



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:21 PM GMT

PDB ID : 1T83
Title : CRYSTAL STRUCTURE OF A HUMAN TYPE III FC GAMMA RECEPTOR IN COMPLEX WITH AN FC FRAGMENT OF IGG1 (ORTHORHOMBIC)
Authors : Radaev, S.; Motyka, S.; Fridman, W.-H.; Sautes-Fridman, C.; Sun, P.D.
Deposited on : 2004-05-11
Resolution : 3.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

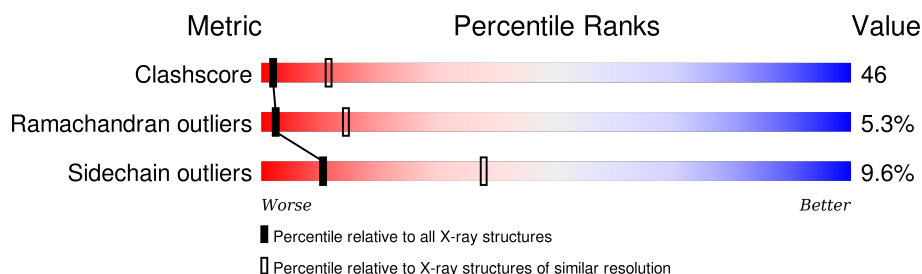
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	224	
1	B	224	
2	C	176	

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	NAG	B	448	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NDG	B	449	-	-	X	-
5	HG2	A	456	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5037 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 IGG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	1	0	0
			1677	1067	282	321	7			
1	B	212	Total	C	N	O	S	0	0	0
			1695	1080	284	324	7			

- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	167	Total	C	N	O	S	0	0	0
			1347	856	231	256	4			

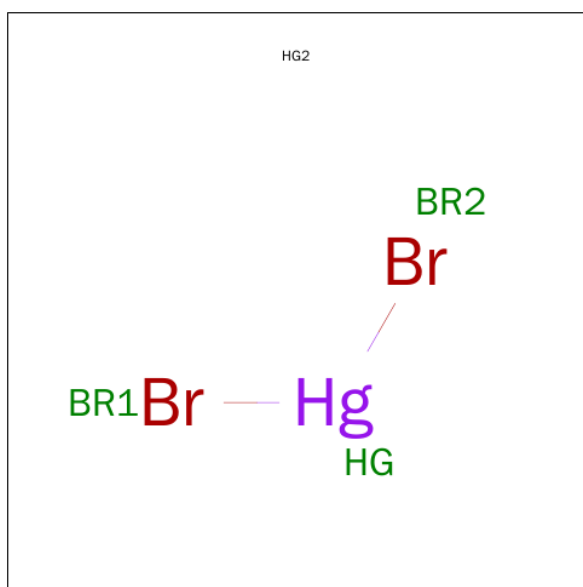
- Molecule 3 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	8	Total	C	N	O	0	0
			96	54	3	39		

- Molecule 4 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	8	Total	C	N	O	0	0
			99	56	4	39		

- Molecule 5 is DIBROMOMERCURY (three-letter code: HG2) (formula: Br₂Hg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Br	Hg	0	0
			3	2	1		

- Molecule 6 is water.

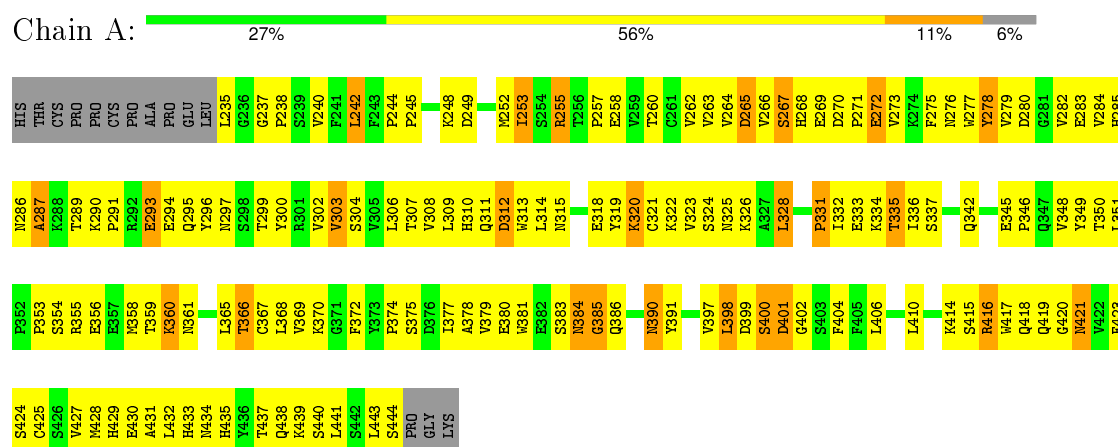
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	54	Total	O	0	0
			54	54		
6	C	30	Total	O	0	0
			30	30		

3 Residue-property plots

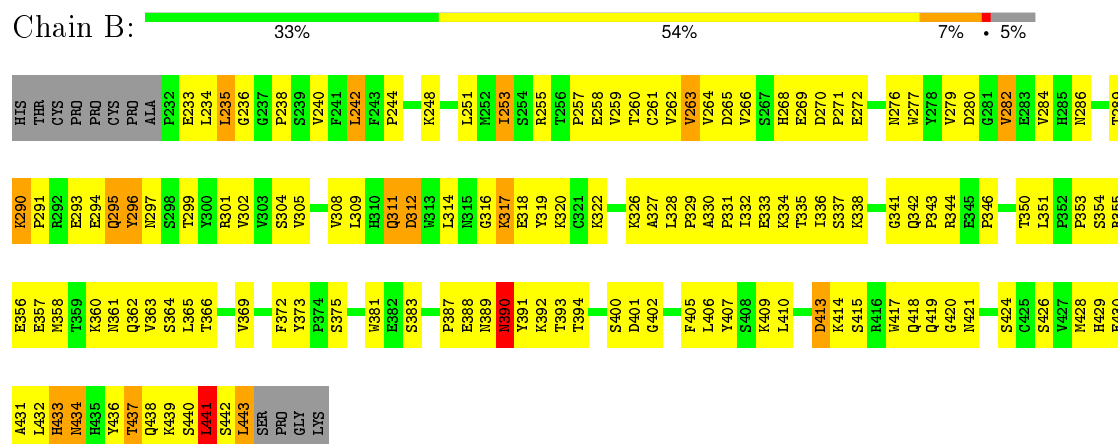
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

