



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:40 AM UTC

PDB ID : 7ZQT / pdb_00007zqt
Title : Helicobacter pylori adhesin BabA bound to neutralising human antibody.
Authors : Moonens, K.; Boren, T.
Deposited on : 2022-05-03
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

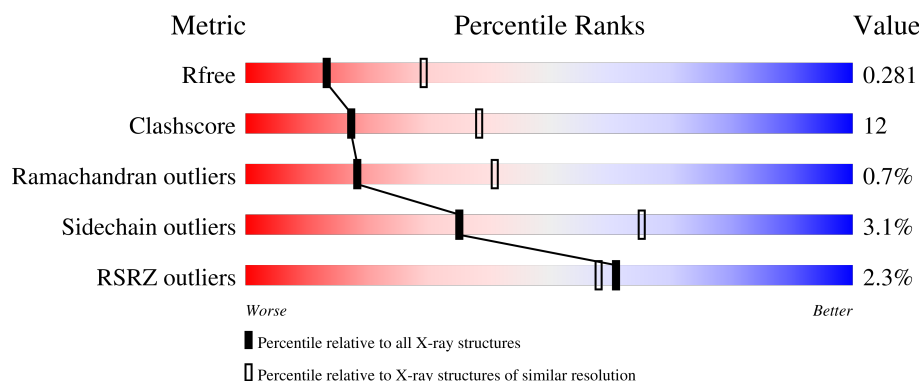
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	466	
1	E	466	
2	B	120	
2	F	120	
3	C	222	

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Mol	Chain	Length	Quality of chain
3	G	222	3% 66% 28%
4	D	211	2% 67% 30%
4	H	211	% 72% 27%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13999 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 Adhesin binding fucosylated histo-blood group antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			2983	1840	513	617	13			
1	E	413	Total	C	N	O	S	0	0	0
			3077	1900	528	636	13			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	expression tag	UNP O52269
A	4	SER	-	expression tag	UNP O52269
A	5	TRP	-	expression tag	UNP O52269
A	6	SER	-	expression tag	UNP O52269
A	7	HIS	-	expression tag	UNP O52269
A	8	PRO	-	expression tag	UNP O52269
A	9	GLN	-	expression tag	UNP O52269
A	10	PHE	-	expression tag	UNP O52269
A	11	GLU	-	expression tag	UNP O52269
A	12	LYS	-	expression tag	UNP O52269
A	13	SER	-	expression tag	UNP O52269
A	14	GLY	-	expression tag	UNP O52269
A	15	GLY	-	expression tag	UNP O52269
A	16	GLY	-	expression tag	UNP O52269
A	17	GLY	-	expression tag	UNP O52269
A	18	GLY	-	expression tag	UNP O52269
A	19	LEU	-	expression tag	UNP O52269
A	20	VAL	-	expression tag	UNP O52269
A	21	PRO	-	expression tag	UNP O52269
A	22	ARG	-	expression tag	UNP O52269
A	23	GLY	-	expression tag	UNP O52269
A	24	SER	-	expression tag	UNP O52269
A	461	GLY	-	expression tag	UNP O52269
A	462	SER	-	expression tag	UNP O52269
A	463	HIS	-	expression tag	UNP O52269

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Chain	Residue	Modelled	Actual	Comment	Reference
A	464	HIS	-	expression tag	UNP O52269
A	465	HIS	-	expression tag	UNP O52269
A	466	HIS	-	expression tag	UNP O52269
A	467	HIS	-	expression tag	UNP O52269
A	468	HIS	-	expression tag	UNP O52269
E	3	ALA	-	expression tag	UNP O52269
E	4	SER	-	expression tag	UNP O52269
E	5	TRP	-	expression tag	UNP O52269
E	6	SER	-	expression tag	UNP O52269
E	7	HIS	-	expression tag	UNP O52269
E	8	PRO	-	expression tag	UNP O52269
E	9	GLN	-	expression tag	UNP O52269
E	10	PHE	-	expression tag	UNP O52269
E	11	GLU	-	expression tag	UNP O52269
E	12	LYS	-	expression tag	UNP O52269
E	13	SER	-	expression tag	UNP O52269
E	14	GLY	-	expression tag	UNP O52269
E	15	GLY	-	expression tag	UNP O52269
E	16	GLY	-	expression tag	UNP O52269
E	17	GLY	-	expression tag	UNP O52269
E	18	GLY	-	expression tag	UNP O52269
E	19	LEU	-	expression tag	UNP O52269
E	20	VAL	-	expression tag	UNP O52269
E	21	PRO	-	expression tag	UNP O52269
E	22	ARG	-	expression tag	UNP O52269
E	23	GLY	-	expression tag	UNP O52269
E	24	SER	-	expression tag	UNP O52269
E	461	GLY	-	expression tag	UNP O52269
E	462	SER	-	expression tag	UNP O52269
E	463	HIS	-	expression tag	UNP O52269
E	464	HIS	-	expression tag	UNP O52269
E	465	HIS	-	expression tag	UNP O52269
E	466	HIS	-	expression tag	UNP O52269
E	467	HIS	-	expression tag	UNP O52269
E	468	HIS	-	expression tag	UNP O52269

- Molecule 2 is a protein called Nanobody Nb19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	110	Total	C	N	O	S	0	0	0
			844	529	152	158	5			
2	F	111	Total	C	N	O	S	0	0	0
			851	534	153	159	5			

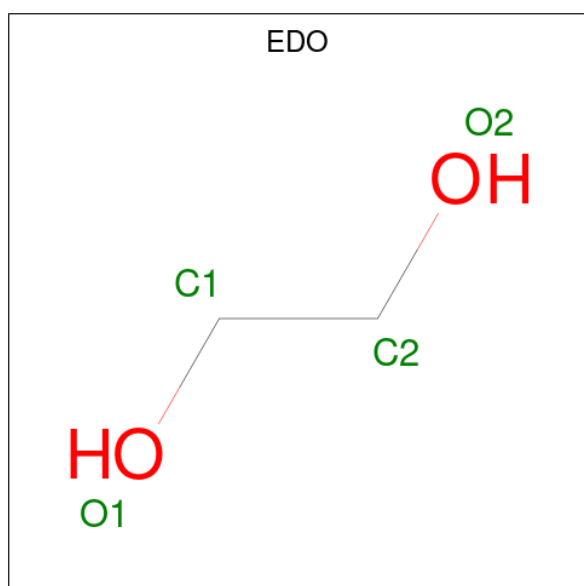
- Molecule 3 is a protein called VH domain human IgG antibody ABbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	189	Total	C	N	O	S	0	0	0
			1392	877	236	274	5			
3	G	213	Total	C	N	O	S	0	0	0
			1580	994	270	310	6			

