



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:35 AM GMT

PDB ID : 4JM2
Title : Crystal Structure of PGT 135 Fab in Complex with gp120 Core Protein from HIV-1 Strain JR-FL Bound to CD4 and 17b Fab
Authors : Kong, L.; Wilson, I.A.
Deposited on : 2013-03-13
Resolution : 3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

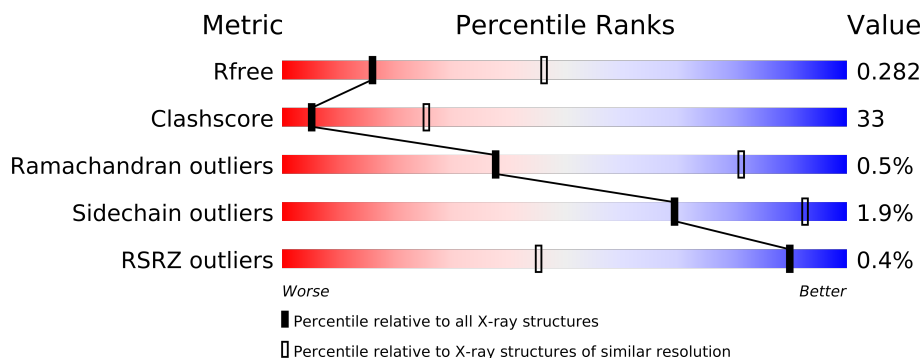
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.10 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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	236	
2	B	214	
3	C	214	
4	D	229	
5	E	321	
6	F	185	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10907 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PGT 135 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1744	1106	308	323	7			

- Molecule 2 is a protein called PGT 135 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1672	1050	279	336	7			

- Molecule 3 is a protein called 17b Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1646	1028	282	331	5			

- Molecule 4 is a protein called 17b Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	220	Total	C	N	O	S	0	0	0
			1668	1056	279	328	5			

- Molecule 5 is a protein called gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	315	Total	C	N	O	S	0	0	0
			2467	1539	437	470	21			

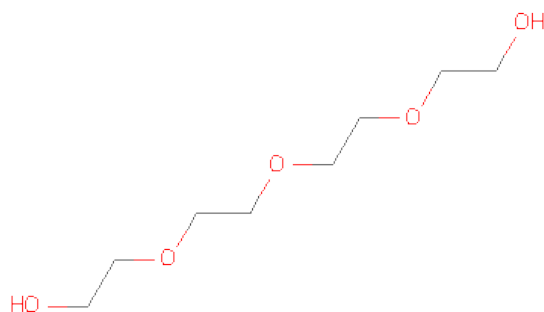
- Molecule 6 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	175	Total	C	N	O	S	0	0	0
			1363	851	239	269	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	184	ASN	-	EXPRESSION TAG	UNP P01730
F	185	THR	-	EXPRESSION TAG	UNP P01730

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			13	8	5		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	8	Total	C	N	O	0	0
			94	52	2	40		

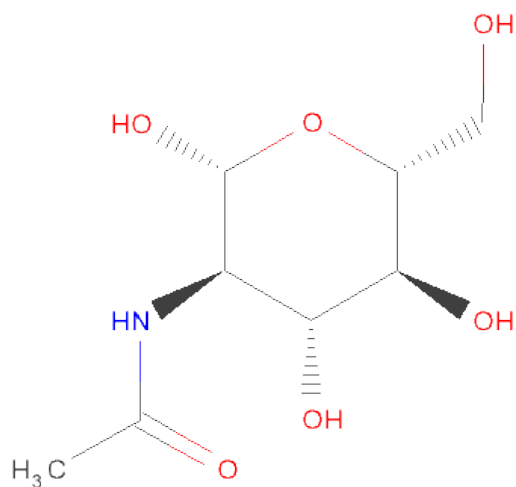
- Molecule 9 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	E	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	E	1	Total	C	N	O	0	0
			14	8	1	5		
11	E	1	Total	C	N	O	0	0
			14	8	1	5		
11	E	1	Total	C	N	O	0	0
			14	8	1	5		
11	E	1	Total	C	N	O	0	0
			14	8	1	5		
11	E	1	Total	C	N	O	0	0
			14	8	1	5		
11	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	O	0	0
			1	1		

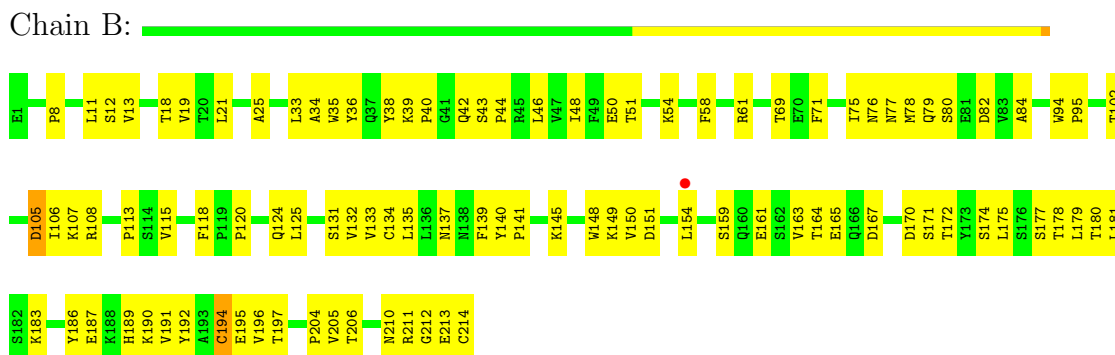
3 Residue-property plots

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.

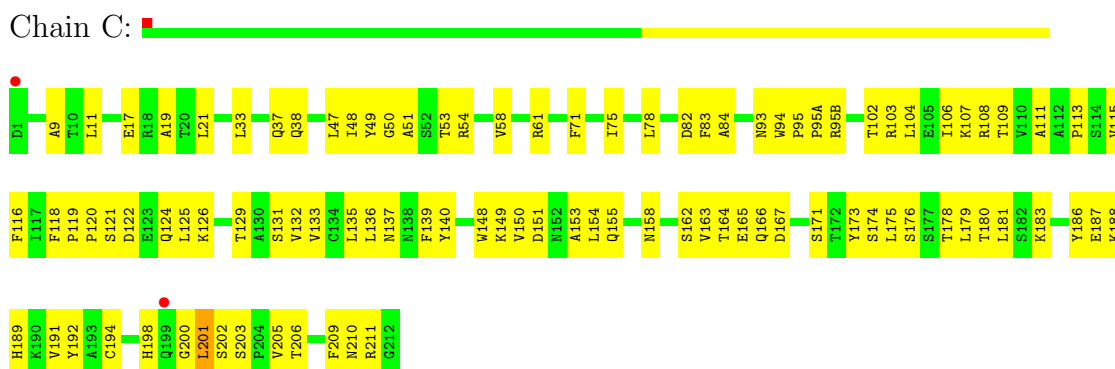
- Molecule 1: PGT 135 Heavy chain



- Molecule 2: PGT 135 Light chain

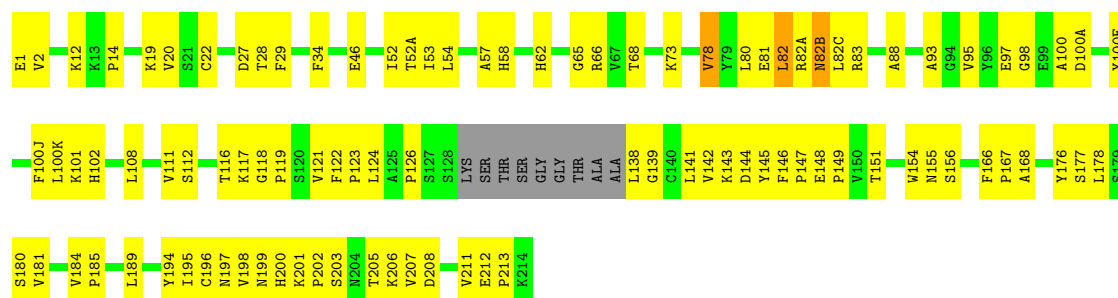


- Molecule 3: 17b Light chain



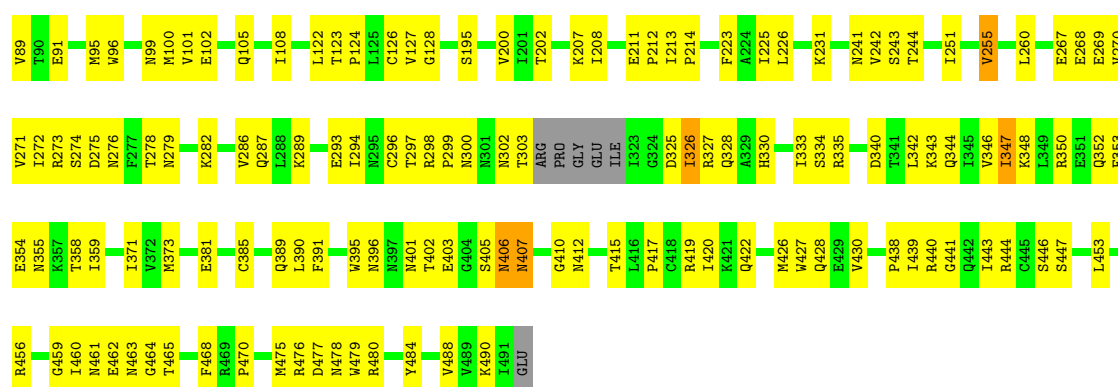
- Molecule 4: 17b Heavy chain

Chain D:



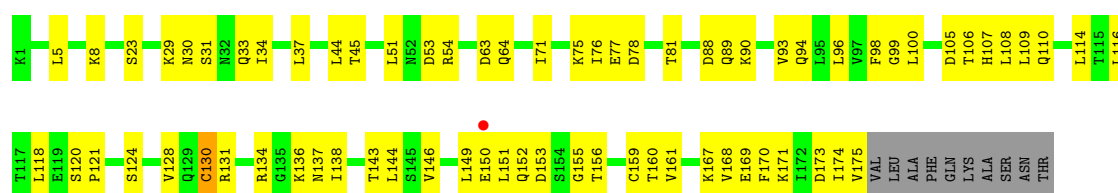
- Molecule 5: gp120

Chain E:



- Molecule 6: T-cell surface glycoprotein CD4

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.41Å 92.15Å 88.19Å 90.00° 104.75° 90.00°	Depositor
Resolution (Å)	43.58 – 3.10 43.58 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.58-3.10) 99.7 (43.58-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.238 , 0.285 0.241 , 0.282	Depositor DCC
R_{free} test set	1562 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	104.8	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 70.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30862 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10907	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, BMA, NAG, 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	0.43	0/1795	0.67	0/2447
2	B	0.45	0/1709	0.70	0/2323
3	C	0.41	0/1683	0.63	0/2288
4	D	0.51	0/1707	0.69	0/2325
5	E	0.48	0/2514	0.70	1/3404 (0.0%)
6	F	0.37	0/1382	0.62	0/1863
All	All	0.45	0/10790	0.67	1/14650 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	406	ASN	N-CA-C	-5.47	96.23	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1744	0	1700	126	0
2	B	1672	0	1619	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1646	0	1595	124	0
4	D	1668	0	1637	116	0
5	E	2467	0	2412	159	0
6	F	1363	0	1389	92	0
7	C	13	0	18	0	0
8	E	94	0	79	7	0
9	E	116	0	97	4	0
10	E	39	0	34	0	0
11	E	84	0	78	10	0
12	A	1	0	0	0	0
All	All	10907	0	10658	710	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