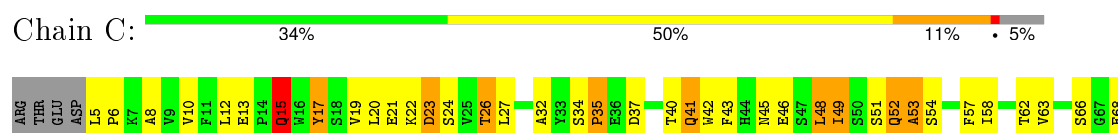
• Molecule 1: IGG1

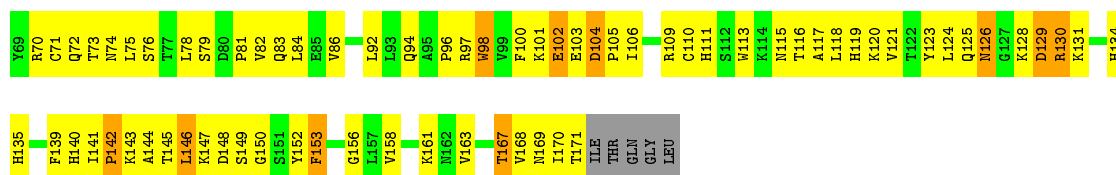


• Molecule 1: IGG1



• Molecule 2: Low affinity immunoglobulin gamma Fc region receptor III-B





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.85Å 102.39Å 123.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.226 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5037	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

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: BMA, NAG, HG2, NDG, GAL, FUL, MAN

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	0.49	1/1723 (0.1%)	0.71	0/2346
1	B	0.52	1/1742 (0.1%)	0.73	1/2372 (0.0%)
2	C	0.40	0/1385	0.67	0/1884
All	All	0.47	2/4850 (0.0%)	0.71	1/6602 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	272	GLU	CD-OE2	7.25	1.33	1.25
1	A	272	GLU	CD-OE2	7.05	1.33	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	441	LEU	CA-CB-CG	5.32	127.54	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	1677	0	1644	162	0
1	B	1695	0	1663	169	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1347	0	1288	119	0
3	A	96	0	82	6	0
4	B	99	0	85	28	0
5	A	3	0	0	0	0
6	A	36	0	0	4	0
6	B	54	0	0	9	0
6	C	30	0	0	4	0
All	All	5037	0	4762	447	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 46.

