Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 02:42 PM EDT

PDB ID	:	2I60
Title	:	Crystal structure of [Phe23]M47, a scorpion-toxin mimic of CD4, in complex with HIV-1 YU2 GP120 envelope glycoprotein and anti-HIV-1 antibody 17B
Authors	:	Huang, C.-C.; Kwong, P.D.
Deposited on	:	2006-08-26
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

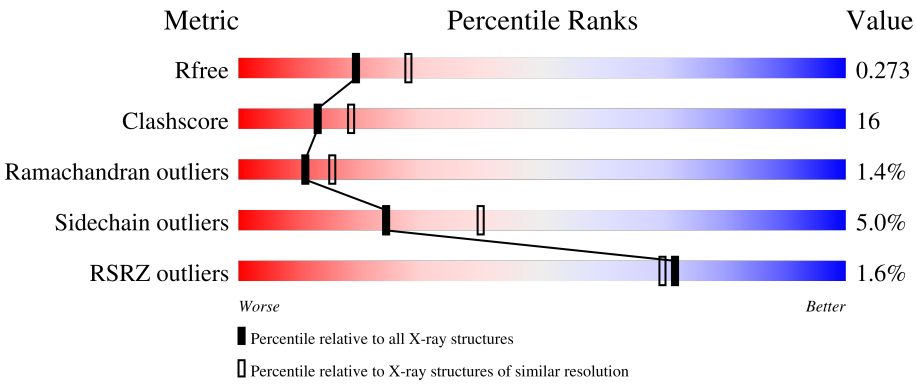
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	G	313	2%, 65%, 29%, • •
1	P	313	4%, 55%, 38%, • •
2	L	214	71%, 28%, •
2	Q	214	2%, 67%, 28%, 5%
3	H	229	69%, 24%, • •

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Mol	Chain	Length	Quality of chain
3	R	229	% 67% 28%
4	M	27	70% 30%
4	S	27	67% 26% 7%

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
5	NAG	G	886	X	-	-	-
5	NAG	P	734	X	-	-	-
5	NAG	P	741	X	-	-	X
5	NAG	P	789	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12434 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 EXTERIOR MEMBRANE GLYCOPROTEIN(GP120).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	301	2342	1468	407	447	20	0	0	0
1	P	300	2332	1463	405	444	20	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	79	GLY	-	cloning artifact	UNP P35961
G	80	ALA	-	cloning artifact	UNP P35961
G	81	ARG	-	cloning artifact	UNP P35961
G	82	SER	-	cloning artifact	UNP P35961
G	128	GLY	-	linker	UNP P35961
G	129	ALA	-	linker	UNP P35961
G	194	GLY	-	linker	UNP P35961
G	298	GLY	-	linker	UNP P35961
G	299	ALA	-	linker	UNP P35961
G	329	GLY	-	linker	UNP P35961
P	79	GLY	-	cloning artifact	UNP P35961
P	80	ALA	-	cloning artifact	UNP P35961
P	81	ARG	-	cloning artifact	UNP P35961
P	82	SER	-	cloning artifact	UNP P35961
P	128	GLY	-	linker	UNP P35961
P	129	ALA	-	linker	UNP P35961
P	194	GLY	-	linker	UNP P35961
P	298	GLY	-	linker	UNP P35961
P	299	ALA	-	linker	UNP P35961
P	329	GLY	-	linker	UNP P35961

- Molecule 2 is a protein called ANTIBODY 17B LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1647	1028	282	332	5	0	0	0
2	Q	214	1647	1028	282	332	5	0	0	0

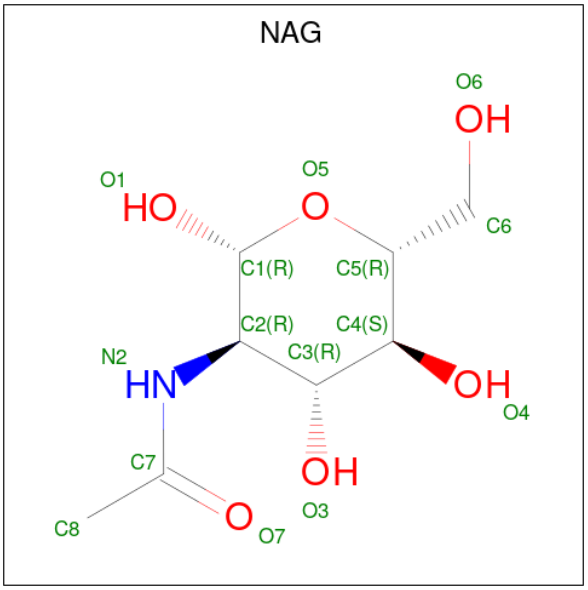
- Molecule 3 is a protein called ANTIBODY 17B HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	221	1669	1057	280	327	5	0	0	0
3	R	222	1678	1062	281	330	5	0	0	0