All (710) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:268:GLU:CG	5:E:269:GLU:H	1.32	1.34
4:D:82(C):LEU:O	4:D:111:VAL:HG11	1.35	1.26
1:A:33:GLU:HG3	1:A:34:TRP:N	1.37	1.12
5:E:268:GLU:HG2	5:E:269:GLU:N	1.61	1.11
3:C:151:ASP:OD1	3:C:191:VAL:HG12	1.50	1.10
5:E:268:GLU:CG	5:E:269:GLU:N	2.09	1.06
1:A:212:GLU:HG3	1:A:213:PRO:HD2	1.39	1.04
5:E:268:GLU:HG2	5:E:269:GLU:H	0.88	1.02
2:B:187:GLU:HA	2:B:211:ARG:HH22	1.21	1.00
6:F:5:LEU:CD1	6:F:98:PHE:CD1	2.46	0.98
5:E:101:VAL:HG13	5:E:102:GLU:OE1	1.63	0.98
5:E:326:ILE:HG13	5:E:327:ARG:H	1.24	0.98
1:A:87:THR:HG22	1:A:111:VAL:H	1.27	0.98
4:D:200:HIS:HB3	4:D:205:THR:OG1	1.63	0.97
5:E:231:LYS:HE3	5:E:267:GLU:OE1	1.64	0.97
1:A:33:GLU:HG3	1:A:34:TRP:H	0.98	0.96
2:B:150:VAL:HG12	2:B:189:HIS:CG	2.00	0.96
2:B:213:GLU:HG2	2:B:214:CYS:H	1.29	0.96
1:A:33:GLU:CG	1:A:34:TRP:N	2.29	0.95
1:A:100(B):MET:HE3	1:A:100(E):PRO:HA	1.49	0.95
6:F:37:LEU:HD21	6:F:44:LEU:HD11	1.49	0.94
1:A:29:ILE:HG21	1:A:71:ILE:HD11	1.48	0.94
3:C:151:ASP:HA	3:C:191:VAL:CG1	1.98	0.93
5:E:350:ARG:HG2	5:E:355:ASN:HA	1.49	0.93
3:C:201:LEU:HD12	3:C:202:SER:H	1.34	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:268:GLU:HG3	5:E:269:GLU:H	1.33	0.92
4:D:141:LEU:HD21	4:D:143:LYS:HB2	1.50	0.92
6:F:134:ARG:NH2	6:F:152:GLN:HB2	1.86	0.91
3:C:162:SER:HB2	4:D:167:PRO:HG2	1.52	0.90
3:C:201:LEU:HD12	3:C:202:SER:N	1.86	0.90
6:F:161:VAL:O	6:F:167:LYS:HA	1.74	0.88
1:A:171:GLN:HE21	1:A:177:SER:HB2	1.38	0.88
4:D:82(C):LEU:O	4:D:111:VAL:CG1	2.20	0.88
2:B:42:GLN:HG2	2:B:43:SER:H	1.38	0.88
5:E:358:THR:HG22	5:E:465:THR:CB	2.05	0.87
5:E:346:VAL:HG13	5:E:359:ILE:HD11	1.56	0.87
3:C:180:THR:O	3:C:181:LEU:HD23	1.75	0.87
3:C:125:LEU:O	3:C:183:LYS:HE2	1.75	0.86
4:D:154:TRP:HE1	4:D:180:SER:HG	1.21	0.86
5:E:327:ARG:HD3	5:E:420:ILE:O	1.76	0.86
2:B:187:GLU:HA	2:B:211:ARG:NH2	1.90	0.85
5:E:325:ASP:O	5:E:326:ILE:HB	1.75	0.84
1:A:171:GLN:NE2	1:A:177:SER:HB2	1.92	0.84
3:C:11:LEU:O	3:C:104:LEU:HD12	1.76	0.83
1:A:33:GLU:CG	1:A:34:TRP:H	1.88	0.83
3:C:120:PRO:HG3	3:C:131:SER:O	1.76	0.83
2:B:118:PHE:HB2	2:B:133:VAL:HG22	1.61	0.82
1:A:212:GLU:CG	1:A:213:PRO:HD2	2.09	0.82
5:E:346:VAL:HA	5:E:359:ILE:CD1	2.10	0.81
2:B:213:GLU:HG2	2:B:214:CYS:N	1.95	0.81
5:E:358:THR:HG22	5:E:465:THR:HB	1.62	0.81
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.63	0.81
8:E:503:BMA:H2	8:E:507:MAN:O6	1.81	0.80
5:E:108:ILE:HG22	5:E:427:TRP:HH2	1.44	0.80
2:B:125:LEU:HA	2:B:183:LYS:HZ1	1.46	0.80
2:B:80:SER:HA	2:B:106:ILE:CD1	2.13	0.79
3:C:48:ILE:HD13	3:C:54:ARG:HA	1.61	0.79
1:A:100(C):LEU:CD1	5:E:415:THR:HG21	2.12	0.79
5:E:326:ILE:HG13	5:E:327:ARG:N	1.97	0.79
1:A:34:TRP:CH2	5:E:419:ARG:HG2	2.18	0.79
6:F:134:ARG:HH22	6:F:152:GLN:HB2	1.45	0.79
6:F:116:LEU:HD11	6:F:144:LEU:HD13	1.65	0.78
2:B:164:THR:HG22	2:B:174:SER:H	1.48	0.78
5:E:346:VAL:HG22	5:E:359:ILE:HD11	1.66	0.78
1:A:39:HIS:HB2	1:A:45:LEU:CD2	2.13	0.78
4:D:184:VAL:HG13	4:D:185:PRO:HD2	1.66	0.78
4:D:138:LEU:HD11	4:D:211:VAL:HG21	1.65	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:5:LEU:HD21	6:F:168:VAL:HB	1.65	0.77
4:D:138:LEU:HD11	4:D:211:VAL:CG2	2.14	0.77
2:B:149:LYS:HG2	2:B:154:LEU:HD23	1.66	0.77
1:A:29:ILE:CG2	1:A:71:ILE:HD11	2.14	0.77
5:E:270:VAL:O	5:E:348:LYS:HE2	1.85	0.77
5:E:358:THR:CG2	5:E:465:THR:HB	2.14	0.76
3:C:108:ARG:NH2	3:C:140:TYR:HB2	2.00	0.76
1:A:214:LYS:HB3	2:B:214:CYS:SG	2.25	0.76
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.68	0.76
5:E:358:THR:CG2	5:E:465:THR:CB	2.64	0.76
2:B:145:LYS:HB3	2:B:197:THR:OG1	1.86	0.75
4:D:167:PRO:C	4:D:178:LEU:HD21	2.08	0.75
1:A:171:GLN:HE21	1:A:177:SER:CB	1.99	0.75
5:E:346:VAL:HA	5:E:359:ILE:HD11	1.67	0.75
4:D:2:VAL:HG12	4:D:102:HIS:ND1	2.02	0.74
5:E:461:ASN:OD1	5:E:462:GLU:N	2.19	0.74
5:E:350:ARG:CG	5:E:355:ASN:HA	2.16	0.74
1:A:6:GLU:OE1	1:A:105:PRO:HD2	1.86	0.74
5:E:126:CYS:HB3	5:E:195:SER:O	1.86	0.74
6:F:160:THR:CG2	6:F:167:LYS:HB2	2.17	0.74
6:F:108:LEU:HB3	6:F:175:VAL:C	2.08	0.74
2:B:125:LEU:HA	2:B:183:LYS:NZ	2.01	0.74
6:F:37:LEU:CD2	6:F:44:LEU:HD11	2.18	0.74
1:A:2:LEU:HD21	1:A:4:MET:HE3	1.67	0.74
4:D:138:LEU:HD21	4:D:211:VAL:HG21	1.67	0.73
2:B:125:LEU:HD23	2:B:183:LYS:HZ1	1.54	0.73
6:F:53:ASP:OD1	6:F:54:ARG:HG3	1.89	0.73
1:A:33:GLU:O	1:A:34:TRP:HB2	1.88	0.73
5:E:297:THR:OG1	5:E:444:ARG:HD3	1.88	0.73
2:B:151:ASP:CB	2:B:189:HIS:HD2	2.01	0.73
3:C:151:ASP:H	3:C:191:VAL:HG13	1.52	0.72
2:B:125:LEU:HD23	2:B:183:LYS:NZ	2.05	0.72
4:D:12:LYS:CB	4:D:82(C):LEU:HD12	2.19	0.72
5:E:371:ILE:CD1	6:F:45:THR:HG22	2.20	0.71
3:C:108:ARG:HG2	3:C:109:THR:N	2.05	0.71
5:E:335:ARG:NE	5:E:410:GLY:O	2.22	0.71
6:F:5:LEU:HD11	6:F:98:PHE:CD1	2.25	0.71
3:C:158:ASN:HD22	3:C:181:LEU:HD21	1.56	0.71
2:B:164:THR:CG2	2:B:174:SER:H	2.02	0.71
6:F:30:ASN:HD21	6:F:34:ILE:HD12	1.56	0.71
6:F:5:LEU:CD1	6:F:98:PHE:CE1	2.73	0.71
3:C:151:ASP:HA	3:C:191:VAL:HG12	1.73	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:289:LYS:HD3	5:E:289:LYS:O	1.91	0.71
6:F:5:LEU:HD12	6:F:98:PHE:CD1	2.26	0.71
1:A:16:GLU:O	1:A:82(C):VAL:HG23	1.91	0.70
2:B:40:PRO:HG3	2:B:165:GLU:HG2	1.74	0.70
2:B:161:GLU:OE2	2:B:175:LEU:HD22	1.91	0.70
3:C:17:GLU:O	3:C:78:LEU:HD13	1.91	0.70
4:D:156:SER:H	4:D:195:ILE:HD11	1.56	0.70
5:E:342:LEU:O	5:E:346:VAL:HG23	1.90	0.70
3:C:47:LEU:HA	3:C:58:VAL:HG21	1.74	0.70
5:E:459:GLY:HA2	6:F:33:GLN:HB2	1.73	0.70
5:E:346:VAL:CG1	5:E:359:ILE:HD11	2.21	0.70
6:F:96:LEU:HD23	6:F:98:PHE:HZ	1.57	0.69
6:F:128:VAL:HB	6:F:144:LEU:HD11	1.75	0.69
1:A:201:LYS:N	1:A:202:PRO:HD2	2.07	0.69
5:E:260:LEU:HD21	5:E:453:LEU:HD11	1.74	0.69
4:D:121:VAL:HG22	4:D:142:VAL:HG13	1.73	0.69
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.73	0.69
5:E:279:ASN:HA	11:E:526:NAG:H83	1.73	0.69
3:C:151:ASP:CA	3:C:191:VAL:CG1	2.69	0.69
6:F:5:LEU:HD13	6:F:98:PHE:CE1	2.27	0.69
3:C:158:ASN:ND2	3:C:179:LEU:HD11	2.08	0.69
2:B:197:THR:HG22	2:B:204:PRO:HB3	1.75	0.69
1:A:2:LEU:HD23	1:A:3:GLN:N	2.08	0.68
6:F:31:SER:HB3	6:F:81:THR:HB	1.74	0.68
1:A:168:ALA:HA	1:A:178:LEU:HB3	1.75	0.68
2:B:54:LYS:HE2	2:B:58:PHE:O	1.93	0.68
2:B:135:LEU:HD21	2:B:137:ASN:HB2	1.74	0.68
1:A:100(C):LEU:HD11	5:E:415:THR:HG21	1.76	0.68
5:E:335:ARG:HD2	5:E:410:GLY:O	1.94	0.68
3:C:95:PRO:HG3	5:E:202:THR:HG22	1.74	0.68
3:C:108:ARG:HG2	3:C:109:THR:H	1.59	0.67
2:B:25:ALA:O	2:B:69:THR:HG23	1.94	0.67
4:D:82(A):ARG:O	4:D:82(B):ASN:HB2	1.95	0.67
5:E:268:GLU:O	5:E:289:LYS:HG3	1.94	0.67
5:E:326:ILE:CG1	5:E:327:ARG:H	1.98	0.67
4:D:139:GLY:HA2	4:D:154:TRP:HH2	1.59	0.67
1:A:2:LEU:HD23	1:A:2:LEU:C	2.16	0.67
2:B:150:VAL:HG12	2:B:189:HIS:CD2	2.30	0.66
6:F:110:GLN:HG2	6:F:151:LEU:HB2	1.76	0.66
5:E:335:ARG:CD	5:E:410:GLY:O	2.43	0.66
1:A:100(C):LEU:HD12	5:E:415:THR:HG21	1.78	0.66
4:D:118:GLY:HA3	4:D:205:THR:HG21	1.78	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:23:SER:HB2	6:F:63:ASP:HA	1.77	0.66
4:D:148:GLU:OE2	4:D:149:PRO:HA	1.95	0.66
2:B:205:VAL:HG12	2:B:206:THR:N	2.09	0.66
3:C:135:LEU:HD12	4:D:181:VAL:HG11	1.77	0.66
4:D:34:PHE:HD2	4:D:52(A):THR:HG21	1.61	0.66
5:E:207:LYS:O	5:E:208:ILE:HD13	1.96	0.66
5:E:346:VAL:CB	5:E:359:ILE:HD11	2.26	0.65
6:F:106:THR:HG22	6:F:106:THR:O	1.94	0.65
3:C:122:ASP:O	3:C:126:LYS:HG3	1.96	0.65
5:E:346:VAL:HG13	5:E:359:ILE:CD1	2.26	0.65
4:D:141:LEU:CD2	4:D:143:LYS:HB2	2.26	0.65
6:F:5:LEU:CD2	6:F:168:VAL:HB	2.26	0.65
5:E:298:ARG:HH11	5:E:443:ILE:HD12	1.62	0.65
1:A:2:LEU:HD22	1:A:102:VAL:HG11	1.79	0.64
1:A:13:LYS:O	1:A:16:GLU:HB2	1.98	0.64
5:E:463:ASN:O	5:E:463:ASN:ND2	2.30	0.64
3:C:188:LYS:C	3:C:189:HIS:HD2	2.01	0.64
5:E:91:GLU:CD	5:E:242:VAL:HG21	2.18	0.64
3:C:94:TRP:HA	3:C:95:PRO:C	2.17	0.64
5:E:108:ILE:HG22	5:E:427:TRP:CH2	2.31	0.64
1:A:82(C):VAL:CG1	1:A:111:VAL:HG21	2.28	0.64
6:F:110:GLN:HA	6:F:149:LEU:HD11	1.80	0.64
5:E:346:VAL:CA	5:E:359:ILE:HD11	2.28	0.64
3:C:106:ILE:HD11	3:C:171:SER:OG	1.97	0.64
1:A:4:MET:HG2	1:A:22:CYS:SG	2.38	0.63
3:C:151:ASP:HA	3:C:191:VAL:HG11	1.80	0.63
5:E:358:THR:CG2	5:E:465:THR:OG1	2.46	0.63