- Molecule 4 is a protein called VL domain human IgG antibody ABbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	211	Total	C	N	O	S	0	0	0
			1624	1017	271	331	5			
4	H	211	Total	C	N	O	S	0	0	0
			1624	1017	271	331	5			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

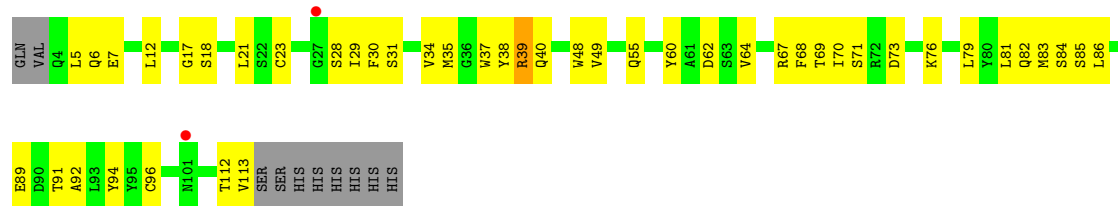
- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



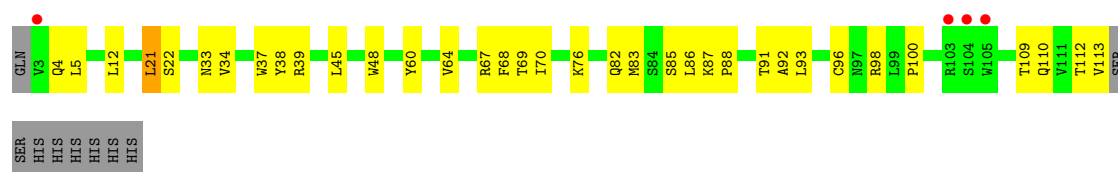
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

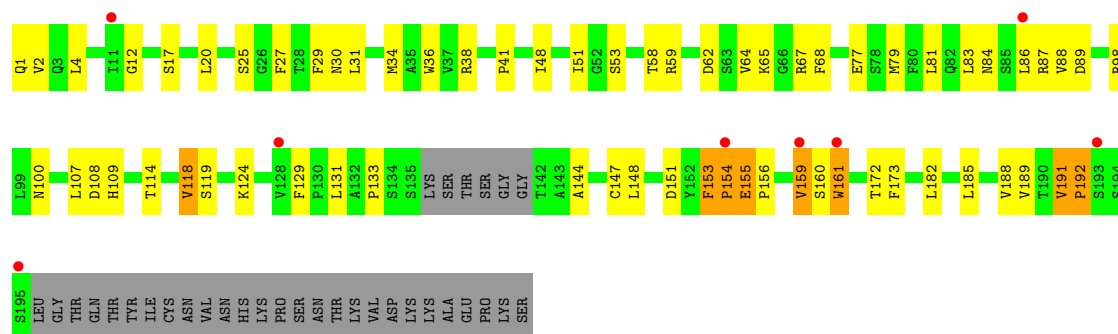
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	E	1	Total	O	0	0
			1	1		
7	H	2	Total	O	0	0
			2	2		



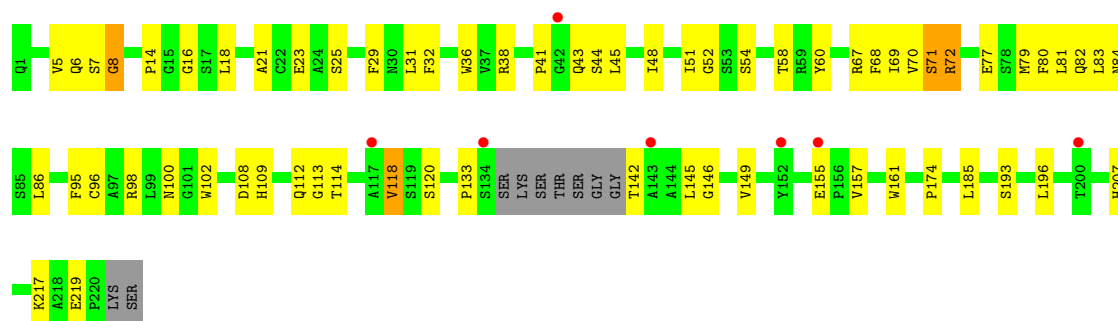
• Molecule 2: Nanobody Nb19



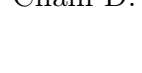
• Molecule 3: VH domain human IgG antibody ABbA

