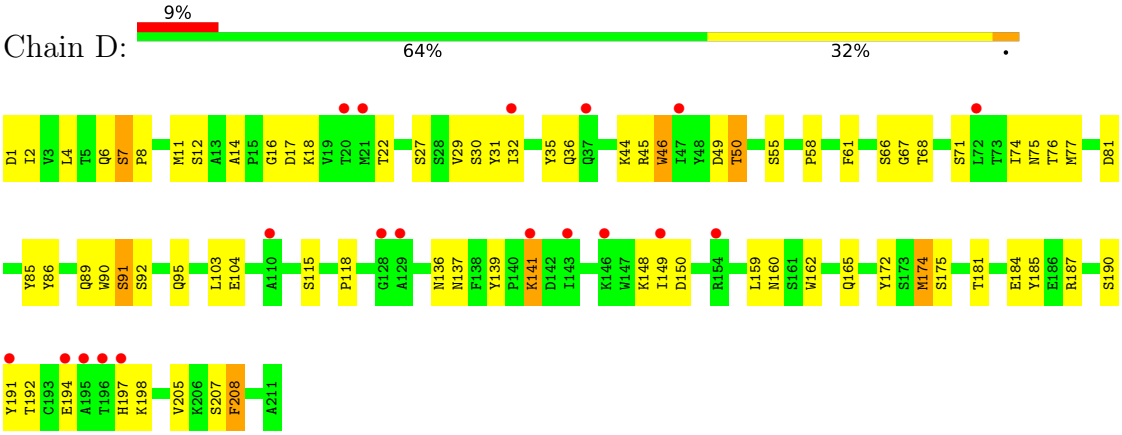
• Molecule 2: antibody Fab fragment, heavy chain

Chain E:



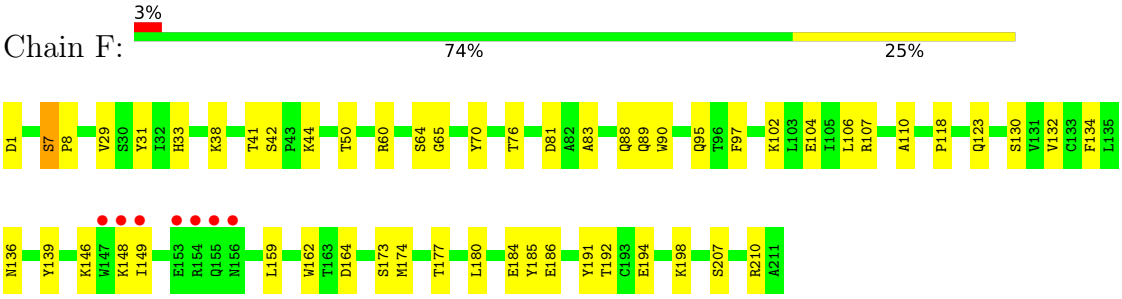
• Molecule 3: antibody Fab fragment, light chain

Chain D:



• Molecule 3: antibody Fab fragment, light chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	233.25Å 96.73Å 169.78Å 90.00° 131.45° 90.00°	Depositor
Resolution (Å)	34.85 – 3.06 49.92 – 3.06	Depositor EDS
% Data completeness (in resolution range)	97.6 (34.85-3.06) 97.8 (49.92-3.06)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.226 , 0.275 0.228 , 0.276	Depositor DCC
R_{free} test set	2651 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	103.1	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 58.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.002 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	13237	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BXA

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	0.46	0/3383	0.72	1/4592 (0.0%)
1	B	0.45	0/3383	0.69	2/4592 (0.0%)
2	C	0.55	0/1730	0.71	0/2367
2	E	0.52	0/1721	0.70	0/2355
3	D	0.52	0/1660	0.70	0/2257
3	F	0.48	0/1660	0.71	0/2257
All	All	0.49	0/13537	0.71	3/18420 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	430	LEU	CA-CB-CG	-6.56	100.21	115.30
1	A	430	LEU	CA-CB-CG	-5.78	102.00	115.30
1	B	319	LEU	CA-CB-CG	5.09	127.02	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3311	0	3469	111	0
1	B	3311	0	3469	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1681	0	1663	32	0
2	E	1672	0	1654	37	0
3	D	1621	0	1546	58	0
3	F	1621	0	1546	40	0
4	A	10	0	0	5	0
4	B	10	0	0	8	0
All	All	13237	0	13347	341	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 13.