1:A:123:PRO:HB3	1:A:211:VAL:HG12	1.79	0.63
4:D:82:LEU:HD12	4:D:82(A):ARG:N	2.14	0.63
2:B:125:LEU:CD2	2:B:183:LYS:HZ1	2.12	0.63
4:D:65:GLY:O	4:D:82(A):ARG:NH1	2.30	0.63
4:D:34:PHE:CD2	4:D:52(A):THR:HG21	2.33	0.63
3:C:21:LEU:HD23	3:C:102:THR:HG23	1.79	0.63
9:E:513:MAN:C1	9:E:514:MAN:H5	2.28	0.63
3:C:148:TRP:CE3	3:C:179:LEU:HD22	2.34	0.63
6:F:160:THR:HG22	6:F:167:LYS:HB2	1.79	0.63
4:D:143:LYS:HG2	4:D:144:ASP:OD2	1.99	0.63
5:E:346:VAL:CG2	5:E:359:ILE:HD11	2.28	0.63
2:B:124:GLN:NE2	2:B:131:SER:H	1.97	0.63
6:F:156:THR:HG21	6:F:171:LYS:HE2	1.80	0.63
5:E:241:ASN:C	5:E:241:ASN:OD1	2.36	0.62
1:A:184:VAL:HG13	1:A:185:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:1:GLU:OE1	4:D:1:GLU:N	2.30	0.62
2:B:150:VAL:HG12	2:B:189:HIS:CB	2.30	0.62
1:A:212:GLU:CG	1:A:213:PRO:CD	2.76	0.62
2:B:190:LYS:HD3	2:B:211:ARG:HB3	1.81	0.62
1:A:124:LEU:HB3	2:B:118:PHE:CD1	2.34	0.62
1:A:2:LEU:HD21	1:A:4:MET:CE	2.29	0.62
2:B:150:VAL:CG1	2:B:189:HIS:CG	2.79	0.62
1:A:87:THR:CG2	1:A:111:VAL:H	2.08	0.62
1:A:14:PRO:O	1:A:15:SER:CB	2.45	0.62
5:E:279:ASN:HB2	11:E:526:NAG:HN2	1.65	0.62
4:D:12:LYS:HB2	4:D:82(C):LEU:HD12	1.82	0.62
3:C:21:LEU:HD23	3:C:102:THR:CG2	2.29	0.62
2:B:151:ASP:HB3	2:B:189:HIS:HD2	1.64	0.61
4:D:194:TYR:HB2	4:D:211:VAL:HG11	1.82	0.61
4:D:203:SER:HB2	4:D:205:THR:HG23	1.82	0.61
2:B:39:LYS:HB3	2:B:40:PRO:HD2	1.82	0.61
2:B:190:LYS:CD	2:B:211:ARG:HB3	2.30	0.61
4:D:53:ILE:HG23	4:D:54:LEU:N	2.15	0.61
1:A:123:PRO:CB	1:A:211:VAL:HG12	2.31	0.61
1:A:35(B):LYS:HD2	1:A:35(B):LYS:N	2.16	0.61
3:C:189:HIS:O	3:C:211:ARG:HD2	2.01	0.61
1:A:144:ASP:OD1	1:A:171:GLN:NE2	2.33	0.61
2:B:42:GLN:HG2	2:B:43:SER:N	2.13	0.61
1:A:189:LEU:HD11	1:A:213:PRO:HG3	1.83	0.61
2:B:151:ASP:HB2	2:B:189:HIS:HD2	1.64	0.61
2:B:118:PHE:HB2	2:B:133:VAL:CG2	2.30	0.61
4:D:119:PRO:HB3	4:D:145:TYR:HB3	1.81	0.61
6:F:96:LEU:HD23	6:F:98:PHE:CZ	2.35	0.61
4:D:82(C):LEU:HB3	4:D:111:VAL:HG21	1.83	0.60
3:C:107:LYS:HA	3:C:140:TYR:OH	2.01	0.60
4:D:68:THR:HG23	4:D:82(A):ARG:NH2	2.15	0.60
2:B:205:VAL:CG1	2:B:206:THR:N	2.64	0.60
1:A:108:GLN:HB3	1:A:149:PRO:HD3	1.84	0.60
6:F:105:ASP:O	6:F:106:THR:HB	2.02	0.60
3:C:164:THR:HG22	3:C:174:SER:H	1.65	0.60
3:C:150:VAL:HG11	3:C:155:GLN:NE2	2.17	0.60
6:F:136:LYS:HG3	6:F:138:ILE:HD11	1.83	0.60
5:E:344:GLN:O	5:E:347:ILE:HB	2.01	0.60
8:E:503:BMA:H2	8:E:507:MAN:C5	2.32	0.60
2:B:124:GLN:HE22	2:B:131:SER:CB	2.15	0.60
3:C:93:ASN:ND2	3:C:95(B):ARG:HB2	2.17	0.59
2:B:187:GLU:CA	2:B:211:ARG:HH22	2.05	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35(C):ASP:O	1:A:52:HIS:CD2	2.55	0.59
5:E:278:THR:HG22	11:E:526:NAG:H82	1.84	0.59
5:E:475:MET:O	5:E:478:ASN:HB2	2.02	0.59
2:B:11:LEU:HD23	2:B:19:VAL:CG2	2.32	0.59
1:A:82(C):VAL:HG12	1:A:111:VAL:HG21	1.84	0.59
4:D:168:ALA:HA	4:D:178:LEU:CD2	2.32	0.59
2:B:120:PRO:HD3	2:B:132:VAL:CG2	2.32	0.59
2:B:21:LEU:CD2	2:B:102:THR:HG21	2.33	0.59
1:A:11:LEU:HD23	1:A:11:LEU:H	1.68	0.59
3:C:19:ALA:HB3	3:C:75:ILE:HG23	1.85	0.59
1:A:97:HIS:ND1	1:A:98:HIS:N	2.43	0.59
1:A:114:ALA:HB3	1:A:146:PHE:CE2	2.38	0.59
2:B:135:LEU:HD23	2:B:135:LEU:C	2.23	0.58
3:C:49:TYR:CZ	3:C:53:THR:HG21	2.38	0.58
6:F:5:LEU:CD1	6:F:98:PHE:HD1	2.11	0.58
4:D:168:ALA:HA	4:D:178:LEU:HD21	1.84	0.58
3:C:151:ASP:CA	3:C:191:VAL:HG12	2.34	0.58
6:F:106:THR:O	6:F:107:HIS:ND1	2.36	0.58
4:D:19:LYS:HA	4:D:80:LEU:O	2.04	0.58
1:A:138:LEU:HD23	1:A:139:GLY:H	1.68	0.58
4:D:82(C):LEU:HB3	4:D:111:VAL:CG2	2.34	0.58
6:F:143:THR:C	6:F:144:LEU:HD12	2.23	0.58
3:C:155:GLN:HB3	3:C:158:ASN:HD21	1.69	0.58
1:A:87:THR:HG22	1:A:111:VAL:N	2.09	0.58
6:F:109:LEU:HD12	6:F:110:GLN:H	1.68	0.58
3:C:151:ASP:CG	3:C:191:VAL:HG12	2.24	0.58
3:C:187:GLU:HA	3:C:211:ARG:NH2	2.19	0.57
5:E:358:THR:O	5:E:358:THR:CG2	2.50	0.57
3:C:19:ALA:HB3	3:C:75:ILE:CG2	2.34	0.57
6:F:120:SER:HB3	6:F:121:PRO:HD2	1.84	0.57
2:B:61:ARG:HD2	2:B:76:ASN:O	2.03	0.57
3:C:131:SER:OG	3:C:180:THR:HG22	2.04	0.57
5:E:353:PHE:O	5:E:354:GLU:HG2	2.04	0.57
1:A:105:PRO:HA	2:B:43:SER:OG	2.04	0.57
3:C:187:GLU:HA	3:C:211:ARG:CZ	2.35	0.57
6:F:114:LEU:O	6:F:146:VAL:HG12	2.05	0.57
4:D:58:HIS:HE1	5:E:202:THR:HG21	1.68	0.57
4:D:66:ARG:O	4:D:82:LEU:HD12	2.05	0.57
3:C:54:ARG:HG2	3:C:58:VAL:HB	1.85	0.57
4:D:58:HIS:CE1	5:E:202:THR:HG21	2.40	0.56
1:A:95:HIS:ND1	1:A:100(G):ALA:HB1	2.20	0.56
2:B:178:THR:O	2:B:178:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:96:LEU:HB3	6:F:98:PHE:HE1	1.71	0.56
6:F:160:THR:HA	6:F:168:VAL:O	2.05	0.56
2:B:78:MET:SD	2:B:82:ASP:HB2	2.45	0.56
3:C:33:LEU:HD13	3:C:71:PHE:CD1	2.40	0.56
5:E:420:ILE:HG21	5:E:438:PRO:HG3	1.87	0.56
3:C:151:ASP:N	3:C:191:VAL:HG13	2.21	0.56
4:D:167:PRO:O	4:D:178:LEU:HD21	2.05	0.56
5:E:350:ARG:HG2	5:E:355:ASN:OD1	2.05	0.56
5:E:223:PHE:CE1	5:E:490:LYS:HB2	2.41	0.56
5:E:446:SER:O	11:E:524:NAG:H83	2.06	0.56
5:E:326:ILE:HG23	5:E:327:ARG:N	2.21	0.56
6:F:100:LEU:HD11	6:F:118:LEU:HD12	1.87	0.56
2:B:180:THR:O	2:B:181:LEU:HD23	2.05	0.56
5:E:477:ASP:HA	5:E:480:ARG:HG3	1.88	0.56
6:F:109:LEU:O	6:F:149:LEU:HD11	2.06	0.56
4:D:29:PHE:CD2	4:D:73:LYS:HA	2.41	0.56
6:F:89:GLN:HG3	6:F:90:LYS:N	2.22	0.55
3:C:175:LEU:C	4:D:166:PHE:CE2	2.80	0.55
3:C:116:PHE:HD2	3:C:135:LEU:HD22	1.71	0.55
3:C:175:LEU:CA	4:D:166:PHE:HE2	2.19	0.55
3:C:133:VAL:HG12	3:C:178:THR:OG1	2.07	0.55
3:C:150:VAL:HG23	3:C:192:TYR:CE1	2.42	0.55
6:F:131:ARG:HA	6:F:136:LYS:O	2.07	0.55
6:F:108:LEU:HD22	6:F:174:ILE:HG13	1.89	0.55
2:B:8:PRO:CG	2:B:11:LEU:HD13	2.37	0.55
3:C:150:VAL:O	3:C:151:ASP:HB2	2.07	0.55
4:D:68:THR:OG1	4:D:81:GLU:HB3	2.07	0.55
3:C:164:THR:HG23	3:C:165:GLU:O	2.07	0.54
5:E:268:GLU:HG3	5:E:269:GLU:N	1.99	0.54
6:F:5:LEU:HD12	6:F:98:PHE:HD1	1.68	0.54
3:C:94:TRP:CE3	3:C:95(A):PRO:HD3	2.42	0.54
4:D:20:VAL:HG13	4:D:80:LEU:HB3	1.90	0.54
1:A:18:LEU:O	1:A:81:ARG:HA	2.07	0.54
6:F:134:ARG:NH1	6:F:150:GLU:HG3	2.22	0.54
5:E:406:ASN:O	5:E:407:ASN:HB2	2.07	0.54
6:F:161:VAL:HB	6:F:168:VAL:HG12	1.88	0.54
4:D:95:VAL:HG21	4:D:100(J):PHE:O	2.07	0.54
2:B:94:TRP:CD1	8:E:506:MAN:H2	2.42	0.54
4:D:112:SER:OG	4:D:146:PHE:CZ	2.61	0.54
5:E:102:GLU:O	5:E:105:GLN:HB3	2.08	0.54
6:F:37:LEU:HD21	6:F:44:LEU:CD1	2.32	0.54
2:B:35:TRP:HD1	2:B:48:ILE:HB	1.73	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:163:VAL:O	1:A:164:HIS:CD2	2.61	0.54
4:D:34:PHE:HD2	4:D:52(A):THR:CG2	2.20	0.54
5:E:327:ARG:NE	5:E:422:GLN:OE1	2.40	0.54
3:C:191:VAL:O	3:C:191:VAL:HG13	2.07	0.54
1:A:212:GLU:HG3	1:A:213:PRO:CD	2.23	0.54
3:C:188:LYS:C	3:C:189:HIS:CD2	2.80	0.54
2:B:125:LEU:O	2:B:183:LYS:HE3	2.08	0.54
3:C:106:ILE:HG12	3:C:166:GLN:NE2	2.23	0.54
1:A:189:LEU:HG	1:A:213:PRO:HG2	1.90	0.54
3:C:83:PHE:CE1	3:C:106:ILE:HG22	2.42	0.54
2:B:148:TRP:CD1	2:B:159:SER:HB3	2.43	0.54
4:D:12:LYS:HB3	4:D:82(C):LEU:HD12	1.89	0.53
4:D:145:TYR:CZ	4:D:176:TYR:HB2	2.43	0.53
2:B:69:THR:HG22	2:B:69:THR:O	2.09	0.53
6:F:99:GLY:O	6:F:100:LEU:HD12	2.08	0.53
5:E:241:ASN:OD1	5:E:242:VAL:N	2.42	0.53
1:A:58:HIS:ND1	8:E:505:MAN:H3	2.24	0.53
2:B:139:PHE:CZ	2:B:175:LEU:HD12	2.44	0.53
3:C:75:ILE:HD11	3:C:82:ASP:OD2	2.08	0.53
6:F:120:SER:HB3	6:F:124:SER:OG	2.08	0.53
5:E:214:PRO:HA	5:E:251:ILE:O	2.08	0.53
5:E:346:VAL:HG22	5:E:359:ILE:CD1	2.38	0.53
3:C:11:LEU:O	3:C:104:LEU:CD1	2.54	0.53
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.44	0.53
3:C:120:PRO:HG3	3:C:131:SER:C	2.29	0.53
6:F:51:LEU:HD13	6:F:71:ILE:HD13	1.90	0.53
4:D:116:THR:HG22	4:D:147:PRO:HD3	1.89	0.52
4:D:119:PRO:CB	4:D:145:TYR:HB3	2.39	0.52
3:C:135:LEU:C	3:C:135:LEU:HD23	2.29	0.52
2:B:34:ALA:HA	2:B:48:ILE:O	2.08	0.52
2:B:12:SER:HA	2:B:105:ASP:OD1	2.09	0.52
6:F:150:GLU:H	6:F:150:GLU:CD	2.13	0.52
4:D:184:VAL:HG12	4:D:185:PRO:O	2.09	0.52
5:E:462:GLU:HG3	5:E:462:GLU:O	2.09	0.52
1:A:95:HIS:CE1	1:A:100(G):ALA:HB1	2.44	0.52
2:B:77:ASN:ND2	2:B:77:ASN:O	2.42	0.52
3:C:148:TRP:CE2	3:C:179:LEU:HB2	2.45	0.52
4:D:139:GLY:HA3	4:D:180:SER:O	2.09	0.52
5:E:124:PRO:HD2	5:E:430:VAL:O	2.09	0.52
6:F:93:VAL:HG12	6:F:94:GLN:N	2.25	0.52
3:C:50:GLY:O	3:C:51:ALA:HB3	2.10	0.52
