Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:56 PM GMT

PDB ID	:	1MQL
Title	:	BHA of Ukr/63
Authors	:	ha, y.; stevens, d.j.; skehel, j.j.; wiley, d.c.
Deposited on	:	2002-09-16
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

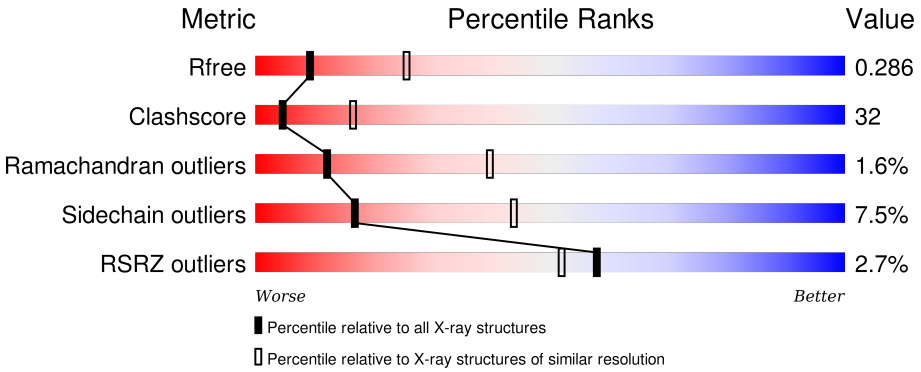
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	329	3% 43% 48% 6%
1	D	329	% 52% 40%
1	G	329	3% 46% 47%
2	B	221	2% 45% 29% 22%
2	E	221	3% 41% 32% 5% 22%

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Mol	Chain	Length	Quality of chain
2	H	221	2% 45% 29% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	333	-	-	X	-
3	NAG	A	335	-	-	X	-
3	NAG	H	341	-	-	-	X
4	NDG	A	334	-	-	X	X
4	NDG	B	223	-	-	-	X
4	NDG	D	332	-	-	X	-
4	NDG	G	330	-	-	X	-
4	NDG	G	333	-	-	-	X
4	NDG	G	334	-	-	X	-
4	NDG	G	336	-	-	-	X
5	MAN	A	336	-	-	X	-
5	MAN	D	334	X	-	X	-
5	MAN	D	335	X	-	-	-
5	MAN	G	331	X	-	X	-
5	MAN	G	332	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11890 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.

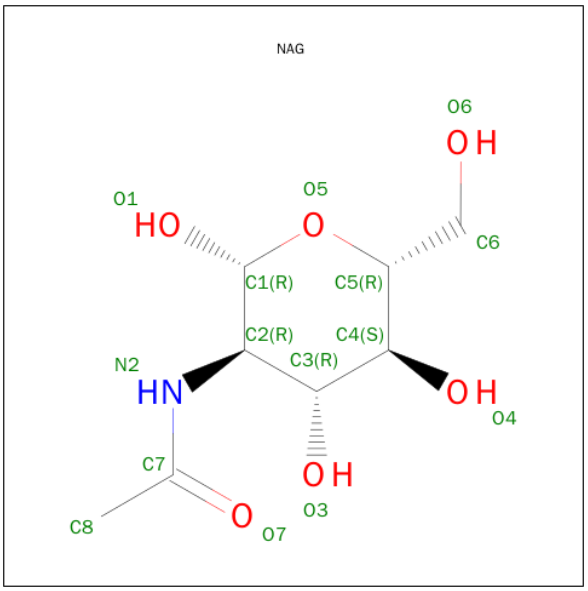
- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2425	1522	424	466	13			
1	D	318	Total	C	N	O	S	0	0	0
			2432	1526	425	468	13			
1	G	318	Total	C	N	O	S	0	0	0
			2426	1523	424	466	13			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

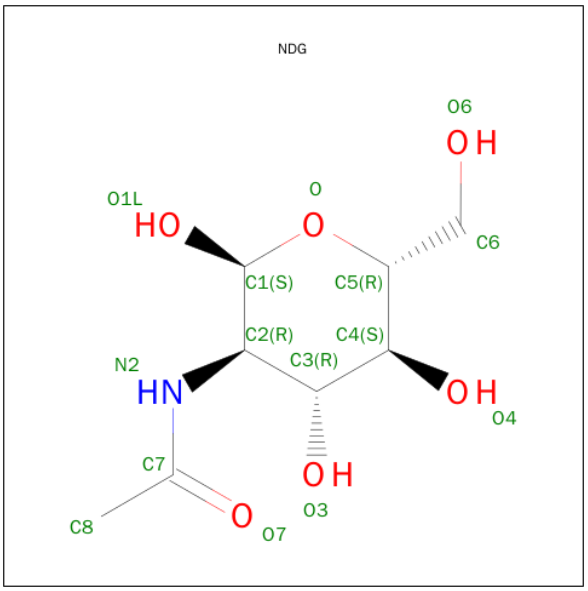
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1398	867	247	278	6			
2	E	172	Total	C	N	O	S	0	0	0
			1401	869	248	278	6			
2	H	172	Total	C	N	O	S	0	0	0
			1404	871	249	278	6			

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



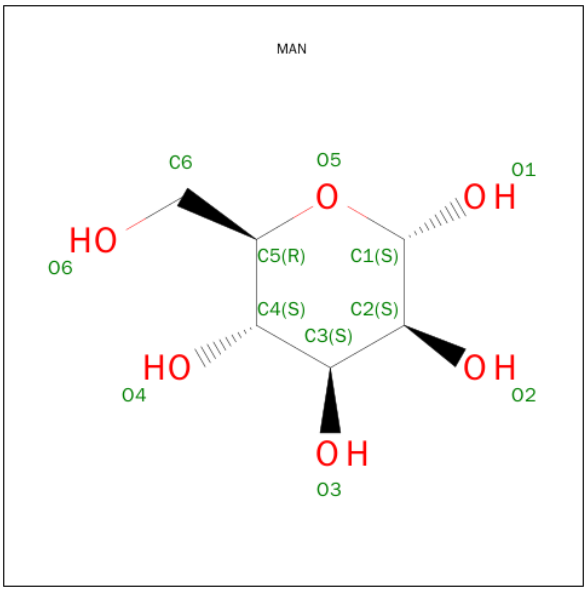
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 15 8 1 6	0	0
3	A	1	Total C N O 15 8 1 6	0	0
3	A	1	Total C N O 15 8 1 6	0	0
3	D	1	Total C N O 15 8 1 6	0	0
3	A	1	Total C N O 15 8 1 6	0	0
3	G	1	Total C N O 15 8 1 6	0	0
3	H	1	Total C N O 15 8 1 6	0	0

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 15 8 1 6	0	0
4	G	1	Total C N O 15 8 1 6	0	0
4	A	1	Total C N O 15 8 1 6	0	0
4	B	1	Total C N O 15 8 1 6	0	0
4	B	1	Total C N O 15 8 1 6	0	0
4	D	1	Total C N O 15 8 1 6	0	0
4	D	1	Total C N O 15 8 1 6	0	0
4	E	1	Total C N O 15 8 1 6	0	0
4	G	1	Total C N O 15 8 1 6	0	0
4	G	1	Total C N O 15 8 1 6	0	0
4	D	1	Total C N O 15 8 1 6	0	0
4	G	1	Total C N O 15 8 1 6	0	0

- Molecule 5 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total C O 12 6 6	0	0
5	G	1	Total C O 12 6 6	0	0
5	A	1	Total C O 12 6 6	0	0
5	A	1	Total C O 12 6 6	0	0
5	D	1	Total C O 12 6 6	0	0
5	D	1	Total C O 12 6 6	0	0

- Molecule 6 is water.

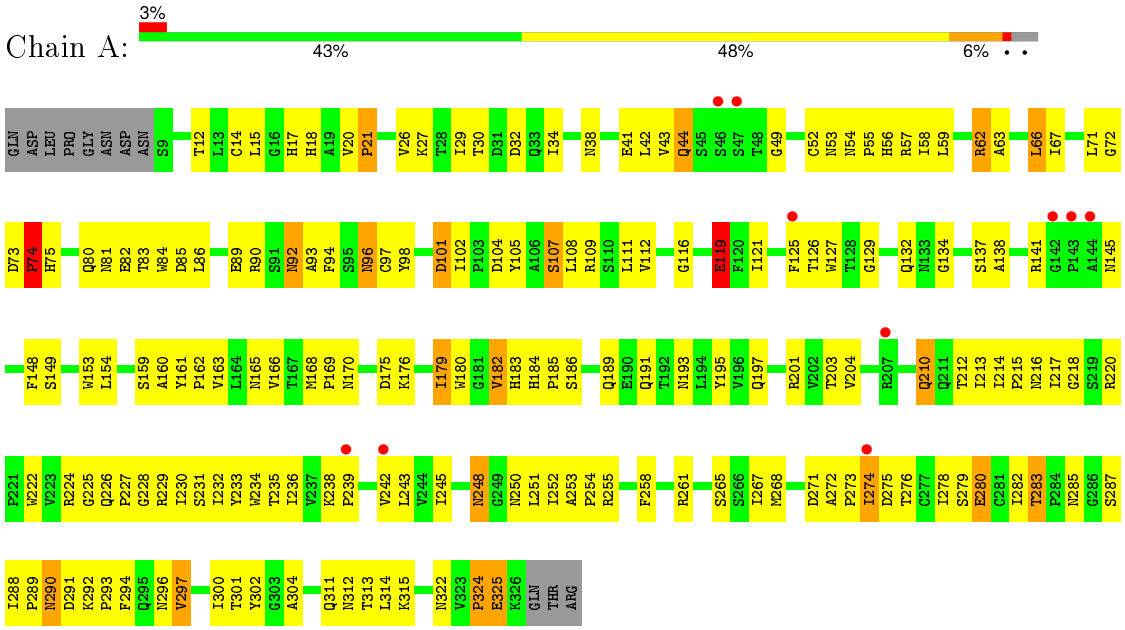
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	10	Total O 10 10	0	0
6	B	5	Total O 5 5	0	0
6	D	11	Total O 11 11	0	0
6	E	7	Total O 7 7	0	0
6	G	9	Total O 9 9	0	0
6	H	5	Total O 5 5	0	0

3 Residue-property plots (i)

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.

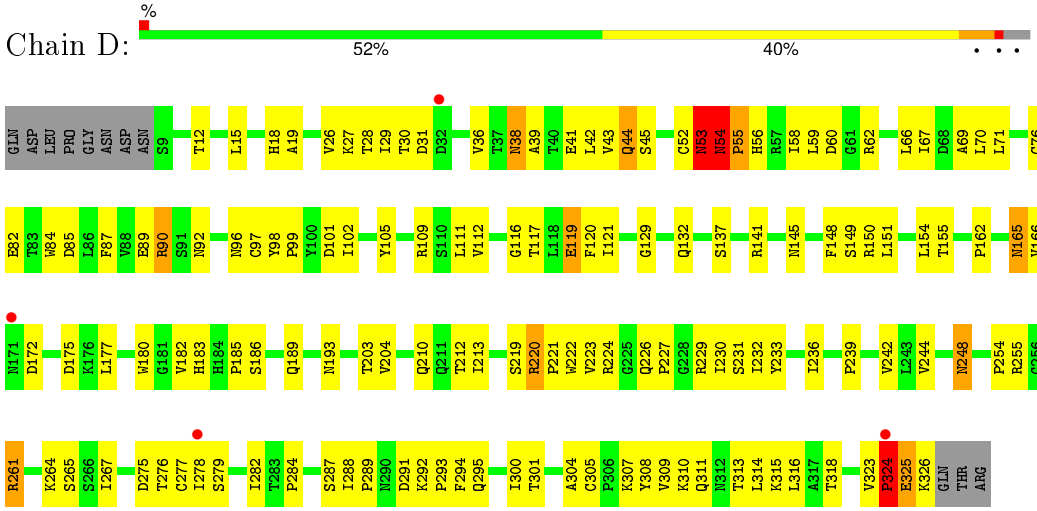
- Molecule 1: Hemagglutinin HA1 chain

Chain A:

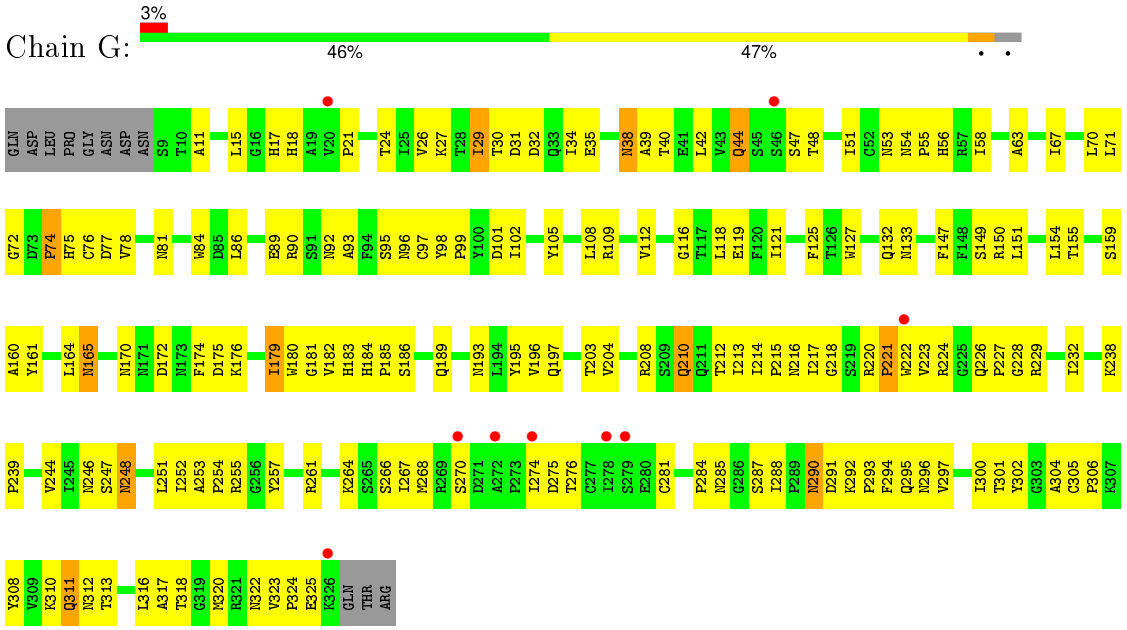


- Molecule 1: Hemagglutinin HA1 chain

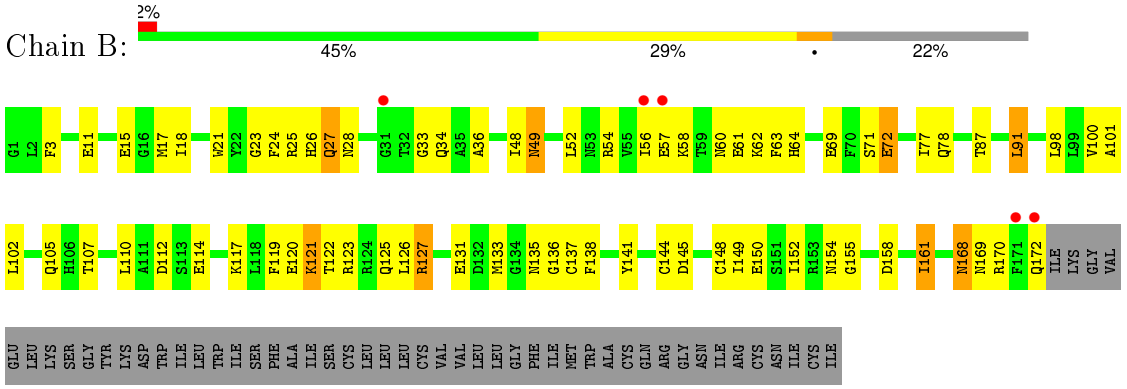
Chain D:



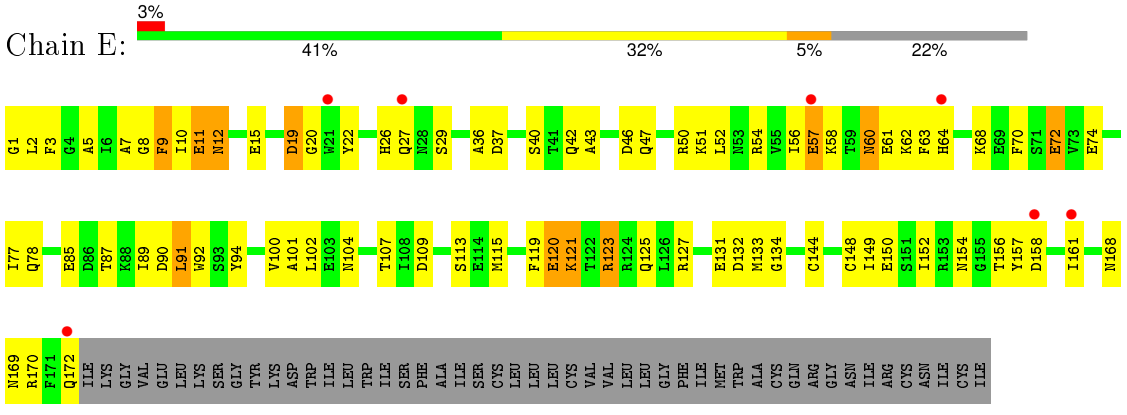
- Molecule 1: Hemagglutinin HA1 chain



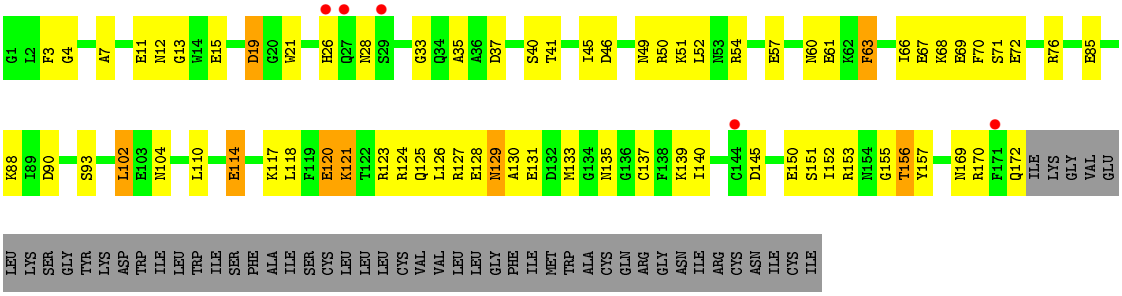
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain


G1 L2 F3 G4 A7 E11 N12 G13 W14 E15 D19 G20 W21 H26 Q27 N28 S29 G33 Q34 A35 A36 D37 S40 T41 I45 D46 N49 R50 K51 L52 N53 R54 E57 N60 E61 K62 F63 I66 E67 K68 E69 F70 S71 E72 R76 E85
K88 I89 D90 S93 L102 E103 N104 L110 E114 K117 L118 F119 E120 K121 T122 R123 R124 Q125 L126 R127 E128 N129 A130 E131 D132 M133 G134 N135 G136 C137 F138 K139 I140 C144 D145 E150 S151 I152 R153 N154 G155 T156 Y157 N169 R170 F171 Q172 ILE LYS GLY VAL GLU
LEU LYS SER GLY TYR LYS ASP TRP ILE LEU TRP ILE SER PHE ALA ILE SER CYS LEU LEU LEU CYS VAL VAL LEU LEU GLY PHE ILE MET TRP ALA CYS GLN ARG GLY ASN ILE ARG CYS ASN ILE CYS ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	147.68Å 147.10Å 251.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 40.15 – 2.91	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.90) 90.4 (40.15-2.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.269 , 0.306 0.251 , 0.286	Depositor DCC
R_{free} test set	2979 reflections (5.77%)	DCC
Wilson B-factor (Å^2)	64.4	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.1	EDS
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 58926 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11890	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NDG, 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	0.45	1/2482 (0.0%)	0.68	0/3390
1	D	0.46	1/2489 (0.0%)	0.75	3/3398 (0.1%)
1	G	0.47	1/2483 (0.0%)	0.72	0/3391
2	B	0.45	0/1422	0.63	0/1912
2	E	0.42	0/1425	0.63	0/1915
2	H	0.40	0/1428	0.65	0/1918
All	All	0.45	3/11729 (0.0%)	0.69	3/15924 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	119	GLU	CB-CG	-5.29	1.42	1.52
1	D	119	GLU	CB-CG	-5.07	1.42	1.52
1	A	119	GLU	CB-CG	-5.07	1.42	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	54	ASN	N-CA-C	7.32	130.76	111.00
1	D	54	ASN	C-N-CD	6.18	141.37	128.40
1	D	53	ASN	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2425	0	2339	185	0
1	D	2432	0	2352	160	0
1	G	2426	0	2341	191	0
2	B	1398	0	1309	90	0
2	E	1401	0	1318	89	0
2	H	1404	0	1327	80	0
3	A	60	0	60	24	0
3	D	15	0	15	1	0
3	G	15	0	15	4	0
3	H	15	0	15	2	0
4	A	30	0	30	15	0
4	B	30	0	30	9	0
4	D	45	0	44	15	0
4	E	15	0	15	5	0
4	G	60	0	60	28	0
5	A	24	0	24	8	0
5	D	24	0	24	6	0
5	G	24	0	24	6	0
6	A	10	0	0	6	0
6	B	5	0	0	0	0
6	D	11	0	0	0	0
6	E	7	0	0	2	0
6	G	9	0	0	6	0
6	H	5	0	0	1	0
All	All	11890	0	11342	743	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (743) 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:A:334:NDG:O4	4:B:222:NDG:H1	1.36	1.25
1:A:165:ASN:OD1	3:A:333:NAG:H1	1.40	1.19
2:B:125:GLN:HE22	2:B:155:GLY:HA2	1.09	1.18
4:D:333:NDG:H1	3:G:335:NAG:C4	1.81	1.10
4:D:333:NDG:O4	5:D:334:MAN:H1	1.51	1.10
3:A:333:NAG:H4	4:G:330:NDG:H1	1.33	1.08
3:A:333:NAG:H4	4:G:330:NDG:C1	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:333:NDG:C1	3:G:335:NAG:H4	1.86	1.04
1:A:81:ASN:ND2	4:A:331:NDG:H1	1.73	1.04
3:A:333:NAG:H61	4:G:330:NDG:H1	1.37	1.03
3:A:335:NAG:H4	5:A:336:MAN:H1	1.42	1.01
4:D:333:NDG:H1	3:G:335:NAG:H4	1.00	0.99
2:B:125:GLN:NE2	2:B:155:GLY:HA2	1.77	0.98
1:G:81:ASN:ND2	4:G:334:NDG:H1	1.78	0.96
1:A:29:ILE:HD11	2:B:102:LEU:HD12	1.44	0.95
1:A:285:ASN:HD21	4:A:334:NDG:H1	1.29	0.95
1:A:201:ARG:HA	6:A:345:HOH:O	1.69	0.93
1:A:214:ILE:HG12	6:A:345:HOH:O	1.69	0.92
1:G:44:GLN:HG2	1:G:292:LYS:HD3	1.51	0.92
1:A:285:ASN:ND2	4:A:334:NDG:H1	1.86	0.90
2:E:169:ASN:HA	2:E:172:GLN:HE21	1.37	0.90
1:A:81:ASN:ND2	1:A:119:GLU:HA	1.87	0.90
1:G:275:ASP:CG	1:G:276:THR:H	1.75	0.90
3:A:333:NAG:C4	4:G:330:NDG:H1	2.00	0.89
2:B:154:ASN:ND2	4:B:223:NDG:H1	1.88	0.89
2:B:154:ASN:HD21	4:B:223:NDG:H1	1.39	0.88
1:A:165:ASN:OD1	3:A:333:NAG:C1	2.23	0.87
1:G:248:ASN:H	1:G:248:ASN:HD22	1.21	0.87
2:B:144:CYS:SG	2:B:149:ILE:HD12	2.15	0.86
2:H:150:GLU:HG3	3:H:341:NAG:O1	1.76	0.84
3:A:335:NAG:H4	5:A:336:MAN:C1	2.06	0.84
3:A:335:NAG:C4	5:A:336:MAN:H1	2.07	0.84
4:A:334:NDG:O4	4:B:222:NDG:C1	2.26	0.83
1:D:165:ASN:HD21	4:D:332:NDG:C1	1.91	0.83
1:A:111:LEU:HD12	1:A:112:VAL:N	1.92	0.83
2:B:57:GLU:HG3	2:B:57:GLU:O	1.77	0.83
1:G:161:TYR:HB3	1:G:197:GLN:HE22	1.43	0.83
3:A:335:NAG:H82	4:D:332:NDG:H6C1	1.61	0.82
1:D:165:ASN:ND2	4:D:332:NDG:H1	1.94	0.82
1:D:89:GLU:HG3	1:D:267:ILE:HD11	1.63	0.81
4:A:334:NDG:C4	4:B:222:NDG:H1	2.11	0.80
2:E:12:ASN:HD22	2:E:12:ASN:N	1.76	0.80
2:H:57:GLU:HG3	2:H:57:GLU:O	1.80	0.80
3:A:333:NAG:H4	4:G:330:NDG:O	1.80	0.80
1:A:27:LYS:HE2	2:E:54:ARG:HH12	1.45	0.80
1:G:189:GLN:O	1:G:193:ASN:HB2	1.82	0.80
2:H:41:THR:O	2:H:45:ILE:HG13	1.82	0.80
3:A:333:NAG:C6	4:G:330:NDG:H1	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:ASN:HD21	4:G:334:NDG:C7	1.94	0.80
1:D:165:ASN:ND2	4:D:332:NDG:C1	2.45	0.79
2:E:57:GLU:HG3	2:E:57:GLU:O	1.84	0.78
1:A:170:ASN:OD1	1:A:176:LYS:HE3	1.83	0.78
1:G:316:LEU:HD23	2:H:52:LEU:HD13	1.65	0.78
1:D:43:VAL:HA	1:D:294:PHE:O	1.84	0.78
1:A:81:ASN:CG	4:A:331:NDG:H1	2.04	0.78
2:E:154:ASN:ND2	4:E:241:NDG:H1	2.01	0.76
1:G:67:ILE:HG13	1:G:105:TYR:CZ	2.21	0.76
1:G:39:ALA:O	4:G:333:NDG:H2	1.86	0.75
2:B:54:ARG:HG3	6:G:339:HOH:O	1.85	0.75
1:G:24:THR:OG1	4:G:333:NDG:H6C2	1.86	0.75
2:E:125:GLN:HE21	2:E:157:TYR:HB3	1.50	0.75
2:E:134:GLY:HA2	2:H:124:ARG:HD3	1.67	0.75
1:G:102:ILE:HG12	1:G:232:ILE:HB	1.66	0.75
1:D:169:PRO:CA	1:D:242:VAL:HG23	2.17	0.75
2:H:133:MET:SD	2:H:139:LYS:HB2	2.26	0.75
5:G:331:MAN:H2	5:G:332:MAN:H1	1.69	0.75
1:G:275:ASP:CG	1:G:276:THR:N	2.38	0.75
1:D:98:TYR:CD2	1:D:230:ILE:HD13	2.22	0.74
1:A:185:PRO:HG2	1:A:191:GLN:OE1	1.87	0.74
1:A:285:ASN:HD21	4:A:334:NDG:C1	1.98	0.74
2:E:72:GLU:HG2	1:G:238:LYS:NZ	2.02	0.74
1:G:11:ALA:HB3	2:H:140:ILE:HB	1.69	0.73
5:A:336:MAN:HO2	5:A:337:MAN:HO1	1.06	0.73
1:G:38:ASN:HD22	1:G:39:ALA:N	1.85	0.73
1:D:148:PHE:HB2	1:D:151:LEU:HD12	1.71	0.73
1:G:38:ASN:ND2	1:G:39:ALA:N	2.36	0.73
1:D:109:ARG:NH1	1:D:267:ILE:HD13	2.04	0.72
1:G:71:LEU:HD23	1:G:179:ILE:HD11	1.72	0.72
5:D:334:MAN:O2	5:D:335:MAN:H5	1.90	0.72
1:D:248:ASN:HD22	1:D:248:ASN:H	1.36	0.72
2:E:144:CYS:SG	2:E:149:ILE:HD12	2.30	0.72
1:A:304:ALA:HB2	2:B:61:GLU:HG2	1.72	0.71
1:D:52:CYS:HB2	1:D:279:SER:HB3	1.72	0.71
1:G:109:ARG:NH1	1:G:267:ILE:HD13	2.06	0.71
3:A:335:NAG:O1	4:D:332:NDG:O4	2.08	0.70
2:H:151:SER:HA	2:H:156:THR:HG23	1.74	0.70
1:A:71:LEU:HD23	1:A:179:ILE:HD11	1.74	0.70
1:A:96:ASN:HA	1:A:224:ARG:HE	1.56	0.69
1:G:292:LYS:O	1:G:306:PRO:HB3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD22	1:A:293:PRO:HG2	1.75	0.69
1:A:214:ILE:HA	6:A:345:HOH:O	1.92	0.69
1:A:180:TRP:HB3	1:A:254:PRO:HG3	1.74	0.69
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.73	0.69
1:A:17:HIS:HA	2:B:21:TRP:O	1.91	0.69
1:G:291:ASP:OD1	1:G:292:LYS:HG3	1.93	0.69
2:E:37:ASP:OD2	2:E:40:SER:HB2	1.92	0.69
1:D:66:LEU:HD21	1:D:112:VAL:HG12	1.75	0.69
3:A:333:NAG:H61	4:G:330:NDG:C1	2.18	0.69
5:G:331:MAN:C2	5:G:332:MAN:H1	2.23	0.69
1:A:185:PRO:HB2	1:A:217:ILE:HG13	1.75	0.69
2:H:169:ASN:HA	2:H:172:GLN:NE2	2.08	0.69
1:A:30:THR:O	2:E:50:ARG:HD2	1.94	0.68
1:G:151:LEU:HA	6:G:341:HOH:O	1.91	0.68
1:G:183:HIS:HB2	1:G:252:ILE:HD11	1.75	0.68
1:G:293:PRO:HB2	1:G:294:PHE:CE1	2.28	0.68
1:D:90:ARG:HD2	1:D:90:ARG:N	2.08	0.68
1:G:325:GLU:HG2	2:H:12:ASN:HD22	1.58	0.68
4:G:330:NDG:O4	5:G:331:MAN:H1	1.94	0.68
1:D:167:THR:OG1	4:D:332:NDG:H6C2	1.94	0.67
1:D:29:ILE:HD11	2:E:102:LEU:HD12	1.74	0.67
1:G:220:ARG:HB2	1:G:227:PRO:O	1.94	0.67
1:A:71:LEU:CD2	1:A:179:ILE:HD11	2.24	0.67
1:G:255:ARG:HG3	6:G:341:HOH:O	1.93	0.67
1:D:165:ASN:OD1	4:D:332:NDG:O1L	2.13	0.67
2:H:71:SER:C	2:H:72:GLU:HG3	2.15	0.67
1:A:175:ASP:OD1	1:A:239:PRO:HD3	1.95	0.67
1:A:184:HIS:HB3	1:A:220:ARG:HH21	1.60	0.67
2:B:158:ASP:HB3	2:B:161:ILE:HD12	1.76	0.66
1:A:12:THR:HG23	2:B:133:MET:HE3	1.78	0.66
2:B:28:ASN:HD22	2:B:145:ASP:HA	1.60	0.66
2:B:131:GLU:OE2	2:B:170:ARG:HD2	1.96	0.66
2:B:169:ASN:HA	2:B:172:GLN:HE21	1.61	0.66
4:A:331:NDG:O4	3:A:332:NAG:H1	1.96	0.65
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.77	0.65
1:D:169:PRO:N	1:D:242:VAL:HG23	2.11	0.65
2:B:77:ILE:HG23	2:B:78:GLN:N	2.10	0.65
2:B:54:ARG:HD3	1:G:32:ASP:HB3	1.78	0.65
1:A:96:ASN:HA	1:A:224:ARG:NE	2.11	0.65
1:G:290:ASN:C	1:G:290:ASN:HD22	1.99	0.65
2:B:11:GLU:OE1	2:B:11:GLU:HA	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLY:HA3	1:A:162:PRO:HG2	1.79	0.65
1:D:81:ASN:N	1:D:81:ASN:HD22	1.93	0.64
1:A:220:ARG:HD2	1:A:229:ARG:HG3	1.79	0.64
1:A:27:LYS:HE2	2:E:54:ARG:NH1	2.12	0.64
1:A:104:ASP:CG	1:A:107:SER:HB2	2.18	0.64
1:A:29:ILE:H	2:B:105:GLN:HE21	1.44	0.64
1:G:71:LEU:CD2	1:G:179:ILE:HD11	2.27	0.64
1:D:44:GLN:HG2	1:D:292:LYS:HD2	1.79	0.63
1:G:121:ILE:HD12	1:G:257:TYR:OH	1.98	0.63
1:D:54:ASN:O	1:D:55:PRO:C	2.29	0.63
2:E:51:LYS:HE3	2:E:107:THR:OG1	1.98	0.63
1:G:81:ASN:HD21	4:G:334:NDG:H1	1.64	0.63
1:D:97:CYS:O	1:D:224:ARG:NH1	2.31	0.63
1:D:180:TRP:HB3	1:D:254:PRO:HG3	1.79	0.63
1:A:166:VAL:HG22	1:A:245:ILE:HB	1.81	0.63
1:D:169:PRO:HA	1:D:242:VAL:HG23	1.80	0.62
1:G:220:ARG:CB	1:G:229:ARG:HH11	2.13	0.62
1:G:161:TYR:HB3	1:G:197:GLN:NE2	2.13	0.62
1:A:12:THR:HG23	2:B:133:MET:CE	2.30	0.62
1:A:170:ASN:HD22	1:A:238:LYS:C	2.02	0.62
2:H:21:TRP:H	2:H:41:THR:CG2	2.13	0.62
1:G:86:LEU:HD21	1:G:268:MET:HE3	1.82	0.62
1:G:161:TYR:CE1	1:G:195:TYR:HD2	2.18	0.62
2:H:35:ALA:HB2	2:H:153:ARG:NH1	2.14	0.62
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.33	0.62
2:H:151:SER:O	2:H:156:THR:HG23	1.99	0.62
1:D:97:CYS:H	1:D:224:ARG:NH1	1.98	0.62
1:A:125:PHE:O	1:A:126:THR:HG23	1.99	0.62
1:A:302:TYR:HE2	2:B:63:PHE:HB3	1.64	0.62
1:D:169:PRO:HA	1:D:242:VAL:HA	1.80	0.62
1:D:264:LYS:HB2	2:E:63:PHE:CG	2.35	0.62
2:E:154:ASN:CG	4:E:241:NDG:H1	2.20	0.61
1:D:279:SER:OG	1:D:287:SER:HB3	2.00	0.61
2:H:125:GLN:HE21	2:H:157:TYR:HB3	1.64	0.61
1:D:175:ASP:OD1	1:D:239:PRO:HD3	2.01	0.61
3:A:335:NAG:H1	4:D:332:NDG:H4	1.83	0.61
2:H:71:SER:O	2:H:72:GLU:HG3	2.00	0.61
2:B:26:HIS:CE1	2:B:33:GLY:HA3	2.36	0.61
2:E:43:ALA:O	2:E:47:GLN:HG3	2.00	0.61
2:E:12:ASN:ND2	2:E:12:ASN:N	2.49	0.61
1:G:15:LEU:HD23	2:H:118:LEU:HG	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:LEU:HD23	2:E:52:LEU:HD13	1.83	0.61
1:A:217:ILE:HD12	1:A:217:ILE:N	2.16	0.60
2:H:131:GLU:OE2	2:H:170:ARG:HD2	2.01	0.60
2:E:11:GLU:C	2:E:12:ASN:HD22	2.03	0.60
1:D:27:LYS:HB3	2:H:54:ARG:NH1	2.17	0.60
1:G:285:ASN:OD1	4:G:336:NDG:H1	2.01	0.60
1:A:248:ASN:HD22	1:A:248:ASN:H	1.48	0.60
2:H:19:ASP:N	2:H:19:ASP:OD1	2.35	0.60
1:D:326:LYS:N	2:E:12:ASN:OD1	2.31	0.60
1:G:220:ARG:HB3	1:G:229:ARG:NH1	2.17	0.60
2:B:102:LEU:HD21	2:E:102:LEU:HD23	1.83	0.60
1:G:53:ASN:HB3	1:G:275:ASP:O	2.02	0.60
1:G:220:ARG:CB	1:G:229:ARG:NH1	2.65	0.59
2:B:77:ILE:HG23	2:B:78:GLN:H	1.67	0.59
1:A:182:VAL:HG11	1:A:213:ILE:HG21	1.85	0.59
2:B:98:LEU:HD12	2:B:102:LEU:HD13	1.83	0.59
1:G:316:LEU:HD23	2:H:52:LEU:CD1	2.32	0.59
2:B:110:LEU:HD23	2:B:110:LEU:C	2.23	0.59
1:D:111:LEU:HD12	1:D:111:LEU:C	2.22	0.59
2:B:102:LEU:HD23	2:H:102:LEU:HD21	1.85	0.59
2:E:91:LEU:O	2:E:94:TYR:HB3	2.03	0.59
1:A:86:LEU:HD21	1:A:268:MET:HE3	1.83	0.59
2:B:149:ILE:HG22	2:B:150:GLU:N	2.17	0.58
1:G:38:ASN:HD22	1:G:38:ASN:C	2.06	0.58
1:A:300:ILE:HD11	2:B:69:GLU:HG3	1.85	0.58
2:E:3:PHE:CE1	2:E:113:SER:HB2	2.39	0.58
1:A:38:ASN:ND2	3:A:330:NAG:H1	2.18	0.58
1:G:311:GLN:NE2	2:H:93:SER:HB3	2.18	0.58
1:G:29:ILE:HG22	1:G:30:THR:HG23	1.85	0.58
1:G:56:HIS:O	1:G:58:ILE:HG13	2.03	0.58
1:G:220:ARG:HB2	1:G:229:ARG:HH11	1.67	0.58
1:G:42:LEU:O	1:G:292:LYS:HB3	2.03	0.58
1:D:220:ARG:HD2	1:D:229:ARG:HG2	1.84	0.58
1:D:30:THR:HG22	2:H:51:LYS:HB2	1.86	0.58
4:A:334:NDG:C3	4:B:222:NDG:H1	2.33	0.58
1:G:248:ASN:N	1:G:248:ASN:HD22	1.96	0.58
1:A:63:ALA:HA	1:A:93:ALA:HA	1.85	0.58
1:A:102:ILE:HG12	1:A:232:ILE:HB	1.86	0.58
1:G:183:HIS:O	1:G:185:PRO:HD3	2.04	0.57
1:A:184:HIS:HB3	1:A:220:ARG:NH2	2.19	0.57