All (341) 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:207:GLN:HG2	1:B:28:ARG:HD2	1.48	0.95
3:D:6:GLN:NE2	3:D:85:TYR:O	2.07	0.87
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.40	0.86
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.57	0.86
1:A:28:ARG:HD2	1:B:207:GLN:HG2	1.57	0.85
3:D:95:GLN:OE1	3:D:95:GLN:N	2.08	0.85
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.43	0.82
1:A:234:HIS:HD1	1:A:235:GLU:HG3	1.46	0.81
2:E:52:ASN:HD21	2:E:56:SER:HB3	1.47	0.79
1:A:205:ARG:HH12	1:B:205:ARG:HH12	1.31	0.78
1:A:206:PRO:HG2	1:A:211:THR:HG21	1.67	0.77
1:A:180:THR:HG22	1:A:218:VAL:HG22	1.66	0.77
3:D:191:TYR:HB2	3:D:208:PHE:HE1	1.49	0.77
1:B:206:PRO:HG2	1:B:211:THR:HG21	1.68	0.75
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.16	0.75
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.19	0.74
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.22	0.74
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.71	0.73
2:E:2:VAL:HA	2:E:26:GLY:HA3	1.71	0.73
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.89	0.72
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.69	0.72
3:D:191:TYR:HB2	3:D:208:PHE:CE1	2.24	0.72
3:F:148:LYS:HB2	3:F:192:THR:HG23	1.70	0.72
2:E:137:ALA:O	2:E:139:ALA:N	2.22	0.72
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.06	0.70
2:E:221:ARG:NH2	3:F:118:PRO:O	2.24	0.70
1:B:355:GLY:HA3	4:B:501[B]:BXA:C1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.75	0.69
3:F:95:GLN:H	3:F:95:GLN:CD	1.96	0.68
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.28	0.67
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.77	0.66
2:E:19:LYS:HG3	2:E:82:GLN:HG2	1.78	0.66
1:A:146:GLY:HA3	4:A:501[A]:BXA:BR2	2.51	0.66
3:D:1:ASP:OD1	3:D:1:ASP:N	2.27	0.65
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.30	0.65
3:D:197:HIS:CD2	3:D:198:LYS:H	2.15	0.65
3:D:14:ALA:O	3:D:17:ASP:HB3	1.97	0.64
1:B:101:ALA:HB3	1:B:130:VAL:HG11	1.79	0.64
1:A:180:THR:HG22	1:A:218:VAL:CG2	2.27	0.64
3:F:89:GLN:O	3:F:95:GLN:HB2	1.97	0.64
3:D:197:HIS:CG	3:D:198:LYS:H	2.16	0.63
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.34	0.63
2:C:163:ASN:HD22	2:C:167:LEU:HD13	1.62	0.63
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.81	0.62
1:A:360:MET:HG2	1:A:397:LEU:HD13	1.82	0.62
1:A:422:ILE:HA	1:A:425:MET:HE3	1.81	0.62
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.37	0.60
3:F:106:LEU:HA	3:F:139:TYR:OH	2.02	0.60
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.82	0.60
2:C:176:ALA:HB2	2:C:185:LEU:HD23	1.83	0.60
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.85	0.59
1:A:279:LEU:HA	1:A:282:ARG:HH11	1.66	0.59
1:B:148:ALA:HB3	4:B:501[A]:BXA:C2	2.33	0.59
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.67	0.59
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.85	0.59
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.38	0.59
3:D:187:ARG:HH11	3:D:187:ARG:HG2	1.68	0.58
1:A:333:LEU:HD11	1:A:369:THR:HG22	1.85	0.58
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.69	0.58