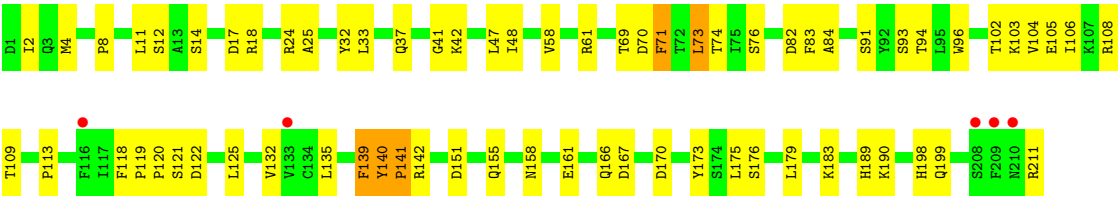


• Molecule 3: VH domain human IgG antibody ABbA

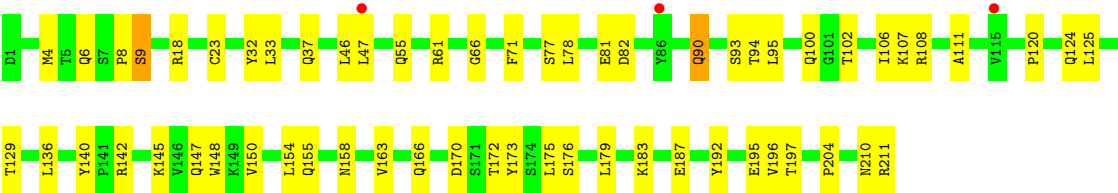


• Molecule 4: VL domain human IgG antibody ABbA





● Molecule 4: VL domain human IgG antibody ABbA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.70Å 68.40Å 176.60Å 90.00° 104.40° 90.00°	Depositor
Resolution (Å)	48.28 – 2.70 48.28 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.28-2.70) 99.2 (48.28-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.225 , 0.281 0.227 , 0.281	Depositor DCC
R_{free} test set	3132 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	72.4	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13999	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/3027	0.70	0/4114
1	E	0.47	0/3122	0.72	0/4243
2	B	0.34	0/863	0.66	0/1169
2	F	0.37	0/870	0.66	0/1179
3	C	0.47	0/1423	0.84	1/1936 (0.1%)
3	G	0.41	0/1615	0.75	1/2197 (0.0%)
4	D	0.40	0/1659	0.77	2/2253 (0.1%)
4	H	0.38	0/1659	0.68	0/2253
All	All	0.43	0/14238	0.73	4/19344 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	161	TRP	N-CA-C	6.01	120.12	113.21
4	D	139	PHE	CA-C-N	-5.50	108.37	121.80
4	D	139	PHE	C-N-CA	-5.50	108.37	121.80
3	G	155	GLU	N-CA-C	5.29	121.51	109.81

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	2983	0	2904	56	1
1	E	3077	0	3010	50	0
2	B	844	0	826	31	0
2	F	851	0	835	22	0
3	C	1392	0	1354	56	0
3	G	1580	0	1544	45	1
4	D	1624	0	1581	63	0
4	H	1624	0	1581	46	0
5	A	4	0	6	0	0
5	E	4	0	6	0	0
6	A	6	0	8	1	0
6	E	6	0	8	1	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
7	H	2	0	0	0	0
All	All	13999	0	13663	345	1

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 12.

