



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:40 PM UTC

PDB ID : 6ADC / pdb_00006adc
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 ⓘ 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

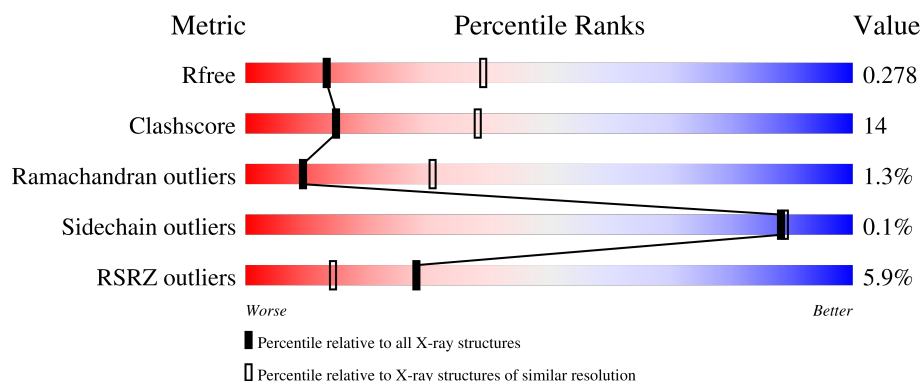
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (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 $\leq 5\%$. 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	442	7% 72% 28%
1	B	442	10% 70% 30%
2	C	222	4% 75% 24% .
2	E	222	6% 73% 25% .
3	D	211	4% 63% 36% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	211	% 75% 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

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
1	A	442	Total	C	N	O	S	0	0	0
			3311	2178	557	556	20			
1	B	442	Total	C	N	O	S	0	0	0
			3311	2178	557	556	20			

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

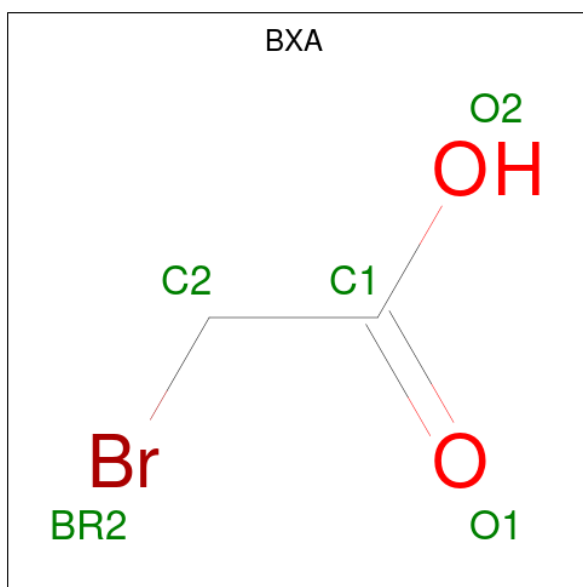
- Molecule 2 is a protein called antibody Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 bromoacetic acid (CCD ID: BXA) (formula: C₂H₃BrO₂).

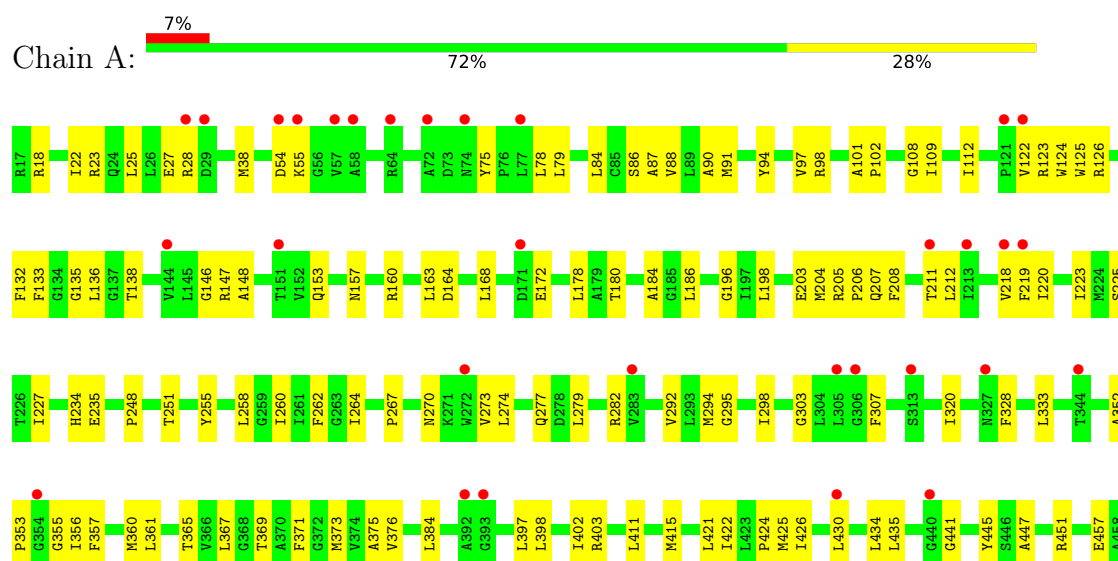


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Br	C	O	0	1
			10	2	4	4		
4	B	1	Total	Br	C	O	0	1
			10	2	4	4		

3 Residue-property plots

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.