1:B:374:VAL:O	1:B:378:LEU:HG	2.03	0.58
1:A:88:VAL:HA	1:A:91:MET:HE2	1.85	0.57
1:A:360:MET:HE3	1:A:398:LEU:HD23	1.86	0.57
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.86	0.57
2:C:151:LYS:HA	2:C:184:THR:HG23	1.85	0.57
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.40	0.57
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.86	0.56
1:A:163:LEU:HD12	1:A:168:LEU:HB2	1.87	0.56
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:NH1	1:A:27:GLU:HG3	2.21	0.56
3:F:192:THR:HB	3:F:207:SER:HB2	1.86	0.56
1:A:260:ILE:O	1:A:264:ILE:HG23	2.05	0.56
3:D:31:TYR:HA	3:D:50:THR:OG1	2.05	0.56
1:B:146:GLY:HA3	4:B:501[A]:BXA:BR2	2.60	0.56
1:A:220:ILE:HG12	1:B:430:LEU:HD23	1.88	0.56
3:D:149:ILE:HG23	3:D:191:TYR:CE1	2.41	0.56
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.88	0.56
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.21	0.55
1:A:219:PHE:CD2	1:B:430:LEU:HD11	2.40	0.55
3:F:31:TYR:HA	3:F:50:THR:OG1	2.06	0.55
1:B:355:GLY:HA3	4:B:501[A]:BXA:C1	2.36	0.55
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.41	0.55
1:B:357:PHE:HB3	4:B:501[A]:BXA:C2	2.37	0.55
3:F:89:GLN:NE2	3:F:95:GLN:HA	2.21	0.55
3:D:118:PRO:HB3	3:D:208:PHE:CE2	2.42	0.55
1:B:41:VAL:O	1:B:45:LEU:HG	2.07	0.54
2:E:135:GLY:O	2:E:137:ALA:N	2.39	0.54
3:F:7:SER:CB	3:F:8:PRO:HD3	2.38	0.54
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.17	0.54
1:B:176:THR:O	1:B:180:THR:HG23	2.07	0.54
3:D:162:TRP:CE2	3:D:174:MET:HG3	2.42	0.54
1:B:370:ALA:O	1:B:374:VAL:HG23	2.08	0.54
3:D:6:GLN:HA	3:D:22:THR:O	2.08	0.54
1:B:172:GLU:HG3	1:B:212:LEU:O	2.08	0.54
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.07	0.54
3:D:192:THR:HG22	3:D:207:SER:CB	2.38	0.54
1:B:38:MET:O	1:B:42:VAL:HG23	2.07	0.54
1:A:133:PHE:HA	1:A:136:LEU:HD12	1.90	0.54
2:E:188:SER:HB2	3:F:134:PHE:CE2	2.43	0.54
2:C:172:HIS:O	2:C:174:PHE:CE1	2.60	0.54
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.43	0.53
3:F:95:GLN:CD	3:F:95:GLN:N	2.61	0.53
1:A:112:ILE:HD11	1:A:153:GLN:HG3	1.89	0.53
1:A:219:PHE:CG	1:B:430:LEU:HD11	2.42	0.53
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.88	0.53
1:B:163:LEU:HD22	1:B:174:ARG:HA	1.91	0.53
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.89	0.53
2:C:18:LEU:HD11	2:C:83:ILE:HD12	1.89	0.53
2:C:91:THR:HG23	2:C:118:THR:HA	1.90	0.53
2:E:6:GLU:OE1	2:E:112:GLY:HA3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.43	0.53
1:A:148:ALA:HB1	1:A:186:LEU:HD12	1.91	0.53
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.90	0.53
2:E:24:ALA:HB1	2:E:27:PHE:CE1	2.44	0.53
1:A:430:LEU:HD23	1:B:220:ILE:HG12	1.91	0.52
2:C:93:LEU:HD11	2:C:114:GLY:HA3	1.92	0.52
2:C:176:ALA:HA	2:C:185:LEU:HB3	1.90	0.52
1:A:148:ALA:N	4:A:501[A]:BXA:BR2	2.97	0.52
1:A:447:ALA:O	1:A:451:ARG:HG3	2.10	0.52
1:A:198:LEU:HD11	1:B:198:LEU:HD11	1.92	0.52
1:A:160:ARG:HE	1:A:163:LEU:HD23	1.75	0.52
1:A:422:ILE:HD12	1:A:425:MET:HE3	1.92	0.52
2:E:17:SER:HB3	2:E:84:SER:HA	1.90	0.52
3:F:7:SER:HB2	3:F:8:PRO:HD3	1.92	0.52
1:A:86:SER:OG	1:A:303:GLY:HA3	2.10	0.52