All (345) 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)
4:H:197:THR:HG22	4:H:204:PRO:HB3	1.37	1.06
1:A:215:THR:HG22	1:A:224:THR:HG22	1.40	1.03
3:C:38:ARG:HD3	3:C:48:ILE:HD11	1.53	0.89
3:G:142:THR:N	3:G:193:SER:HG	1.70	0.89
3:C:147:CYS:HG	3:C:161:TRP:CD1	1.94	0.86
1:A:381:THR:HG21	2:F:76:LYS:HG3	1.55	0.86
1:A:213:THR:HG22	1:A:226:THR:HG22	1.60	0.84
1:E:174:LEU:HD12	1:E:174:LEU:H	1.43	0.83
4:D:189:HIS:O	4:D:211:ARG:NH1	2.13	0.82
1:E:329:GLU:OE2	1:E:331:SER:N	2.13	0.80
2:F:87:LYS:HG2	2:F:88:PRO:HD2	1.62	0.80
1:E:63:ARG:NH2	1:E:332:THR:O	2.15	0.79
3:C:147:CYS:SG	3:C:161:TRP:NE1	2.55	0.79
4:D:18:ARG:HG3	4:D:76:SER:HA	1.64	0.78
2:B:91:THR:HG22	2:B:113:VAL:H	1.49	0.78
1:E:202:THR:OG1	1:E:204:VAL:HG22	1.84	0.78
4:D:2:ILE:HD13	4:D:93:SER:HB3	1.65	0.77
4:D:61:ARG:NH1	4:D:82:ASP:OD2	2.20	0.75
4:D:140:TYR:O	4:D:142:ARG:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:PHE:H	3:C:154:PRO:HD2	1.52	0.74
4:D:70:ASP:C	4:D:71:PHE:HD1	1.96	0.73
3:C:62:ASP:OD1	3:C:65:LYS:NZ	2.15	0.73
4:H:108:ARG:HH12	4:H:111:ALA:HB2	1.55	0.71
3:G:82:GLN:HG3	3:G:84:ASN:ND2	2.06	0.71
1:A:343:ASN:OD1	1:A:346:THR:OG1	2.08	0.70
1:E:72:ASN:HA	1:E:76:ASP:OD2	1.90	0.70
2:B:39:ARG:HG2	2:B:94:TYR:HE1	1.56	0.69
4:D:161:GLU:HG3	4:D:175:LEU:HD21	1.74	0.69
1:E:321:GLN:NE2	1:E:363:LYS:HD3	2.07	0.68
3:C:188:VAL:HG21	4:D:135:LEU:HD11	1.75	0.68
3:G:82:GLN:HG3	3:G:84:ASN:HD21	1.59	0.68
4:D:198:HIS:HD2	4:D:199:GLN:H	1.41	0.68
2:B:49:VAL:HG13	2:B:64:VAL:HG21	1.75	0.67
3:G:51:ILE:HG22	3:G:79:MET:HE3	1.76	0.67
3:C:131:LEU:HD21	3:C:148:LEU:HB2	1.75	0.67
4:H:120:PRO:HB2	4:H:125:LEU:HD11	1.77	0.66
2:B:91:THR:HA	2:B:112:THR:HA	1.78	0.66
3:G:108:ASP:OD2	3:G:109:HIS:ND1	2.27	0.66
2:B:60:TYR:HE1	2:B:70:ILE:HG22	1.61	0.65
2:F:67:ARG:NH1	2:F:85:SER:O	2.30	0.64
4:D:105:GLU:OE1	4:D:173:TYR:OH	2.14	0.64
1:E:171:LEU:HD13	1:E:262:LEU:HD12	1.80	0.64
4:D:37:GLN:HB2	4:D:47:LEU:HD11	1.81	0.63
4:H:155:GLN:HG3	4:H:179:LEU:HD11	1.80	0.63
3:C:147:CYS:SG	3:C:161:TRP:CD1	2.91	0.63
2:B:86:LEU:HB3	2:B:113:VAL:HG21	1.80	0.63
3:G:5:VAL:HG22	3:G:23:GLU:CG	2.29	0.63
3:C:48:ILE:HG23	3:C:64:VAL:HG11	1.82	0.62
2:F:21:LEU:HD22	2:F:37:TRP:CH2	2.35	0.62
3:C:68:PHE:CZ	3:C:83:LEU:HD23	2.36	0.61
4:H:211:ARG:HG2	4:H:211:ARG:HH11	1.66	0.61
3:C:59:ARG:HE	4:D:94:THR:HG23	1.65	0.61
4:D:113:PRO:HD3	4:D:198:HIS:HD1	1.65	0.61
4:D:151:ASP:OD2	4:D:189:HIS:ND1	2.33	0.61
4:D:24:ARG:NH1	4:D:70:ASP:OD1	2.34	0.61
1:A:166:ALA:HB1	1:A:262:LEU:HD11	1.83	0.60
1:A:242:ARG:HD2	4:D:32:TYR:CZ	2.36	0.60
1:A:312:ILE:O	1:A:316:GLN:HG3	2.02	0.60
1:E:52:LEU:HD11	2:F:45:LEU:HD21	1.84	0.60
1:E:220:GLY:O	1:E:221:LYS:HE2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:ARG:HD2	4:H:32:TYR:CE2	2.37	0.59
1:E:438:ALA:HB2	2:F:34:VAL:HG11	1.84	0.59
1:A:215:THR:CG2	1:A:224:THR:HG22	2.25	0.59
3:C:1:GLN:O	3:C:1:GLN:NE2	2.36	0.59
3:C:88:VAL:HA	3:C:118:VAL:HG22	1.84	0.59
3:C:129:PHE:HB3	4:D:121:SER:OG	2.03	0.59
3:C:161:TRP:HA	3:C:161:TRP:CE3	2.38	0.59
3:G:71:SER:HB2	3:G:80:PHE:HB2	1.85	0.59
1:A:112:GLY:O	1:A:142:PRO:HD2	2.02	0.58
4:D:122:ASP:HA	4:D:125:LEU:HD22	1.85	0.58
2:B:68:PHE:HB3	2:B:81:LEU:HD11	1.85	0.58
4:D:83:PHE:CD1	4:D:106:ILE:HG22	2.37	0.58
1:E:164:GLN:OE1	1:E:412:GLY:HA2	2.03	0.58
3:G:133:PRO:HG3	3:G:145:LEU:HB3	1.85	0.58
4:H:148:TRP:O	4:H:154:LEU:HA	2.02	0.58
1:A:230:LYS:NZ	1:A:247:GLU:OE2	2.31	0.58
3:G:29:PHE:CD2	3:G:77:GLU:HA	2.39	0.57
3:C:155:GLU:HB3	3:C:156:PRO:HD3	1.85	0.57
2:F:4:GLN:O	2:F:5:LEU:HD23	2.05	0.57
1:E:171:LEU:HD12	1:E:172:PRO:HD2	1.86	0.57
3:C:38:ARG:CD	3:C:48:ILE:HD11	2.32	0.57
4:D:198:HIS:CD2	4:D:199:GLN:H	2.22	0.57
1:A:453:ILE:O	1:A:457:LEU:HD13	2.05	0.56
3:G:8:GLY:HA3	3:G:114:THR:HG21	1.86	0.56
6:A:1002:GOL:H12	3:C:31:LEU:HD13	1.88	0.56