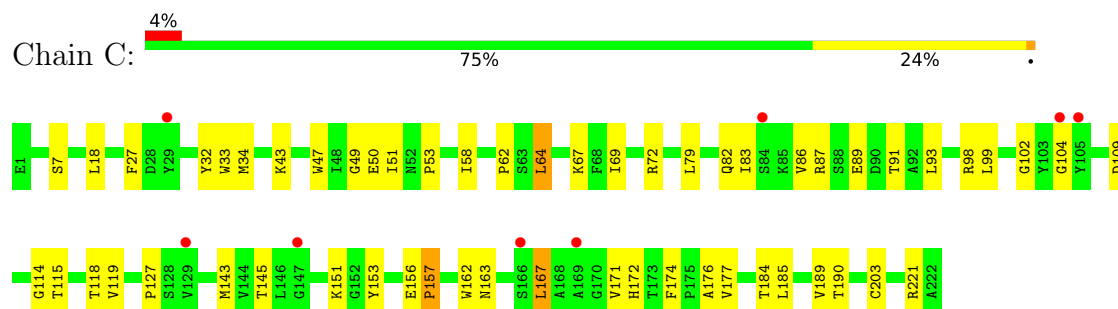
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



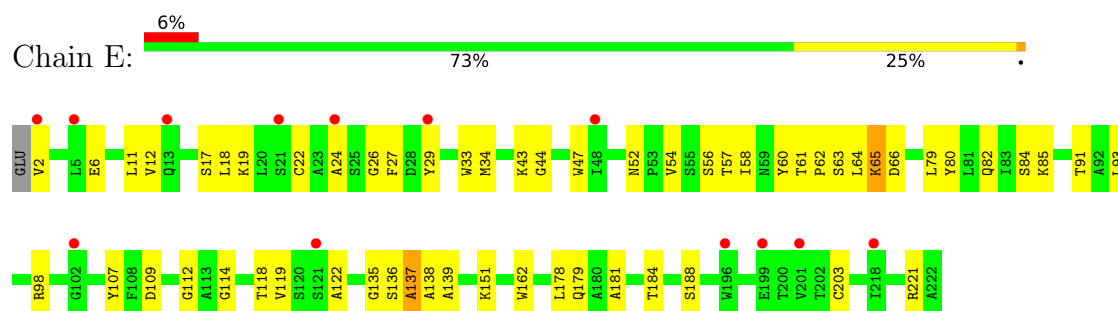
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



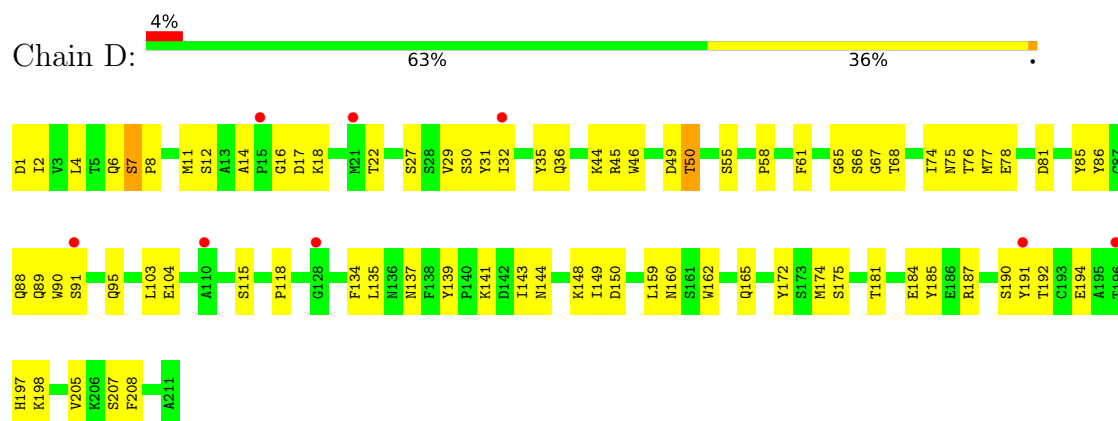
- Molecule 2: antibody Fab fragment, heavy chain