1:D:120:PHE:CE2	1:D:150:ARG:HD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ASN:OD1	1:A:313:THR:HG22	2.04	0.57
1:G:98:TYR:CD2	1:G:99:PRO:HD2	2.39	0.57
1:G:24:THR:CG2	4:G:333:NDG:H6C2	2.35	0.57
1:G:81:ASN:ND2	4:G:334:NDG:C7	2.66	0.57
1:A:111:LEU:HD12	1:A:111:LEU:C	2.25	0.57
2:E:150:GLU:HA	2:E:150:GLU:OE2	2.04	0.57
1:A:302:TYR:CZ	2:B:63:PHE:HD2	2.23	0.57
2:E:100:VAL:HG23	2:E:101:ALA:N	2.20	0.57
2:E:131:GLU:OE2	2:E:170:ARG:HD2	2.04	0.57
1:G:99:PRO:HG3	1:G:223:VAL:HG12	1.87	0.57
1:D:167:THR:HG23	1:D:244:VAL:CG2	2.35	0.57
2:E:52:LEU:O	2:E:56:ILE:HG22	2.04	0.57
1:G:170:ASN:HA	1:G:176:LYS:NZ	2.19	0.56
1:A:125:PHE:HD1	1:A:127:TRP:H	1.53	0.56
1:A:280:GLU:OE1	1:A:280:GLU:HA	2.05	0.56
2:E:72:GLU:CG	1:G:238:LYS:NZ	2.68	0.56
5:G:331:MAN:O2	5:G:332:MAN:H1	2.03	0.56
1:G:281:CYS:HB2	1:G:304:ALA:O	2.04	0.56
2:H:68:LYS:HE2	2:H:85:GLU:OE1	2.05	0.56
1:G:288:ILE:HG21	1:G:297:VAL:HG21	1.88	0.56
1:A:81:ASN:CG	4:A:331:NDG:C1	2.74	0.56
1:A:54:ASN:HA	1:A:56:HIS:N	2.20	0.56
1:A:132:GLN:HG2	1:A:154:LEU:CD2	2.36	0.56
1:A:285:ASN:CG	4:A:334:NDG:H1	2.25	0.56
1:G:109:ARG:NH1	1:G:267:ILE:CD1	2.68	0.56
1:D:301:THR:HB	1:D:305:CYS:SG	2.46	0.56
2:E:169:ASN:HA	2:E:172:GLN:NE2	2.14	0.56
1:A:71:LEU:O	1:A:148:PHE:HB3	2.05	0.56
2:B:100:VAL:HG23	2:B:101:ALA:N	2.20	0.56
1:G:15:LEU:CD2	2:H:118:LEU:HG	2.37	0.55
2:B:121:LYS:HD2	2:B:121:LYS:O	2.06	0.55
1:A:159:SER:O	1:A:160:ALA:HB2	2.06	0.55
2:B:54:ARG:NH1	1:G:27:LYS:HE2	2.22	0.55
1:G:266:SER:OG	1:G:267:ILE:N	2.38	0.55
1:G:217:ILE:N	1:G:217:ILE:HD12	2.22	0.55
1:A:222:TRP:CZ3	5:A:336:MAN:O1	2.59	0.55
1:D:304:ALA:HB2	2:E:61:GLU:HG2	1.88	0.55
2:B:150:GLU:OE2	2:B:150:GLU:HA	2.07	0.55
1:A:275:ASP:CG	1:A:276:THR:N	2.60	0.55
1:A:42:LEU:HD22	1:A:293:PRO:CG	2.37	0.55
2:E:156:THR:HG1	4:E:241:NDG:H1L	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ALA:HB2	2:B:61:GLU:CG	2.37	0.55
1:A:74:PRO:HA	1:A:141:ARG:HH21	1.72	0.55
2:B:98:LEU:CD1	2:B:102:LEU:HD13	2.36	0.55
2:E:40:SER:O	2:E:43:ALA:HB3	2.05	0.55
1:A:189:GLN:O	1:A:193:ASN:HB2	2.06	0.55
2:H:151:SER:CA	2:H:156:THR:HG23	2.37	0.55
1:A:302:TYR:CE2	2:B:63:PHE:HB3	2.42	0.55
2:H:125:GLN:NE2	2:H:155:GLY:HA2	2.21	0.54
1:G:285:ASN:ND2	4:G:336:NDG:H1	2.23	0.54
1:A:274:ILE:HG12	1:A:274:ILE:O	2.05	0.54
1:G:81:ASN:ND2	4:G:334:NDG:C1	2.62	0.54
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.89	0.54
2:B:54:ARG:HA	2:B:58:LYS:NZ	2.23	0.54
1:D:102:ILE:HG12	1:D:232:ILE:HB	1.89	0.54
1:G:221:PRO:HA	4:G:330:NDG:O7	2.07	0.54
1:A:238:LYS:NZ	2:H:72:GLU:HG2	2.23	0.54
1:G:17:HIS:HB2	1:G:320:MET:SD	2.48	0.54
1:D:148:PHE:CB	1:D:151:LEU:HD12	2.36	0.54
1:A:38:ASN:HD21	3:A:330:NAG:H1	1.73	0.54
1:D:15:LEU:HD22	2:E:119:PHE:HA	1.90	0.54
1:G:165:ASN:CG	3:G:335:NAG:O1	2.46	0.54
2:E:154:ASN:HD21	4:E:241:NDG:H1	1.69	0.54
1:A:222:TRP:NE1	1:A:227:PRO:HG3	2.23	0.54
1:D:119:GLU:HB2	1:D:259:LYS:HG2	1.90	0.54
1:G:325:GLU:HG2	2:H:12:ASN:ND2	2.23	0.54
2:E:125:GLN:NE2	2:E:157:TYR:HB3	2.21	0.53
2:E:74:GLU:HG3	2:E:78:GLN:NE2	2.23	0.53
1:G:71:LEU:HD23	1:G:179:ILE:CD1	2.38	0.53
1:A:216:ASN:CB	1:D:212:THR:HG21	2.38	0.53
1:G:39:ALA:HB2	1:G:317:ALA:HA	1.89	0.53
1:A:43:VAL:HA	1:A:294:PHE:O	2.08	0.53
4:D:333:NDG:O4	5:D:334:MAN:C1	2.42	0.53
1:D:291:ASP:O	2:E:56:ILE:HG13	2.09	0.53
1:A:44:GLN:NE2	1:A:289:PRO:HD2	2.24	0.53
1:D:12:THR:O	2:E:26:HIS:HA	2.08	0.53
1:A:72:GLY:HA3	1:A:149:SER:OG	2.09	0.53
1:D:38:ASN:ND2	1:D:39:ALA:N	2.57	0.53
2:B:127:ARG:NH1	2:H:131:GLU:OE1	2.40	0.53
1:G:285:ASN:HD21	4:G:336:NDG:H1	1.73	0.53
1:A:26:VAL:O	1:A:34:ILE:HG22	2.08	0.53
1:A:304:ALA:CB	2:B:61:GLU:HG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:169:ASN:HA	2:H:172:GLN:HE21	1.74	0.53
1:D:53:ASN:HD22	1:D:54:ASN:N	2.07	0.53
2:E:77:ILE:HG23	2:E:78:GLN:N	2.23	0.53
1:A:204:VAL:CG1	1:A:243:LEU:HD11	2.37	0.53
2:B:87:THR:O	2:B:91:LEU:HD22	2.08	0.53
1:A:82:GLU:HG3	1:A:83:THR:H	1.74	0.53
1:D:28:THR:N	1:D:31:ASP:O	2.31	0.53
2:B:57:GLU:C	2:B:58:LYS:HG3	2.29	0.53
1:G:165:ASN:HD22	1:G:165:ASN:C	2.12	0.52
1:G:150:ARG:C	1:G:255:ARG:HD2	2.29	0.52
1:A:228:GLY:O	1:A:229:ARG:HG2	2.08	0.52
2:B:158:ASP:HB3	2:B:161:ILE:CD1	2.39	0.52
1:D:117:THR:HG21	1:D:261:ARG:HD2	1.91	0.52
1:D:129:GLY:HA3	1:D:162:PRO:HG2	1.91	0.52
2:E:22:TYR:HE2	2:E:115:MET:HB2	1.74	0.52
2:B:154:ASN:HD21	4:B:223:NDG:C1	2.16	0.52
2:B:150:GLU:HG3	4:B:223:NDG:O	2.10	0.52
1:A:43:VAL:HG23	6:A:347:HOH:O	2.08	0.52
1:D:183:HIS:O	1:D:185:PRO:HD3	2.10	0.52
2:H:123:ARG:HB3	2:H:123:ARG:HH11	1.75	0.52
1:D:304:ALA:CA	2:E:61:GLU:HG2	2.39	0.52
2:B:114:GLU:OE2	2:B:117:LYS:HD2	2.10	0.52
2:B:131:GLU:CG	2:B:170:ARG:HH11	2.22	0.52
1:D:180:TRP:CD2	1:D:204:VAL:HG21	2.45	0.52
1:D:119:GLU:HB2	1:D:259:LYS:CG	2.40	0.52
2:H:28:ASN:ND2	2:H:145:ASP:HA	2.25	0.52
2:B:48:ILE:HG12	2:B:107:THR:HG23	1.90	0.52
1:D:295:GLN:NE2	1:D:308:TYR:HD1	2.08	0.52
2:E:132:ASP:OD2	2:H:124:ARG:NE	2.40	0.52
1:A:233:TYR:CD1	1:A:233:TYR:N	2.76	0.52
1:D:98:TYR:CD2	1:D:99:PRO:HD2	2.44	0.52
1:G:323:VAL:HG21	2:H:7:ALA:HB2	1.92	0.52
1:A:203:THR:HG23	1:A:212:THR:HB	1.92	0.52
1:G:293:PRO:HB2	1:G:294:PHE:CD1	2.45	0.52
1:G:264:LYS:HB2	2:H:63:PHE:CG	2.45	0.52
1:G:84:TRP:CE2	1:G:116:GLY:HA2	2.45	0.52
1:G:228:GLY:C	1:G:229:ARG:HD2	2.31	0.52
2:B:126:LEU:HD21	2:B:152:ILE:HD13	1.91	0.52
1:D:167:THR:HG22	1:D:242:VAL:CG2	2.40	0.51
2:H:126:LEU:HD21	2:H:152:ILE:HD13	1.91	0.51
1:A:67:ILE:HG13	1:A:105:TYR:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:325:GLU:OE2	2:H:15:GLU:HG3	2.09	0.51
1:D:36:VAL:HG23	1:D:38:ASN:H	1.75	0.51
1:G:42:LEU:HD11	1:G:316:LEU:HB2	1.92	0.51
1:A:170:ASN:ND2	1:A:239:PRO:HA	2.24	0.51
1:G:154:LEU:HD12	1:G:251:LEU:HD23	1.92	0.51
1:A:92:ASN:HD22	1:A:93:ALA:N	2.07	0.51
1:G:99:PRO:HG3	1:G:223:VAL:CG1	2.40	0.51
1:A:275:ASP:CG	1:A:276:THR:H	2.13	0.51
1:A:279:SER:OG	1:A:287:SER:HB3	2.11	0.51
2:E:85:GLU:O	2:E:89:ILE:HG13	2.11	0.51
1:D:55:PRO:HG3	1:D:278:ILE:HG23	1.91	0.51
1:D:295:GLN:HE21	1:D:308:TYR:HB2	1.74	0.51
1:D:310:LYS:NZ	2:E:90:ASP:OD1	2.42	0.51
1:A:203:THR:HG21	1:G:220:ARG:NH1	2.25	0.51
5:D:334:MAN:HO2	5:D:335:MAN:H5	1.74	0.51
1:G:31:ASP:N	6:G:339:HOH:O	2.42	0.51
1:D:221:PRO:O	1:D:229:ARG:NH2	2.40	0.51
1:D:99:PRO:CB	1:D:229:ARG:HE	2.24	0.51
1:A:29:ILE:O	1:A:29:ILE:HG22	2.10	0.51
1:D:99:PRO:HG3	1:D:223:VAL:CG1	2.41	0.51
2:H:11:GLU:OE2	2:H:11:GLU:HA	2.11	0.51
1:A:236:ILE:N	1:A:236:ILE:HD12	2.26	0.51
1:D:53:ASN:HB3	1:D:275:ASP:O	2.11	0.51
1:D:311:GLN:HG3	1:D:314:LEU:HD11	1.92	0.51
2:H:135:ASN:OD1	2:H:137:CYS:SG	2.69	0.51
2:H:21:TRP:H	2:H:41:THR:HG23	1.74	0.50
1:G:290:ASN:ND2	1:G:290:ASN:O	2.44	0.50
2:H:46:ASP:O	2:H:50:ARG:HG3	2.11	0.50
2:B:135:ASN:OD1	2:B:137:CYS:HB2	2.11	0.50
1:A:228:GLY:C	1:A:229:ARG:HG2	2.32	0.50
1:G:220:ARG:HD2	1:G:229:ARG:HD3	1.93	0.50
3:A:335:NAG:H4	5:A:336:MAN:O1	2.09	0.50
2:E:57:GLU:C	2:E:58:LYS:HG3	2.30	0.50
1:D:54:ASN:C	1:D:56:HIS:N	2.58	0.50
1:G:108:LEU:O	1:G:112:VAL:HG23	2.10	0.50
1:D:58:ILE:HD11	1:D:282:ILE:CD1	2.41	0.50
2:E:8:GLY:O	2:E:10:ILE:N	2.45	0.50
2:B:158:ASP:OD1	2:B:161:ILE:HG13	2.12	0.50
1:D:80:GLN:O	1:D:81:ASN:HB2	2.10	0.50
1:D:264:LYS:HB2	2:E:63:PHE:CD1	2.46	0.50
1:G:127:TRP:CZ2	1:G:253:ALA:HB1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:LYS:HD2	2:B:121:LYS:C	2.32	0.50
1:A:235:THR:C	1:A:236:ILE:HD12	2.32	0.50
2:E:9:PHE:CD1	2:E:10:ILE:HG13	2.47	0.50
1:A:283:THR:C	1:A:285:ASN:H	2.15	0.50
1:G:90:ARG:HH22	1:G:274:ILE:HG13	1.77	0.50
2:B:125:GLN:HE22	2:B:155:GLY:CA	2.00	0.50
1:D:97:CYS:SG	1:D:98:TYR:N	2.84	0.50
1:G:180:TRP:HB3	1:G:254:PRO:HG3	1.94	0.50
1:D:42:LEU:O	1:D:293:PRO:HD2	2.11	0.50
1:G:89:GLU:HG3	1:G:267:ILE:HD11	1.93	0.49
1:G:325:GLU:HG2	2:H:13:GLY:O	2.12	0.49
1:G:63:ALA:HA	1:G:93:ALA:HA	1.93	0.49
1:G:81:ASN:HD21	4:G:334:NDG:C1	2.24	0.49
1:G:48:THR:HG23	1:G:287:SER:O	2.12	0.49
1:A:80:GLN:O	1:A:81:ASN:HB2	2.12	0.49
1:G:44:GLN:O	1:G:295:GLN:HA	2.12	0.49
1:A:195:TYR:CE2	1:A:250:ASN:HA	2.47	0.49
1:A:290:ASN:HD22	1:A:290:ASN:H	1.60	0.49
1:G:297:VAL:O	4:G:336:NDG:H8C1	2.12	0.49
1:G:304:ALA:HB2	2:H:61:GLU:HG2	1.95	0.49
2:H:110:LEU:HD23	2:H:110:LEU:C	2.32	0.49
1:G:222:TRP:CD1	1:G:227:PRO:HG3	2.48	0.49
1:A:96:ASN:ND2	1:A:96:ASN:C	2.64	0.49
1:D:60:ASP:HB3	1:D:62:ARG:NH1	2.27	0.49
1:A:220:ARG:NH1	1:D:203:THR:HG21	2.28	0.49
2:H:35:ALA:CB	2:H:153:ARG:NH1	2.75	0.49
1:A:134:GLY:CA	1:A:153:TRP:HB3	2.43	0.49
2:H:110:LEU:HD23	2:H:110:LEU:O	2.12	0.49
1:G:175:ASP:OD1	1:G:239:PRO:HD3	2.13	0.49
2:H:126:LEU:HD13	2:H:130:ALA:CB	2.43	0.49
1:D:71:LEU:HD11	1:D:232:ILE:CD1	2.43	0.49
1:A:163:VAL:O	1:A:163:VAL:HG12	2.13	0.49
3:A:335:NAG:C1	4:D:332:NDG:HC	2.23	0.49
1:G:295:GLN:NE2	1:G:308:TYR:HB2	2.28	0.49
2:E:54:ARG:HA	2:E:58:LYS:NZ	2.28	0.49
1:D:59:LEU:HD22	1:D:82:GLU:CG	2.43	0.48
1:G:222:TRP:CZ3	5:G:331:MAN:H3	2.48	0.48
1:D:26:VAL:CG1	1:D:27:LYS:N	2.76	0.48
1:A:279:SER:CB	1:A:287:SER:HB3	2.43	0.48
1:D:177:LEU:HD13	1:D:236:ILE:HD11	1.95	0.48
2:E:121:LYS:HD2	2:E:121:LYS:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:CYS:N	1:D:224:ARG:HH11	2.11	0.48
1:A:222:TRP:CD1	1:A:227:PRO:HG3	2.47	0.48
3:A:335:NAG:H1	4:D:332:NDG:C4	2.44	0.48
1:A:138:ALA:HB1	1:A:224:ARG:HB2	1.96	0.48
2:B:125:GLN:NE2	2:B:155:GLY:CA	2.64	0.48
1:G:305:CYS:HA	1:G:306:PRO:HD3	1.67	0.48
1:G:38:ASN:CG	4:G:333:NDG:H1	2.33	0.48
1:D:27:LYS:HB3	2:H:54:ARG:HH12	1.77	0.48
1:A:186:SER:HA	1:A:218:GLY:O	2.13	0.48
1:G:26:VAL:CG1	2:H:104:ASN:ND2	2.77	0.48
2:B:131:GLU:CD	2:B:170:ARG:HH11	2.16	0.48
1:G:290:ASN:C	1:G:290:ASN:ND2	2.66	0.48
1:G:97:CYS:SG	1:G:98:TYR:N	2.83	0.48
1:G:86:LEU:HD22	1:G:302:TYR:CD1	2.48	0.48
2:E:120:GLU:OE1	2:E:123:ARG:NH1	2.47	0.48
1:G:27:LYS:HG2	1:G:32:ASP:O	2.14	0.48
1:G:170:ASN:ND2	1:G:239:PRO:HA	2.28	0.48
1:G:251:LEU:HD21	1:G:253:ALA:HB2	1.96	0.48
1:A:73:ASP:OD1	1:A:74:PRO:HD2	2.14	0.48
1:D:55:PRO:HG3	1:D:278:ILE:CG2	2.44	0.48
1:D:213:ILE:HG12	1:D:233:TYR:CZ	2.49	0.48
2:E:154:ASN:OD1	4:E:241:NDG:H1	2.14	0.47
1:A:182:VAL:HG11	1:A:213:ILE:CG2	2.42	0.47
1:A:59:LEU:CD2	1:A:82:GLU:HG2	2.43	0.47
1:D:59:LEU:HD22	1:D:82:GLU:HG3	1.96	0.47
1:D:323:VAL:HG21	2:E:7:ALA:HB2	1.95	0.47
1:G:54:ASN:CG	1:G:55:PRO:HA	2.34	0.47
1:A:94:PHE:CD1	1:A:94:PHE:C	2.88	0.47
1:A:111:LEU:HD12	1:A:112:VAL:HG23	1.96	0.47
1:G:38:ASN:ND2	1:G:318:THR:OG1	2.47	0.47
1:D:294:PHE:HB3	1:D:309:VAL:HG22	1.95	0.47
1:G:95:SER:O	1:G:224:ARG:NH2	2.36	0.47
1:G:222:TRP:NE1	1:G:227:PRO:HG3	2.29	0.47
1:G:295:GLN:HE21	1:G:308:TYR:HB2	1.79	0.47
1:D:248:ASN:N	1:D:248:ASN:HD22	2.05	0.47
2:B:145:ASP:O	2:B:148:CYS:HB3	2.14	0.47
1:A:75:HIS:NE2	1:A:94:PHE:CE1	2.82	0.47
1:D:97:CYS:H	1:D:224:ARG:HH11	1.62	0.47
1:D:99:PRO:HB2	1:D:229:ARG:HE	1.79	0.47
1:A:104:ASP:OD1	1:A:107:SER:HB2	2.14	0.47
2:H:114:GLU:OE2	2:H:117:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:PHE:HB2	2:B:112:ASP:OD2	2.14	0.47
1:G:164:LEU:HB2	1:G:247:SER:O	2.15	0.47
1:G:179:ILE:O	1:G:179:ILE:HG12	2.13	0.47
1:A:216:ASN:HB2	1:D:212:THR:HG21	1.95	0.47
1:G:86:LEU:HD22	1:G:302:TYR:CG	2.49	0.47
1:A:55:PRO:HD3	1:A:278:ILE:HG23	1.96	0.47
2:E:9:PHE:CE1	2:E:10:ILE:HG13	2.49	0.47
6:A:340:HOH:O	1:G:216:ASN:HB3	2.14	0.47
1:G:222:TRP:CE2	4:G:330:NDG:H4	2.49	0.47
1:D:26:VAL:HG12	1:D:27:LYS:N	2.29	0.47
1:A:204:VAL:HG13	1:A:243:LEU:HD11	1.97	0.47
2:H:28:ASN:HD22	2:H:145:ASP:HA	1.80	0.47
1:G:220:ARG:HB2	1:G:229:ARG:NH1	2.27	0.47
1:G:81:ASN:CG	4:G:334:NDG:H1	2.31	0.47
2:B:141:TYR:CG	2:B:170:ARG:HG2	2.50	0.47
1:A:230:ILE:HD12	1:A:252:ILE:HG12	1.97	0.47
1:D:81:ASN:CG	3:D:331:NAG:HO1	2.10	0.47
2:B:17:MET:O	2:B:18:ILE:HD13	2.15	0.47
2:H:37:ASP:OD2	2:H:40:SER:HB2	2.15	0.47
1:G:67:ILE:HG13	1:G:105:TYR:OH	2.15	0.46
1:D:53:ASN:CG	1:D:276:THR:HA	2.35	0.46
2:H:129:ASN:OD1	2:H:129:ASN:N	2.47	0.46