1:E:260:GLN:O	1:E:260:GLN:NE2	2.37	0.56
1:A:137:LEU:HD22	1:A:147:PRO:HG3	1.87	0.56
1:A:105:GLN:HE22	1:E:287:GLY:HA2	1.70	0.56
2:B:40:GLN:H	2:B:92:ALA:HB1	1.71	0.55
4:D:12:SER:HA	4:D:105:GLU:O	2.07	0.55
3:C:36:TRP:CE2	3:C:81:LEU:HB2	2.41	0.55
4:D:33:LEU:HD22	4:D:71:PHE:HD2	1.71	0.55
2:B:69:THR:HB	2:B:82:GLN:HG3	1.89	0.55
1:E:174:LEU:H	1:E:174:LEU:CD1	2.18	0.55
1:A:63:ARG:NH1	1:A:330:GLN:OE1	2.39	0.55
4:H:94:THR:HG23	4:H:95:LEU:HD13	1.89	0.55
2:B:23:CYS:HB3	2:B:79:LEU:HB3	1.88	0.55
1:A:105:GLN:HG2	1:A:147:PRO:HB3	1.89	0.54
3:C:188:VAL:HG11	4:D:135:LEU:HD13	1.89	0.54
4:H:124:GLN:HE21	4:H:129:THR:HG23	1.72	0.54
4:D:47:LEU:HA	4:D:58:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32:PHE:O	3:G:72:ARG:NH2	2.40	0.54
1:E:163:LEU:HD21	1:E:265:GLN:HB2	1.89	0.54
1:A:66:LEU:HD21	1:A:358:ALA:HB2	1.90	0.53
3:C:68:PHE:CE2	3:C:83:LEU:HD23	2.43	0.53
2:F:21:LEU:HD21	2:F:109:THR:HG21	1.91	0.53
3:G:68:PHE:CE2	3:G:83:LEU:HD22	2.44	0.53
2:B:7:GLU:N	2:B:7:GLU:OE1	2.42	0.53
4:D:121:SER:O	4:D:125:LEU:HD13	2.08	0.53
3:G:5:VAL:HG22	3:G:23:GLU:HG3	1.89	0.53
3:G:52:GLY:O	3:G:72:ARG:NH1	2.42	0.53
4:D:83:PHE:CG	4:D:106:ILE:HG22	2.44	0.53
1:E:69:SER:OG	1:E:361:GLN:OE1	2.24	0.53
1:E:369:HIS:NE2	2:F:33:ASN:OD1	2.41	0.53
1:A:84:GLN:HB2	1:A:433:LEU:HD13	1.89	0.52
2:B:38:TYR:CD2	2:B:48:TRP:HA	2.44	0.52
1:E:141:LYS:HD3	1:E:142:PRO:O	2.09	0.52
4:H:170:ASP:HB3	4:H:172:THR:HG23	1.92	0.52
1:E:213:THR:HG23	1:E:226:THR:HG22	1.91	0.52
3:G:133:PRO:HG2	3:G:196:LEU:HD21	1.92	0.52
2:F:98:ARG:HG3	2:F:100:PRO:O	2.10	0.52
4:D:41:GLY:O	4:D:42:LYS:HE2	2.10	0.52
4:H:94:THR:HG23	4:H:95:LEU:CD1	2.40	0.52
3:G:6:GLN:OE1	3:G:113:GLY:N	2.40	0.52
4:D:14:SER:HB3	4:H:18:ARG:NH1	2.25	0.51
1:E:216:GLN:HG3	1:E:218:ILE:HD11	1.91	0.51
1:A:431:THR:OG1	2:B:55:GLN:NE2	2.44	0.51
3:G:133:PRO:HG2	3:G:196:LEU:CD2	2.41	0.51
4:H:155:GLN:HB3	4:H:158:ASN:HD21	1.76	0.51
1:A:438:ALA:HB2	2:B:34:VAL:HG21	1.92	0.50
3:C:191:VAL:HG13	3:C:192:PRO:HD2	1.94	0.50
4:D:120:PRO:HD3	4:D:132:VAL:HG22	1.93	0.50
4:H:175:LEU:HD23	4:H:176:SER:N	2.27	0.50
3:G:6:GLN:H	3:G:112:GLN:HE22	1.58	0.50
4:D:113:PRO:HD3	4:D:198:HIS:ND1	2.27	0.50
1:E:49:LEU:HD21	1:E:452:ASN:HB3	1.94	0.50
3:C:17:SER:HB3	3:C:84:ASN:HA	1.95	0.49
1:E:395:CYS:SG	1:E:397:ASN:ND2	2.85	0.49
3:C:188:VAL:HG21	4:D:135:LEU:CD1	2.41	0.49
2:F:87:LYS:CG	2:F:88:PRO:HD2	2.39	0.49
3:C:12:GLY:O	3:C:118:VAL:HA	2.12	0.49
1:A:206:ASP:OD2	3:C:30:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:GLN:HB2	1:E:364:MET:HG3	1.94	0.49
1:E:329:GLU:OE2	1:E:330:GLN:N	2.46	0.49
2:F:93:LEU:HD23	2:F:110:GLN:HA	1.94	0.49
3:C:151:ASP:HB3	3:C:182:LEU:HD22	1.95	0.49
4:D:198:HIS:CD2	4:D:199:GLN:N	2.81	0.49
1:A:273:ILE:HG23	1:A:298:LEU:HD13	1.95	0.48
2:B:5:LEU:O	2:B:6:GLN:HG3	2.13	0.48
4:D:175:LEU:HD23	4:D:176:SER:N	2.28	0.48
2:F:69:THR:HB	2:F:82:GLN:CG	2.44	0.48
3:C:159:VAL:HG21	3:C:172:THR:OG1	2.14	0.48
4:D:8:PRO:O	4:D:102:THR:OG1	2.23	0.48
1:A:63:ARG:HD2	1:A:330:GLN:OE1	2.14	0.48
1:A:208:ASN:ND2	3:C:53:SER:HB3	2.28	0.48
4:D:70:ASP:C	4:D:71:PHE:CD1	2.86	0.48
6:E:1002:GOL:H12	3:G:31:LEU:HD13	1.96	0.48
1:E:174:LEU:HD12	1:E:174:LEU:N	2.20	0.48
1:E:312:ILE:O	1:E:316:GLN:HG3	2.14	0.48
1:A:46:LEU:HD12	1:A:49:LEU:HB3	1.95	0.48
4:H:66:GLY:HA3	4:H:71:PHE:HA	1.96	0.48
4:H:90:GLN:HE22	4:H:93:SER:CB	2.27	0.47
3:C:2:VAL:HB	3:C:109:HIS:CD2	2.49	0.47
3:C:36:TRP:CG	3:C:81:LEU:HD22	2.49	0.47
1:E:334:VAL:HG21	1:E:350:PHE:CE1	2.49	0.47
2:B:83:MET:SD	2:B:94:TYR:HE2	2.38	0.47
2:F:60:TYR:CE1	2:F:70:ILE:HG22	2.49	0.47
3:G:68:PHE:CD1	3:G:83:LEU:HA	2.50	0.47
4:D:11:LEU:HD12	4:D:12:SER:N	2.29	0.47
1:A:310:LYS:NZ	1:A:314:ASP:OD1	2.47	0.47
3:C:2:VAL:HG13	3:C:27:PHE:CD1	2.50	0.47
1:A:289:PRO:HB2	1:A:391:PHE:CZ	2.49	0.47