1:A:122:VAL:HG11	1:A:160:ARG:HB2	1.92	0.52
1:A:160:ARG:NE	1:A:163:LEU:HD23	2.24	0.51
3:D:11:MET:HG3	3:D:103:LEU:HD12	1.93	0.51
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.92	0.51
2:C:171:VAL:HG22	2:C:189:VAL:HG23	1.93	0.51
1:A:180:THR:HG22	1:A:218:VAL:HA	1.92	0.51
2:C:69:ILE:HB	2:C:82:GLN:HB2	1.91	0.51
1:A:208:PHE:CE2	1:B:24:GLN:HB3	2.46	0.51
2:E:91:THR:HG1	2:E:119:VAL:H	1.55	0.51
1:A:219:PHE:O	1:A:223:ILE:HG13	2.11	0.51
1:B:114:GLY:O	1:B:117:GLU:N	2.40	0.50
1:B:148:ALA:O	1:B:152:VAL:HG23	2.12	0.50
2:C:87:ARG:NH2	2:C:89:GLU:OE1	2.38	0.50
1:A:294:MET:O	1:A:298:ILE:HG13	2.11	0.50
1:B:206:PRO:CG	1:B:211:THR:HG21	2.39	0.50
1:A:94:TYR:CE1	1:A:295:GLY:HA3	2.47	0.50
1:A:262:PHE:CE1	1:A:367:LEU:HD23	2.46	0.50
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.94	0.50
2:E:162:TRP:CH2	2:E:203:CYS:HB3	2.46	0.50
3:D:12:SER:HA	3:D:104:GLU:O	2.12	0.50
1:A:91:MET:HG2	1:A:292:VAL:O	2.12	0.49
3:D:148:LYS:HB2	3:D:192:THR:HG1	1.75	0.49
1:A:248:PRO:O	1:A:251:THR:HB	2.11	0.49
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.94	0.49
1:A:376:VAL:HG22	1:A:384:LEU:HB2	1.94	0.49
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:TYR:CE2	1:A:424:PRO:HB3	2.48	0.49
1:B:198:LEU:HG	1:B:410:ILE:HD12	1.94	0.49
1:A:219:PHE:CE1	1:B:426:ILE:HG23	2.47	0.49
1:A:90:ALA:O	1:A:94:TYR:HD1	1.95	0.49
1:B:42:VAL:O	1:B:46:VAL:HG23	2.13	0.49
1:B:267:PRO:HB3	1:B:441:GLY:HA3	1.93	0.49
1:A:355:GLY:HA3	4:A:501[B]:BXA:BR2	2.68	0.49
3:D:77:MET:SD	3:D:103:LEU:HD21	2.53	0.49
3:F:186:GLU:HG2	3:F:210:ARG:NH1	2.28	0.48
1:A:430:LEU:HD11	1:B:219:PHE:CG	2.48	0.48
1:A:25:LEU:HD11	1:B:449:LEU:HD23	1.95	0.48
2:E:52:ASN:CG	2:E:57:THR:H	2.16	0.48
3:D:29:VAL:CG1	3:D:32:ILE:HD11	2.44	0.48
3:D:30:SER:H	3:D:91:SER:CB	2.26	0.48
1:B:148:ALA:N	4:B:501[B]:BXA:O2	2.46	0.48
3:F:88:GLN:HG3	3:F:97:PHE:CE1	2.49	0.48
1:A:180:THR:CG2	1:A:218:VAL:HA	2.44	0.48
1:B:149:GLY:H	4:B:501[A]:BXA:C2	2.26	0.48
2:E:178:LEU:HD11	2:E:181:ALA:HA	1.95	0.48
3:F:107:ARG:NH2	3:F:110:ALA:HB2	2.29	0.48
1:B:248:PRO:O	1:B:251:THR:HB	2.14	0.47
3:F:192:THR:HB	3:F:207:SER:CB	2.44	0.47
1:A:203:GLU:OE1	1:B:28:ARG:NH2	2.43	0.47
1:B:90:ALA:HB2	1:B:299:GLY:HA3	1.96	0.47
2:E:93:LEU:HD11	2:E:114:GLY:HA3	1.95	0.47
1:B:150:PRO:HG3	1:B:354:GLY:HA2	1.95	0.47
3:D:74:ILE:HG21	3:D:81:ASP:OD2	2.14	0.47
3:F:64:SER:OG	3:F:65:GLY:N	2.48	0.47
1:A:78:LEU:HD11	1:A:307:PHE:CE2	2.49	0.47
1:A:434:LEU:HD11	1:B:220:ILE:HD11	1.95	0.47
1:B:311:ALA:O	1:B:340:ARG:HD2	2.14	0.47
3:F:102:LYS:HE3	3:F:104:GLU:OE2	2.14	0.47
1:A:258:LEU:HD13	1:A:371:PHE:CG	2.49	0.47
1:B:53:PHE:O	1:B:57:VAL:HG23	2.15	0.47
1:B:152:VAL:HG13	1:B:182:ALA:HB1	1.96	0.47
1:B:184:ALA:HB1	1:B:225:SER:CB	2.44	0.47
1:A:220:ILE:CG1	1:B:430:LEU:HD23	2.45	0.47
1:B:324:THR:C	1:B:326:GLY:H	2.18	0.47
2:C:7:SER:HA	2:C:115:THR:HG21	1.96	0.47
2:C:50:GLU:OE1	3:D:90:TRP:HH2	1.97	0.47
3:D:7:SER:HB3	3:D:22:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.96	0.47
3:D:29:VAL:HG12	3:D:32:ILE:HD11	1.97	0.47
1:B:92:PHE:O	1:B:96:LEU:HD23	2.15	0.47
1:B:132:PHE:CE1	1:B:136:LEU:HD11	2.50	0.47