1:A:251:LEU:HD12	1:A:252:ILE:N	2.30	0.46
1:D:165:ASN:ND2	1:D:165:ASN:C	2.68	0.46
1:A:285:ASN:OD1	4:A:334:NDG:H1	2.16	0.46
1:D:111:LEU:HD12	1:D:112:VAL:N	2.30	0.46
2:H:70:PHE:CD1	2:H:70:PHE:N	2.83	0.46
2:E:37:ASP:OD2	2:E:40:SER:CB	2.63	0.46
1:G:180:TRP:CE2	1:G:204:VAL:HG21	2.51	0.46
1:D:85:ASP:O	1:D:265:SER:HA	2.16	0.46
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.31	0.46
1:D:180:TRP:N	1:D:180:TRP:CD1	2.83	0.46
1:A:54:ASN:HA	1:A:56:HIS:H	1.79	0.46
1:G:34:ILE:HG12	1:G:35:GLU:N	2.31	0.46
1:D:27:LYS:HE2	2:H:54:ARG:CZ	2.46	0.46
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.80	0.46
1:A:90:ARG:HH11	1:A:271:ASP:HA	1.80	0.46
2:B:49:ASN:O	2:B:52:LEU:HB3	2.15	0.46
1:D:167:THR:HG22	1:D:242:VAL:HG21	1.98	0.46
1:G:285:ASN:CG	4:G:336:NDG:H1	2.36	0.46
1:G:311:GLN:HG2	1:G:311:GLN:H	1.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:ARG:HD2	1:D:229:ARG:CG	2.45	0.46
1:D:220:ARG:HH11	1:G:210:GLN:HG3	1.80	0.46
1:A:54:ASN:ND2	1:A:55:PRO:HA	2.30	0.46
1:G:90:ARG:HD3	1:G:270:SER:O	2.16	0.46
2:E:70:PHE:CD1	2:E:70:PHE:N	2.84	0.46
1:G:295:GLN:NE2	1:G:308:TYR:HD1	2.14	0.45
1:D:325:GLU:HA	2:E:12:ASN:HB3	1.97	0.45
2:E:8:GLY:C	2:E:10:ILE:N	2.69	0.45
1:A:288:ILE:HG21	1:A:297:VAL:HG21	1.98	0.45
2:E:60:ASN:HD22	2:E:60:ASN:C	2.17	0.45
1:G:228:GLY:O	1:G:229:ARG:HD2	2.16	0.45
3:A:333:NAG:C5	4:G:330:NDG:H1	2.45	0.45
1:G:34:ILE:CG1	1:G:35:GLU:N	2.79	0.45
1:A:291:ASP:OD1	1:A:292:LYS:HG3	2.17	0.45
1:A:324:PRO:O	1:A:325:GLU:CB	2.64	0.45
1:A:234:TRP:HD1	1:A:236:ILE:CD1	2.29	0.45
1:D:58:ILE:HD11	1:D:282:ILE:HD13	1.98	0.45
1:A:291:ASP:O	2:B:56:ILE:HG13	2.16	0.45
1:G:125:PHE:CE1	1:G:254:PRO:HB2	2.52	0.45
1:D:120:PHE:CD2	1:D:150:ARG:HD2	2.51	0.45
1:D:165:ASN:HD22	1:D:165:ASN:C	2.20	0.45
1:G:38:ASN:ND2	1:G:38:ASN:C	2.69	0.45
1:D:60:ASP:OD2	1:D:90:ARG:NH1	2.50	0.45
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.81	0.45
1:A:82:GLU:HG3	1:A:83:THR:N	2.32	0.45
1:G:220:ARG:O	1:G:227:PRO:HA	2.16	0.45
1:D:87:PHE:O	1:D:267:ILE:HG13	2.17	0.45
1:D:222:TRP:NE1	1:D:227:PRO:HG3	2.31	0.45
1:G:186:SER:HA	1:G:218:GLY:O	2.17	0.45
1:D:137:SER:HA	1:D:145:ASN:OD1	2.17	0.45
2:E:19:ASP:OD1	2:E:19:ASP:N	2.47	0.45
2:B:27:GLN:HB3	2:B:27:GLN:HE21	1.51	0.45
1:A:27:LYS:HG2	1:A:32:ASP:O	2.17	0.45
1:D:66:LEU:HD21	1:D:112:VAL:CG1	2.44	0.45
1:G:147:PHE:CE2	1:G:151:LEU:HB2	2.51	0.45
1:D:12:THR:HG23	2:E:133:MET:CE	2.47	0.45
1:G:161:TYR:HE1	1:G:195:TYR:HD2	1.62	0.45
1:A:217:ILE:CD1	1:A:217:ILE:N	2.80	0.45
1:G:181:GLY:O	1:G:252:ILE:HB	2.17	0.45
1:A:53:ASN:OD1	1:A:276:THR:HA	2.17	0.45
1:A:314:LEU:HB2	6:A:347:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:THR:C	1:A:285:ASN:N	2.70	0.44
2:H:156:THR:HG21	3:H:341:NAG:H1	1.99	0.44
2:E:121:LYS:HD2	2:E:121:LYS:C	2.37	0.44
1:D:67:ILE:O	1:D:70:LEU:HB3	2.17	0.44
5:D:334:MAN:O2	5:D:335:MAN:C5	2.62	0.44
1:A:108:LEU:O	1:A:109:ARG:C	2.55	0.44
1:D:109:ARG:NH1	1:D:267:ILE:CD1	2.78	0.44
1:D:324:PRO:O	1:D:325:GLU:CB	2.65	0.44
1:A:89:GLU:HG3	1:A:267:ILE:HD11	2.00	0.44
1:D:41:GLU:HG2	1:D:315:LYS:NZ	2.32	0.44
1:D:19:ALA:O	2:E:15:GLU:HA	2.17	0.44
1:D:167:THR:HG23	1:D:244:VAL:HG22	1.98	0.44
1:A:302:TYR:CE2	2:B:63:PHE:HD2	2.35	0.44
2:E:77:ILE:CG2	2:E:78:GLN:N	2.80	0.44
1:G:195:TYR:O	1:G:196:VAL:HB	2.18	0.44
1:D:304:ALA:CB	2:E:61:GLU:HG2	2.48	0.44
1:G:159:SER:O	1:G:160:ALA:HB2	2.18	0.44
1:D:29:ILE:HD11	2:E:102:LEU:CD1	2.44	0.44
1:G:67:ILE:O	1:G:70:LEU:N	2.50	0.44
1:D:186:SER:HB3	1:D:227:PRO:HB2	1.99	0.44
1:A:253:ALA:HA	1:A:254:PRO:HD3	1.77	0.44
1:G:252:ILE:HG22	1:G:252:ILE:O	2.18	0.44
1:D:203:THR:OG1	1:D:212:THR:HB	2.18	0.44
2:B:158:ASP:CG	2:B:161:ILE:HG13	2.37	0.44
2:B:169:ASN:HA	2:B:172:GLN:NE2	2.31	0.44
1:G:47:SER:HA	1:G:288:ILE:HG22	1.99	0.44
1:G:213:ILE:HG22	1:G:214:ILE:N	2.32	0.44
1:D:307:LYS:HE2	2:E:60:ASN:HD21	1.81	0.44
1:G:264:LYS:HB2	2:H:63:PHE:CD1	2.53	0.44
2:E:8:GLY:C	2:E:10:ILE:H	2.21	0.44
2:B:71:SER:C	2:B:72:GLU:HG3	2.37	0.44
1:G:291:ASP:OD1	1:G:292:LYS:HD2	2.17	0.44
1:G:253:ALA:HA	1:G:254:PRO:HD3	1.70	0.44
1:D:189:GLN:O	1:D:193:ASN:HB2	2.18	0.44
1:G:132:GLN:HG2	1:G:154:LEU:CD2	2.48	0.44
2:B:131:GLU:CG	2:B:170:ARG:NH1	2.81	0.44
1:D:167:THR:HG23	1:D:244:VAL:HG23	2.00	0.43
1:A:111:LEU:CD1	1:A:112:VAL:HG23	2.48	0.43
1:G:67:ILE:O	1:G:70:LEU:HB3	2.17	0.43
1:D:221:PRO:HG3	1:G:244:VAL:CG2	2.48	0.43
2:B:168:ASN:O	2:B:172:GLN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2:LEU:HB3	2:H:3:PHE:CZ	2.53	0.43
2:B:23:GLY:HA3	2:B:36:ALA:HA	2.00	0.43
1:G:300:ILE:HD11	2:H:69:GLU:HG3	2.00	0.43
1:G:248:ASN:H	1:G:248:ASN:ND2	2.02	0.43
2:B:168:ASN:ND2	2:B:168:ASN:O	2.50	0.43
1:A:125:PHE:HB2	1:A:127:TRP:CD1	2.54	0.43
1:A:92:ASN:C	1:A:92:ASN:HD22	2.19	0.43
1:G:76:CYS:C	1:G:78:VAL:H	2.20	0.43
1:A:212:THR:HG21	1:G:216:ASN:HB2	2.00	0.43
1:D:98:TYR:CE2	1:D:230:ILE:HD13	2.52	0.43
1:D:77:ASP:OD2	1:D:141:ARG:NH1	2.51	0.43
1:A:272:ALA:HA	1:A:273:PRO:HD3	1.90	0.43
1:A:165:ASN:HA	1:A:245:ILE:O	2.18	0.43
1:A:119:GLU:O	1:A:258:PHE:HA	2.19	0.43
1:D:166:VAL:HG12	1:D:167:THR:N	2.34	0.43
1:A:29:ILE:HD11	2:B:102:LEU:CD1	2.31	0.43
1:G:26:VAL:HG12	1:G:27:LYS:O	2.18	0.43
2:B:77:ILE:CG2	2:B:78:GLN:N	2.79	0.43
1:G:310:LYS:HE2	2:H:90:ASP:OD1	2.18	0.43
1:D:294:PHE:HA	1:D:307:LYS:O	2.18	0.43
2:H:21:TRP:CG	2:H:41:THR:HG23	2.54	0.43
1:G:172:ASP:HB3	1:G:174:PHE:CE2	2.54	0.43
1:A:96:ASN:HD22	1:A:96:ASN:C	2.22	0.43
1:G:323:VAL:CG2	2:H:7:ALA:HB2	2.48	0.43
1:G:84:TRP:HZ3	1:G:118:LEU:HG	1.84	0.43
1:A:121:ILE:HG22	1:A:121:ILE:O	2.19	0.43
1:G:322:ASN:O	1:G:324:PRO:HD3	2.19	0.43
1:A:73:ASP:OD1	1:A:96:ASN:ND2	2.52	0.43
1:A:116:GLY:HA3	1:A:265:SER:OG	2.19	0.43
2:B:15:GLU:O	2:B:18:ILE:HD11	2.18	0.43
1:D:84:TRP:CE2	1:D:116:GLY:HA2	2.53	0.43
2:E:87:THR:HG23	2:H:88:LYS:HG3	2.00	0.43
1:G:72:GLY:HA3	1:G:149:SER:OG	2.18	0.43
1:A:41:GLU:HG2	1:A:315:LYS:NZ	2.34	0.43
1:G:44:GLN:N	1:G:292:LYS:HZ2	2.17	0.43
1:D:53:ASN:OD1	1:D:276:THR:HA	2.19	0.43
2:H:125:GLN:HE22	2:H:152:ILE:HA	1.83	0.43
1:G:98:TYR:CE1	1:G:226:GLN:HG3	2.54	0.43
1:A:67:ILE:HG13	1:A:105:TYR:CE1	2.54	0.43
1:G:224:ARG:HG3	1:G:224:ARG:NH1	2.34	0.43
1:D:132:GLN:HG2	1:D:154:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:SER:HA	1:A:145:ASN:OD1	2.18	0.43
2:H:127:ARG:HB3	2:H:128:GLU:H	1.53	0.43
1:G:291:ASP:OD1	1:G:292:LYS:CG	2.65	0.43
1:G:325:GLU:OE2	2:H:15:GLU:CG	2.67	0.43
1:A:210:GLN:HE21	1:A:210:GLN:HB3	1.54	0.43
2:B:91:LEU:HD13	2:E:92:TRP:CE2	2.54	0.42
1:A:52:CYS:SG	1:A:279:SER:HB2	2.59	0.42
5:D:334:MAN:C2	5:D:335:MAN:H1	2.49	0.42
1:A:214:ILE:HA	1:A:215:PRO:HD3	1.94	0.42
2:B:168:ASN:ND2	2:B:168:ASN:C	2.72	0.42
2:E:5:ALA:O	2:E:10:ILE:HB	2.19	0.42
2:E:1:GLY:HA2	2:E:109:ASP:OD1	2.19	0.42
1:G:320:MET:CE	2:H:21:TRP:HB3	2.49	0.42
1:D:220:ARG:HB2	1:D:227:PRO:O	2.19	0.42
2:B:133:MET:HE2	2:B:138:PHE:C	2.39	0.42
1:D:311:GLN:HE21	1:D:314:LEU:HD11	1.84	0.42
1:G:214:ILE:HA	1:G:215:PRO:HD3	1.91	0.42
1:A:20:VAL:N	1:A:322:ASN:OD1	2.49	0.42
1:G:67:ILE:HG13	1:G:105:TYR:CE1	2.54	0.42
1:A:29:ILE:O	1:A:29:ILE:CG2	2.68	0.42
1:A:34:ILE:O	1:A:34:ILE:HG23	2.20	0.42
2:B:18:ILE:O	2:B:18:ILE:HG22	2.19	0.42
1:D:69:ALA:HA	1:D:76:CYS:HB3	2.02	0.42
1:G:312:ASN:OD1	1:G:313:THR:HG22	2.19	0.42
2:H:4:GLY:HA2	6:H:345:HOH:O	2.18	0.42
1:A:168:MET:C	1:A:242:VAL:HG23	2.40	0.42
3:A:335:NAG:C4	5:A:336:MAN:C1	2.82	0.42
1:D:53:ASN:ND2	1:D:54:ASN:N	2.68	0.42
1:D:149:SER:O	1:D:255:ARG:HD2	2.20	0.42
1:G:301:THR:HB	1:G:305:CYS:SG	2.60	0.42
2:B:25:ARG:NE	2:B:34:GLN:OE1	2.37	0.42
2:H:66:ILE:HG13	2:H:67:GLU:O	2.20	0.42
2:B:122:THR:O	2:B:123:ARG:C	2.58	0.42
1:G:311:GLN:HE21	2:H:93:SER:HB3	1.84	0.42
1:D:304:ALA:HA	2:E:61:GLU:HG2	2.02	0.42
1:D:29:ILE:O	1:D:29:ILE:HG22	2.18	0.42
1:A:138:ALA:HB2	1:A:226:GLN:HG2	2.02	0.42
2:B:100:VAL:CG2	2:B:101:ALA:N	2.82	0.42
1:D:67:ILE:HA	1:D:67:ILE:HD13	1.89	0.42
2:B:150:GLU:O	2:B:154:ASN:ND2	2.53	0.41
2:B:61:GLU:O	2:B:62:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:ASN:HD22	2:B:168:ASN:C	2.22	0.41
1:G:184:HIS:HB3	1:G:220:ARG:NH2	2.35	0.41
1:A:108:LEU:HD12	1:A:111:LEU:HD11	2.02	0.41
2:E:152:ILE:HA	2:E:157:TYR:HB2	2.01	0.41
2:E:149:ILE:HG22	2:E:150:GLU:N	2.35	0.41
1:D:55:PRO:HD3	1:D:278:ILE:HA	2.02	0.41
2:E:68:LYS:HA	6:E:242:HOH:O	2.20	0.41
2:E:20:GLY:HA3	2:E:36:ALA:HB1	2.00	0.41
1:D:219:SER:H	1:G:246:ASN:ND2	2.18	0.41
2:E:57:GLU:CG	2:E:57:GLU:O	2.61	0.41
1:D:99:PRO:HB3	1:D:229:ARG:NE	2.35	0.41
1:D:98:TYR:HA	1:D:99:PRO:HD3	1.92	0.41
2:H:126:LEU:HD13	2:H:130:ALA:HB3	2.02	0.41
1:A:300:ILE:O	1:A:301:THR:CG2	2.68	0.41
1:D:284:PRO:CG	1:D:300:ILE:HB	2.51	0.41
1:A:62:ARG:HH11	1:A:62:ARG:HG2	1.85	0.41
2:E:148:CYS:O	2:E:152:ILE:HG13	2.21	0.41
1:D:26:VAL:CG1	2:E:104:ASN:ND2	2.83	0.41
1:A:58:ILE:HD11	1:A:282:ILE:CD1	2.51	0.41
1:A:97:CYS:SG	1:A:98:TYR:N	2.93	0.41
1:G:170:ASN:HD22	1:G:238:LYS:C	2.23	0.41
1:D:26:VAL:HG11	2:E:104:ASN:CG	2.41	0.41
1:G:203:THR:HG23	1:G:212:THR:HB	2.02	0.41
1:A:49:GLY:O	1:A:273:PRO:HD2	2.21	0.41
1:A:169:PRO:HA	1:A:242:VAL:HG23	2.02	0.41
1:A:101:ASP:O	1:A:231:SER:HA	2.21	0.41
1:G:248:ASN:N	1:G:248:ASN:ND2	2.67	0.41
1:D:284:PRO:HG2	1:D:300:ILE:HB	2.02	0.41
2:B:71:SER:OG	2:B:72:GLU:OE2	2.39	0.41
1:A:14:CYS:O	2:B:24:PHE:HA	2.20	0.41
4:A:334:NDG:H3	4:B:222:NDG:O1L	2.20	0.41
1:A:222:TRP:CE3	1:A:225:GLY:HA2	2.56	0.41
1:A:26:VAL:CG1	1:A:27:LYS:N	2.83	0.41
1:D:99:PRO:CB	1:D:229:ARG:NE	2.83	0.41
2:B:119:PHE:CE1	2:B:136:GLY:HA2	2.55	0.41
1:A:125:PHE:CD1	1:A:126:THR:N	2.89	0.41
1:D:172:ASP:O	1:D:239:PRO:HB3	2.20	0.41
1:D:27:LYS:HE2	2:H:54:ARG:NH2	2.36	0.41
1:A:300:ILE:C	1:A:301:THR:HG23	2.42	0.41
1:A:53:ASN:O	1:A:54:ASN:HB3	2.20	0.41
2:E:61:GLU:O	2:E:62:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:GLU:HG3	2:H:123:ARG:NH1	2.36	0.41
1:D:67:ILE:HG13	1:D:105:TYR:CZ	2.56	0.41
2:H:26:HIS:CE1	2:H:33:GLY:HA3	2.56	0.41
6:E:248:HOH:O	1:G:208:ARG:CG	2.68	0.41
2:E:158:ASP:HB3	2:E:161:ILE:HD12	2.02	0.41
3:A:335:NAG:O3	5:A:336:MAN:C1	2.69	0.41
1:G:295:GLN:HG3	1:G:306:PRO:O	2.21	0.41
1:D:226:GLN:HA	1:D:227:PRO:HD3	1.84	0.41
1:G:254:PRO:HA	6:G:341:HOH:O	2.21	0.41
1:G:304:ALA:HA	2:H:61:GLU:HA	2.03	0.41
1:G:212:THR:O	1:G:213:ILE:HD13	2.21	0.41
1:D:313:THR:O	1:D:313:THR:HG23	2.21	0.41
4:G:330:NDG:O4	5:G:331:MAN:C1	2.65	0.40
2:H:151:SER:HA	2:H:156:THR:CG2	2.48	0.40
1:G:101:ASP:O	1:G:232:ILE:N	2.52	0.40
1:D:44:GLN:HG2	1:D:292:LYS:CD	2.50	0.40
1:A:57:ARG:O	1:A:85:ASP:HB2	2.22	0.40
1:G:77:ASP:HA	6:G:343:HOH:O	2.19	0.40
1:A:283:THR:O	1:A:285:ASN:N	2.54	0.40
1:A:285:ASN:HD21	4:A:334:NDG:C2	2.34	0.40
2:B:122:THR:O	2:B:125:GLN:N	2.54	0.40
2:B:102:LEU:HD21	2:E:102:LEU:CD2	2.48	0.40
1:G:292:LYS:HA	1:G:293:PRO:HD3	1.94	0.40
1:D:324:PRO:O	1:D:325:GLU:HB2	2.21	0.40
1:D:99:PRO:HG3	1:D:223:VAL:HG12	2.02	0.40
1:G:121:ILE:HD12	1:G:257:TYR:CZ	2.56	0.40
2:E:42:GLN:HG3	2:E:46:ASP:OD2	2.22	0.40
1:A:66:LEU:HG	1:A:66:LEU:O	2.22	0.40
1:D:288:ILE:HA	1:D:289:PRO:HD3	1.84	0.40
2:B:150:GLU:CA	2:B:150:GLU:OE2	2.69	0.40
1:G:170:ASN:ND2	1:G:238:LYS:C	2.75	0.40
2:E:74:GLU:HG3	2:E:78:GLN:HE21	1.86	0.40
2:H:117:LYS:O	2:H:121:LYS:HB2	2.22	0.40
1:A:20:VAL:HB	1:A:21:PRO:CD	2.52	0.40
1:A:220:ARG:HH12	1:D:203:THR:HG21	1.86	0.40
1:D:27:LYS:CB	2:H:54:ARG:HH12	2.35	0.40
1:G:51:ILE:HG22	1:G:58:ILE:CD1	2.51	0.40
2:E:100:VAL:CG2	2:E:101:ALA:N	2.85	0.40
1:D:121:ILE:HD12	1:D:257:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	316/329 (96%)	268 (85%)	40 (13%)	8 (2%)	7 27
1	D	316/329 (96%)	283 (90%)	30 (10%)	3 (1%)	21 57
1	G	316/329 (96%)	276 (87%)	35 (11%)	5 (2%)	12 40
2	B	170/221 (77%)	145 (85%)	24 (14%)	1 (1%)	30 67
2	E	170/221 (77%)	153 (90%)	13 (8%)	4 (2%)	7 29
2	H	170/221 (77%)	150 (88%)	18 (11%)	2 (1%)	16 48
All	All	1458/1650 (88%)	1275 (87%)	160 (11%)	23 (2%)	12 40