- Molecule 4 is a protein called [PHE23]M47, SCORPION-TOXIN MIMIC OF CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	27	201	126	38	31	6	0	0	0
4	S	27	201	126	38	31	6	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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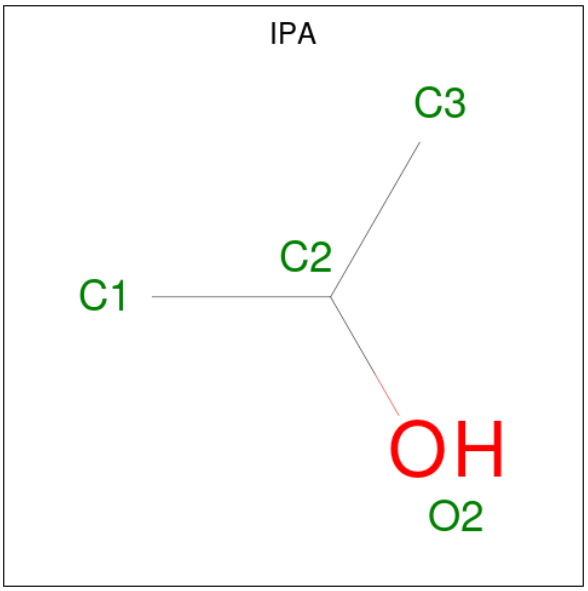
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	P	1	14	8	1	5	0	0
			Total	C	N	O		
5	P	1	14	8	1	5	0	0
			Total	C	N	O		
5	P	1	14	8	1	5	0	0
			Total	C	N	O		
5	P	1	14	8	1	5	0	0
			Total	C	N	O		
5	P	1	14	8	1	5	0	0
			Total	C	N	O		
5	P	1	14	8	1	5	0	0
			Total	C	N	O		
5	P	1	14	8	1	5	0	0
			Total	C	N	O		
5	P	1	14	8	1	5	0	0

- Molecule 6 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	G	1	4	3	1	0	0
			Total	C	O		
6	P	1	4	3	1	0	0

- Molecule 7 is water.

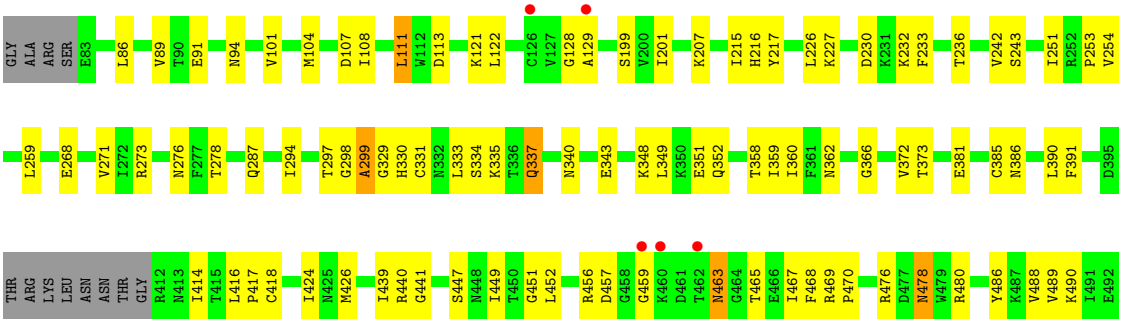
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	G	83	83	83	0	0
			Total	O		
7	L	85	85	85	0	0
			Total	O		
7	H	112	112	112	0	0
			Total	O		
7	M	7	7	7	0	0
			Total	O		
7	P	59	59	59	0	0
			Total	O		
7	Q	70	70	70	0	0
			Total	O		
7	R	61	61	61	0	0
			Total	O		
7	S	8	8	8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

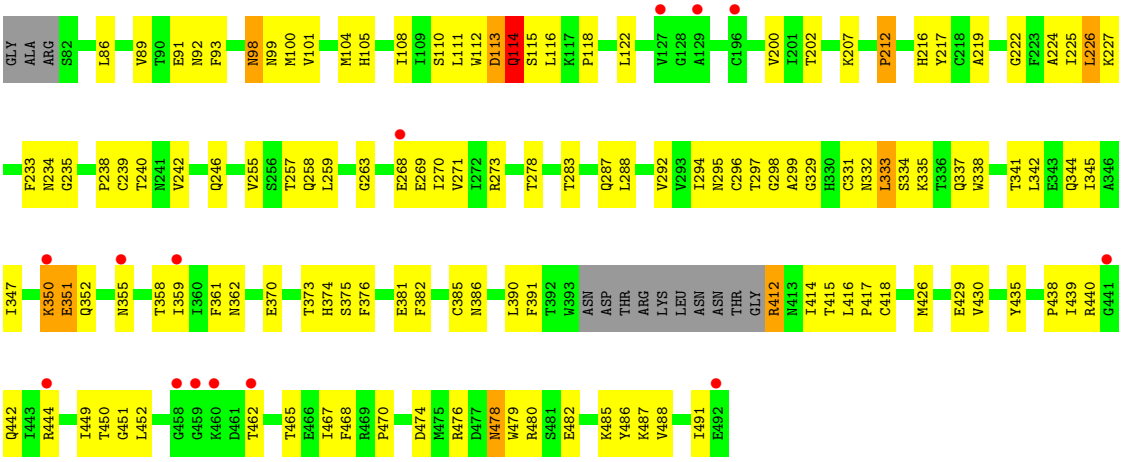
• Molecule 1: EXTERIOR MEMBRANE GLYCOPROTEIN(GP120)