1:A:379:ASN:ND2	2:B:31:SER:OG	2.47	0.47
3:C:64:VAL:HG21	3:C:68:PHE:CD2	2.50	0.47
4:H:33:LEU:HD13	4:H:71:PHE:CD2	2.49	0.47
4:H:147:GLN:HB2	4:H:195:GLU:HB3	1.96	0.47
3:C:153:PHE:O	3:C:154:PRO:C	2.58	0.47
4:D:91:SER:HA	4:D:96:TRP:CD1	2.50	0.47
3:G:6:GLN:HE22	3:G:95:PHE:HA	1.79	0.47
2:F:87:LYS:HG2	2:F:88:PRO:CD	2.38	0.47
4:D:166:GLN:HG3	4:D:173:TYR:CZ	2.50	0.46
3:G:36:TRP:CZ3	3:G:96:CYS:HB3	2.51	0.46
4:D:106:ILE:HD13	4:D:106:ILE:HG21	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:TYR:HD2	1:E:84:GLN:NE2	2.13	0.46
3:C:131:LEU:HB3	4:D:118:PHE:CD2	2.51	0.46
1:A:188:THR:HA	1:A:246:THR:O	2.16	0.46
2:B:17:GLY:O	2:B:84:SER:HA	2.15	0.46
3:G:5:VAL:HG22	3:G:23:GLU:HG2	1.95	0.46
2:B:12:LEU:CD2	2:B:112:THR:OG1	2.64	0.46
4:H:154:LEU:HD23	4:H:155:GLN:O	2.16	0.46
4:H:37:GLN:HB2	4:H:47:LEU:HD11	1.97	0.46
4:D:14:SER:HB3	4:H:18:ARG:HH12	1.80	0.46
2:F:21:LEU:HD23	2:F:22:SER:H	1.79	0.46
2:B:23:CYS:HB2	2:B:37:TRP:CH2	2.51	0.46
2:B:73:ASP:CG	2:B:76:LYS:HB2	2.41	0.46
4:D:71:PHE:CD1	4:D:71:PHE:N	2.84	0.46
1:A:304:GLU:OE1	1:A:304:GLU:N	2.46	0.46
3:C:100:ASN:HB2	3:C:108:ASP:HB2	1.97	0.46
1:E:83:TYR:OH	1:E:171:LEU:O	2.17	0.46
4:H:211:ARG:HG2	4:H:211:ARG:NH1	2.31	0.46
2:F:69:THR:HB	2:F:82:GLN:HG3	1.97	0.45
3:G:44:SER:OG	3:G:45:LEU:N	2.49	0.45
4:H:150:VAL:HG12	4:H:192:TYR:CD2	2.50	0.45
1:A:211:THR:HG22	1:A:228:SER:HB3	1.98	0.45
1:E:329:GLU:CD	1:E:329:GLU:C	2.84	0.45
4:H:166:GLN:HG3	4:H:173:TYR:CZ	2.52	0.45
1:A:454:ALA:O	1:A:458:VAL:HG23	2.16	0.45
4:D:190:LYS:HA	4:D:211:ARG:HD3	1.97	0.45
1:A:82:ALA:HB1	1:A:318:LEU:HD21	1.99	0.45
4:D:11:LEU:HD12	4:D:12:SER:H	1.81	0.45
1:A:395:CYS:SG	1:A:397:ASN:ND2	2.89	0.45
4:H:108:ARG:HB3	4:H:140:TYR:CD1	2.52	0.45
1:A:208:ASN:HD21	3:C:53:SER:CB	2.30	0.45
3:C:4:LEU:HD21	3:C:34:MET:HE1	1.98	0.45
1:E:452:ASN:O	1:E:456:THR:HG23	2.17	0.45
3:C:153:PHE:N	3:C:154:PRO:HD2	2.26	0.45
4:D:47:LEU:O	4:D:48:ILE:HD13	2.17	0.45
1:E:317:GLU:OE2	1:E:321:GLN:NE2	2.50	0.45
2:B:86:LEU:HA	2:B:86:LEU:HD23	1.79	0.44
3:C:124:LYS:HE3	3:C:151:ASP:O	2.17	0.44
4:D:14:SER:HB2	4:D:17:ASP:OD2	2.17	0.44
4:D:71:PHE:HD1	4:D:71:PHE:N	2.14	0.44
2:B:12:LEU:HD23	2:B:112:THR:OG1	2.17	0.44
3:G:217:LYS:HG2	3:G:219:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:78:LEU:CD2	4:H:82:ASP:HB2	2.48	0.44
4:H:210:ASN:OD1	4:H:210:ASN:N	2.51	0.44
1:A:186:THR:HG22	1:A:249:THR:HA	1.99	0.44
3:G:51:ILE:CG2	3:G:79:MET:HE3	2.46	0.44
3:G:146:GLY:HA2	3:G:161:TRP:CH2	2.52	0.44
1:A:70:ALA:HB2	1:A:361:GLN:NE2	2.33	0.44
4:D:167:ASP:HB3	4:D:170:ASP:HB2	2.00	0.44
3:G:16:GLY:C	3:G:86:LEU:HD12	2.43	0.44
4:H:77:SER:O	4:H:77:SER:OG	2.35	0.44
2:B:18:SER:HA	2:B:83:MET:O	2.18	0.44
4:H:142:ARG:HB2	4:H:173:TYR:CE2	2.53	0.44
4:H:183:LYS:O	4:H:187:GLU:HG3	2.18	0.44
1:A:443:GLN:O	1:A:447:ILE:HG13	2.18	0.44
3:C:51:ILE:CG2	3:C:79:MET:HE3	2.48	0.44
2:F:91:THR:HG22	2:F:113:VAL:N	2.32	0.44
4:D:73:LEU:HD23	4:D:74:THR:N	2.32	0.43
1:A:380:LEU:HD23	1:A:380:LEU:HA	1.82	0.43
4:D:155:GLN:HG3	4:D:158:ASN:OD1	2.19	0.43
1:A:78:LYS:HG3	1:A:79:ASN:N	2.33	0.43
2:F:83:MET:HE2	2:F:86:LEU:HD21	2.01	0.43
1:A:241:THR:O	1:A:243:VAL:HG23	2.18	0.43
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.90	0.43
1:E:164:GLN:CD	1:E:412:GLY:HA2	2.43	0.43
3:C:87:ARG:NH2	3:C:89:ASP:OD2	2.48	0.43
4:D:125:LEU:O	4:D:183:LYS:HD3	2.19	0.43
4:H:150:VAL:HG22	4:H:155:GLN:OE1	2.19	0.43
3:C:133:PRO:HB3	3:C:144:ALA:O	2.19	0.43
4:H:9:SER:O	4:H:102:THR:HA	2.19	0.43
1:A:223:VAL:HG22	1:A:254:GLY:O	2.18	0.43
3:C:51:ILE:HG22	3:C:79:MET:HE3	1.99	0.43
3:G:98:ARG:HH21	3:G:100:ASN:ND2	2.17	0.43
4:H:145:LYS:O	4:H:196:VAL:HA	2.19	0.43
1:E:237:LYS:HE3	1:E:237:LYS:HB3	1.78	0.43
1:E:426:VAL:O	1:E:430:ILE:HG13	2.19	0.43
3:G:60:TYR:OH	3:G:69:ILE:HA	2.19	0.43