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	PRO
1	A	325	GLU
1	D	324	PRO
1	D	325	GLU
1	G	133	ASN
2	H	63	PHE
1	A	21	PRO
1	A	119	GLU
2	E	11	GLU
1	G	74	PRO
1	G	75	HIS
2	H	76	ARG
1	D	54	ASN
2	E	29	SER
2	E	57	GLU
1	A	66	LEU
1	A	74	PRO
2	B	161	ILE
1	A	62	ARG
2	E	9	PHE

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Mol	Chain	Res	Type
1	A	297	VAL
1	G	21	PRO
1	G	221	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/288 (93%)	248 (92%)	20 (8%)	17	44
1	D	270/288 (94%)	247 (92%)	23 (8%)	13	37
1	G	268/288 (93%)	249 (93%)	19 (7%)	18	47
2	B	145/190 (76%)	135 (93%)	10 (7%)	19	48
2	E	146/190 (77%)	134 (92%)	12 (8%)	14	39
2	H	147/190 (77%)	138 (94%)	9 (6%)	23	56
All	All	1244/1434 (87%)	1151 (92%)	93 (8%)	17	44

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	44	GLN
1	A	74	PRO
1	A	92	ASN
1	A	96	ASN
1	A	101	ASP
1	A	107	SER
1	A	161	TYR
1	A	179	ILE
1	A	182	VAL
1	A	197	GLN
1	A	210	GLN
1	A	248	ASN
1	A	261	ARG
1	A	274	ILE