Chain G: 2% 65% 29%



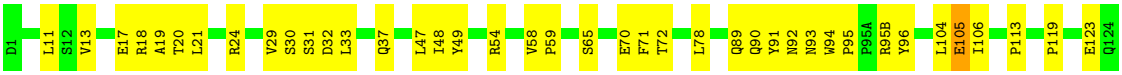
• Molecule 1: EXTERIOR MEMBRANE GLYCOPROTEIN(GP120)

Chain P: 4% 55% 38%



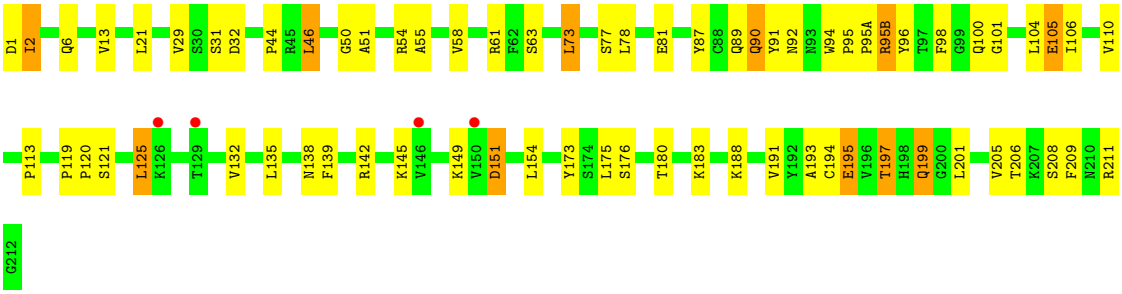
• Molecule 2: ANTIBODY 17B LIGHT CHAIN

Chain L: 71% 28%



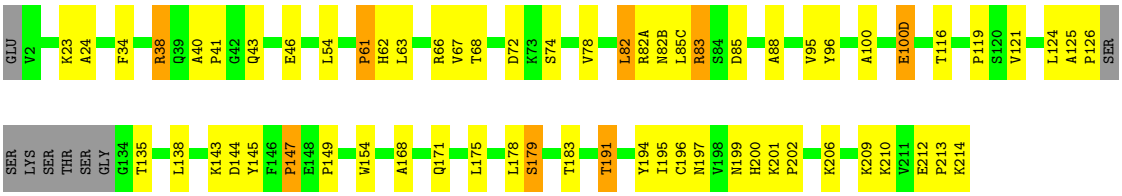
• Molecule 2: ANTIBODY 17B LIGHT CHAIN

Chain Q:



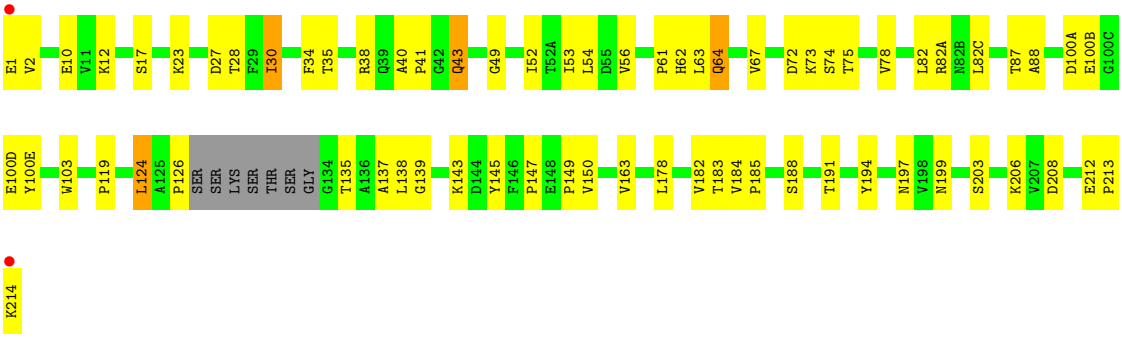
• Molecule 3: ANTIBODY 17B HEAVY CHAIN

Chain H:



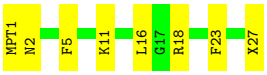
• Molecule 3: ANTIBODY 17B HEAVY CHAIN

Chain R:



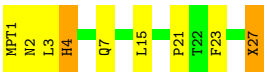
• Molecule 4: [PHE23]M47, SCORPION-TOXIN MIMIC OF CD4

Chain M:



• Molecule 4: [PHE23]M47, SCORPION-TOXIN MIMIC OF CD4

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.44Å 157.76Å 109.85Å 90.00° 93.74° 90.00°	Depositor
Resolution (Å)	19.98 – 2.40 45.65 – 2.08	Depositor EDS
% Data completeness (in resolution range)	83.6 (19.98-2.40) 61.7 (45.65-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.281 0.207 , 0.273	Depositor DCC
R_{free} test set	6863 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12434	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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, 0.333 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: IPA, NAG, DPR, MPT, VLM

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	G	0.35	0/2387	0.63	0/3234
1	P	0.32	0/2377	0.59	0/3220
2	L	0.40	0/1684	0.64	0/2288
2	Q	0.37	0/1684	0.64	0/2288
3	H	0.39	0/1708	0.67	0/2326
3	R	0.37	0/1717	0.62	0/2338
4	M	0.40	0/182	0.62	0/240
4	S	0.39	0/182	0.68	0/240
All	All	0.37	0/11921	0.63	0/16174

There are no bond length outliers.