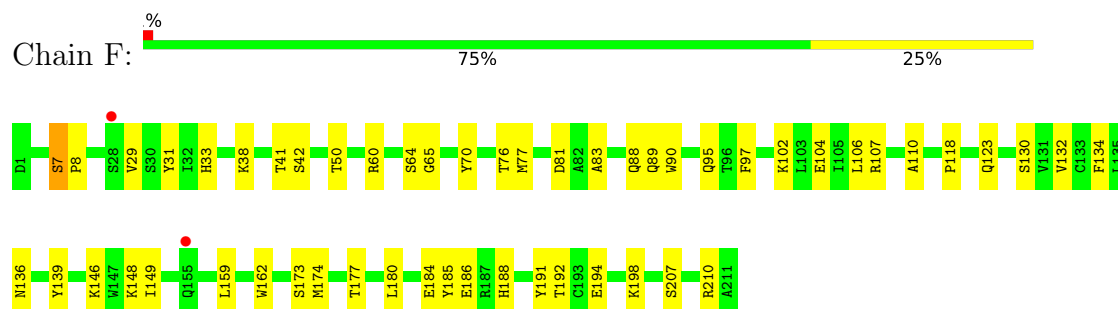
- Molecule 2: antibody Fab fragment, heavy chain



- 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	233.25Å 96.73Å 169.78Å 90.00° 131.45° 90.00°	Depositor
Resolution (Å)	34.85 – 3.06 34.85 – 3.06	Depositor EDS
% Data completeness (in resolution range)	97.6 (34.85-3.06) 97.7 (34.85-3.06)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.226 , 0.275 0.232 , 0.278	Depositor DCC
R_{free} test set	2654 reflections (4.92%)	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)	0.30 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	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.*

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: 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	0.44	0/3383	0.71	0/4592
1	B	0.42	0/3383	0.70	0/4592
2	C	0.50	0/1730	0.73	0/2367
2	E	0.45	0/1721	0.67	0/2355
3	D	0.47	0/1660	0.74	1/2257 (0.0%)
3	F	0.46	0/1660	0.75	0/2257
All	All	0.45	0/13537	0.71	1/18420 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	65	GLY	N-CA-C	5.38	117.56	111.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3311	0	3469	116	0
1	B	3311	0	3469	107	0
2	C	1681	0	1663	34	0
2	E	1672	0	1654	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1621	0	1546	64	0
3	F	1621	0	1546	43	0
4	A	10	0	0	5	0
4	B	10	0	0	8	0
All	All	13237	0	13347	366	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 14.

All (366) 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:A:88:VAL:HA	1:A:91:MET:HE2	1.67	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
3:F:95:GLN:H	3:F:95:GLN:CD	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.75	0.69
1:B:200:ILE:HD11	1:B:204:MET:HE2	1.74	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
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
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.78	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: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
1:A:361:LEU:HD13	1:A:415:MET:HE1	1.84	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:411:LEU:HG	1:A:415:MET:HE2	1.86	0.58
1:A:422:ILE:HA	1:A:425:MET:HE3	1.86	0.58
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

Continued on next page...

Continued from previous page...