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Mol	Chain	Res	Type
1	A	280	GLU
1	A	283	THR
1	A	290	ASN
1	A	296	ASN
1	A	311	GLN
2	B	27	GLN
2	B	49	ASN
2	B	60	ASN
2	B	64	HIS
2	B	72	GLU
2	B	91	LEU
2	B	120	GLU
2	B	121	LYS
2	B	127	ARG
2	B	168	ASN
1	D	18	HIS
1	D	38	ASN
1	D	44	GLN
1	D	45	SER
1	D	53	ASN
1	D	55	PRO
1	D	81	ASN
1	D	90	ARG
1	D	92	ASN
1	D	96	ASN
1	D	101	ASP
1	D	155	THR
1	D	165	ASN
1	D	167	THR
1	D	182	VAL
1	D	210	GLN
1	D	220	ARG
1	D	231	SER
1	D	248	ASN
1	D	261	ARG
1	D	277	CYS
1	D	318	THR
1	D	324	PRO
2	E	12	ASN
2	E	19	ASP
2	E	27	GLN
2	E	60	ASN

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Mol	Chain	Res	Type
2	E	64	HIS
2	E	72	GLU
2	E	91	LEU
2	E	120	GLU
2	E	121	LYS
2	E	123	ARG
2	E	127	ARG
2	E	168	ASN
1	G	18	HIS
1	G	29	ILE
1	G	38	ASN
1	G	40	THR
1	G	44	GLN
1	G	74	PRO
1	G	92	ASN
1	G	96	ASN
1	G	155	THR
1	G	165	ASN
1	G	179	ILE
1	G	182	VAL
1	G	210	GLN
1	G	248	ASN
1	G	261	ARG
1	G	284	PRO
1	G	290	ASN
1	G	296	ASN
1	G	311	GLN
2	H	19	ASP
2	H	49	ASN
2	H	60	ASN
2	H	102	LEU
2	H	114	GLU
2	H	120	GLU
2	H	121	LYS
2	H	129	ASN
2	H	156	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	38	ASN

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Mol	Chain	Res	Type
1	A	44	GLN
1	A	54	ASN
1	A	81	ASN
1	A	92	ASN
1	A	96	ASN
1	A	170	ASN
1	A	193	ASN
1	A	210	GLN
1	A	211	GLN
1	A	216	ASN
1	A	248	ASN
1	A	285	ASN
1	A	290	ASN
2	B	27	GLN
2	B	60	ASN
2	B	105	GLN
2	B	154	ASN
2	B	168	ASN
2	B	169	ASN
2	B	172	GLN
1	D	44	GLN
1	D	53	ASN
1	D	54	ASN
1	D	92	ASN
1	D	96	ASN
1	D	165	ASN
1	D	171	ASN
1	D	210	GLN
1	D	248	ASN
1	D	296	ASN
2	E	12	ASN
2	E	27	GLN
2	E	60	ASN
2	E	105	GLN
2	E	125	GLN
2	E	146	ASN
2	E	168	ASN
2	E	172	GLN
1	G	18	HIS
1	G	38	ASN
1	G	44	GLN
1	G	81	ASN