1:A:375:ILE:O	1:A:375:ILE:HG13	2.19	0.42
3:C:20:LEU:HD13	3:C:36:TRP:CZ3	2.54	0.42
4:D:139:PHE:HB2	4:D:198:HIS:HE1	1.84	0.42
2:F:64:VAL:HB	2:F:68:PHE:CD2	2.54	0.42
1:A:211:THR:HG22	1:A:228:SER:CB	2.49	0.42
2:B:71:SER:O	2:B:79:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:TRP:HA	3:C:161:TRP:HE3	1.82	0.42
1:E:169:LYS:HD2	1:E:181:VAL:HG23	2.01	0.42
4:D:141:PRO:HD2	4:D:198:HIS:NE2	2.34	0.42
3:G:98:ARG:HH21	3:G:100:ASN:HD22	1.66	0.42
3:G:100:ASN:HB2	3:G:108:ASP:HB2	2.00	0.42
3:G:36:TRP:CE2	3:G:81:LEU:HB2	2.54	0.42
3:G:174:PRO:HG2	4:H:163:VAL:O	2.19	0.42
4:D:140:TYR:HB3	4:D:141:PRO:HD3	2.00	0.42
1:E:291:MET:HG3	1:E:292:GLU:N	2.35	0.42
1:E:318:LEU:C	1:E:318:LEU:HD23	2.45	0.42
1:A:91:ASN:HB3	1:A:424:ALA:HB1	2.01	0.42
4:D:4:MET:HE1	4:D:25:ALA:HB2	2.01	0.42
4:D:139:PHE:HB2	4:D:198:HIS:CE1	2.55	0.42
3:G:43:GLN:OE1	3:G:43:GLN:HA	2.19	0.42
3:C:20:LEU:HB2	3:C:81:LEU:HB3	2.01	0.42
4:H:94:THR:C	4:H:95:LEU:HD12	2.44	0.42
4:H:107:LYS:HG2	4:H:108:ARG:N	2.35	0.42
3:C:67:ARG:CZ	3:C:87:ARG:HD3	2.49	0.42
4:D:69:THR:HG23	4:D:70:ASP:OD2	2.20	0.42
1:E:277:CYS:SG	1:E:297:LYS:HB2	2.60	0.42
4:D:84:ALA:O	4:D:104:VAL:HG22	2.19	0.41
1:E:267:SER:O	1:E:271:ASN:HB2	2.20	0.41
1:E:348:ALA:HA	1:E:350:PHE:CE1	2.54	0.41
3:G:7:SER:HB2	3:G:21:ALA:HB3	2.02	0.41
1:A:242:ARG:HD2	4:D:32:TYR:CE2	2.54	0.41
3:C:29:PHE:CD2	3:C:77:GLU:HA	2.55	0.41
1:E:212:LYS:HE3	1:E:214:LYS:HG3	2.02	0.41
4:H:6:GLN:H	4:H:100:GLN:HE22	1.68	0.41
1:E:391:PHE:O	1:E:394:THR:OG1	2.35	0.41
3:G:86:LEU:HB3	3:G:118:VAL:HG11	2.02	0.41
1:A:68:ALA:O	1:A:72:ASN:HB2	2.20	0.41
3:C:20:LEU:HD12	3:C:81:LEU:HD23	2.01	0.41
3:C:83:LEU:HB3	3:C:86:LEU:HD21	2.02	0.41
4:D:108:ARG:HG2	4:D:109:THR:N	2.35	0.41
4:D:155:GLN:HG2	4:D:179:LEU:HD11	2.03	0.41
1:E:139:ARG:HE	1:E:139:ARG:HB3	1.71	0.41
1:E:304:GLU:OE2	1:E:304:GLU:N	2.49	0.41
3:G:67:ARG:O	3:G:68:PHE:HD1	2.04	0.41
4:H:148:TRP:CE3	4:H:179:LEU:HD12	2.56	0.41
1:A:87:LEU:HD12	1:A:87:LEU:HA	1.91	0.41
2:B:67:ARG:HD2	2:B:85:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:PHE:O	3:C:185:LEU:HG	2.20	0.41
4:H:148:TRP:O	4:H:154:LEU:HG	2.21	0.41
1:A:459:ASN:O	1:A:463:HIS:ND1	2.54	0.41
3:C:88:VAL:HA	3:C:118:VAL:CG2	2.51	0.41
4:D:106:ILE:H	4:D:106:ILE:HG23	1.65	0.41
3:G:18:LEU:HB2	3:G:83:LEU:HD12	2.03	0.41
4:H:106:ILE:HG22	4:H:166:GLN:OE1	2.20	0.41
4:H:140:TYR:O	4:H:142:ARG:N	2.54	0.41
1:A:148:MET:HE2	1:A:278:PRO:HG3	2.01	0.41
1:A:321:GLN:HB2	1:A:364:MET:HE2	2.02	0.41
2:B:62:ASP:C	2:B:64:VAL:H	2.27	0.41
2:B:5:LEU:HD21	2:B:96:CYS:SG	2.60	0.41
2:B:30:PHE:HA	2:B:35:MET:HE3	2.02	0.41
3:C:98:ARG:HH21	3:C:100:ASN:HD22	1.69	0.41
1:E:66:LEU:HD23	1:E:66:LEU:HA	1.91	0.41
3:G:32:PHE:CE2	3:G:102:TRP:HD1	2.39	0.41
3:G:38:ARG:NE	3:G:48:ILE:HD11	2.36	0.41
3:G:16:GLY:O	3:G:86:LEU:HD12	2.20	0.41
3:G:157:VAL:HG22	3:G:207:HIS:HD2	1.85	0.41
1:A:445:GLN:HA	1:A:445:GLN:OE1	2.20	0.40
2:F:38:TYR:CD1	2:F:48:TRP:HA	2.56	0.40
4:H:166:GLN:HG3	4:H:173:TYR:CE1	2.56	0.40
2:B:29:ILE:HG22	2:B:35:MET:HE1	2.03	0.40
3:C:1:GLN:O	3:C:1:GLN:CD	2.64	0.40
4:D:118:PHE:HA	4:D:119:PRO:HD3	1.93	0.40
3:G:149:VAL:CG2	3:G:185:LEU:HB3	2.50	0.40
4:H:145:LYS:HB3	4:H:197:THR:OG1	2.22	0.40
1:A:66:LEU:HD12	1:A:66:LEU:HA	1.89	0.40
1:A:397:ASN:HD22	1:A:409:SER:HB2	1.85	0.40
1:E:88:LEU:HD13	1:E:429:THR:HG22	2.04	0.40
4:H:4:MET:HE3	4:H:23:CYS:SG	2.61	0.40
3:C:107:LEU:HA	3:C:107:LEU:HD23	1.82	0.40
4:H:46:LEU:HD23	4:H:55:GLN:HE21	1.86	0.40
1:A:242:ARG:HH21	1:A:242:ARG:HG2	1.85	0.40
1:A:442:THR:HG23	2:B:48:TRP:CE3	2.57	0.40
1:E:125:GLU:OE2	1:E:157:ASN:ND2	2.35	0.40
2:F:39:ARG:HB2	2:F:92:ALA:HB3	2.03	0.40
3:G:6:GLN:NE2	3:G:96:CYS:H	2.20	0.40
4:H:90:GLN:HE22	4:H:93:SER:HB3	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:NH2	3:G:14:PRO:O[2_555]	1.91	0.29