All (447) 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:301:ARG:NH1	4:B:449:NDG:H8C3	1.54	1.19
1:B:233:GLU:HG3	1:B:235:LEU:HD22	1.28	1.14
1:B:301:ARG:HH11	4:B:449:NDG:H8C3	0.93	1.07
1:A:320:LYS:HG3	1:A:335:THR:HG22	1.33	1.06
4:B:448:NAG:H61	4:B:449:NDG:HA	1.10	1.04
4:B:448:NAG:H4	4:B:455:FUL:O2	1.62	1.00
1:B:443:LEU:H	1:B:443:LEU:HD12	1.26	0.97
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.46	0.95
4:B:448:NAG:H61	4:B:449:NDG:N2	1.80	0.95
1:A:264:VAL:HG11	3:A:449:NAG:H2	1.50	0.94
1:A:240:VAL:HG12	1:A:263:VAL:HG22	1.50	0.93
2:C:103:GLU:HG3	2:C:143:LYS:HG2	1.47	0.92
1:A:293:GLU:HB3	1:A:300:TYR:CD1	2.05	0.91
2:C:10:VAL:HB	2:C:82:VAL:HG21	1.53	0.90
1:B:279:VAL:HG23	1:B:284:VAL:HG21	1.58	0.84
1:A:276:ASN:HB3	1:A:278:TYR:HE1	1.43	0.83
1:A:322:LYS:HG3	1:A:333:GLU:HB3	1.61	0.81
2:C:102:GLU:O	2:C:144:ALA:HB3	1.80	0.81
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.60	0.81
1:A:346:PRO:HG3	1:A:372:PHE:HB3	1.62	0.81
1:B:299:THR:HG21	4:B:448:NAG:C8	2.10	0.81
1:B:235:LEU:HD23	1:B:235:LEU:H	1.46	0.81
1:B:297:ASN:HB2	4:B:448:NAG:O7	1.80	0.80
4:B:448:NAG:C6	4:B:449:NDG:N2	2.44	0.80
1:B:443:LEU:HD12	1:B:443:LEU:N	1.96	0.80
1:B:400:SER:HB3	6:B:90:HOH:O	1.80	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:448:NAG:C6	4:B:449:NDG:HA	1.93	0.80
1:B:295:GLN:HG3	1:B:296:TYR:H	1.46	0.79
1:A:309:LEU:O	1:A:312:ASP:HB2	1.82	0.78
1:B:301:ARG:HH11	4:B:449:NDG:C8	1.87	0.77
2:C:103:GLU:O	2:C:104:ASP:HB2	1.83	0.77
4:B:448:NAG:H62	4:B:449:NDG:H8C1	1.66	0.76
1:A:267:SER:HB2	1:A:269:GLU:HG2	1.66	0.76
1:B:234:LEU:HD11	4:B:448:NAG:H81	1.66	0.76
1:B:260:THR:HG22	1:B:305:VAL:HG22	1.67	0.76
1:B:234:LEU:HD21	4:B:448:NAG:H83	1.67	0.76
1:A:414:LYS:HG2	1:A:418:GLN:HE21	1.52	0.75
1:B:415:SER:O	1:B:419:GLN:HG3	1.87	0.75
1:B:420:GLY:HA2	1:B:443:LEU:HD13	1.68	0.74
1:B:290:LYS:HB2	6:B:75:HOH:O	1.87	0.74
2:C:26:THR:HG23	2:C:57:PHE:HD1	1.53	0.74
1:A:350:THR:HB	1:A:441:LEU:HG	1.70	0.74
1:A:321:CYS:O	1:A:333:GLU:HA	1.88	0.73
1:A:242:LEU:HD13	1:A:336:ILE:HG22	1.68	0.73
1:B:299:THR:HG21	4:B:448:NAG:H82	1.70	0.73
1:B:429:HIS:HB3	1:B:432:LEU:CD1	2.19	0.73
2:C:168:VAL:HG12	2:C:169:ASN:N	2.04	0.73
4:B:452:MAN:H4	4:B:453:NAG:H83	1.71	0.73
1:B:235:LEU:CD2	1:B:235:LEU:H	2.03	0.72
2:C:100:PHE:CE2	2:C:106:ILE:HG12	2.24	0.72
1:B:383:SER:HB2	1:B:388:GLU:OE1	1.90	0.72
1:B:355:ARG:O	1:B:358:MET:HG2	1.90	0.72
2:C:27:LEU:N	2:C:27:LEU:HD12	2.05	0.71
2:C:116:THR:HG21	2:C:158:VAL:HG13	1.72	0.71
1:A:263:VAL:HG21	1:A:323:VAL:HG11	1.72	0.71
1:B:248:LYS:HG3	1:B:428:MET:CE	2.21	0.71
1:B:443:LEU:CD1	1:B:443:LEU:H	2.04	0.70
1:A:238:PRO:HD2	1:A:328:LEU:HD13	1.72	0.70
2:C:94:GLN:OE1	2:C:111:HIS:HB2	1.92	0.70
1:A:240:VAL:HG23	1:A:334:LYS:HE2	1.75	0.69
2:C:126:ASN:N	2:C:126:ASN:HD22	1.90	0.69
1:B:253:ILE:HD12	1:B:253:ILE:C	2.12	0.69
1:B:353:PRO:HD3	1:B:365:LEU:HD23	1.75	0.69
2:C:126:ASN:O	2:C:128:LYS:HG2	1.92	0.69
4:B:448:NAG:H62	4:B:449:NDG:C8	2.22	0.69
1:B:356:GLU:O	1:B:356:GLU:HG2	1.92	0.69
1:A:293:GLU:O	1:A:293:GLU:HG3	1.90	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:HIS:HB3	1:B:432:LEU:HD11	1.75	0.68
1:B:294:GLU:HG3	6:B:172:HOH:O	1.92	0.68
2:C:34:SER:OG	2:C:37:ASP:HB3	1.93	0.68
1:A:238:PRO:HB3	1:A:265:ASP:O	1.93	0.67
1:A:289:THR:HG22	1:A:303:VAL:O	1.94	0.67
2:C:146:LEU:HG	6:C:193:HOH:O	1.94	0.67
1:A:294:GLU:HG3	1:A:295:GLN:HG3	1.77	0.67
1:B:257:PRO:HG2	1:B:308:VAL:O	1.95	0.67
1:B:390:ASN:O	1:B:410:LEU:HD12	1.94	0.67
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.76	0.66
1:B:235:LEU:HD23	1:B:235:LEU:N	2.10	0.66
1:A:276:ASN:HB3	1:A:278:TYR:CE1	2.29	0.66
2:C:42:TRP:CB	2:C:49:ILE:HG13	2.26	0.66
2:C:45:ASN:O	2:C:46:GLU:HB2	1.95	0.66
1:B:432:LEU:HD12	1:B:432:LEU:N	2.09	0.66
1:B:234:LEU:HD21	4:B:448:NAG:C8	2.25	0.66
2:C:70:ARG:HD3	2:C:79:SER:O	1.96	0.65
1:B:233:GLU:HG3	1:B:235:LEU:CD2	2.18	0.65
2:C:42:TRP:CZ3	2:C:71:CYS:HB3	2.31	0.65
2:C:153:PHE:HB3	2:C:167:THR:HA	1.78	0.65
1:A:278:TYR:HA	1:A:283:GLU:HA	1.77	0.65
1:A:264:VAL:O	1:A:265:ASP:HB2	1.96	0.65
2:C:66:SER:HA	2:C:84:LEU:O	1.96	0.65
1:B:238:PRO:HD2	1:B:327:ALA:HB3	1.78	0.65
1:A:271:PRO:O	1:A:272:GLU:HG2	1.98	0.64
1:A:262:VAL:HG22	1:A:303:VAL:CG1	2.28	0.64
2:C:48:LEU:HD12	2:C:48:LEU:N	2.12	0.64
1:A:279:VAL:O	1:A:282:VAL:HG22	1.98	0.64
1:B:309:LEU:HB3	1:B:311:GLN:OE1	1.98	0.63
1:A:324:SER:HA	1:A:331:PRO:HB3	1.81	0.63
1:B:264:VAL:O	1:B:265:ASP:HB2	1.99	0.63
1:B:279:VAL:O	1:B:282:VAL:HG23	1.99	0.63
1:B:299:THR:HG21	4:B:448:NAG:H81	1.80	0.63
2:C:83:GLN:HG2	6:C:188:HOH:O	1.98	0.62
1:B:248:LYS:HG3	1:B:428:MET:HE1	1.80	0.62
1:A:258:GLU:HB3	1:A:307:THR:HA	1.81	0.62
2:C:118:LEU:HG	2:C:121:VAL:HG22	1.81	0.62
1:A:399:ASP:HA	1:B:392:LYS:HE3	1.82	0.62
1:A:255:ARG:HH11	1:A:255:ARG:HB3	1.65	0.62
2:C:34:SER:HA	2:C:75:LEU:HD11	1.82	0.61
2:C:106:ILE:HB	2:C:141:ILE:HB	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:GLN:O	2:C:71:CYS:HA	2.00	0.61
1:B:417:TRP:O	1:B:443:LEU:HD11	1.98	0.61
1:B:438:GLN:HG2	6:B:111:HOH:O	2.00	0.61
1:A:320:LYS:HG3	1:A:335:THR:CG2	2.21	0.61
1:A:284:VAL:HG12	1:A:285:HIS:N	2.15	0.61
1:B:270:ASP:HB3	1:B:326:LYS:HB2	1.83	0.61
2:C:117:ALA:HB1	2:C:119:HIS:HE1	1.66	0.61
1:B:351:LEU:HB2	1:B:366:THR:HB	1.83	0.61
1:B:328:LEU:N	1:B:328:LEU:HD12	2.16	0.61
1:A:414:LYS:CG	1:A:418:GLN:HE21	2.14	0.60
2:C:105:PRO:HA	2:C:142:PRO:O	2.01	0.60
2:C:63:VAL:HA	2:C:86:VAL:HB	1.82	0.60
1:A:384:ASN:O	1:A:386:GLN:N	2.34	0.60
1:B:297:ASN:ND2	4:B:448:NAG:C7	2.64	0.60
1:A:249:ASP:OD2	1:A:255:ARG:NH1	2.35	0.60
1:A:378:ALA:HB3	1:A:428:MET:HB2	1.82	0.60
2:C:104:ASP:H	2:C:143:LYS:HA	1.67	0.60
2:C:94:GLN:OE1	2:C:109:ARG:HD3	2.02	0.59
1:B:365:LEU:HD22	1:B:441:LEU:HD11	1.83	0.59
1:B:279:VAL:HG23	1:B:284:VAL:CG2	2.30	0.59
2:C:74:ASN:OD1	2:C:75:LEU:HG	2.02	0.59
1:A:351:LEU:CD2	1:B:354:SER:HB2	2.31	0.59
1:B:341:GLY:O	1:B:343:PRO:HD3	2.02	0.59
1:B:234:LEU:CD2	4:B:448:NAG:H83	2.32	0.59
2:C:119:HIS:CD2	2:C:135:HIS:ND1	2.71	0.58
1:B:314:LEU:HD22	1:B:430:GLU:HG3	1.84	0.58
1:B:260:THR:HG22	1:B:305:VAL:HG13	1.86	0.58
2:C:168:VAL:HG12	2:C:169:ASN:H	1.65	0.58
1:A:244:PRO:HB3	1:A:336:ILE:HD11	1.85	0.58
1:B:235:LEU:HD12	2:C:117:ALA:HB3	1.85	0.57
1:B:320:LYS:HG3	1:B:335:THR:HG22	1.86	0.57
1:B:426:SER:HB3	1:B:436:TYR:CE2	2.39	0.57
1:A:279:VAL:HA	1:A:318:GLU:O	2.04	0.57
1:A:276:ASN:HB2	1:A:322:LYS:CB	2.28	0.57
1:A:429:HIS:O	1:A:435:HIS:HA	2.05	0.57
1:A:248:LYS:HG2	1:A:428:MET:SD	2.45	0.56
1:B:264:VAL:HG11	4:B:449:NDG:H2	1.85	0.56
1:B:360:LYS:O	1:B:414:LYS:HD2	2.05	0.56
1:A:398:LEU:HB2	1:A:404:PHE:CE1	2.41	0.56
1:A:353:PRO:HD3	1:A:365:LEU:CD2	2.35	0.56