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Mol	Chain	Res	Type
1	G	92	ASN
1	G	96	ASN
1	G	170	ASN
1	G	171	ASN
1	G	197	GLN
1	G	210	GLN
1	G	211	GLN
1	G	248	ASN
1	G	290	ASN
1	G	296	ASN
2	H	12	ASN
2	H	26	HIS
2	H	27	GLN
2	H	60	ASN
2	H	105	GLN
2	H	125	GLN
2	H	168	ASN
2	H	172	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

25 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	$\#\|Z\| > 2$
3	NAG	A	330	-	15,15,15	0.87	1 (6%)	17,21,21	1.31	2 (11%)
4	NDG	A	331	-	15,15,15	1.12	2 (13%)	17,21,21	0.99	1 (5%)
3	NAG	A	332	-	15,15,15	1.34	1 (6%)	17,21,21	0.98	0
3	NAG	A	333	-	15,15,15	0.54	0	17,21,21	1.50	2 (11%)
4	NDG	A	334	-	15,15,15	0.78	0	17,21,21	0.98	1 (5%)
3	NAG	A	335	-	15,15,15	0.70	0	17,21,21	1.81	2 (11%)
5	MAN	A	336	5	12,12,12	1.14	1 (8%)	17,17,17	0.71	0
5	MAN	A	337	5	12,12,12	0.67	0	17,17,17	1.04	1 (5%)
4	NDG	B	222	-	15,15,15	0.58	0	17,21,21	0.71	0
4	NDG	B	223	-	15,15,15	0.59	0	17,21,21	0.67	0
4	NDG	D	330	-	15,15,15	0.79	0	17,21,21	0.68	0
3	NAG	D	331	-	15,15,15	0.58	0	17,21,21	0.91	0
4	NDG	D	332	-	15,15,15	1.64	1 (6%)	17,21,21	1.69	2 (11%)
4	NDG	D	333	-	15,15,15	1.06	2 (13%)	17,21,21	1.29	3 (17%)
5	MAN	D	334	-	12,12,12	0.75	0	17,17,17	2.09	3 (17%)
5	MAN	D	335	-	12,12,12	0.53	0	17,17,17	0.51	0
4	NDG	E	241	-	15,15,15	0.49	0	17,21,21	0.55	0
4	NDG	G	330	-	15,15,15	0.82	1 (6%)	17,21,21	0.89	0
5	MAN	G	331	-	12,12,12	0.55	0	17,17,17	0.98	1 (5%)
5	MAN	G	332	-	12,12,12	0.45	0	17,17,17	0.43	0
4	NDG	G	333	-	15,15,15	0.67	0	17,21,21	0.93	1 (5%)
4	NDG	G	334	-	15,15,15	0.67	0	17,21,21	0.66	0
3	NAG	G	335	-	15,15,15	0.68	0	17,21,21	1.89	4 (23%)
4	NDG	G	336	-	15,15,15	0.69	0	17,21,21	0.67	0
3	NAG	H	341	-	15,15,15	0.50	0	17,21,21	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	330	-	-	0/6/26/26	0/1/1/1
4	NDG	A	331	-	-	0/6/26/26	0/1/1/1
3	NAG	A	332	-	-	0/6/26/26	0/1/1/1
3	NAG	A	333	-	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDG	A	334	-	-	0/6/26/26	0/1/1/1
3	NAG	A	335	-	-	0/6/26/26	0/1/1/1
5	MAN	A	336	5	-	0/2/22/22	0/1/1/1
5	MAN	A	337	5	-	0/2/22/22	0/1/1/1
4	NDG	B	222	-	-	0/6/26/26	0/1/1/1
4	NDG	B	223	-	-	0/6/26/26	0/1/1/1
4	NDG	D	330	-	-	0/6/26/26	0/1/1/1
3	NAG	D	331	-	-	0/6/26/26	0/1/1/1
4	NDG	D	332	-	-	0/6/26/26	0/1/1/1
4	NDG	D	333	-	-	0/6/26/26	0/1/1/1
5	MAN	D	334	-	1/1/5/5	0/2/22/22	0/1/1/1
5	MAN	D	335	-	1/1/5/5	0/2/22/22	0/1/1/1
4	NDG	E	241	-	-	0/6/26/26	0/1/1/1
4	NDG	G	330	-	-	0/6/26/26	0/1/1/1
5	MAN	G	331	-	1/1/5/5	0/2/22/22	0/1/1/1
5	MAN	G	332	-	1/1/5/5	0/2/22/22	0/1/1/1
4	NDG	G	333	-	-	0/6/26/26	0/1/1/1
4	NDG	G	334	-	-	0/6/26/26	0/1/1/1
3	NAG	G	335	-	-	0/6/26/26	0/1/1/1
4	NDG	G	336	-	-	0/6/26/26	0/1/1/1
3	NAG	H	341	-	-	0/6/26/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	332	NDG	C1-C2	-5.67	1.46	1.53
5	A	336	MAN	C1-C2	-2.97	1.47	1.52
4	D	333	NDG	C1-C2	-2.85	1.49	1.53
4	A	331	NDG	C1-C2	-2.31	1.50	1.53
4	G	330	NDG	C4-C5	2.09	1.57	1.53
4	D	333	NDG	C4-C5	2.10	1.57	1.53
3	A	330	NAG	C1-C2	2.18	1.55	1.53
4	A	331	NDG	C4-C5	3.04	1.59	1.53
3	A	332	NAG	C1-C2	4.69	1.58	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	334	NDG	C4-C3-C2	-2.68	106.71	110.43
4	G	333	NDG	C4-C3-C2	-2.54	106.91	110.43
3	A	330	NAG	C3-C4-C5	-2.34	106.13	110.20
3	G	335	NAG	C2-N2-C7	-2.16	117.56	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	333	NDG	C2-N2-C7	-2.06	117.82	123.10
5	G	331	MAN	C1-C2-C3	-2.05	107.38	110.43
4	D	333	NDG	C6-C5-C4	-2.03	108.01	113.02
3	G	335	NAG	C8-C7-N2	2.15	120.23	116.11
3	A	335	NAG	C3-C4-C5	2.17	113.98	110.20
4	A	331	NDG	O-C5-C4	2.20	113.82	109.68
5	A	337	MAN	O5-C1-C2	2.37	113.57	109.80
4	D	332	NDG	C3-C4-C5	2.37	114.33	110.20
5	D	334	MAN	C1-O5-C5	2.44	117.99	113.47
4	D	333	NDG	C8-C7-N2	2.46	120.82	116.11
3	A	330	NAG	C1-O5-C5	3.15	119.30	113.47
3	A	333	NAG	C3-C4-C5	3.27	115.90	110.20
3	G	335	NAG	C3-C4-C5	3.31	115.96	110.20
3	A	333	NAG	C4-C3-C2	3.77	115.66	110.43
5	D	334	MAN	C1-C2-C3	4.91	117.73	110.43
3	G	335	NAG	C4-C3-C2	5.13	117.55	110.43
4	D	332	NDG	C4-C3-C2	5.37	117.88	110.43
5	D	334	MAN	O5-C1-C2	5.82	119.08	109.80
3	A	335	NAG	C4-C3-C2	5.96	118.70	110.43

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	331	MAN	C1
5	D	335	MAN	C1
5	G	332	MAN	C1
5	D	334	MAN	C1

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	330	NAG	2	0
4	A	331	NDG	4	0
3	A	332	NAG	1	0
3	A	333	NAG	10	0
4	A	334	NDG	11	0
3	A	335	NAG	11	0
5	A	336	MAN	8	0
5	A	337	MAN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	222	NDG	5	0
4	B	223	NDG	4	0
3	D	331	NAG	1	0
4	D	332	NDG	10	0
4	D	333	NDG	5	0
5	D	334	MAN	6	0
5	D	335	MAN	4	0
4	E	241	NDG	5	0
4	G	330	NDG	12	0
5	G	331	MAN	6	0
5	G	332	MAN	3	0
4	G	333	NDG	4	0
4	G	334	NDG	7	0
3	G	335	NAG	4	0
4	G	336	NDG	5	0
3	H	341	NAG	2	0

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, 95^{th} 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	318/329 (96%)	0.15	10 (3%)	52	45	46, 71, 87, 98	0
1	D	318/329 (96%)	-0.04	4 (1%)	79	78	41, 59, 75, 95	0
1	G	318/329 (96%)	0.23	9 (2%)	56	50	47, 65, 82, 101	0
2	B	172/221 (77%)	0.07	5 (2%)	55	49	40, 64, 82, 100	0
2	E	172/221 (77%)	0.15	7 (4%)	41	34	41, 67, 85, 100	0
2	H	172/221 (77%)	0.28	5 (2%)	55	49	40, 66, 87, 101	0
All	All	1470/1650 (89%)	0.13	40 (2%)	58	52	40, 65, 84, 101	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	46	SER	4.7
2	B	57	GLU	4.4
2	H	27	GLN	4.2
2	H	29	SER	4.1
1	A	143	PRO	3.9
2	B	172	GLN	3.7
2	E	57	GLU	3.6
2	H	171	PHE	3.5
1	G	326	LYS	3.5
1	A	125	PHE	3.4
2	H	26	HIS	3.1
1	A	47	SER	3.0
1	G	278	ILE	3.0
1	A	144	ALA	3.0
1	G	270	SER	3.0
1	D	324	PRO	2.9
2	B	56	ILE	2.8
2	B	31	GLY	2.8
1	G	272	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	161	ILE	2.8
1	G	222	TRP	2.6
1	A	242	VAL	2.6
1	A	239	PRO	2.5
2	H	144	CYS	2.5
1	D	32	ASP	2.5
1	A	46	SER	2.4
1	G	20	VAL	2.4
2	E	172	GLN	2.3
1	A	207	ARG	2.3
1	D	278	ILE	2.2
1	D	171	ASN	2.2
1	A	142	GLY	2.2
2	B	171	PHE	2.1
1	G	279	SER	2.1
1	A	274	ILE	2.1
2	E	158	ASP	2.1
2	E	64	HIS	2.0
1	G	274	ILE	2.0
2	E	21	TRP	2.0
2	E	27	GLN	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 carbohydrates 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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	NDG	B	223	15/15	0.81	0.45	8.75	98,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NDG	G	336	15/15	0.76	0.41	4.69	99,100,100,100	0
4	NDG	G	333	15/15	0.69	0.41	4.00	99,100,100,100	0
4	NDG	A	334	15/15	0.86	0.39	2.74	98,100,100,100	0
3	NAG	H	341	15/15	0.77	0.41	2.55	99,100,100,100	0
4	NDG	A	331	15/15	0.84	0.29	1.94	100,100,100,100	0
3	NAG	G	335	15/15	0.91	0.26	1.84	51,58,63,65	0
3	NAG	A	335	15/15	0.84	0.28	1.64	86,95,99,100	0
4	NDG	D	332	15/15	0.91	0.25	1.18	75,76,82,82	0
4	NDG	D	330	15/15	0.79	0.30	1.11	99,100,100,100	0
3	NAG	A	333	15/15	0.87	0.27	0.51	84,88,93,93	0
4	NDG	G	334	15/15	0.78	0.23	0.37	82,84,85,89	0
4	NDG	G	330	15/15	0.93	0.35	0.12	92,93,96,96	0
5	MAN	A	337	12/12	0.53	0.30	-	99,100,100,100	0
5	MAN	D	334	12/12	0.73	0.32	-	83,89,91,93	0
3	NAG	D	331	15/15	0.80	0.25	-	99,100,100,100	0
3	NAG	A	332	15/15	0.51	0.54	-	100,100,100,100	0
5	MAN	G	331	12/12	0.77	0.38	-	100,100,100,100	0
5	MAN	D	335	12/12	0.77	0.39	-	96,100,100,100	0
4	NDG	E	241	15/15	0.71	0.50	-	98,100,100,100	0
4	NDG	B	222	15/15	0.81	0.33	-	99,100,100,100	0
3	NAG	A	330	15/15	0.57	0.45	-	97,100,100,100	0
4	NDG	D	333	15/15	0.93	0.21	-	54,57,66,66	0
5	MAN	A	336	12/12	0.83	0.32	-	92,99,100,100	0
5	MAN	G	332	12/12	0.66	0.41	-	100,100,100,100	0

6.5 Other polymers (i)

There are no such residues in this entry.