3:F:38:LYS:HG2	3:F:83:ALA:HB2	1.96	0.47
2:C:221:ARG:NE	3:D:118:PRO:HG2	2.30	0.46
3:F:60:ARG:NH2	3:F:81:ASP:OD1	2.48	0.46
1:A:18:ARG:O	1:A:22:ILE:HG13	2.15	0.46
1:B:234:HIS:ND1	1:B:235:GLU:HG3	2.30	0.46
1:A:112:ILE:HG13	1:A:153:GLN:HA	1.96	0.46
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.97	0.46
3:F:123:GLN:HE22	3:F:130:SER:HB2	1.81	0.46
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.97	0.46
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.81	0.46
2:C:102:GLY:C	2:C:104:GLY:H	2.19	0.46
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.51	0.46
1:B:180:THR:HG22	1:B:218:VAL:HG22	1.98	0.46
2:E:61:THR:O	2:E:63:SER:N	2.47	0.46
1:B:270:ASN:HA	1:B:273:VAL:HG12	1.98	0.46
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.98	0.45
1:A:55:LYS:HA	1:A:55:LYS:HD3	1.69	0.45
1:A:109:ILE:HG23	1:A:204:MET:SD	2.57	0.45
1:B:109:ILE:HG23	1:B:204:MET:SD	2.57	0.45
2:E:188:SER:HB2	3:F:134:PHE:CD2	2.52	0.45
1:A:87:ALA:O	1:A:91:MET:HG3	2.16	0.45
1:B:398:LEU:HD23	1:B:398:LEU:HA	1.59	0.45
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.98	0.45
3:D:141:LYS:HB3	3:D:172:TYR:CE2	2.50	0.45
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.51	0.45
1:B:150:PRO:CG	1:B:354:GLY:HA2	2.46	0.45
1:A:172:GLU:HG3	1:A:212:LEU:O	2.16	0.45
2:C:86:VAL:HG12	2:C:119:VAL:HG11	1.97	0.45
3:F:41:THR:HG22	3:F:42:SER:O	2.17	0.45
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.97	0.44
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.80	0.44
1:B:118:ASP:CG	1:B:174:ARG:HH21	2.19	0.44
1:A:160:ARG:HA	1:A:160:ARG:HD2	1.75	0.44
1:A:186:LEU:HD23	1:A:196:GLY:HA2	1.99	0.44
1:B:86:SER:OG	1:B:303:GLY:HA3	2.16	0.44
3:F:180:LEU:HD22	3:F:184:GLU:HG2	1.99	0.44
2:E:54:VAL:HG23	2:E:56:SER:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:162:TRP:CE2	3:F:174:MET:HG3	2.52	0.44
1:A:160:ARG:NH2	1:A:164:ASP:OD1	2.51	0.44
2:C:177:VAL:HG21	3:D:159:LEU:HD13	2.00	0.44
1:A:54:ASP:OD1	1:A:147:ARG:NE	2.51	0.44
1:A:264:ILE:O	1:A:267:PRO:HD2	2.18	0.44
1:B:54:ASP:OD1	1:B:147:ARG:NE	2.47	0.44
3:D:46:TRP:HA	3:D:46:TRP:CE3	2.53	0.44
2:E:19:LYS:HE2	2:E:80:TYR:CD1	2.52	0.44
1:B:33:LEU:HD23	1:B:33:LEU:O	2.18	0.43
1:B:36:LEU:HD23	1:B:217:ALA:HB2	2.00	0.43
1:B:72:ALA:HA	1:B:78:LEU:HD23	1.99	0.43
1:B:94:TYR:OH	1:B:352:ALA:HB2	2.17	0.43
1:A:320:ILE:HG23	1:A:365:THR:HG21	1.99	0.43
1:A:402:ILE:HG21	1:A:402:ILE:HD13	1.73	0.43
3:D:17:ASP:OD1	3:D:18:LYS:N	2.50	0.43
1:B:75:TYR:O	1:B:79:LEU:HG	2.18	0.43
2:E:24:ALA:HB3	2:E:29:TYR:CD1	2.54	0.43
3:F:89:GLN:HE22	3:F:95:GLN:HA	1.83	0.43
2:E:65:LYS:HB3	2:E:66:ASP:H	1.48	0.43
1:B:346:LEU:O	1:B:350:SER:HB3	2.18	0.43
1:A:357:PHE:HE1	1:A:411:LEU:HD22	1.83	0.43
1:A:403:ARG:HH12	1:A:441:GLY:C	2.22	0.43
1:A:430:LEU:HD22	1:B:223:ILE:HD12	2.00	0.43
1:B:77:LEU:O	1:B:81:VAL:HG13	2.18	0.43
1:B:172:GLU:HG3	1:B:212:LEU:HB3	2.01	0.43
1:A:132:PHE:CE1	1:A:136:LEU:HD11	2.53	0.43
1:B:98:ARG:HB2	1:B:288:ILE:HG13	2.01	0.43
2:C:145:THR:HB	3:D:115:SER:OG	2.19	0.43
1:A:426:ILE:HG22	1:B:223:ILE:HD11	2.01	0.43