There are no bond angle outliers.

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	G	2342	0	2294	73	0
1	P	2332	0	2289	120	0
2	L	1647	0	1593	46	0
2	Q	1647	0	1593	53	0
3	H	1669	0	1638	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	1678	0	1647	40	0
4	M	201	0	201	7	0
4	S	201	0	201	7	0
5	G	112	0	104	7	0
5	P	112	0	104	12	0
6	G	4	0	8	0	0
6	P	4	0	8	2	0
7	G	83	0	0	2	0
7	H	112	0	0	1	0
7	L	85	0	0	3	0
7	M	7	0	0	0	0
7	P	59	0	0	5	0
7	Q	70	0	0	1	0
7	R	61	0	0	2	0
7	S	8	0	0	0	0
All	All	12434	0	11680	388	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 16.

All (388) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:439:ILE:HG13	1:P:440:ARG:H	1.18	1.04
3:H:199:ASN:HD21	3:H:206:LYS:HG3	1.30	0.94
3:H:199:ASN:ND2	3:H:206:LYS:HG3	1.84	0.92
1:P:442:GLN:HE21	1:P:444:ARG:HD2	1.33	0.92
2:L:106:ILE:H	2:L:166:GLN:HE22	1.20	0.88
2:Q:145:LYS:HB3	2:Q:197:THR:HG23	1.53	0.88
3:H:135:THR:HG23	3:H:183:THR:HG23	1.59	0.82
3:H:63:LEU:HD13	3:H:67:VAL:HG11	1.64	0.80
3:R:135:THR:HG23	3:R:183:THR:HG23	1.63	0.79
2:Q:94:TRP:HA	2:Q:95:PRO:C	2.01	0.78
1:G:440:ARG:HD3	1:G:441:GLY:H	1.48	0.77
2:Q:105:GLU:HG2	2:Q:106:ILE:N	2.00	0.77
1:G:386:ASN:ND2	5:G:886:NAG:C7	2.48	0.77
2:L:94:TRP:HA	2:L:95:PRO:C	2.06	0.75
3:R:191:THR:HG22	7:R:273:HOH:O	1.86	0.74
1:P:439:ILE:HG13	1:P:440:ARG:N	1.97	0.74
1:G:439:ILE:HG13	1:G:440:ARG:H	1.50	0.74
3:R:1:GLU:HG2	3:R:2:VAL:H	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:271:VAL:HG11	1:P:273:ARG:NH1	2.04	0.73
2:L:105:GLU:HG3	2:L:173:TYR:OH	1.88	0.72
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.74	0.69
1:G:386:ASN:O	1:G:416:LEU:HD23	1.92	0.69
2:L:21:LEU:HD12	2:L:21:LEU:N	2.07	0.68
3:H:38:ARG:HG3	3:H:46:GLU:HB3	1.75	0.68
1:P:122:LEU:CD2	1:P:200:VAL:HG22	2.23	0.68
2:L:32:ASP:HB2	2:L:92:ASN:HB2	1.75	0.67
1:G:107:ASP:O	1:G:111:LEU:HD22	1.93	0.67
1:G:439:ILE:HG13	1:G:440:ARG:N	2.08	0.67
3:H:83:ARG:HG3	3:H:85:ASP:OD1	1.93	0.67
1:G:207:LYS:HE3	1:G:381:GLU:OE2	1.94	0.67
1:G:440:ARG:HD3	1:G:441:GLY:N	2.10	0.66
1:P:444:ARG:HH11	1:P:444:ARG:HB3	1.61	0.66
1:P:98:ASN:ND2	1:P:100:MET:H	1.94	0.66
1:P:219:ALA:HB2	1:P:225:ILE:HG13	1.78	0.65
5:G:886:NAG:H3	5:G:886:NAG:C8	2.27	0.65
2:Q:91:TYR:HA	2:Q:96:TYR:CD1	2.32	0.65
4:S:3:LEU:O	4:S:7:GLN:HG3	1.97	0.64
3:R:30:ILE:HD11	3:R:73:LYS:HD3	1.79	0.64
1:P:98:ASN:C	1:P:98:ASN:HD22	1.99	0.64
1:P:390:LEU:HD11	1:P:416:LEU:HD11	1.80	0.64
1:G:227:LYS:HD2	1:G:486:TYR:CE2	2.34	0.63
2:L:105:GLU:HG2	2:L:106:ILE:N	2.12	0.63
3:H:171:GLN:HG3	3:H:175:LEU:O	1.98	0.63
2:Q:120:PRO:HD3	2:Q:132:VAL:HG22	1.80	0.63
1:P:442:GLN:HG2	1:P:444:ARG:HG3	1.80	0.63
3:R:1:GLU:HG2	3:R:2:VAL:N	2.14	0.63