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:95:GLN:CD	3:F:95:GLN:N	2.61	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:A:422:ILE:HD12	1:A:425:MET:HE3	1.87	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
1:B:200:ILE:CD1	1:B:204:MET:HE2	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
1:B:394:MET:HE2	1:B:412:VAL:HG22	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
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
1:B:422:ILE:HA	1:B:425:MET:HE3	1.91	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:52:ASN:CG	2:E:57:THR:H	2.16	0.53
2:E:6:GLU:OE1	2:E:112:GLY:HA3	2.07	0.53
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
2:E:91:THR:HG1	2:E:119:VAL:H	1.54	0.52
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:356:ILE:HG23	1:A:360:MET:HE2	1.90	0.52
1:A:160:ARG:HE	1:A:163:LEU:HD23	1.75	0.52
1:B:324:THR:C	1:B:326:GLY:H	2.18	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:C:102:GLY:C	2:C:104:GLY:H	2.19	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
1:A:328:PHE:O	1:A:373:MET:HE1	2.11	0.50
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:B:118:ASP:CG	1:B:174:ARG:HH21	2.19	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
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
3:D:148:LYS:HB2	3:D:192:THR:HG1	1.77	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:A:403:ARG:HH12	1:A:441:GLY:C	2.22	0.48
3:D:1:ASP:OD1	3:D:1:ASP:N	2.27	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:77:MET:HE2	3:F:77:MET:HB3	1.56	0.47
1:A:220:ILE:CG1	1:B:430:LEU:HD23	2.45	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:8:PRO:HD3	1.96	0.47
3:D:7:SER:HB3	3:D:22:THR:HB	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
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
3:D:104:GLU:OE2	3:D:172:TYR:OH	2.31	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:360:MET:HE3	1:A:398:LEU:HD23	1.99	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: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
3:D:95:GLN:H	3:D:95:GLN:CD	2.13	0.44
2:E:54:VAL:HG23	2:E:56:SER:H	1.82	0.44
3:D:77:MET:HE3	3:D:78:GLU:O	2.17	0.44
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:7:SER:O	3:F:8:PRO:C	2.60	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:B:411:LEU:HG	1:B:415:MET:HE2	2.01	0.43
1:A:357:PHE:HE1	1:A:411:LEU:HD22	1.83	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:328:PHE:O	1:B:373:MET:HE1	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
1:B:361:LEU:HD13	1:B:415:MET:HE1	2.01	0.42
3:D:143:ILE:C	3:D:144:ASN:HD22	2.27	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
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
1:B:356:ILE:C	1:B:359:PRO:HD2	2.44	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: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:294:MET:HE2	1:A:294:MET:HB3	1.90	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:134:PHE:C	3:D:135:LEU:HD23	2.44	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
2:C:143:MET:HE3	2:C:190:THR:HG22	2.01	0.41
1:A:148:ALA:HB3	4:A:501[A]:BXA:BR2	2.76	0.41
1:A:307:PHE:CD1	1:A:307:PHE:C	2.99	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:89:GLN:CD	3:F:89:GLN:C	2.88	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
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:77:MET:HE2	3:D:77:MET:HB3	1.67	0.41
3:D:88:GLN:HE21	3:D:89:GLN:C	2.29	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
2:C:102:GLY:C	2:C:104:GLY:N	2.79	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:186:GLU:C	3:F:188:HIS:H	2.29	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/442 (100%)	404 (92%)	35 (8%)	1 (0%)	43	70
1	B	440/442 (100%)	406 (92%)	32 (7%)	2 (0%)	24	52
2	C	220/222 (99%)	202 (92%)	14 (6%)	4 (2%)	6	24
2	E	219/222 (99%)	196 (90%)	16 (7%)	7 (3%)	3	14
3	D	209/211 (99%)	187 (90%)	17 (8%)	5 (2%)	4	18
3	F	209/211 (99%)	195 (93%)	11 (5%)	3 (1%)	9	29
All	All	1737/1750 (99%)	1590 (92%)	125 (7%)	22 (1%)	9	31

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	64	LEU
2	E	65	LYS
2	E	136	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	332 (100%)	0	100	100
1	B	332/332 (100%)	331 (100%)	1 (0%)	86	85
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	1397/1398 (100%)	1396 (100%)	1 (0%)	88	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	73	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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
2	C	172	HIS
3	D	88	GLN
3	D	137	ASN
3	D	144	ASN
3	D	189	ASN
2	E	179	GLN
3	F	36	GLN
3	F	75	ASN
3	F	123	GLN
3	F	136	ASN
3	F	189	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 oligosaccharides 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	B	501[A]	-	4,4,4	1.17	0	3,4,4	2.74	2 (66%)
4	BXA	B	501[B]	-	4,4,4	1.32	0	3,4,4	3.29	2 (66%)
4	BXA	A	501[A]	-	4,4,4	1.10	0	3,4,4	4.02	2 (66%)
4	BXA	A	501[B]	-	4,4,4	1.31	0	3,4,4	3.21	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	B	501[A]	-	-	0/1/2/2	-
4	BXA	B	501[B]	-	-	0/1/2/2	-
4	BXA	A	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(°)	Ideal(°)
4	A	501[A]	BXA	BR2-C2-C1	5.87	131.61	110.86
4	B	501[B]	BXA	BR2-C2-C1	4.55	126.95	110.86
4	A	501[B]	BXA	BR2-C2-C1	4.08	125.30	110.86
4	B	501[A]	BXA	BR2-C2-C1	3.80	124.28	110.86
4	A	501[B]	BXA	O2-C1-O1	-3.76	113.66	123.33
4	B	501[B]	BXA	O2-C1-O1	-3.40	114.58	123.33
4	A	501[A]	BXA	O2-C1-O1	-3.25	114.97	123.33
4	B	501[A]	BXA	O2-C1-O1	-2.85	116.00	123.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