1:B:50:ALA:O	1:B:54:ASP:HB2	2.19	0.43
3:F:38:LYS:O	3:F:41:THR:HB	2.19	0.43
2:E:85:LYS:HA	2:E:85:LYS:HD3	1.88	0.43
2:C:33:TRP:HB2	2:C:99:LEU:HB2	2.00	0.43
3:D:35:TYR:HA	3:D:44:LYS:O	2.19	0.43
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.79	0.42
2:E:91:THR:OG1	2:E:119:VAL:HG23	2.19	0.42
2:E:58:ILE:HG22	2:E:60:TYR:CE1	2.55	0.42
1:A:227:ILE:HD11	1:B:427:ILE:HD11	2.01	0.42
1:A:421:LEU:O	1:A:425:MET:HG3	2.20	0.42
3:D:197:HIS:CG	3:D:198:LYS:N	2.84	0.42
1:A:357:PHE:CE1	1:A:398:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LEU:HD22	1:B:223:ILE:CD1	2.50	0.42
1:B:123:ARG:HH21	1:B:126:ARG:HD3	1.84	0.42
3:D:58:PRO:HG2	3:D:61:PHE:HE2	1.83	0.42
3:D:75:ASN:O	3:D:76:THR:HB	2.18	0.42
3:F:136:ASN:HD22	3:F:173:SER:HB3	1.85	0.42
1:A:135:GLY:O	1:A:138:THR:N	2.52	0.42
1:B:423:LEU:HD12	1:B:423:LEU:HA	1.81	0.42
3:D:104:GLU:OE2	3:D:172:TYR:OH	2.31	0.42
3:D:181:THR:OG1	3:D:184:GLU:HG3	2.19	0.42
1:A:108:GLY:O	1:A:112:ILE:HG12	2.20	0.42
1:A:274:LEU:O	1:A:277:GLN:HB2	2.19	0.42
3:D:17:ASP:H	3:D:77:MET:H	1.66	0.42
3:F:7:SER:OG	3:F:8:PRO:HD3	2.20	0.42
1:A:426:ILE:HG22	1:B:223:ILE:CD1	2.50	0.42
1:B:44:THR:O	1:B:48:LEU:HG	2.19	0.42
1:A:430:LEU:CD2	1:B:220:ILE:HG12	2.50	0.42
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.55	0.42
1:A:270:ASN:HA	1:A:273:VAL:HG12	2.01	0.42
2:E:151:LYS:HA	2:E:184:THR:HG23	2.02	0.42
1:A:357:PHE:H	4:A:501[A]:BXA:C1	2.33	0.41
3:D:58:PRO:HG2	3:D:61:PHE:CE2	2.54	0.41
3:D:150:ASP:HA	3:D:190:SER:OG	2.19	0.41
3:D:160:ASN:HA	3:D:175:SER:O	2.20	0.41
2:E:11:LEU:HD12	2:E:118:THR:O	2.20	0.41
3:F:29:VAL:HG23	3:F:70:TYR:HE1	1.85	0.41
1:B:445:TYR:OH	4:B:501[B]:BXA:BR2	2.80	0.41
1:B:128:LEU:HD21	1:B:158:ILE:HG13	2.03	0.41
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.55	0.41
1:B:241:VAL:HG21	1:B:324:THR:HG21	2.02	0.41
3:D:36:GLN:HG3	3:D:85:TYR:CE1	2.56	0.41
3:D:66:SER:O	3:D:68:THR:N	2.53	0.41
3:D:141:LYS:HB3	3:D:172:TYR:CD2	2.56	0.41
1:A:75:TYR:CZ	1:A:79:LEU:HD21	2.55	0.41
2:C:51:ILE:HG13	2:C:58:ILE:HG12	2.03	0.41
3:D:139:TYR:HE2	3:D:165:GLN:NE2	2.19	0.41
1:A:112:ILE:HG23	1:A:178:LEU:HD11	2.02	0.41
1:A:148:ALA:HB3	4:A:501[A]:BXA:BR2	2.76	0.41
1:B:120:ARG:HE	1:B:120:ARG:HB3	1.61	0.41
2:C:51:ILE:CD1	2:C:72:ARG:HG2	2.49	0.41
3:F:149:ILE:HG12	3:F:191:TYR:CD1	2.56	0.41
1:A:54:ASP:OD1	1:A:147:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:MET:HE2	1:A:91:MET:HB2	1.93	0.41
1:A:109:ILE:HD12	1:A:445:TYR:CZ	2.56	0.41
1:A:375:ALA:O	1:A:384:LEU:HD12	2.21	0.41
1:B:284:HIS:CD2	1:B:291:TRP:HA	2.56	0.41
2:C:43:LYS:HE2	2:C:43:LYS:HB3	1.68	0.41
3:D:185:TYR:CE1	3:D:191:TYR:CE2	3.09	0.41
2:E:43:LYS:HB3	2:E:43:LYS:HE2	1.82	0.41
2:E:179:GLN:NE2	3:F:159:LEU:HD11	2.36	0.41
3:F:132:VAL:HG22	3:F:177:THR:HG23	2.02	0.41
1:A:97:VAL:HG13	1:A:101:ALA:O	2.21	0.41
1:A:251:THR:HG22	1:A:255:TYR:HE2	1.85	0.41
3:D:74:ILE:HG22	3:D:76:THR:O	2.21	0.41
3:F:146:LYS:HB3	3:F:194:GLU:HB2	2.03	0.41
3:F:185:TYR:O	3:F:191:TYR:OH	2.36	0.41
2:C:27:PHE:HD2	2:C:32:TYR:CE2	2.39	0.40
2:C:53:PRO:HA	2:C:72:ARG:CZ	2.51	0.40
3:D:4:LEU:HD21	3:D:89:GLN:HG2	2.02	0.40