1:P:412:ARG:HD2	1:P:412:ARG:N	2.14	0.63
1:P:474:ASP:OD2	4:S:21:DPR:HG3	1.99	0.62
1:G:232:LYS:O	1:G:232:LYS:HG3	1.99	0.62
4:M:2:ASN:HD22	4:M:5:PHE:HB3	1.65	0.62
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.82	0.62
1:P:224:ALA:HB2	1:P:491:ILE:HD11	1.82	0.62
1:P:297:THR:HG23	1:P:299:ALA:H	1.64	0.61
1:G:476:ARG:HB3	1:G:480:ARG:HH12	1.64	0.61
1:P:100:MET:HE1	1:P:486:TYR:C	2.21	0.61
1:G:94:ASN:HA	1:G:236:THR:HG22	1.82	0.61
1:P:98:ASN:HD22	1:P:99:ASN:N	1.99	0.61
1:P:295:ASN:ND2	5:P:795:NAG:H82	2.16	0.61
2:Q:211:ARG:HH11	2:Q:211:ARG:HB3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:478:ASN:N	1:G:478:ASN:HD22	1.99	0.60
3:H:121:VAL:O	3:H:209:LYS:HE3	2.00	0.60
1:G:337:GLN:C	1:G:337:GLN:HE21	2.05	0.60
7:L:214:HOH:O	3:H:179:SER:HB2	2.01	0.60
1:G:334:SER:OG	1:G:337:GLN:HB2	2.01	0.60
1:P:263:GLY:O	1:P:450:THR:HG21	2.00	0.60
3:R:119:PRO:HB3	3:R:145:TYR:HB3	1.83	0.60
1:P:118:PRO:HG3	1:P:435:TYR:CZ	2.36	0.60
1:P:258:GLN:HE21	1:P:470:PRO:HB2	1.66	0.60
1:G:233:PHE:O	1:G:273:ARG:NH1	2.35	0.60
3:R:100(A):ASP:OD1	3:R:100(B):GLU:HG3	2.02	0.59
3:R:35:THR:HG23	3:R:49:GLY:O	2.03	0.59
2:Q:105:GLU:HG3	2:Q:173:TYR:OH	2.01	0.59
2:Q:149:LYS:HE2	2:Q:195:GLU:HG3	1.84	0.58
1:G:91:GLU:HG3	1:G:226:LEU:CD2	2.32	0.58
2:L:135:LEU:HD22	2:L:136:LEU:N	2.19	0.58
1:P:373:THR:HB	1:P:385:CYS:O	2.04	0.58
1:P:478:ASN:N	1:P:478:ASN:HD22	2.02	0.58
1:P:338:TRP:O	1:P:342:LEU:HG	2.04	0.58
1:G:488:VAL:HG12	7:G:965:HOH:O	2.03	0.57
2:L:29:VAL:O	2:L:29:VAL:HG12	2.04	0.57
1:P:442:GLN:HE21	1:P:444:ARG:CD	2.12	0.57
2:Q:29:VAL:CG2	2:Q:90:GLN:HG3	2.34	0.57
3:R:178:LEU:HD12	3:R:178:LEU:C	2.24	0.57
1:P:332:ASN:HB3	1:P:415:THR:HA	1.85	0.57
1:G:297:THR:HG22	1:G:298:GLY:N	2.20	0.57
3:H:210:LYS:HE3	3:H:212:GLU:OE2	2.05	0.57
1:P:207:LYS:HE3	1:P:381:GLU:OE2	2.05	0.57
1:G:89:VAL:HG13	1:G:89:VAL:O	2.05	0.57
1:G:463:ASN:HB2	1:G:465:THR:HG22	1.87	0.57
2:L:183:LYS:O	2:L:187:GLU:HG2	2.05	0.56
3:H:61:PRO:O	3:H:63:LEU:N	2.38	0.56
5:P:734:NAG:H3	5:P:734:NAG:H82	1.88	0.56
4:S:2:ASN:HB3	4:S:4:HIS:CD2	2.40	0.56
1:G:331:CYS:SG	1:G:418:CYS:SG	3.03	0.56
1:P:271:VAL:HG11	1:P:273:ARG:HH12	1.71	0.56
1:P:100:MET:HE1	1:P:486:TYR:CB	2.36	0.56
1:P:233:PHE:O	1:P:273:ARG:NH1	2.39	0.56
1:P:258:GLN:NE2	1:P:470:PRO:HB2	2.21	0.56
2:Q:29:VAL:HG12	2:Q:29:VAL:O	2.05	0.56
1:G:201:ILE:HG13	7:G:927:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:330:HIS:HA	1:G:416:LEU:O	2.06	0.56
1:G:108:ILE:HA	1:G:111:LEU:HD23	1.88	0.56
5:G:886:NAG:H3	5:G:886:NAG:H82	1.87	0.56
3:R:212:GLU:HG3	3:R:213:PRO:HD2	1.88	0.55
1:G:391:PHE:CG	1:G:470:PRO:HG3	2.40	0.55
1:G:489:VAL:HG22	1:G:490:LYS:N	2.21	0.55
2:L:154:LEU:HD23	7:L:281:HOH:O	2.05	0.55