3:C:175:LEU:HD23	3:C:176:SER:N	2.25	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:203:SER:OG	3:C:205:VAL:HG23	2.10	0.52
4:D:194:TYR:HB2	4:D:211:VAL:CG1	2.40	0.51
3:C:48:ILE:HG21	3:C:51:ALA:O	2.09	0.51
3:C:108:ARG:HH12	3:C:111:ALA:HB2	1.74	0.51
1:A:200:HIS:NE2	1:A:202:PRO:HG2	2.25	0.51
1:A:138:LEU:HD21	1:A:211:VAL:HB	1.92	0.51
2:B:124:GLN:NE2	2:B:131:SER:N	2.58	0.51
1:A:97:HIS:HB2	1:A:100(F):ILE:O	2.10	0.51
4:D:139:GLY:HA2	4:D:154:TRP:CH2	2.44	0.51
2:B:80:SER:HA	2:B:106:ILE:HD11	1.92	0.51
3:C:83:PHE:CZ	3:C:106:ILE:HG22	2.45	0.51
1:A:184:VAL:HG11	1:A:194:TYR:OH	2.10	0.51
6:F:118:LEU:HD21	6:F:120:SER:OG	2.10	0.51
1:A:18:LEU:HD12	1:A:19:SER:N	2.26	0.51
2:B:124:GLN:HE22	2:B:131:SER:H	1.58	0.51
2:B:167:ASP:HB3	2:B:170:ASP:OD1	2.09	0.51
5:E:95:MET:SD	5:E:484:TYR:HB2	2.50	0.51
3:C:186:TYR:CE1	3:C:192:TYR:HE2	2.28	0.51
5:E:373:MET:HB3	5:E:385:CYS:O	2.09	0.51
6:F:108:LEU:HG	6:F:109:LEU:N	2.25	0.51
3:C:113:PRO:HB3	3:C:139:PHE:HB3	1.92	0.51
3:C:124:GLN:HG2	3:C:129:THR:O	2.10	0.51
4:D:124:LEU:HD11	4:D:138:LEU:HA	1.93	0.51
2:B:124:GLN:HE22	2:B:131:SER:N	2.08	0.51
2:B:131:SER:HA	2:B:179:LEU:O	2.10	0.51
2:B:11:LEU:HD23	2:B:19:VAL:HG21	1.92	0.51
1:A:39:HIS:HB2	1:A:45:LEU:HD23	1.88	0.51
6:F:106:THR:CG2	6:F:106:THR:O	2.58	0.51
3:C:21:LEU:N	3:C:21:LEU:HD12	2.25	0.51
1:A:35(A):ASP:OD1	1:A:35(B):LYS:NZ	2.43	0.51
2:B:190:LYS:HD3	2:B:211:ARG:HD2	1.93	0.51
2:B:19:VAL:CG1	2:B:75:ILE:HB	2.41	0.51
6:F:159:CYS:O	6:F:169:GLU:HA	2.11	0.51
1:A:167:PRO:HG2	2:B:163:VAL:O	2.11	0.50
2:B:150:VAL:CG1	2:B:189:HIS:HB2	2.40	0.50
1:A:107:VAL:O	1:A:107:VAL:HG13	2.11	0.50
6:F:5:LEU:HD21	6:F:168:VAL:CB	2.40	0.50
1:A:13:LYS:N	1:A:13:LYS:HD3	2.27	0.50
2:B:150:VAL:CG1	2:B:189:HIS:CB	2.89	0.50
6:F:149:LEU:C	6:F:149:LEU:HD12	2.31	0.50
1:A:163:VAL:C	1:A:164:HIS:HD2	2.14	0.50
3:C:149:LYS:HA	3:C:153:ALA:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:186:TYR:CD1	3:C:192:TYR:HE2	2.29	0.50
4:D:168:ALA:N	4:D:178:LEU:HD21	2.26	0.50
4:D:58:HIS:HE1	5:E:202:THR:CG2	2.23	0.50
5:E:396:ASN:OD1	5:E:402:THR:O	2.30	0.50
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.47	0.50
5:E:276:ASN:ND2	5:E:279:ASN:HB2	2.25	0.50
5:E:275:ASP:HB3	5:E:282:LYS:HD2	1.93	0.50
1:A:40:SER:O	1:A:43:LYS:O	2.30	0.50
5:E:293:GLU:OE1	11:E:527:NAG:H4	2.12	0.50
2:B:50:GLU:O	2:B:51:THR:HB	2.12	0.50
3:C:94:TRP:CZ3	3:C:95(A):PRO:HD3	2.46	0.50
5:E:381:GLU:HG3	5:E:443:ILE:HD13	1.94	0.50
2:B:18:THR:HG22	2:B:18:THR:O	2.10	0.50
5:E:403:GLU:O	5:E:403:GLU:OE1	2.30	0.50
2:B:124:GLN:HE22	2:B:131:SER:HB2	1.77	0.49
5:E:272:ILE:HD11	5:E:352:GLN:HG3	1.94	0.49
3:C:125:LEU:HD23	3:C:183:LYS:HD3	1.95	0.49
2:B:164:THR:HG23	2:B:165:GLU:O	2.12	0.49
5:E:333:ILE:HD12	5:E:390:LEU:HD21	1.93	0.49
3:C:150:VAL:HG13	3:C:150:VAL:O	2.12	0.49
5:E:358:THR:HG22	5:E:465:THR:CA	2.42	0.49
6:F:100:LEU:HD22	6:F:170:PHE:CD1	2.47	0.49
5:E:294:ILE:HG23	5:E:294:ILE:O	2.12	0.49
6:F:96:LEU:HB3	6:F:98:PHE:CE1	2.47	0.49
4:D:82:LEU:HD12	4:D:82(A):ARG:H	1.77	0.49
3:C:132:VAL:O	3:C:132:VAL:HG13	2.13	0.49
5:E:462:GLU:OE1	5:E:462:GLU:HA	2.13	0.49
5:E:126:CYS:CB	5:E:195:SER:O	2.59	0.49
5:E:340:ASP:O	5:E:343:LYS:HB3	2.12	0.49
2:B:140:TYR:CD1	2:B:141:PRO:HA	2.47	0.49
1:A:14:PRO:O	1:A:15:SER:OG	2.30	0.49
2:B:191:VAL:HG22	2:B:210:ASN:OD1	2.12	0.49
5:E:226:LEU:CD2	5:E:244:THR:HG22	2.43	0.49
4:D:200:HIS:HB3	4:D:205:THR:HG1	1.71	0.49
3:C:135:LEU:HD21	3:C:137:ASN:HB2	1.95	0.49
5:E:358:THR:HG23	5:E:465:THR:OG1	2.12	0.48
3:C:115:VAL:HG12	3:C:116:PHE:N	2.28	0.48
3:C:198:HIS:CD2	3:C:200:GLY:H	2.30	0.48
1:A:34:TRP:HE3	5:E:417:PRO:HB2	1.78	0.48
1:A:87:THR:HA	1:A:109:VAL:O	2.13	0.48
1:A:35(B):LYS:HG3	1:A:35(D):TYR:CE2	2.48	0.48
6:F:138:ILE:N	6:F:138:ILE:HD12	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:97:GLU:HG3	4:D:100(E):TYR:CZ	2.49	0.48
5:E:346:VAL:HG21	5:E:395:TRP:CD2	2.48	0.48
2:B:13:VAL:O	2:B:106:ILE:HA	2.14	0.48
5:E:371:ILE:HD13	6:F:45:THR:HG22	1.94	0.48
6:F:75:LYS:HD2	6:F:77:GLU:OE1	2.13	0.48
4:D:27:ASP:OD1	4:D:28:THR:N	2.42	0.48
4:D:143:LYS:HG3	4:D:177:SER:HB3	1.95	0.48
2:B:21:LEU:HD23	2:B:102:THR:HG21	1.95	0.48
1:A:4:MET:CE	1:A:35(F):TRP:HZ3	2.27	0.48
6:F:30:ASN:ND2	6:F:34:ILE:HB	2.28	0.48
1:A:35(A):ASP:CG	1:A:35(B):LYS:HD3	2.34	0.48
1:A:169:VAL:HG22	1:A:177:SER:O	2.13	0.48
4:D:124:LEU:HG	4:D:139:GLY:O	2.14	0.48
4:D:93:ALA:HA	4:D:102:HIS:O	2.13	0.48
5:E:476:ARG:HA	5:E:479:TRP:CD1	2.49	0.48
2:B:151:ASP:HB3	2:B:189:HIS:CD2	2.47	0.47
1:A:35(C):ASP:O	1:A:52:HIS:NE2	2.47	0.47
2:B:35:TRP:CD1	2:B:48:ILE:HB	2.49	0.47
4:D:22:CYS:HB3	4:D:78:VAL:HG13	1.96	0.47
4:D:168:ALA:CA	4:D:178:LEU:HD21	2.44	0.47
5:E:99:ASN:O	5:E:100:MET:C	2.51	0.47
2:B:36:TYR:CE1	2:B:46:LEU:HD13	2.49	0.47
1:A:163:VAL:O	1:A:164:HIS:HD2	1.98	0.47
4:D:145:TYR:CZ	4:D:176:TYR:CB	2.98	0.47
6:F:120:SER:CB	6:F:121:PRO:HD2	2.44	0.47
5:E:96:TRP:CE3	5:E:275:ASP:HB2	2.49	0.47
1:A:183:THR:O	1:A:183:THR:HG22	2.13	0.47
6:F:64:GLN:O	6:F:64:GLN:HG3	2.15	0.47
1:A:35(B):LYS:CD	1:A:35(B):LYS:N	2.77	0.47
5:E:282:LYS:HD3	5:E:282:LYS:HA	1.68	0.47
1:A:100(D):VAL:HG22	8:E:502:NAG:C7	2.45	0.47
5:E:89:VAL:O	5:E:89:VAL:HG22	2.13	0.47
5:E:412:ASN:OD1	5:E:412:ASN:O	2.33	0.47
6:F:155:GLY:O	6:F:173:ASP:HA	2.14	0.47
2:B:125:LEU:CD2	2:B:183:LYS:NZ	2.75	0.47
5:E:279:ASN:OD1	6:F:29:LYS:NZ	2.47	0.47
2:B:194:CYS:O	2:B:206:THR:HA	2.14	0.47
5:E:271:VAL:HG13	5:E:287:GLN:HB3	1.97	0.47
3:C:125:LEU:HD23	3:C:183:LYS:CD	2.45	0.47
1:A:82(C):VAL:HG11	1:A:111:VAL:HG21	1.96	0.47
3:C:194:CYS:O	3:C:206:THR:HB	2.15	0.47
6:F:116:LEU:HD11	6:F:144:LEU:CD1	2.40	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35(C):ASP:HA	1:A:53:TRP:HE1	1.80	0.47
1:A:163:VAL:HG22	1:A:182:VAL:HG13	1.95	0.47
5:E:391:PHE:CE2	5:E:470:PRO:HB3	2.50	0.47
4:D:201:LYS:N	4:D:202:PRO:CD	2.78	0.47
1:A:212:GLU:HG2	1:A:213:PRO:N	2.30	0.47
1:A:36:TRP:CZ3	1:A:92:CYS:HB3	2.50	0.47
3:C:106:ILE:HG13	3:C:106:ILE:O	2.13	0.47
6:F:8:LYS:HD2	6:F:76:ILE:CD1	2.45	0.47
2:B:196:VAL:HG13	2:B:196:VAL:O	2.13	0.47
1:A:155:ASN:HD22	1:A:159:LEU:HD13	1.80	0.47
3:C:150:VAL:CG2	3:C:192:TYR:HE1	2.28	0.46
4:D:154:TRP:NE1	4:D:180:SER:OG	2.34	0.46
5:E:300:ASN:HB2	5:E:441:GLY:O	2.15	0.46
5:E:350:ARG:HH21	5:E:350:ARG:HG3	1.80	0.46
1:A:144:ASP:HB3	1:A:175:LEU:HD13	1.97	0.46
2:B:38:TYR:CD1	2:B:44:PRO:HG3	2.51	0.46
1:A:35(A):ASP:O	1:A:35(B):LYS:HB2	2.15	0.46
2:B:11:LEU:CD2	2:B:19:VAL:HG23	2.45	0.46
2:B:39:LYS:HG2	2:B:84:ALA:HB2	1.98	0.46
2:B:8:PRO:HG3	2:B:11:LEU:HD13	1.97	0.46
1:A:100(D):VAL:HG22	8:E:502:NAG:O7	2.15	0.46
3:C:119:PRO:HG2	3:C:209:PHE:CD1	2.50	0.46
4:D:155:ASN:HD21	4:D:194:TYR:HD1	1.60	0.46
2:B:149:LYS:NZ	2:B:195:GLU:HB2	2.30	0.46
5:E:298:ARG:HG2	5:E:298:ARG:O	2.15	0.46
5:E:271:VAL:HG11	5:E:273:ARG:NH2	2.30	0.46
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.98	0.46
5:E:213:ILE:HG23	5:E:214:PRO:HD2	1.98	0.46
4:D:54:LEU:HA	4:D:54:LEU:HD23	1.55	0.46
5:E:358:THR:HG22	5:E:465:THR:HA	1.98	0.46
3:C:11:LEU:O	3:C:104:LEU:HA	2.16	0.46
4:D:124:LEU:HG	4:D:139:GLY:H	1.81	0.46
1:A:163:VAL:C	1:A:164:HIS:CD2	2.90	0.46
3:C:108:ARG:CG	3:C:109:THR:H	2.28	0.45
3:C:108:ARG:CG	3:C:109:THR:N	2.77	0.45
1:A:200:HIS:CE1	1:A:202:PRO:HG2	2.52	0.45
6:F:100:LEU:HD13	6:F:170:PHE:CZ	2.51	0.45
4:D:122:PHE:HA	4:D:123:PRO:HD3	1.82	0.45
2:B:108:ARG:HD2	2:B:171:SER:HG	1.81	0.45
4:D:12:LYS:HB2	4:D:82(C):LEU:CD1	2.46	0.45
3:C:151:ASP:N	3:C:191:VAL:CG1	2.78	0.45
5:E:242:VAL:HG12	5:E:243:SER:N	2.30	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:138:LEU:CD1	4:D:211:VAL:HG21	2.41	0.45
1:A:96:ARG:NH2	9:E:515:MAN:H4	2.32	0.45
6:F:110:GLN:OE1	6:F:150:GLU:HA	2.17	0.45
3:C:54:ARG:HD2	3:C:58:VAL:HG12	1.99	0.45
1:A:2:LEU:CD2	1:A:4:MET:HE3	2.43	0.45
4:D:195:ILE:CD1	4:D:197:ASN:HB2	2.47	0.45
4:D:145:TYR:CE1	4:D:176:TYR:HB2	2.51	0.45
3:C:9:ALA:O	3:C:102:THR:HA	2.17	0.45
5:E:447:SER:HA	11:E:524:NAG:C8	2.46	0.45
1:A:100(D):VAL:HG23	1:A:100(D):VAL:O	2.15	0.45