3:D:187:ARG:HH11	3:D:187:ARG:CG	2.34	0.40
2:E:43:LYS:HB3	2:E:44:GLY:H	1.72	0.40
2:E:47:TRP:CG	3:F:95:GLN:NE2	2.89	0.40
1:A:28:ARG:HH11	1:B:207:GLN:HG2	1.86	0.40
2:E:33:TRP:CH2	2:E:52:ASN:HB3	2.56	0.40
3:F:7:SER:O	3:F:8:PRO:C	2.60	0.40
1:B:430:LEU:HA	1:B:433:THR:HG22	2.02	0.40
1:A:78:LEU:HD11	1:A:307:PHE:CD2	2.57	0.40
1:A:180:THR:HG22	1:A:218:VAL:CA	2.51	0.40
3:D:35:TYR:CD2	3:D:45:ARG:HA	2.56	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	440/442 (100%)	404 (92%)	35 (8%)	1 (0%)	47	77
1	B	440/442 (100%)	406 (92%)	32 (7%)	2 (0%)	29	60
2	C	220/222 (99%)	202 (92%)	14 (6%)	4 (2%)	8	30
2	E	219/222 (99%)	196 (90%)	16 (7%)	7 (3%)	4	18
3	D	209/211 (99%)	187 (90%)	17 (8%)	5 (2%)	6	23
3	F	209/211 (99%)	195 (93%)	11 (5%)	3 (1%)	11	36
All	All	1737/1750 (99%)	1590 (92%)	125 (7%)	22 (1%)	12	38

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	64	LEU
2	E	65	LYS
2	E	136	SER
2	E	138	ALA
3	F	7	SER
3	D	67	GLY
3	D	137	ASN
3	F	76	THR
3	D	50	THR
3	D	55	SER
2	E	62	PRO
2	E	64	LEU
2	E	137	ALA
3	F	198	LYS
2	C	167	LEU
2	E	122	ALA
1	A	457	GLU
1	B	443	PRO
3	D	7	SER
2	C	62	PRO
1	B	309	ALA
2	C	157	PRO

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	332/332 (100%)	325 (98%)	7 (2%)	53	77
1	B	332/332 (100%)	329 (99%)	3 (1%)	78	90
2	C	182/182 (100%)	180 (99%)	2 (1%)	73	88
2	E	181/182 (100%)	178 (98%)	3 (2%)	60	82
3	D	185/185 (100%)	177 (96%)	8 (4%)	29	59
3	F	185/185 (100%)	182 (98%)	3 (2%)	62	83
All	All	1397/1398 (100%)	1371 (98%)	26 (2%)	57	79

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	160	ARG
1	A	204	MET
1	A	219	PHE
1	A	246	ASP
1	A	304	LEU
1	A	397	LEU
1	B	219	PHE
1	B	304	LEU
1	B	397	LEU
2	C	66	ASP
2	C	72	ARG
3	D	46	TRP
3	D	71	SER
3	D	91	SER
3	D	92	SER
3	D	136	ASN
3	D	141	LYS
3	D	174	MET
3	D	208	PHE
2	E	32	TYR
2	E	87	ARG
2	E	188	SER
3	F	1	ASP
3	F	44	LYS
3	F	164	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	157	ASN
1	A	207	GLN
1	A	270	ASN
1	A	284	HIS
1	B	157	ASN
1	B	207	GLN
1	B	270	ASN
1	B	284	HIS
2	C	172	HIS
3	D	137	ASN
3	D	144	ASN
2	E	179	GLN
3	F	36	GLN
3	F	123	GLN
3	F	136	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BXA	A	501[A]	-	4,4,4	1.07	0	3,4,4	4.02	2 (66%)
4	BXA	B	501[B]	-	4,4,4	1.28	0	3,4,4	3.30	2 (66%)
4	BXA	B	501[A]	-	4,4,4	1.14	0	3,4,4	2.76	2 (66%)
4	BXA	A	501[B]	-	4,4,4	1.28	0	3,4,4	3.24	2 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BXA	A	501[A]	-	-	1/1/2/2	-
4	BXA	B	501[B]	-	-	0/1/2/2	-
4	BXA	B	501[A]	-	-	0/1/2/2	-
4	BXA	A	501[B]	-	-	0/1/2/2	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501[A]	BXA	BR2-C2-C1	5.81	131.61	110.74
4	B	501[B]	BXA	BR2-C2-C1	4.51	126.95	110.74
4	A	501[B]	BXA	BR2-C2-C1	4.05	125.30	110.74
4	A	501[B]	BXA	O2-C1-O1	-3.87	113.66	123.30
4	B	501[A]	BXA	BR2-C2-C1	3.77	124.28	110.74
4	B	501[B]	BXA	O2-C1-O1	-3.50	114.58	123.30
4	A	501[A]	BXA	O2-C1-O1	-3.34	114.97	123.30
4	B	501[A]	BXA	O2-C1-O1	-2.93	116.00	123.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501[A]	BXA	O1-C1-C2-BR2