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	393/466 (84%)	374 (95%)	19 (5%)	0	100	100
1	E	407/466 (87%)	387 (95%)	19 (5%)	1 (0%)	43	68
2	B	108/120 (90%)	102 (94%)	6 (6%)	0	100	100
2	F	109/120 (91%)	107 (98%)	2 (2%)	0	100	100
3	C	185/222 (83%)	162 (88%)	17 (9%)	6 (3%)	3	7
3	G	209/222 (94%)	186 (89%)	20 (10%)	3 (1%)	9	23
4	D	209/211 (99%)	195 (93%)	12 (6%)	2 (1%)	12	32
4	H	209/211 (99%)	193 (92%)	15 (7%)	1 (0%)	24	48
All	All	1829/2038 (90%)	1706 (93%)	110 (6%)	13 (1%)	18	41

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	155	GLU
3	C	192	PRO
4	D	141	PRO
3	G	8	GLY
4	H	8	PRO
4	D	140	TYR
3	G	41	PRO
3	G	54	SER
3	C	153	PHE
1	E	129	ARG
3	C	41	PRO
3	C	154	PRO

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Mol	Chain	Res	Type
3	C	191	VAL

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	331/381 (87%)	319 (96%)	12 (4%)	31	60
1	E	342/381 (90%)	337 (98%)	5 (2%)	57	81
2	B	89/99 (90%)	85 (96%)	4 (4%)	24	52
2	F	90/99 (91%)	86 (96%)	4 (4%)	25	53
3	C	153/182 (84%)	145 (95%)	8 (5%)	21	47
3	G	175/182 (96%)	168 (96%)	7 (4%)	28	56
4	D	187/187 (100%)	184 (98%)	3 (2%)	55	80
4	H	187/187 (100%)	182 (97%)	5 (3%)	39	69
All	All	1554/1698 (92%)	1506 (97%)	48 (3%)	35	65

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	66	LEU
1	A	111	ASN
1	A	137	LEU
1	A	182	SER
1	A	230	LYS
1	A	252	LEU
1	A	282	VAL
1	A	294	THR
1	A	334	VAL
1	A	347	ASP
1	A	457	LEU
2	B	21	LEU
2	B	28	SER

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Mol	Chain	Res	Type
2	B	39	ARG
2	B	89	GLU
3	C	25	SER
3	C	58	THR
3	C	114	THR
3	C	118	VAL
3	C	119	SER
3	C	159	VAL
3	C	160	SER
3	C	189	VAL
4	D	71	PHE
4	D	73	LEU
4	D	103	LYS
1	E	94	VAL
1	E	140	TYR
1	E	151	GLU
1	E	292	GLU
1	E	329	GLU
2	F	12	LEU
2	F	21	LEU
2	F	96	CYS
2	F	112	THR
3	G	25	SER
3	G	58	THR
3	G	70	VAL
3	G	71	SER
3	G	72	ARG
3	G	118	VAL
3	G	120	SER
4	H	9	SER
4	H	61	ARG
4	H	81	GLU
4	H	90	GLN
4	H	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	105	GLN
1	A	123	ASN
1	A	124	ASN

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Mol	Chain	Res	Type
1	A	177	ASN
1	A	208	ASN
1	A	366	ASN
1	A	379	ASN
1	A	397	ASN
1	A	417	GLN
1	A	448	GLN
2	B	55	GLN
3	C	43	GLN
3	C	84	ASN
4	D	124	GLN
4	D	155	GLN
4	D	160	GLN
4	D	198	HIS
1	E	60	ASN
1	E	124	ASN
1	E	161	GLN
1	E	207	GLN
1	E	271	ASN
1	E	320	ASN
1	E	326	ASN
1	E	379	ASN
1	E	386	ASN
3	G	84	ASN
4	H	90	GLN
4	H	124	GLN
4	H	147	GLN
4	H	152	ASN
4	H	155	GLN
4	H	160	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GOL	A	1002	-	5,5,5	1.17	0	5,5,5	1.07	0
5	EDO	A	1001	-	3,3,3	0.59	0	2,2,2	0.10	0
6	GOL	E	1002	-	5,5,5	0.90	0	5,5,5	1.23	1 (20%)
5	EDO	E	1001	-	3,3,3	0.68	0	2,2,2	0.45	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
6	GOL	A	1002	-	-	2/4/4/4	-
5	EDO	A	1001	-	-	1/1/1/1	-
6	GOL	E	1002	-	-	2/4/4/4	-
5	EDO	E	1001	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1002	GOL	C3-C2-C1	-2.13	103.99	111.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1002	GOL	C1-C2-C3-O3
6	E	1002	GOL	C1-C2-C3-O3
6	A	1002	GOL	O2-C2-C3-O3
6	E	1002	GOL	O2-C2-C3-O3
5	A	1001	EDO	O1-C1-C2-O2
5	E	1001	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1002	GOL	1	0
6	E	1002	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	401/466 (86%)	0.11	7 (1%) 69 67	57, 88, 129, 157	0
1	E	413/466 (88%)	0.13	7 (1%) 69 67	62, 84, 136, 171	0
2	B	110/120 (91%)	0.65	2 (1%) 67 65	112, 150, 165, 182	0
2	F	111/120 (92%)	0.21	4 (3%) 46 42	82, 111, 142, 167	0
3	C	189/222 (85%)	0.43	8 (4%) 40 37	70, 99, 152, 170	0
3	G	213/222 (95%)	0.23	7 (3%) 49 45	75, 95, 117, 125	0
4	D	211/211 (100%)	0.21	5 (2%) 59 56	70, 106, 142, 153	0
4	H	211/211 (100%)	0.24	3 (1%) 73 72	79, 116, 140, 154	0
All	All	1859/2038 (91%)	0.22	43 (2%) 61 58	57, 97, 149, 182	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	GLY	5.3
4	D	208	SER	4.8
1	E	335	GLY	4.2
3	C	128	VAL	3.8
1	A	341	PRO	3.8
3	G	155	GLU	3.4
4	H	47	LEU	3.4
1	E	341	PRO	3.3
4	H	115	VAL	3.2
1	A	286	SER	3.1
3	G	152	TYR	3.1
1	A	54	ALA	3.1
1	A	340	LYS	2.8
2	F	3	VAL	2.8
2	B	27	GLY	2.8
3	G	117	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	344	PRO	2.7
2	F	103	ARG	2.6
3	G	143	ALA	2.5
1	A	426	VAL	2.5
4	D	209	PHE	2.5
3	C	11	ILE	2.4
3	C	159	VAL	2.4
1	E	396	ASN	2.4
3	C	154	PRO	2.3
2	B	101	ASN	2.3
3	C	195	SER	2.3
2	F	104	SER	2.3
3	C	86	LEU	2.3
3	C	193	SER	2.2
3	G	134	SER	2.2
1	E	420	ALA	2.2
4	H	86	TYR	2.2
2	F	105	TRP	2.1
4	D	210	ASN	2.1
3	G	42	GLY	2.1
1	A	50	ILE	2.1
4	D	133	VAL	2.1
3	C	161	TRP	2.0
1	E	372	GLY	2.0
4	D	116	PHE	2.0
3	G	200	THR	2.0
1	E	179	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	E	1001	4/4	0.87	0.14	68,71,74,79	0
6	GOL	A	1002	6/6	0.90	0.19	80,82,85,86	0
5	EDO	A	1001	4/4	0.92	0.12	78,79,79,83	0
6	GOL	E	1002	6/6	0.96	0.08	83,85,85,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.