4:D:203:SER:HB2	4:D:205:THR:CG2	2.44	0.45
6:F:144:LEU:N	6:F:144:LEU:HD12	2.31	0.45
4:D:95:VAL:CG2	4:D:101:LYS:H	2.30	0.45
2:B:205:VAL:CG1	2:B:206:THR:H	2.29	0.45
4:D:151:THR:OG1	4:D:199:ASN:HB3	2.17	0.45
1:A:4:MET:HE2	1:A:35(F):TRP:HZ3	1.81	0.45
1:A:34:TRP:CE3	5:E:417:PRO:HB2	2.52	0.45
5:E:358:THR:O	5:E:358:THR:HG23	2.15	0.45
6:F:131:ARG:HD3	6:F:137:ASN:HD21	1.81	0.45
5:E:447:SER:HA	11:E:524:NAG:H82	1.99	0.45
2:B:148:TRP:HD1	2:B:159:SER:HB3	1.82	0.45
1:A:155:ASN:ND2	1:A:159:LEU:HD13	2.32	0.45
4:D:178:LEU:HA	4:D:178:LEU:HD23	1.68	0.45
5:E:456:ARG:HB2	5:E:468:PHE:CE1	2.52	0.45
6:F:150:GLU:OE2	6:F:153:ASP:OD2	2.34	0.45
3:C:113:PRO:O	3:C:115:VAL:HG23	2.16	0.45
6:F:106:THR:O	6:F:107:HIS:CG	2.70	0.45
3:C:174:SER:O	3:C:175:LEU:HB2	2.17	0.45
2:B:115:VAL:HG21	2:B:196:VAL:HG11	1.99	0.45
5:E:389:GLN:HG2	9:E:509:NAG:H81	1.99	0.45
5:E:326:ILE:HG12	5:E:419:ARG:HH22	1.81	0.44
4:D:138:LEU:CD2	4:D:211:VAL:HG21	2.42	0.44
3:C:116:PHE:CD2	3:C:135:LEU:HD22	2.50	0.44
5:E:298:ARG:HH11	5:E:443:ILE:CD1	2.29	0.44
4:D:212:GLU:HA	4:D:213:PRO:HD3	1.86	0.44
3:C:150:VAL:HG13	3:C:153:ALA:HB3	2.00	0.44
3:C:209:PHE:CE1	3:C:210:ASN:O	2.71	0.44
4:D:95:VAL:HG23	4:D:100(K):LEU:HA	1.99	0.44
1:A:184:VAL:HG12	1:A:185:PRO:O	2.18	0.44
3:C:93:ASN:N	3:C:93:ASN:OD1	2.41	0.44
5:E:122:LEU:HD22	5:E:200:VAL:HG22	1.98	0.44
4:D:196:CYS:O	4:D:198:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:57:ALA:C	4:D:58:HIS:HD2	2.20	0.44
2:B:80:SER:HA	2:B:106:ILE:HD12	1.96	0.44
4:D:14:PRO:HD3	4:D:112:SER:C	2.38	0.44
6:F:134:ARG:HH12	6:F:150:GLU:HG3	1.83	0.44
5:E:459:GLY:O	5:E:460:ILE:CG1	2.66	0.44
6:F:75:LYS:O	6:F:78:ASP:HB2	2.17	0.44
5:E:350:ARG:NH2	5:E:350:ARG:HG3	2.33	0.44
3:C:135:LEU:C	3:C:136:LEU:HD12	2.38	0.44
1:A:192:GLN:HG2	1:A:194:TYR:CZ	2.53	0.44
1:A:77:TRP:CE3	1:A:77:TRP:C	2.90	0.44
3:C:119:PRO:HA	3:C:120:PRO:HD3	1.80	0.44
1:A:144:ASP:HB3	1:A:175:LEU:CD1	2.47	0.44
1:A:51:ILE:HB	1:A:69:MET:HE2	1.99	0.44
5:E:255:VAL:HG12	5:E:255:VAL:O	2.16	0.44
3:C:121:SER:O	3:C:125:LEU:HD12	2.18	0.43
1:A:78:PHE:CZ	1:A:92:CYS:HB2	2.52	0.43
5:E:91:GLU:OE2	5:E:242:VAL:HG21	2.18	0.43
4:D:12:LYS:CB	4:D:82(C):LEU:CD1	2.92	0.43
4:D:184:VAL:HG13	4:D:185:PRO:CD	2.45	0.43
6:F:131:ARG:HB2	6:F:137:ASN:HD22	1.82	0.43
3:C:103:ARG:CG	3:C:104:LEU:N	2.82	0.43
6:F:53:ASP:OD1	6:F:53:ASP:C	2.56	0.43
2:B:178:THR:O	2:B:178:THR:CG2	2.66	0.43
4:D:29:PHE:CE2	4:D:73:LYS:HA	2.54	0.43
1:A:94:ARG:NH2	1:A:101:ASP:OD2	2.36	0.43
4:D:82(C):LEU:C	4:D:111:VAL:HG11	2.25	0.43
3:C:61:ARG:NH1	3:C:82:ASP:OD1	2.52	0.43
5:E:405:SER:HB3	11:E:525:NAG:C7	2.48	0.43
5:E:439:ILE:HG13	5:E:439:ILE:H	1.56	0.43
3:C:38:GLN:O	3:C:84:ALA:HB1	2.18	0.43
6:F:110:GLN:HA	6:F:149:LEU:CD1	2.47	0.43
5:E:358:THR:HG21	5:E:465:THR:HB	1.97	0.43
4:D:194:TYR:O	4:D:211:VAL:HG12	2.18	0.43
1:A:82(C):VAL:HG12	1:A:83:THR:N	2.34	0.43
1:A:47:TRP:O	1:A:60:LYS:HD2	2.18	0.43
1:A:148:GLU:OE1	1:A:149:PRO:HA	2.19	0.43
4:D:146:PHE:HA	4:D:147:PRO:HA	1.75	0.43
5:E:225:ILE:HG12	5:E:488:VAL:HG22	1.99	0.43
5:E:127:VAL:HG22	5:E:128:GLY:N	2.33	0.43
4:D:46:GLU:OE2	4:D:62:HIS:NE2	2.37	0.43
1:A:6:GLU:HG3	1:A:92:CYS:SG	2.59	0.43
3:C:49:TYR:CZ	3:C:53:THR:CG2	3.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:103:ARG:HG2	3:C:104:LEU:N	2.34	0.43
3:C:163:VAL:HG12	3:C:164:THR:O	2.19	0.43
1:A:198:VAL:O	1:A:206:LYS:HD2	2.19	0.43
4:D:189:LEU:HD12	4:D:189:LEU:N	2.34	0.43
4:D:119:PRO:HB2	4:D:142:VAL:HG12	2.01	0.42
2:B:69:THR:CG2	2:B:69:THR:O	2.67	0.42
1:A:60:LYS:HG3	2:B:95:PRO:HB2	2.00	0.42
1:A:152:VAL:HA	1:A:197:ASN:O	2.19	0.42
3:C:108:ARG:HH22	3:C:140:TYR:HB2	1.81	0.42
5:E:279:ASN:HA	11:E:526:NAG:C8	2.45	0.42
4:D:82(A):ARG:O	4:D:82(B):ASN:CB	2.66	0.42
4:D:100(A):ASP:OD1	4:D:100(A):ASP:N	2.51	0.42
4:D:206:LYS:O	4:D:207:VAL:HG13	2.19	0.42
4:D:141:LEU:HD23	4:D:141:LEU:O	2.19	0.42
6:F:108:LEU:HD12	6:F:109:LEU:H	1.84	0.42
1:A:96:ARG:HD3	1:A:101:ASP:CG	2.39	0.42
1:A:14:PRO:O	1:A:15:SER:HB3	2.18	0.42
3:C:150:VAL:HG21	3:C:189:HIS:ND1	2.35	0.42
2:B:43:SER:HA	2:B:44:PRO:HD3	1.96	0.42
4:D:98:GLY:O	4:D:100:ALA:N	2.50	0.42
4:D:2:VAL:HG12	4:D:102:HIS:CE1	2.55	0.42
6:F:93:VAL:CG1	6:F:94:GLN:N	2.82	0.42
5:E:100:MET:HB3	5:E:100:MET:HE2	1.91	0.42
2:B:186:TYR:O	2:B:192:TYR:OH	2.38	0.42
3:C:191:VAL:HG23	3:C:210:ASN:OD1	2.20	0.42
4:D:101:LYS:HG3	4:D:102:HIS:CD2	2.55	0.42
5:E:213:ILE:HA	5:E:213:ILE:HD13	1.91	0.42
1:A:100(D):VAL:HG21	8:E:502:NAG:O3	2.20	0.42
5:E:296:CYS:HA	5:E:330:HIS:O	2.19	0.42
2:B:211:ARG:HG2	2:B:212:GLY:N	2.35	0.42
2:B:38:TYR:HD1	2:B:44:PRO:HG3	1.85	0.42
1:A:201:LYS:N	1:A:202:PRO:CD	2.79	0.42
3:C:106:ILE:HD11	3:C:171:SER:CB	2.49	0.42
3:C:118:PHE:CD2	4:D:124:LEU:HD13	2.55	0.42
6:F:156:THR:CG2	6:F:171:LYS:HE2	2.46	0.42
5:E:123:THR:HG23	5:E:124:PRO:HD2	2.01	0.42
1:A:39:HIS:CB	1:A:45:LEU:HD23	2.49	0.41
2:B:19:VAL:HG12	2:B:75:ILE:HB	2.02	0.41
5:E:412:ASN:OD1	5:E:412:ASN:C	2.58	0.41
4:D:126:PRO:HG2	4:D:213:PRO:HA	2.02	0.41
3:C:210:ASN:O	3:C:211:ARG:C	2.58	0.41
6:F:128:VAL:CB	6:F:144:LEU:HD11	2.47	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:135:LEU:CD2	2:B:137:ASN:HB2	2.49	0.41
2:B:11:LEU:CD2	2:B:19:VAL:CG2	2.98	0.41
3:C:125:LEU:HD21	3:C:186:TYR:CD2	2.54	0.41
4:D:68:THR:CG2	4:D:82(A):ARG:NH2	2.81	0.41
2:B:11:LEU:HD12	2:B:11:LEU:HA	1.81	0.41
5:E:272:ILE:HG22	5:E:286:VAL:HG22	2.02	0.41
5:E:211:GLU:O	5:E:212:PRO:C	2.56	0.41
6:F:109:LEU:O	6:F:149:LEU:HD21	2.20	0.41
4:D:121:VAL:CG2	4:D:142:VAL:HG13	2.47	0.41
3:C:124:GLN:HG3	4:D:122:PHE:CE2	2.55	0.41
4:D:88:ALA:O	4:D:108:LEU:HD12	2.20	0.41
5:E:96:TRP:CH2	5:E:274:SER:HA	2.55	0.41
5:E:302:ASN:HA	5:E:303:THR:HA	1.68	0.41
1:A:192:GLN:OE1	1:A:192:GLN:HA	2.21	0.41
4:D:52:ILE:HG23	4:D:100(E):TYR:CZ	2.55	0.41
5:E:267:GLU:O	5:E:268:GLU:HB3	2.20	0.41
5:E:395:TRP:CZ3	11:E:525:NAG:H82	2.56	0.41
2:B:77:ASN:HD22	2:B:79:GLN:NE2	2.18	0.41
2:B:107:LYS:HA	2:B:140:TYR:OH	2.21	0.41
6:F:149:LEU:HD12	6:F:149:LEU:O	2.21	0.41
5:E:462:GLU:C	5:E:464:GLY:H	2.23	0.41
1:A:184:VAL:CG1	1:A:185:PRO:N	2.83	0.41
2:B:78:MET:HB2	2:B:78:MET:HE2	1.92	0.41
3:C:33:LEU:HD13	3:C:71:PHE:CG	2.56	0.41
5:E:101:VAL:HG13	5:E:102:GLU:N	2.36	0.41
1:A:178:LEU:HD12	1:A:178:LEU:C	2.42	0.41
6:F:130:CYS:O	6:F:137:ASN:HA	2.20	0.41
5:E:353:PHE:C	5:E:354:GLU:HG2	2.42	0.41
3:C:132:VAL:CG1	3:C:179:LEU:HB3	2.50	0.40
1:A:87:THR:HG22	1:A:110:THR:HA	2.03	0.40
5:E:459:GLY:O	5:E:460:ILE:HG13	2.21	0.40
3:C:166:GLN:HB2	3:C:173:TYR:CZ	2.56	0.40
1:A:184:VAL:HG13	1:A:185:PRO:CD	2.50	0.40
6:F:77:GLU:CD	6:F:77:GLU:H	2.24	0.40
5:E:426:MET:HB3	5:E:428:GLN:OE1	2.21	0.40
5:E:268:GLU:HG3	5:E:269:GLU:HG3	2.03	0.40
5:E:326:ILE:HG23	5:E:328:GLN:N	2.36	0.40
5:E:420:ILE:CG2	5:E:438:PRO:HG3	2.50	0.40
3:C:150:VAL:CG2	3:C:192:TYR:CE1	3.01	0.40
5:E:358:THR:OG1	5:E:395:TRP:O	2.24	0.40
3:C:167:ASP:O	3:C:171:SER:HA	2.20	0.40
9:E:512:MAN:O4	9:E:513:MAN:H5	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:82(C):LEU:O	4:D:83:ARG:C	2.56	0.40
1:A:212:GLU:CG	1:A:213:PRO:N	2.85	0.40
5:E:371:ILE:HD12	6:F:45:THR:HG22	2.01	0.40
5:E:208:ILE:HA	5:E:208:ILE:HD13	1.72	0.40
5:E:242:VAL:CG1	5:E:243:SER:N	2.83	0.40
2:B:108:ARG:NH1	2:B:172:THR:CG2	2.85	0.40
3:C:148:TRP:CD2	3:C:179:LEU:HD22	2.56	0.40
1:A:14:PRO:HG3	1:A:111:VAL:HG12	2.04	0.40
5:E:298:ARG:HD3	5:E:443:ILE:HD12	2.04	0.40
5:E:440:ARG:HG2	5:E:441:GLY:H	1.87	0.40
4:D:66:ARG:O	4:D:82:LEU:CD1	2.70	0.40
6:F:146:VAL:O	6:F:146:VAL:HG13	2.22	0.40
5:E:95:MET:HE2	5:E:96:TRP:NE1	2.37	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	223/236 (94%)	201 (90%)	20 (9%)	2 (1%)	25	71
2	B	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
3	C	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
4	D	216/229 (94%)	213 (99%)	2 (1%)	1 (0%)	38	81
5	E	311/321 (97%)	291 (94%)	16 (5%)	4 (1%)	18	60
6	F	173/185 (94%)	165 (95%)	8 (5%)	0	100	100
All	All	1347/1399 (96%)	1273 (94%)	67 (5%)	7 (0%)	38	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	326	ILE
5	E	407	ASN