1:B:291:PRO:HD2	6:B:75:HOH:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:451:MAN:O3	4:B:454:NAG:O5	2.22	0.56
1:A:390:ASN:O	1:A:410:LEU:HD12	2.06	0.56
1:A:380:GLU:O	1:A:425:CYS:HA	2.06	0.56
1:A:245:PRO:HD2	1:A:313:TRP:CH2	2.40	0.56
1:B:362:GLN:HG2	1:B:413:ASP:HA	1.87	0.55
1:B:260:THR:CG2	1:B:305:VAL:HG13	2.35	0.55
2:C:125:GLN:NE2	2:C:152:TYR:OH	2.39	0.55
1:B:242:LEU:HD13	1:B:336:ILE:HG22	1.88	0.55
1:B:233:GLU:CG	1:B:235:LEU:HD22	2.20	0.55
2:C:52:GLN:HB3	6:C:203:HOH:O	2.05	0.55
2:C:72:GLN:HG2	2:C:73:THR:H	1.70	0.55
2:C:168:VAL:CG1	2:C:169:ASN:N	2.70	0.55
2:C:128:LYS:HE2	6:C:182:HOH:O	2.06	0.55
2:C:42:TRP:HB2	2:C:49:ILE:HG13	1.87	0.55
2:C:42:TRP:HB3	2:C:49:ILE:HG13	1.88	0.55
1:B:357:GLU:CD	1:B:364:SER:H	2.09	0.55
1:B:391:TYR:HB3	1:B:410:LEU:CD1	2.37	0.55
1:A:279:VAL:CG2	1:A:284:VAL:HG21	2.37	0.55
1:A:421:ASN:N	1:A:421:ASN:HD22	2.04	0.55
1:A:262:VAL:HG22	1:A:303:VAL:HG13	1.89	0.54
2:C:111:HIS:HE1	2:C:115:ASN:ND2	2.04	0.54
1:A:289:THR:HG22	1:A:304:SER:HA	1.89	0.54
1:A:266:VAL:O	1:A:300:TYR:HB2	2.07	0.54
2:C:126:ASN:N	2:C:126:ASN:ND2	2.55	0.54
1:A:260:THR:HG22	1:A:303:VAL:HG12	1.89	0.54
2:C:68:GLU:HB3	2:C:81:PRO:HB2	1.89	0.54
1:A:328:LEU:HD21	1:A:332:ILE:HG13	1.89	0.54
2:C:32:ALA:O	2:C:75:LEU:HB2	2.08	0.54
1:A:358:MET:HE1	6:A:84:HOH:O	2.08	0.54
1:A:242:LEU:HD13	1:A:336:ILE:CG2	2.37	0.54
1:B:431:ALA:C	1:B:432:LEU:HD12	2.27	0.54
2:C:62:THR:O	2:C:86:VAL:HG11	2.06	0.54
3:A:450:BMA:H62	3:A:452:MAN:H5	1.90	0.54
2:C:15:GLN:NE2	2:C:96:PRO:HB3	2.22	0.54
2:C:119:HIS:CD2	2:C:135:HIS:CE1	2.95	0.54
1:B:301:ARG:NH1	4:B:449:NDG:C8	2.49	0.54
2:C:15:GLN:HE22	2:C:96:PRO:HB3	1.73	0.54
1:A:253:ILE:HD12	6:A:88:HOH:O	2.06	0.54
1:A:263:VAL:HB	1:A:302:VAL:HB	1.89	0.53
2:C:116:THR:CG2	2:C:158:VAL:HG13	2.37	0.53
1:B:391:TYR:HB3	1:B:410:LEU:HD12	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:152:TYR:O	2:C:153:PHE:HB3	2.08	0.53
1:B:353:PRO:HD3	1:B:365:LEU:CD2	2.38	0.53
2:C:70:ARG:CZ	2:C:81:PRO:HD3	2.39	0.53
1:A:420:GLY:HA2	1:A:443:LEU:HD13	1.90	0.53
1:A:263:VAL:HG21	1:A:323:VAL:CG1	2.38	0.53
1:A:296:TYR:HE2	2:C:128:LYS:HZ2	1.51	0.53
1:A:430:GLU:HG2	1:A:430:GLU:O	2.08	0.53
1:B:330:ALA:HB1	1:B:331:PRO:HD2	1.89	0.53
1:B:259:VAL:HG12	1:B:277:TRP:CH2	2.44	0.53
1:B:248:LYS:HG3	1:B:428:MET:HE2	1.90	0.53
1:B:240:VAL:O	1:B:334:LYS:HE3	2.09	0.53
1:A:351:LEU:HD21	1:B:354:SER:HB2	1.89	0.53
2:C:24:SER:HA	2:C:58:ILE:O	2.09	0.53
2:C:10:VAL:HB	2:C:82:VAL:CG2	2.34	0.52
1:B:365:LEU:HD21	1:B:417:TRP:CE3	2.43	0.52
2:C:126:ASN:HD21	2:C:150:GLY:CA	2.21	0.52
1:B:260:THR:CG2	1:B:305:VAL:HG22	2.37	0.52
1:B:327:ALA:C	1:B:328:LEU:HD12	2.29	0.52
2:C:168:VAL:CG1	2:C:169:ASN:H	2.23	0.52
1:B:318:GLU:HA	1:B:337:SER:HB3	1.91	0.52
1:A:293:GLU:HB3	1:A:300:TYR:CE1	2.45	0.52
2:C:34:SER:HB2	2:C:35:PRO:HD2	1.91	0.51
1:A:328:LEU:CD2	1:A:332:ILE:HG13	2.40	0.51
1:B:279:VAL:CG2	1:B:284:VAL:HG21	2.36	0.51
1:A:296:TYR:HE2	2:C:128:LYS:NZ	2.09	0.51
1:A:443:LEU:N	1:A:443:LEU:HD12	2.25	0.51
1:B:266:VAL:HG21	1:B:302:VAL:HG23	1.92	0.51
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.92	0.51
1:B:430:GLU:O	1:B:430:GLU:HG2	2.10	0.51
2:C:72:GLN:HG2	2:C:73:THR:N	2.25	0.51
1:A:379:VAL:C	1:A:380:GLU:HG3	2.31	0.51
1:B:344:ARG:O	1:B:372:PHE:HA	2.10	0.51
1:B:320:LYS:HD2	1:B:333:GLU:OE1	2.10	0.51
1:B:361:ASN:HA	6:B:187:HOH:O	2.11	0.51
1:A:433:HIS:CD2	1:A:434:ASN:ND2	2.79	0.51
1:A:400:SER:O	1:A:402:GLY:N	2.44	0.51
1:A:238:PRO:HA	1:A:265:ASP:HB2	1.92	0.50
2:C:98:TRP:HB3	2:C:170:ILE:HA	1.92	0.50
2:C:34:SER:HB2	2:C:35:PRO:CD	2.42	0.50
2:C:119:HIS:HD2	2:C:135:HIS:CE1	2.30	0.50
1:A:245:PRO:HD2	1:A:313:TRP:CZ2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:GLU:HB2	1:A:431:ALA:O	2.11	0.50
2:C:130:ARG:HE	2:C:141:ILE:HD11	1.75	0.50
1:A:351:LEU:HB2	1:A:366:THR:HB	1.92	0.50
1:A:290:LYS:HG3	1:A:291:PRO:HD2	1.93	0.50
2:C:111:HIS:CE1	2:C:115:ASN:ND2	2.80	0.50
1:B:354:SER:O	1:B:357:GLU:N	2.36	0.50
2:C:98:TRP:HE3	2:C:170:ILE:HG12	1.77	0.50
2:C:72:GLN:HB2	2:C:78:LEU:HD12	1.94	0.50
1:B:312:ASP:O	1:B:317:LYS:HB2	2.11	0.50
1:A:432:LEU:O	1:A:433:HIS:C	2.49	0.50
1:B:279:VAL:O	1:B:282:VAL:CG2	2.60	0.50
1:A:269:GLU:HG3	1:A:270:ASP:N	2.26	0.49
3:A:448:NDG:H8C3	2:C:120:LYS:HB3	1.93	0.49
1:A:349:TYR:HB3	1:B:354:SER:CB	2.42	0.49
1:A:235:LEU:N	6:A:206:HOH:O	2.45	0.49
1:A:372:PHE:HD1	1:A:374:PRO:O	1.95	0.49
1:A:268:HIS:C	1:A:271:PRO:HD3	2.32	0.49
1:A:345:GLU:HA	1:A:431:ALA:HB3	1.94	0.49
1:B:342:GLN:OE1	1:B:343:PRO:HD2	2.12	0.49
1:B:428:MET:HG3	6:B:109:HOH:O	2.13	0.49
1:A:295:GLN:OE1	3:A:455:FUL:O2	2.17	0.49
1:B:238:PRO:HG2	1:B:328:LEU:CD1	2.42	0.49
1:B:269:GLU:C	1:B:271:PRO:HD3	2.32	0.49
1:A:297:ASN:C	1:A:299:THR:H	2.16	0.49
1:A:414:LYS:HG2	1:A:418:GLN:NE2	2.24	0.49
1:B:312:ASP:HB3	1:B:319:TYR:OH	2.13	0.49
1:A:434:ASN:O	1:A:435:HIS:HB2	2.13	0.49
1:B:316:GLY:O	1:B:317:LYS:C	2.51	0.49
1:B:426:SER:HB3	1:B:436:TYR:HE2	1.78	0.48
1:A:324:SER:CA	1:A:331:PRO:HB3	2.43	0.48
1:A:384:ASN:O	1:A:385:GLY:C	2.52	0.48
1:B:400:SER:C	1:B:402:GLY:H	2.16	0.48
1:A:399:ASP:CB	1:B:392:LYS:HG3	2.43	0.48
3:A:452:MAN:O3	3:A:453:NDG:C1	2.62	0.48
2:C:148:ASP:O	2:C:150:GLY:N	2.40	0.48
2:C:97:ARG:HG2	2:C:97:ARG:HH11	1.79	0.48
1:A:244:PRO:HD3	1:A:336:ILE:CD1	2.43	0.48
1:A:416:ARG:O	1:A:417:TRP:C	2.51	0.48
2:C:5:LEU:HD22	2:C:6:PRO:HD2	1.94	0.48
4:B:448:NAG:H4	4:B:455:FUL:HO2	1.72	0.48
1:A:240:VAL:HG23	1:A:334:LYS:CE	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:104:ASP:O	2:C:142:PRO:O	2.32	0.48
1:A:294:GLU:HG3	1:A:295:GLN:N	2.29	0.48
1:A:437:THR:CG2	1:A:438:GLN:N	2.76	0.48
1:A:368:LEU:HD12	1:A:369:VAL:N	2.28	0.48
1:B:240:VAL:HA	1:B:262:VAL:O	2.13	0.48
2:C:117:ALA:HB1	2:C:119:HIS:CE1	2.49	0.48
1:B:391:TYR:CD2	1:B:391:TYR:C	2.87	0.48
1:B:406:LEU:C	1:B:406:LEU:HD12	2.34	0.48
1:A:311:GLN:O	1:A:315:ASN:ND2	2.46	0.48
2:C:110:CYS:HB2	2:C:123:TYR:CE2	2.49	0.47
2:C:103:GLU:HG3	2:C:143:LYS:CG	2.33	0.47
1:A:443:LEU:O	1:A:444:SER:HB2	2.14	0.47
1:B:413:ASP:N	1:B:413:ASP:OD1	2.47	0.47
2:C:8:ALA:HB2	2:C:76:SER:HB2	1.96	0.47
1:B:365:LEU:HD22	1:B:441:LEU:CD1	2.44	0.47
1:B:293:GLU:HG3	1:B:299:THR:O	2.15	0.47
1:A:240:VAL:O	1:A:334:LYS:HE2	2.14	0.47
1:B:279:VAL:O	1:B:280:ASP:C	2.53	0.47
1:B:236:GLY:O	2:C:161:LYS:HD3	2.14	0.47
1:B:355:ARG:NH1	6:B:173:HOH:O	2.48	0.47
1:B:436:TYR:CD1	1:B:436:TYR:C	2.88	0.46
1:A:284:VAL:HG12	1:A:285:HIS:H	1.77	0.46
2:C:52:GLN:HG3	2:C:53:ALA:N	2.31	0.46
1:A:311:GLN:HA	1:A:314:LEU:HD12	1.96	0.46
1:A:384:ASN:O	1:A:386:GLN:O	2.33	0.46
2:C:40:THR:OG1	2:C:54:SER:HA	2.15	0.46
4:B:448:NAG:H61	4:B:455:FUL:H2	1.71	0.46
1:B:358:MET:C	1:B:360:LYS:N	2.69	0.46
1:A:271:PRO:C	1:A:272:GLU:HG2	2.36	0.46