2:Q:119:PRO:HB3	2:Q:209:PHE:CZ	2.41	0.55
1:G:251:ILE:C	1:G:253:PRO:HD3	2.26	0.55
2:Q:89:GLN:HB2	2:Q:98:PHE:CD1	2.41	0.55
4:M:11:LYS:HE2	4:M:16:LEU:HD23	1.89	0.55
2:Q:1:ASP:CG	2:Q:2:ILE:N	2.59	0.55
1:P:444:ARG:HB3	1:P:444:ARG:NH1	2.21	0.55
2:Q:95:PRO:O	2:Q:95(B):ARG:HD3	2.07	0.55
2:L:54:ARG:HD2	2:L:58:VAL:O	2.07	0.54
1:P:331:CYS:SG	1:P:385:CYS:SG	3.05	0.54
2:Q:121:SER:O	2:Q:125:LEU:HD22	2.06	0.54
1:G:451:GLY:C	1:G:452:LEU:HD12	2.28	0.54
2:L:29:VAL:HG13	2:L:92:ASN:HB3	1.89	0.54
2:Q:211:ARG:HB3	2:Q:211:ARG:NH1	2.22	0.54
1:G:297:THR:HG22	1:G:299:ALA:H	1.72	0.54
3:H:23:LYS:HD3	3:H:23:LYS:C	2.28	0.54
1:P:488:VAL:HG12	7:P:914:HOH:O	2.08	0.54
1:P:105:HIS:HA	1:P:479:TRP:HE1	1.73	0.54
1:P:439:ILE:CG1	1:P:440:ARG:H	2.04	0.54
2:Q:94:TRP:CE3	2:Q:95(A):PRO:HD3	2.44	0.53
3:H:195:ILE:HD13	3:H:210:LYS:HA	1.89	0.53
3:R:43:GLN:HE21	3:R:43:GLN:N	2.05	0.53
2:Q:1:ASP:CG	2:Q:2:ILE:H	2.11	0.53
3:R:199:ASN:HD21	3:R:206:LYS:HD3	1.73	0.53
2:L:175:LEU:HD23	2:L:176:SER:N	2.24	0.53
2:L:21:LEU:N	2:L:21:LEU:CD1	2.71	0.53
1:P:122:LEU:HD11	3:R:54:LEU:HG	1.91	0.53
1:G:254:VAL:HG22	5:G:762:NAG:H83	1.91	0.52
1:P:386:ASN:O	1:P:416:LEU:HD22	2.09	0.52
2:Q:193:ALA:CB	2:Q:208:SER:HB3	2.39	0.52
3:R:72:ASP:OD2	3:R:74:SER:HB3	2.09	0.52
1:G:91:GLU:HG3	1:G:226:LEU:HD23	1.91	0.52
1:G:335:LYS:HB2	1:G:414:ILE:HG13	1.90	0.52
2:L:93:ASN:HD21	2:L:95(B):ARG:HB2	1.74	0.52
1:P:358:THR:HB	1:P:465:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:46:LEU:HD13	2:Q:55:ALA:HB2	1.92	0.52
2:Q:54:ARG:HD2	2:Q:58:VAL:HG12	1.91	0.52
1:P:370:GLU:HG2	4:S:23:PHE:CE2	2.44	0.52
2:L:19:ALA:HB2	2:L:78:LEU:HD21	1.92	0.52
1:P:298:GLY:C	1:P:329:GLY:H	2.13	0.52
1:P:334:SER:HB3	1:P:337:GLN:HB2	1.90	0.52
5:P:886:NAG:H83	7:P:938:HOH:O	2.10	0.52
2:L:123:GLU:HB2	7:L:285:HOH:O	2.10	0.52
2:L:147:GLN:HB3	2:L:195:GLU:HB3	1.90	0.52
3:H:82:LEU:HB3	3:H:85(C):LEU:HD21	1.92	0.51
1:P:476:ARG:HD3	7:P:889:HOH:O	2.08	0.51
2:Q:54:ARG:HG2	2:Q:58:VAL:HB	1.92	0.51
3:R:63:LEU:HD13	3:R:67:VAL:HG21	1.92	0.51
2:Q:175:LEU:HD23	2:Q:176:SER:N	2.25	0.51
2:L:32:ASP:HB3	2:L:91:TYR:CD1	2.45	0.51
2:Q:193:ALA:HB2	2:Q:208:SER:HB3	1.92	0.51
3:R:27:ASP:OD2	3:R:28:THR:N	2.42	0.51
1:P:278:THR:HG22	5:P:776:NAG:H62	1.93	0.51
2:Q:113:PRO:HB3	2:Q:139:PHE:HB3	1.92	0.51
3:H:143:LYS:NZ	3:H:171:GLN:HE22	2.09	0.51
1:G:86:LEU:C	1:G:86:LEU:HD23	2.31	0.51
1:P:386:ASN:ND2	5:P:886:NAG:H82	2.27	0.51
1:G:366:GLY:HA2	1:G:372:VAL:HG22	1.92	0.50
2:L:78:LEU:HD11	2:L:104:LEU:HD21	1.93	0.50
3:H:201:LYS:HB2	3:H:202:PRO:HD3	1.93	0.50
2:Q:6:GLN:OE1	2:Q:87:TYR:HA	2.12	0.50
1:P:89:VAL:O	1:P:89:VAL:HG13	2.11	0.50
1:P:104:MET:HA	1:P:217:TYR:OH	2.11	0.50