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501[A]	BXA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501[B]	BXA	3	0
4	B	501[A]	BXA	5	0
4	A	501[B]	BXA	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	442/442 (100%)	0.27	25 (5%) 23 10	77, 102, 139, 173	0
1	B	442/442 (100%)	0.46	43 (9%) 7 2	77, 108, 150, 234	0
2	C	222/222 (100%)	0.21	15 (6%) 17 6	72, 98, 139, 194	0
2	E	221/222 (99%)	0.07	10 (4%) 33 15	71, 100, 134, 170	0
3	D	211/211 (100%)	0.39	19 (9%) 9 3	82, 113, 138, 152	0
3	F	211/211 (100%)	0.20	7 (3%) 46 23	72, 94, 143, 158	0
All	All	1749/1750 (99%)	0.29	119 (6%) 17 6	71, 103, 141, 234	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	THR	10.5
3	F	155	GLN	6.8
1	B	72	ALA	6.5
3	D	196	THR	5.6
1	B	353	PRO	5.3
3	F	147	TRP	5.2
2	C	138	ALA	5.0
3	D	32	ILE	4.8
1	B	68	LEU	4.7
1	A	72	ALA	4.7
1	B	235	GLU	4.6
2	E	24	ALA	4.5
2	C	29	TYR	4.5
2	C	137	ALA	4.4
2	E	218	ILE	4.4
1	B	104	ALA	4.1
1	B	95	PHE	3.8
3	D	195	ALA	3.8
1	A	353	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	140	ALA	3.7
1	B	73	ASP	3.6
1	B	354	GLY	3.5
1	B	407	THR	3.5
3	F	153	GLU	3.5
1	A	354	GLY	3.5
1	A	77	LEU	3.5
2	E	221	ARG	3.5
3	F	148	LYS	3.5
1	A	288	ILE	3.4
1	B	333	LEU	3.4
3	D	20	THR	3.4
2	C	133	ALA	3.3
3	D	110	ALA	3.2
1	B	70	HIS	3.2
1	B	162	VAL	3.2
2	E	201	VAL	3.1
1	B	163	LEU	3.1
2	E	13	GLN	3.1
1	B	75	TYR	3.0
2	E	66	ASP	3.0
2	E	29	TYR	2.9
1	B	74	ASN	2.9
3	D	129	ALA	2.9
3	D	191	TYR	2.9
2	C	57	THR	2.9
1	B	67	ALA	2.9
2	C	48	ILE	2.9
2	E	48	ILE	2.9
1	B	408	GLY	2.9
1	A	407	THR	2.9
1	B	288	ILE	2.9
2	C	81	LEU	2.9
3	D	21	MET	2.9
1	B	195	ALA	2.9
1	B	177	LEU	2.9
3	D	128	GLY	2.8
3	D	47	ILE	2.8
3	F	154	ARG	2.8
3	D	197	HIS	2.8
1	B	332	MET	2.7
1	B	237	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	289	THR	2.6
2	C	66	ASP	2.6
1	A	350	SER	2.6
1	A	291	TRP	2.6
1	A	71	THR	2.6
1	B	159	GLY	2.6
1	A	283	VAL	2.6
3	D	141	LYS	2.5
1	B	139	LEU	2.5
1	B	328	PHE	2.5
1	B	410	ILE	2.5
3	D	149	ILE	2.5
2	C	147	GLY	2.5
1	A	145	LEU	2.5
3	D	194	GLU	2.5
1	A	293	LEU	2.5
2	C	139	ALA	2.5
1	B	138	THR	2.5
1	B	395	GLY	2.5
1	A	74	ASN	2.4
1	A	346	LEU	2.4
1	B	160	ARG	2.4
1	B	411	LEU	2.4
2	C	73	ASP	2.4
3	D	37	GLN	2.4
2	E	18	LEU	2.4
1	A	414	GLU	2.4
1	A	192	ALA	2.4
2	C	111	TRP	2.3
1	A	143	MET	2.3
1	B	414	GLU	2.3
1	B	419	TYR	2.3
1	A	195	ALA	2.3
3	D	143	ILE	2.3
3	D	154	ARG	2.3
3	F	156	ASN	2.3
1	A	193	PRO	2.2
1	B	78	LEU	2.2
3	D	146	LYS	2.2
1	B	307	PHE	2.2
1	A	290	LYS	2.2
1	A	417	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	192	ALA	2.2
3	D	72	LEU	2.2
1	A	73	ASP	2.2
1	B	35	ILE	2.2
1	A	64	ARG	2.1
2	C	186	SER	2.1
1	B	422	ILE	2.1
1	B	420	GLN	2.1
2	E	47	TRP	2.0
2	C	87	ARG	2.0
1	B	164	ASP	2.0
3	F	149	ILE	2.0
1	B	69	VAL	2.0
1	B	240	ASP	2.0
1	B	77	LEU	2.0
1	A	168	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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
4	BXA	A	501[A]	5/5	0.71	0.27	111,119,119,153	5
4	BXA	A	501[B]	5/5	0.71	0.27	102,112,115,122	5
4	BXA	B	501[A]	5/5	0.89	0.25	109,111,114,155	5
4	BXA	B	501[B]	5/5	0.89	0.25	104,114,116,119	5

6.5 Other polymers (i)

There are no such residues in this entry.