1:A:391:TYR:HB3	1:A:410:LEU:HD13	1.98	0.46
1:A:354:SER:O	1:A:355:ARG:C	2.53	0.46
1:A:319:TYR:O	1:A:320:LYS:C	2.54	0.46
1:B:429:HIS:HB3	1:B:432:LEU:HD13	1.97	0.46
1:B:327:ALA:O	2:C:113:TRP:HZ3	1.99	0.46
2:C:139:PHE:CZ	2:C:141:ILE:HD11	2.51	0.46
1:B:240:VAL:HG22	1:B:263:VAL:HG13	1.97	0.46
1:B:428:MET:HG2	1:B:436:TYR:HD2	1.80	0.46
1:B:433:HIS:O	1:B:434:ASN:HB2	2.16	0.46
1:A:275:PHE:CZ	1:A:302:VAL:HG12	2.51	0.46
2:C:27:LEU:N	2:C:27:LEU:CD1	2.76	0.46
1:A:397:VAL:HG21	1:B:394:THR:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:TRP:CE2	1:B:443:LEU:HG	2.50	0.46
2:C:42:TRP:HB3	2:C:49:ILE:CD1	2.47	0.45
1:B:338:LYS:HD2	1:B:430:GLU:OE1	2.16	0.45
1:B:259:VAL:HG12	1:B:277:TRP:HH2	1.81	0.45
1:A:415:SER:OG	1:A:416:ARG:N	2.50	0.45
1:A:384:ASN:C	1:A:386:GLN:N	2.69	0.45
1:B:350:THR:HB	1:B:441:LEU:HG	1.98	0.45
1:A:418:GLN:O	1:A:419:GLN:C	2.55	0.45
2:C:131:LYS:HD2	2:C:139:PHE:CE1	2.51	0.45
1:B:388:GLU:HB3	1:B:410:LEU:HD11	1.98	0.45
1:A:268:HIS:O	1:A:271:PRO:HD3	2.15	0.45
2:C:101:LYS:O	2:C:103:GLU:N	2.50	0.45
3:A:448:NDG:H6C2	3:A:455:FUL:H2	1.45	0.45
1:A:286:ASN:O	1:A:287:ALA:O	2.35	0.45
1:B:328:LEU:N	1:B:328:LEU:CD1	2.78	0.45
1:A:348:VAL:HG12	1:A:439:LYS:HG3	1.97	0.45
1:B:253:ILE:HD12	1:B:253:ILE:O	2.16	0.45
1:A:293:GLU:HB2	1:A:299:THR:O	2.16	0.45
2:C:42:TRP:HB3	2:C:49:ILE:CG1	2.46	0.45
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.52	0.45
2:C:45:ASN:O	2:C:46:GLU:CB	2.63	0.44
2:C:12:LEU:HA	2:C:12:LEU:HD23	1.83	0.44
1:B:432:LEU:HD23	1:B:437:THR:HB	1.99	0.44
1:B:329:PRO:HG3	2:C:113:TRP:CE3	2.52	0.44
1:A:424:SER:OG	1:A:440:SER:HB3	2.18	0.44
1:B:350:THR:HG23	1:B:439:LYS:HG3	2.00	0.44
1:B:424:SER:OG	1:B:438:GLN:HG3	2.18	0.44
1:B:251:LEU:HD21	1:B:430:GLU:HA	1.99	0.44
1:A:359:THR:OG1	1:A:360:LYS:HD2	2.18	0.44
1:A:325:ASN:O	1:A:328:LEU:HB2	2.18	0.44
1:A:244:PRO:HB3	1:A:336:ILE:CD1	2.47	0.44
1:B:432:LEU:CD1	1:B:432:LEU:N	2.80	0.44
1:A:275:PHE:HZ	1:A:302:VAL:HG12	1.82	0.44
1:B:388:GLU:HA	1:B:388:GLU:OE2	2.17	0.44
1:B:248:LYS:HA	1:B:428:MET:CE	2.47	0.44
1:A:399:ASP:CA	1:B:392:LYS:HE3	2.47	0.44
2:C:62:THR:C	2:C:86:VAL:HG11	2.38	0.44
2:C:17:TYR:CD1	2:C:17:TYR:C	2.90	0.44
2:C:103:GLU:O	2:C:104:ASP:CB	2.57	0.44
2:C:158:VAL:HG23	2:C:163:VAL:HG21	2.00	0.44
2:C:19:VAL:HB	2:C:23:ASP:CG	2.39	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:TRP:CD2	2:C:168:VAL:HG11	2.52	0.43
2:C:42:TRP:HB3	2:C:49:ILE:HD11	2.00	0.43
1:A:399:ASP:HB2	1:B:392:LYS:HG3	2.00	0.43
1:A:286:ASN:HB2	1:A:306:LEU:CD1	2.48	0.43
2:C:124:LEU:HA	2:C:129:ASP:HA	1.99	0.43
1:A:414:LYS:HB3	1:A:414:LYS:HE2	1.74	0.43
1:A:377:ILE:HG22	6:A:121:HOH:O	2.18	0.43
4:B:448:NAG:C4	4:B:455:FUL:O2	2.49	0.43
2:C:5:LEU:HB3	2:C:6:PRO:HD2	1.99	0.43
1:B:346:PRO:CD	1:B:432:LEU:HD11	2.48	0.43
1:A:279:VAL:HG23	1:A:284:VAL:CG2	2.47	0.43
1:B:343:PRO:HA	1:B:373:TYR:O	2.18	0.43
1:A:257:PRO:HG2	1:A:308:VAL:O	2.19	0.43
1:B:260:THR:HG22	1:B:305:VAL:CG2	2.45	0.43
1:B:238:PRO:HG2	1:B:328:LEU:HD11	1.99	0.43
1:A:282:VAL:O	1:A:282:VAL:HG23	2.18	0.43
1:B:424:SER:HB2	1:B:440:SER:OG	2.19	0.43
1:B:244:PRO:HD3	1:B:336:ILE:CD1	2.48	0.43
1:A:263:VAL:CG2	1:A:323:VAL:HG11	2.43	0.43
1:A:356:GLU:O	1:A:359:THR:HG23	2.18	0.43
1:B:293:GLU:HG2	1:B:294:GLU:N	2.32	0.43
2:C:123:TYR:CD1	2:C:139:PHE:HB2	2.54	0.43
2:C:158:VAL:HG23	2:C:163:VAL:CG2	2.49	0.43
1:A:427:VAL:N	1:A:437:THR:O	2.45	0.43
1:A:279:VAL:HG23	1:A:284:VAL:HG21	2.01	0.43
2:C:22:LYS:HA	2:C:22:LYS:HD3	1.63	0.42
2:C:21:GLU:O	2:C:22:LYS:HG2	2.19	0.42
1:B:409:LYS:HB3	1:B:409:LYS:HE2	1.73	0.42
2:C:142:PRO:HB2	2:C:143:LYS:H	1.68	0.42
1:A:294:GLU:OE2	1:A:295:GLN:HG3	2.19	0.42
1:B:265:ASP:OD2	4:B:448:NAG:C8	2.68	0.42
1:A:244:PRO:HD3	1:A:336:ILE:HD11	2.01	0.42
1:A:324:SER:OG	1:A:331:PRO:HB3	2.20	0.42
1:A:349:TYR:HB3	1:B:354:SER:HB3	1.99	0.42
1:A:278:TYR:CD1	1:A:278:TYR:N	2.87	0.42
2:C:116:THR:HG21	2:C:158:VAL:CG1	2.47	0.42
1:B:268:HIS:HB2	1:B:269:GLU:OE2	2.19	0.42
1:A:293:GLU:CB	1:A:300:TYR:HA	2.50	0.42
1:A:353:PRO:HD3	1:A:365:LEU:HD22	2.01	0.42
1:A:383:SER:HA	1:A:423:PHE:HA	2.02	0.42
1:B:293:GLU:CG	1:B:294:GLU:N	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLN:HA	1:B:443:LEU:HD21	2.02	0.42
2:C:13:GLU:HB3	2:C:26:THR:OG1	2.20	0.42
1:B:344:ARG:N	1:B:373:TYR:O	2.45	0.42
1:B:388:GLU:O	1:B:391:TYR:HD1	2.03	0.42
1:A:279:VAL:HG21	1:A:284:VAL:HG21	2.00	0.42
1:A:366:THR:HG23	1:B:407:TYR:CZ	2.55	0.42
1:B:393:THR:HG22	1:B:394:THR:O	2.20	0.42
1:B:388:GLU:O	1:B:391:TYR:CD1	2.72	0.42
1:B:350:THR:HB	1:B:441:LEU:HB2	2.02	0.42
1:A:336:ILE:HG12	1:A:337:SER:N	2.35	0.42
1:A:277:TRP:C	1:A:278:TYR:HD1	2.23	0.41
1:A:273:VAL:CG1	1:A:323:VAL:HG13	2.50	0.41
1:A:345:GLU:HA	1:A:346:PRO:HD3	1.74	0.41
2:C:43:PHE:HB2	2:C:70:ARG:HB2	2.01	0.41
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.54	0.41
1:B:357:GLU:O	1:B:363:VAL:HG12	2.19	0.41
1:A:278:TYR:HD1	1:A:278:TYR:N	2.18	0.41
1:A:333:GLU:C	1:A:334:LYS:HG2	2.40	0.41
1:A:238:PRO:HD3	2:C:134:HIS:NE2	2.36	0.41
1:B:389:ASN:CG	1:B:390:ASN:H	2.23	0.41
1:B:314:LEU:HA	1:B:338:LYS:HZ3	1.85	0.41
1:A:374:PRO:O	1:A:429:HIS:HE1	2.04	0.41
2:C:118:LEU:HD11	2:C:156:GLY:HA3	2.03	0.41
1:A:326:LYS:C	1:A:328:LEU:N	2.73	0.41
1:A:429:HIS:N	1:A:432:LEU:HD12	2.36	0.41
2:C:130:ARG:O	2:C:131:LYS:HG3	2.19	0.41
1:A:296:TYR:CE2	2:C:128:LYS:NZ	2.78	0.41
1:B:369:VAL:O	1:B:405:PHE:HA	2.21	0.41
1:B:381:TRP:HB2	1:B:391:TYR:CD1	2.56	0.41
2:C:48:LEU:N	2:C:48:LEU:CD1	2.82	0.41
4:B:448:NAG:C6	4:B:449:NDG:C7	2.99	0.41
1:A:432:LEU:HD23	1:A:432:LEU:HA	1.75	0.41
1:B:248:LYS:CG	1:B:428:MET:HE1	2.49	0.41
1:A:284:VAL:CG1	1:A:285:HIS:N	2.82	0.41
2:C:145:THR:C	2:C:147:LYS:N	2.74	0.41
1:B:289:THR:HG22	1:B:304:SER:CB	2.51	0.41
1:B:255:ARG:HB3	1:B:255:ARG:HE	1.55	0.41
1:B:441:LEU:HD22	1:B:442:SER:N	2.36	0.41
1:B:322:LYS:HA	1:B:332:ILE:O	2.20	0.41
2:C:129:ASP:OD1	2:C:129:ASP:N	2.52	0.41
1:B:350:THR:O	1:B:351:LEU:HD23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:VAL:HG13	1:A:303:VAL:HG13	2.03	0.40
1:A:372:PHE:HE1	1:A:375:SER:HA	1.86	0.40
1:A:391:TYR:HB3	1:A:410:LEU:CD1	2.52	0.40
1:A:244:PRO:HB3	1:A:313:TRP:HH2	1.86	0.40
1:B:432:LEU:HB3	6:B:116:HOH:O	2.21	0.40
2:C:153:PHE:C	2:C:153:PHE:CD1	2.94	0.40
2:C:5:LEU:HD23	2:C:5:LEU:HA	1.90	0.40
2:C:145:THR:O	2:C:147:LYS:N	2.54	0.40
2:C:20:LEU:HD21	2:C:92:LEU:HB2	2.04	0.40
1:B:235:LEU:CD1	2:C:117:ALA:HB3	2.49	0.40
1:A:308:VAL:HG21	1:A:319:TYR:CZ	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	208/224 (93%)	169 (81%)	27 (13%)	12 (6%)	2	12
1	B	210/224 (94%)	168 (80%)	33 (16%)	9 (4%)	3	19
2	C	165/176 (94%)	131 (79%)	24 (14%)	10 (6%)	2	11
All	All	583/624 (93%)	468 (80%)	84 (14%)	31 (5%)	2	14