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Mol	Chain	Res	Type
1	A	62	SER
5	E	299	PRO
4	D	82(B)	ASN
1	A	105	PRO
5	E	347	ILE

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	193/201 (96%)	184 (95%)	9 (5%)	36	78
2	B	190/190 (100%)	187 (98%)	3 (2%)	75	94
3	C	184/184 (100%)	182 (99%)	2 (1%)	84	96
4	D	188/193 (97%)	184 (98%)	4 (2%)	66	92
5	E	282/287 (98%)	279 (99%)	3 (1%)	84	96
6	F	159/167 (95%)	157 (99%)	2 (1%)	80	95
All	All	1196/1222 (98%)	1173 (98%)	23 (2%)	69	92

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	A	66	ARG
1	A	73	THR
1	A	77	TRP
1	A	99	ASP
1	A	100	VAL
1	A	116	THR
1	A	138	LEU
1	A	173	SER
2	B	105	ASP
2	B	177	SER
2	B	194	CYS
3	C	154	LEU
3	C	201	LEU

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Mol	Chain	Res	Type
4	D	78	VAL
4	D	82	LEU
4	D	117	LYS
4	D	208	ASP
5	E	255	VAL
5	E	334	SER
5	E	401	ASN
6	F	88	ASP
6	F	130	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	164	HIS
1	A	171	GLN
2	B	32	ASN
2	B	77	ASN
2	B	124	GLN
2	B	189	HIS
2	B	199	GLN
3	C	92	ASN
3	C	138	ASN
3	C	198	HIS
4	D	58	HIS
5	E	114	GLN
5	E	216	HIS
5	E	249	HIS
5	E	301	ASN
5	E	302	ASN
5	E	463	ASN
6	F	40	GLN
6	F	89	GLN
6	F	129	GLN
6	F	137	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

21 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$
8	NAG	E	501	8,5	12,14,15	1.21	2 (16%)	15,19,21	1.26	2 (13%)
8	NAG	E	502	8	12,14,15	1.53	3 (25%)	15,19,21	4.02	7 (46%)
8	BMA	E	503	8	10,11,12	1.72	1 (10%)	11,15,17	3.27	8 (72%)
8	MAN	E	504	8	10,11,12	1.19	1 (10%)	11,15,17	2.06	3 (27%)
8	MAN	E	505	8	10,11,12	0.68	0	11,15,17	1.36	2 (18%)
8	MAN	E	506	8	10,11,12	0.86	1 (10%)	11,15,17	1.40	3 (27%)
8	MAN	E	507	8	10,11,12	1.07	1 (10%)	11,15,17	0.86	0
8	MAN	E	508	8	10,11,12	1.04	1 (10%)	11,15,17	0.82	0
9	NAG	E	509	9,5	12,14,15	0.65	0	15,19,21	0.95	0
9	NAG	E	510	9	12,14,15	1.20	2 (16%)	15,19,21	2.58	7 (46%)
9	BMA	E	511	9	10,11,12	0.99	0	11,15,17	1.02	0
9	MAN	E	512	9	10,11,12	1.04	1 (10%)	11,15,17	1.16	1 (9%)
9	MAN	E	513	9	10,11,12	1.05	1 (10%)	11,15,17	1.05	1 (9%)
9	MAN	E	514	9	10,11,12	1.13	1 (10%)	11,15,17	2.04	3 (27%)
9	MAN	E	515	9	10,11,12	0.82	1 (10%)	11,15,17	1.20	1 (9%)
9	MAN	E	516	9	10,11,12	0.79	1 (10%)	11,15,17	0.82	0
9	MAN	E	517	9	10,11,12	0.81	0	11,15,17	1.56	2 (18%)
9	MAN	E	518	9	10,11,12	0.86	1 (10%)	11,15,17	1.43	3 (27%)
10	NAG	E	519	10,5	12,14,15	1.08	1 (8%)	15,19,21	1.02	1 (6%)
10	NAG	E	520	10	12,14,15	0.67	0	15,19,21	1.02	0
10	BMA	E	521	10	10,11,12	0.82	1 (10%)	11,15,17	0.88	1 (9%)