1:P:239:CYS:SG	1:P:242:VAL:HG12	2.51	0.50
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.93	0.50
3:H:178:LEU:HD12	3:H:178:LEU:C	2.32	0.50
4:M:2:ASN:HD22	4:M:5:PHE:CB	2.24	0.50
1:G:232:LYS:HE2	1:G:271:VAL:HG13	1.93	0.50
1:G:373:THR:HB	1:G:385:CYS:O	2.12	0.50
1:P:341:THR:HG22	1:P:345:ILE:HD11	1.92	0.50
1:P:362:ASN:HD22	1:P:467:ILE:CG2	2.24	0.50
2:Q:21:LEU:HD12	2:Q:21:LEU:N	2.27	0.50
1:G:294:ILE:HG23	1:G:294:ILE:O	2.11	0.50
3:H:126:PRO:HG3	3:H:138:LEU:HB3	1.94	0.50
3:H:200:HIS:CE1	3:H:202:PRO:HB2	2.47	0.50
2:L:24:ARG:NE	2:L:70:GLU:HG3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:144:ASP:OD1	3:H:171:GLN:NE2	2.45	0.50
5:P:588:NAG:H2	7:P:931:HOH:O	2.12	0.50
1:P:105:HIS:HA	1:P:479:TRP:NE1	2.27	0.49
2:Q:194:CYS:O	2:Q:206:THR:HA	2.12	0.49
3:H:210:LYS:NZ	3:H:212:GLU:HG2	2.27	0.49
1:P:110:SER:O	1:P:114:GLN:HG3	2.12	0.49
3:R:124:LEU:HB2	3:R:139:GLY:C	2.33	0.49
1:P:386:ASN:HB3	1:P:417:PRO:HD2	1.94	0.49
2:Q:63:SER:O	2:Q:73:LEU:HD23	2.12	0.49
2:Q:95:PRO:O	2:Q:95(B):ARG:NH1	2.45	0.49
1:G:215:ILE:C	1:G:215:ILE:HD12	2.32	0.49
1:P:297:THR:C	1:P:299:ALA:H	2.16	0.49
3:H:138:LEU:HD12	3:H:138:LEU:C	2.33	0.49
1:P:288:LEU:HG	1:P:450:THR:O	2.12	0.49
1:P:478:ASN:HD22	1:P:478:ASN:H	1.60	0.49
2:Q:29:VAL:HG21	2:Q:90:GLN:HG3	1.95	0.49
1:G:478:ASN:HD22	1:G:478:ASN:H	1.60	0.49
3:H:40:ALA:HB1	3:H:41:PRO:HD2	1.94	0.48
2:Q:32:ASP:HB3	2:Q:91:TYR:CD1	2.48	0.48
3:R:82(A):ARG:HD2	7:R:223:HOH:O	2.13	0.48
3:H:34:PHE:CG	3:H:78:VAL:HG21	2.49	0.48
1:P:202:THR:HG22	2:Q:95:PRO:HG3	1.95	0.48
3:H:40:ALA:HA	3:H:88:ALA:CB	2.44	0.48
1:P:91:GLU:HG3	1:P:226:LEU:HD23	1.93	0.48
3:R:184:VAL:HG11	3:R:194:TYR:CE1	2.49	0.48
1:G:359:ILE:O	1:G:360:ILE:HD13	2.14	0.48
4:M:2:ASN:ND2	4:M:5:PHE:HB3	2.28	0.48
1:P:255:VAL:HG12	6:P:502:IPA:H32	1.95	0.48
1:G:337:GLN:HE21	1:G:337:GLN:CA	2.26	0.48
1:G:390:LEU:HG	1:G:416:LEU:HD21	1.96	0.48
2:Q:188:LYS:O	2:Q:188:LYS:HG2	2.14	0.48
1:P:207:LYS:HE2	1:P:438:PRO:HA	1.95	0.48
2:Q:44:PRO:HD2	3:R:103:TRP:CE3	2.48	0.48
1:P:333:LEU:N	1:P:333:LEU:HD23	2.29	0.48
1:G:362:ASN:HB3	1:G:469:ARG:NH1	2.28	0.48
2:L:91:TYR:HA	2:L:96:TYR:CD1	2.49	0.48
1:P:118:PRO:HG3	1:P:435:TYR:OH	2.13	0.48
2:L:161:GLU:HG2	2:L:175:LEU:HD21	1.96	0.47
4:M:1:MPT:HB2	4:M:23:PHE:C	2.34	0.47
2:Q:183:LYS:HB3	7:Q:269:HOH:O	2.14	0.47
4:S:15:LEU:HB3	4:S:27:VLM:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:259:LEU:HD13	1:P:449:ILE:HD13	1.96	0.47
1:P:294:ILE:HG23	1:P:294:ILE:O	2.15	0.47
2:Q:61:ARG:HD2	2:Q:77:SER:O	2.14	0.47
1:P:362:ASN:HD22	1:P:467:ILE:HG23	1.80	0.47
1:G:340:ASN:O	1:G:343:GLU:HB3	2.13	0.47
1:G:348:LYS:HD3	1:G:351:GLU:OE1	2.15	0.47
2:L:48:ILE:HG22	2:L:49:TYR:N	2.30	0.47