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ALA
1	B	317	LYS
1	B	434	ASN
2	C	102	GLU
1	A	385	GLY
1	A	401	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	421	ASN
1	B	295	GLN
1	B	421	ASN
2	C	51	SER
2	C	53	ALA
2	C	104	ASP
2	C	142	PRO
1	A	237	GLY
1	A	265	ASP
1	B	296	TYR
1	B	390	ASN
1	B	401	ASP
2	C	35	PRO
2	C	149	SER
1	A	310	HIS
1	A	312	ASP
1	A	320	LYS
1	A	400	SER
2	C	15	GLN
1	A	331	PRO
1	A	416	ARG
1	B	312	ASP
2	C	146	LEU
2	C	153	PHE
1	B	387	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	195/207 (94%)	174 (89%)	21 (11%)	8	30
1	B	197/207 (95%)	181 (92%)	16 (8%)	15	47
2	C	152/160 (95%)	137 (90%)	15 (10%)	10	35
All	All	544/574 (95%)	492 (90%)	52 (10%)	10	38

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	LEU
1	A	252	MET
1	A	253	ILE
1	A	255	ARG
1	A	267	SER
1	A	278	TYR
1	A	280	ASP
1	A	293	GLU
1	A	303	VAL
1	A	328	LEU
1	A	335	THR
1	A	342	GLN
1	A	360	LYS
1	A	361	ASN
1	A	366	THR
1	A	370	LYS
1	A	384	ASN
1	A	390	ASN
1	A	398	LEU
1	A	401	ASP
1	A	406	LEU
1	B	235	LEU
1	B	242	LEU
1	B	253	ILE
1	B	258	GLU
1	B	263	VAL
1	B	282	VAL
1	B	286	ASN
1	B	290	LYS
1	B	311	GLN
1	B	375	SER
1	B	390	ASN
1	B	413	ASP
1	B	433	HIS
1	B	437	THR
1	B	441	LEU
1	B	443	LEU
2	C	15	GLN
2	C	17	TYR
2	C	23	ASP
2	C	26	THR
2	C	41	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	48	LEU
2	C	49	ILE
2	C	52	GLN
2	C	98	TRP
2	C	126	ASN
2	C	129	ASP
2	C	130	ARG
2	C	140	HIS
2	C	167	THR
2	C	171	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	315	ASN
1	A	386	GLN
1	A	418	GLN
1	A	421	ASN
1	A	429	HIS
1	A	433	HIS
1	A	434	ASN
1	A	438	GLN
1	B	315	ASN
1	B	386	GLN
1	B	390	ASN
1	B	419	GLN
1	B	421	ASN
2	C	15	GLN
2	C	72	GLN
2	C	115	ASN
2	C	119	HIS
2	C	125	GLN
2	C	126	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