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
8	NAG	E	501	8,5	-	0/6/23/26	0/1/1/1
8	NAG	E	502	8	-	0/6/23/26	0/1/1/1
8	BMA	E	503	8	-	0/2/19/22	0/1/1/1
8	MAN	E	504	8	-	0/2/19/22	0/1/1/1
8	MAN	E	505	8	-	0/2/19/22	0/1/1/1
8	MAN	E	506	8	-	0/2/19/22	0/1/1/1
8	MAN	E	507	8	-	0/2/19/22	0/1/1/1
8	MAN	E	508	8	-	0/2/19/22	0/1/1/1
9	NAG	E	509	9,5	-	0/6/23/26	0/1/1/1
9	NAG	E	510	9	-	0/6/23/26	0/1/1/1
9	BMA	E	511	9	-	0/2/19/22	0/1/1/1
9	MAN	E	512	9	-	0/2/19/22	0/1/1/1
9	MAN	E	513	9	-	0/2/19/22	0/1/1/1
9	MAN	E	514	9	-	0/2/19/22	0/1/1/1
9	MAN	E	515	9	-	0/2/19/22	0/1/1/1
9	MAN	E	516	9	-	0/2/19/22	0/1/1/1
9	MAN	E	517	9	-	0/2/19/22	0/1/1/1
9	MAN	E	518	9	-	0/2/19/22	0/1/1/1
10	NAG	E	519	10,5	-	0/6/23/26	0/1/1/1
10	NAG	E	520	10	-	0/6/23/26	0/1/1/1
10	BMA	E	521	10	-	0/2/19/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	503	BMA	O5-C5	-4.37	1.37	1.45
8	E	504	MAN	O5-C5	-3.04	1.39	1.45
8	E	502	NAG	C4-C5	-2.87	1.46	1.53
9	E	510	NAG	O5-C5	-2.78	1.40	1.45
8	E	501	NAG	C2-N2	-2.54	1.43	1.46
9	E	514	MAN	O5-C5	-2.45	1.40	1.45
8	E	502	NAG	O5-C5	-2.41	1.40	1.45
9	E	510	NAG	C2-N2	-2.39	1.43	1.46
8	E	502	NAG	O4-C4	-2.22	1.37	1.43
8	E	507	MAN	O2-C2	2.21	1.48	1.43
9	E	513	MAN	O2-C2	2.20	1.48	1.43
9	E	512	MAN	O3-C3	2.18	1.48	1.43
9	E	518	MAN	O5-C5	-2.16	1.41	1.45
8	E	506	MAN	O5-C5	-2.14	1.41	1.45
8	E	501	NAG	O4-C4	2.09	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	519	NAG	O4-C4	2.07	1.48	1.43
10	E	521	BMA	O5-C5	-2.07	1.41	1.45
8	E	508	MAN	O2-C2	2.03	1.48	1.43
9	E	515	MAN	O5-C5	-2.01	1.41	1.45
9	E	516	MAN	O5-C5	-2.00	1.41	1.45

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	502	NAG	O5-C5-C6	12.10	119.68	106.98
9	E	510	NAG	O5-C5-C4	-6.74	102.09	110.65
8	E	502	NAG	C2-N2-C7	-6.74	111.77	123.09
8	E	503	BMA	C4-C3-C2	-6.61	101.63	110.50
8	E	503	BMA	O2-C2-C3	4.78	120.50	110.18
9	E	514	MAN	O5-C5-C6	4.24	111.42	106.98
8	E	504	MAN	O4-C4-C5	4.11	120.12	109.28
9	E	517	MAN	C4-C3-C2	-4.08	105.03	110.50
9	E	514	MAN	O5-C5-C4	-3.87	105.75	110.65
9	E	510	NAG	C4-C3-C2	-3.61	102.48	111.32
9	E	515	MAN	O5-C5-C6	3.44	110.59	106.98
8	E	503	BMA	O3-C3-C2	3.29	115.95	109.94
8	E	503	BMA	O3-C3-C4	-3.24	103.08	110.35
8	E	502	NAG	O4-C4-C5	-3.23	100.78	109.28
8	E	502	NAG	O6-C6-C5	-3.16	100.50	111.36
8	E	503	BMA	O5-C5-C4	-3.05	106.78	110.65
9	E	510	NAG	C3-C2-N2	-3.04	107.13	111.76
9	E	510	NAG	C3-C4-C5	-3.01	104.83	110.20
8	E	504	MAN	O5-C5-C4	-2.96	106.90	110.65
8	E	501	NAG	C4-C3-C2	-2.86	104.33	111.32
9	E	512	MAN	O5-C5-C4	-2.84	107.05	110.65
9	E	518	MAN	O5-C5-C4	-2.81	107.09	110.65
8	E	502	NAG	C3-C2-N2	2.79	116.01	111.76
9	E	518	MAN	O5-C5-C6	2.71	109.82	106.98
9	E	510	NAG	O4-C4-C5	2.70	116.41	109.28
8	E	506	MAN	O5-C5-C4	-2.68	107.25	110.65
8	E	506	MAN	O5-C5-C6	2.68	109.79	106.98
8	E	505	MAN	O2-C2-C3	-2.64	104.47	110.18
8	E	503	BMA	O6-C6-C5	-2.61	102.39	111.36
8	E	501	NAG	C2-N2-C7	-2.48	118.92	123.09
10	E	521	BMA	O5-C5-C6	2.48	109.58	106.98
9	E	514	MAN	C4-C3-C2	-2.46	107.20	110.50
8	E	503	BMA	C3-C4-C5	2.38	114.45	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	510	NAG	C2-N2-C7	-2.34	119.16	123.09
8	E	502	NAG	O4-C4-C3	-2.32	105.16	110.35
10	E	519	NAG	O5-C5-C4	-2.29	107.75	110.65
8	E	504	MAN	O3-C3-C4	2.29	115.48	110.35
8	E	506	MAN	C4-C3-C2	-2.24	107.50	110.50
9	E	510	NAG	O3-C3-C4	-2.19	105.43	110.35
8	E	505	MAN	O3-C3-C2	2.15	113.88	109.94
9	E	517	MAN	O2-C2-C3	-2.15	105.53	110.18
9	E	518	MAN	C4-C3-C2	-2.15	107.62	110.50
8	E	502	NAG	O3-C3-C4	-2.05	105.77	110.35
9	E	513	MAN	C4-C3-C2	2.03	113.22	110.50
8	E	503	BMA	O5-C5-C6	-2.00	104.88	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

7 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
7	PG4	C	301	-	12,12,12	0.66	0	11,11,11	0.79	0
11	NAG	E	522	5	12,14,15	0.70	1 (8%)	15,19,21	0.88	0
11	NAG	E	523	5	12,14,15	0.67	0	15,19,21	0.92	1 (6%)
11	NAG	E	524	5	12,14,15	0.68	0	15,19,21	1.22	2 (13%)
11	NAG	E	525	5	12,14,15	0.67	1 (8%)	15,19,21	0.76	0
11	NAG	E	526	5	12,14,15	0.74	1 (8%)	15,19,21	1.07	2 (13%)
11	NAG	E	527	5	12,14,15	0.76	1 (8%)	15,19,21	0.83	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
7	PG4	C	301	-	-	0/10/10/10	0/0/0/0
11	NAG	E	522	5	-	0/6/23/26	0/1/1/1
11	NAG	E	523	5	-	0/6/23/26	0/1/1/1
11	NAG	E	524	5	-	0/6/23/26	0/1/1/1
11	NAG	E	525	5	-	0/6/23/26	0/1/1/1
11	NAG	E	526	5	-	0/6/23/26	0/1/1/1
11	NAG	E	527	5	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	527	NAG	O5-C5	-2.36	1.41	1.45
11	E	526	NAG	O5-C5	-2.30	1.41	1.45
11	E	522	NAG	O5-C5	-2.07	1.41	1.45
11	E	525	NAG	O5-C5	-2.02	1.41	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	526	NAG	O5-C5-C6	2.59	109.70	106.98
11	E	524	NAG	O5-C5-C4	2.56	113.90	110.65
11	E	524	NAG	C2-N2-C7	-2.39	119.08	123.09
11	E	523	NAG	O5-C5-C6	2.37	109.47	106.98
11	E	526	NAG	O5-C5-C4	-2.25	107.80	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	227/236 (96%)	0.00	1 (0%)	90 45	75, 122, 168, 178	0
2	B	214/214 (100%)	0.09	1 (0%)	88 39	72, 121, 182, 197	0
3	C	214/214 (100%)	0.02	2 (0%)	81 25	81, 145, 187, 197	0
4	D	220/229 (96%)	-0.02	0	100 100	49, 96, 210, 242	0
5	E	315/321 (98%)	-0.05	0	100 100	27, 110, 174, 204	0
6	F	175/185 (94%)	0.13	1 (0%)	86 36	79, 143, 214, 222	0
All	All	1365/1399 (97%)	0.02	5 (0%)	90 45	27, 122, 194, 242	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	THR	2.2
3	C	1	ASP	2.2
2	B	154	LEU	2.2
3	C	199	GLN	2.1
6	F	150	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	MAN	E	517	11/12	0.20	-	80,86,94,100	0
9	MAN	E	518	11/12	0.26	-	100,107,114,114	0
9	MAN	E	512	11/12	0.18	-	89,93,101,107	0
8	MAN	E	504	11/12	0.20	-	85,91,95,101	0
9	BMA	E	511	11/12	0.16	-	83,89,96,96	0
9	MAN	E	516	11/12	0.20	-	86,88,97,97	0
8	MAN	E	508	11/12	0.25	-	148,152,157,159	0
9	NAG	E	509	14/15	0.21	-	87,96,99,101	0
8	MAN	E	505	11/12	0.24	-	94,97,103,110	0
9	MAN	E	513	11/12	0.26	-	116,121,127,128	0
9	MAN	E	515	11/12	0.25	-	87,88,90,93	0
10	NAG	E	520	14/15	0.23	-	116,125,135,139	0
8	NAG	E	501	14/15	0.20	-	75,86,100,106	0
8	MAN	E	506	11/12	0.23	-	86,92,103,104	0
10	NAG	E	519	14/15	0.23	-	104,113,123,136	0
9	MAN	E	514	11/12	0.23	-	135,140,144,152	0
8	MAN	E	507	11/12	0.23	-	121,125,134,144	0
8	NAG	E	502	14/15	0.22	-	77,87,100,110	0
8	BMA	E	503	11/12	0.15	-	88,94,105,110	0
10	BMA	E	521	11/12	0.14	-	131,140,144,146	0
9	NAG	E	510	14/15	0.18	-	94,102,105,118	0

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	NAG	E	526	14/15	0.20	-	114,126,132,132	0
11	NAG	E	523	14/15	0.24	-	86,91,97,100	0
7	PG4	C	301	13/13	0.24	-	85,107,121,123	0
11	NAG	E	527	14/15	0.16	-	115,135,142,144	0
11	NAG	E	524	14/15	0.27	-	120,142,156,156	0
11	NAG	E	525	14/15	0.33	-	148,154,164,165	0
11	NAG	E	522	14/15	0.18	-	100,107,112,115	0

6.5 Other polymers ⓘ

There are no such residues in this entry.