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

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	442/442 (100%)	0.27	31 (7%) 22 11	77, 102, 139, 173	0
1	B	442/442 (100%)	0.51	42 (9%) 14 7	77, 108, 150, 234	0
2	C	222/222 (100%)	0.25	8 (3%) 46 25	72, 98, 139, 194	0
2	E	221/222 (99%)	0.19	13 (5%) 28 14	71, 100, 134, 170	0
3	D	211/211 (100%)	0.36	8 (3%) 44 24	82, 113, 138, 152	0
3	F	211/211 (100%)	0.03	2 (0%) 81 61	72, 94, 143, 158	0
All	All	1749/1750 (99%)	0.30	104 (5%) 28 14	71, 103, 141, 234	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	353	PRO	6.8
1	B	95	PHE	6.6
1	B	104	ALA	5.8
1	B	159	GLY	5.5
1	B	354	GLY	4.7
1	B	139	LEU	4.6
2	E	218	ILE	4.4
1	B	162	VAL	4.1
1	B	164	ASP	4.0
1	A	392	ALA	3.9
2	E	201	VAL	3.7
1	B	177	LEU	3.7
1	A	305	LEU	3.6
1	B	288	ILE	3.5
1	A	213	ILE	3.5
1	B	147	ARG	3.4
1	B	71	THR	3.4
2	E	13	GLN	3.4
1	A	58	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	447	ALA	3.3
3	F	155	GLN	3.3
1	A	29	ASP	3.2
1	A	354	GLY	3.2
3	D	32	ILE	3.2
2	E	199	GLU	3.1
1	B	61	GLN	3.1
2	C	169	ALA	3.1
1	B	351	GLY	3.0
1	B	138	THR	3.0
1	B	145	LEU	3.0
3	D	91	SER	3.0
1	B	333	LEU	2.9
1	B	219	PHE	2.9
2	E	121	SER	2.9
1	A	122	VAL	2.9
2	C	29	TYR	2.9
3	D	128	GLY	2.9
1	B	235	GLU	2.9
1	A	72	ALA	2.8
1	B	442	LYS	2.8
1	A	77	LEU	2.8
2	E	102	GLY	2.8
1	A	219	PHE	2.7
2	E	29	TYR	2.7
2	E	24	ALA	2.7
2	E	2	VAL	2.7
1	B	252	LEU	2.7
1	A	306	GLY	2.6
1	B	163	LEU	2.6
1	A	55	LYS	2.6
3	D	15	PRO	2.6
1	B	72	ALA	2.6
1	A	430	LEU	2.5
2	C	105	TYR	2.5
2	C	104	GLY	2.5
1	A	313	SER	2.5
3	D	110	ALA	2.5
1	B	125	TRP	2.5
1	A	211	THR	2.5
1	B	387	GLY	2.5
1	B	26	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	393	GLY	2.4
2	C	84	SER	2.4
1	A	74	ASN	2.4
1	B	57	VAL	2.4
1	A	151	THR	2.4
1	A	28	ARG	2.4
2	C	129	VAL	2.3
1	B	286	GLY	2.3
2	E	5	LEU	2.3
3	D	196	THR	2.3
1	A	57	VAL	2.3
1	A	171	ASP	2.3
1	A	440	GLY	2.2
2	C	166	SER	2.2
2	C	147	GLY	2.2
1	A	121	PRO	2.2
1	B	211	THR	2.2
1	B	121	PRO	2.2
1	B	242	GLY	2.2
1	B	68	LEU	2.2
1	B	397	LEU	2.2
1	B	298	ILE	2.1
1	B	161	MET	2.1
3	D	191	TYR	2.1
2	E	21	SER	2.1
1	B	269	PHE	2.1
1	B	444	LEU	2.1
1	B	270	ASN	2.1
1	A	144	VAL	2.1
1	A	54	ASP	2.1
1	A	218	VAL	2.1
1	A	327	ASN	2.1
1	A	64	ARG	2.1
1	B	212	LEU	2.1
1	B	289	THR	2.1
1	B	110	PRO	2.1
3	F	28	SER	2.0
2	E	48	ILE	2.0
1	A	272	TRP	2.0
1	A	283	VAL	2.0
2	E	196	TRP	2.0
3	D	21	MET	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	344	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BXA	A	501[A]	5/5	0.92	0.15	111,119,119,153	5
4	BXA	A	501[B]	5/5	0.92	0.15	102,112,115,122	5
4	BXA	B	501[A]	5/5	0.93	0.13	109,111,114,155	5
4	BXA	B	501[B]	5/5	0.93	0.13	104,114,116,119	5

6.5 Other polymers [i](#)

There are no such residues in this entry.