16 carbohydrates 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	$\# Z > 2$
3	NDG	A	448	1,3	14,14,15	1.18	1 (7%)	15,19,21	1.58	3 (20%)
3	NAG	A	449	3	14,14,15	0.76	0	15,19,21	0.70	0
3	BMA	A	450	3	11,11,12	0.39	0	14,15,17	1.27	1 (7%)
3	BMA	A	451	3	11,11,12	0.33	0	14,15,17	0.68	0
3	MAN	A	452	3	11,11,12	1.14	1 (9%)	14,15,17	1.51	4 (28%)
3	NDG	A	453	3	14,14,15	0.83	0	15,19,21	0.84	1 (6%)
3	GAL	A	454	3	11,11,12	0.75	0	14,15,17	0.48	0
3	FUL	A	455	3	10,10,11	0.69	0	14,14,16	1.11	2 (14%)
4	NAG	B	448	1,4	14,14,15	0.85	0	15,19,21	0.85	0
4	NDG	B	449	4	14,14,15	1.22	1 (7%)	15,19,21	1.30	2 (13%)
4	BMA	B	450	4	11,11,12	0.87	0	14,15,17	0.67	0
4	MAN	B	451	4	11,11,12	0.73	0	14,15,17	1.47	3 (21%)
4	MAN	B	452	4	11,11,12	0.89	1 (9%)	14,15,17	1.95	2 (14%)
4	NAG	B	453	4	14,14,15	0.76	0	15,19,21	2.28	4 (26%)
4	NAG	B	454	4	14,14,15	0.86	1 (7%)	15,19,21	1.46	2 (13%)
4	FUL	B	455	4	10,10,11	1.04	1 (10%)	14,14,16	0.59	0

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
3	NDG	A	448	1,3	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	449	3	-	1/6/23/26	0/1/1/1
3	BMA	A	450	3	-	0/2/19/22	0/1/1/1
3	BMA	A	451	3	-	0/2/19/22	0/1/1/1
3	MAN	A	452	3	-	0/2/19/22	0/1/1/1
3	NDG	A	453	3	-	0/6/23/26	0/1/1/1
3	GAL	A	454	3	-	0/2/19/22	0/1/1/1
3	FUL	A	455	3	-	0/0/17/20	0/1/1/1
4	NAG	B	448	1,4	-	0/6/23/26	0/1/1/1
4	NDG	B	449	4	-	0/6/23/26	0/1/1/1
4	BMA	B	450	4	-	0/2/19/22	0/1/1/1
4	MAN	B	451	4	-	0/2/19/22	0/1/1/1
4	MAN	B	452	4	-	0/2/19/22	0/1/1/1
4	NAG	B	453	4	-	0/6/23/26	0/1/1/1
4	NAG	B	454	4	-	0/6/23/26	0/1/1/1
4	FUL	B	455	4	-	0/0/17/20	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	452	MAN	C4-C5	-2.07	1.48	1.53
4	B	454	NAG	O5-C5	2.13	1.48	1.43
4	B	455	FUL	C2-C3	2.26	1.55	1.52
3	A	452	MAN	C2-C3	3.03	1.56	1.52
4	B	449	NDG	C1-C2	3.67	1.57	1.52
3	A	448	NDG	C1-C2	3.83	1.57	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	453	NAG	C6-C5-C4	-4.24	102.55	113.02
4	B	453	NAG	C2-N2-C7	-4.02	117.87	123.04
4	B	454	NAG	C4-C3-C2	-3.55	105.70	111.23
4	B	454	NAG	C2-N2-C7	-3.43	118.64	123.04
3	A	448	NDG	C3-C4-C5	-3.23	104.57	110.20
4	B	449	NDG	C2-N2-C7	-2.35	120.02	123.04
4	B	451	MAN	O2-C2-C1	-2.34	104.52	109.21
3	A	448	NDG	C2-N2-C7	-2.26	120.13	123.04
3	A	453	NDG	C2-N2-C7	-2.25	120.15	123.04
3	A	455	FUL	C3-C4-C5	2.05	113.17	109.72
3	A	452	MAN	C1-O5-C5	2.06	114.86	112.25
4	B	452	MAN	C2-C3-C4	2.06	114.55	111.04
3	A	452	MAN	C2-C3-C4	2.33	114.99	111.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	451	MAN	O5-C1-C2	2.54	114.98	110.86
3	A	455	FUL	C1-C2-C3	2.66	112.69	109.54
3	A	452	MAN	C1-C2-C3	2.69	112.73	109.54
3	A	452	MAN	O2-C2-C3	2.84	115.83	110.12
4	B	453	NAG	C1-O5-C5	3.10	116.18	112.25
4	B	451	MAN	C1-O5-C5	3.23	116.35	112.25
4	B	449	NDG	C4-C3-C2	3.72	117.01	111.23
3	A	448	NDG	C6-C5-C4	3.77	122.31	113.02
3	A	450	BMA	C1-C2-C3	3.96	114.23	109.54
4	B	453	NAG	C3-C4-C5	4.93	118.78	110.20
4	B	452	MAN	C1-C2-C3	6.14	116.81	109.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	449	NAG	O7-C7-N2-C2

There are no ring outliers.

13 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	448	NDG	2	0
3	A	449	NAG	1	0
3	A	450	BMA	1	0
3	A	452	MAN	2	0
3	A	453	NDG	1	0
3	A	455	FUL	2	0
4	B	448	NAG	21	0
4	B	449	NDG	12	0
4	B	451	MAN	1	0
4	B	452	MAN	1	0
4	B	453	NAG	1	0
4	B	454	NAG	1	0
4	B	455	FUL	4	0

5.6 Ligand geometry

1 ligand is 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$
5	HG2	A	456	1	2,2,2	7.03	2 (100%)	0,1,1	0.00	-

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
5	HG2	A	456	1	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	456	HG2	BR2-HG	5.39	2.63	2.41
5	A	456	HG2	BR1-HG	8.35	2.75	2.41

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.