3:R:52:ILE:HG23	3:R:100(E):TYR:OH	2.14	0.47
1:G:91:GLU:HG3	1:G:226:LEU:HD21	1.95	0.47
1:G:251:ILE:O	1:G:253:PRO:HD3	2.15	0.47
1:P:115:SER:C	1:P:116:LEU:HD12	2.35	0.47
1:P:359:ILE:HD12	1:P:359:ILE:N	2.30	0.47
3:R:12:LYS:HD3	3:R:17:SER:O	2.15	0.47
3:R:34:PHE:CG	3:R:78:VAL:HG21	2.49	0.47
2:L:65:SER:HB3	2:L:72:THR:HG23	1.97	0.46
1:P:92:ASN:OD1	1:P:238:PRO:HB3	2.15	0.46
1:P:258:GLN:NE2	1:P:470:PRO:CB	2.78	0.46
2:Q:151:ASP:HA	2:Q:191:VAL:CG1	2.45	0.46
2:L:33:LEU:HG	2:L:71:PHE:CG	2.51	0.46
3:H:135:THR:HG23	3:H:183:THR:CG2	2.39	0.46
4:M:2:ASN:ND2	4:M:5:PHE:CB	2.78	0.46
2:L:175:LEU:HD23	2:L:175:LEU:C	2.36	0.46
1:P:91:GLU:HA	1:P:91:GLU:OE2	2.15	0.46
3:R:82:LEU:HD22	3:R:82(C):LEU:HD23	1.98	0.46
1:P:335:LYS:HA	1:P:414:ILE:CD1	2.46	0.46
3:R:185:PRO:HG2	3:R:188:SER:OG	2.15	0.46
1:G:230:ASP:HB3	5:G:741:NAG:H81	1.96	0.46
1:P:297:THR:HG23	1:P:299:ALA:HB3	1.98	0.46
2:L:119:PRO:HB3	2:L:209:PHE:CZ	2.51	0.46
3:R:1:GLU:HG2	3:R:2:VAL:HG23	1.97	0.46
3:R:63:LEU:HD22	3:R:67:VAL:HG21	1.97	0.46
1:G:278:THR:HG22	5:G:776:NAG:O6	2.16	0.46
2:Q:32:ASP:HB2	2:Q:92:ASN:HB2	1.97	0.46
2:L:30:SER:OG	2:L:31:SER:N	2.49	0.46
1:P:86:LEU:HD23	1:P:86:LEU:C	2.37	0.46
1:G:273:ARG:NH2	1:G:287:GLN:OE1	2.49	0.45
3:H:23:LYS:HD3	3:H:24:ALA:N	2.31	0.45
3:R:212:GLU:HG2	3:R:214:LYS:H	1.80	0.45
1:G:104:MET:HA	1:G:217:TYR:OH	2.16	0.45
1:P:296:CYS:HA	1:P:331:CYS:HA	1.97	0.45
1:P:430:VAL:CG2	4:S:1:MPT:HA1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:13:VAL:CG1	2:Q:104:LEU:HD21	2.45	0.45
1:G:391:PHE:CD2	1:G:470:PRO:HG3	2.51	0.45
1:G:101:VAL:HG21	1:G:480:ARG:HG2	1.99	0.45
1:G:489:VAL:HG22	1:G:490:LYS:H	1.79	0.45
1:P:382:PHE:HD1	7:P:905:HOH:O	1.99	0.45
3:R:1:GLU:CG	3:R:2:VAL:H	2.27	0.45
2:L:20:THR:C	2:L:21:LEU:HD12	2.36	0.45
3:H:154:TRP:CH2	3:H:196:CYS:HB3	2.52	0.45
1:G:113:ASP:O	1:G:113:ASP:OD2	2.35	0.45
1:P:269:GLU:HA	5:P:789:NAG:O5	2.17	0.45
2:Q:105:GLU:HG2	2:Q:106:ILE:H	1.78	0.45
1:P:98:ASN:HD22	1:P:100:MET:H	1.64	0.45
1:P:451:GLY:C	1:P:452:LEU:HD12	2.37	0.45
1:P:104:MET:O	1:P:108:ILE:HG12	2.17	0.45
3:R:53:ILE:HG13	3:R:53:ILE:O	2.15	0.45
2:L:94:TRP:CA	2:L:95:PRO:C	2.82	0.45
3:H:66:ARG:NH2	3:H:83:ARG:HE	2.15	0.45
4:M:1:MPT:HB2	4:M:23:PHE:O	2.16	0.45
1:P:233:PHE:CE2	1:P:235:GLY:HA2	2.52	0.45
2:Q:29:VAL:HG22	2:Q:90:GLN:HG3	1.98	0.45
1:P:376:PHE:HA	6:P:502:IPA:H33	1.98	0.44
3:R:163:VAL:HG12	3:R:182:VAL:CG2	2.47	0.44
1:P:333:LEU:HD23	1:P:333:LEU:H	1.82	0.44
1:G:349:LEU:HD13	1:G:468:PHE:CE1	2.53	0.44
1:P:100:MET:HE1	1:P:487:LYS:N	2.32	0.44
1:G:232:LYS:O	1:G:232:LYS:CG	2.65	0.44
1:P:112:TRP:C	1:P:114:GLN:H	2.21	0.44
1:P:344:GLN:OE1	5:P:789:NAG:H62	2.18	0.44
1:P:101:VAL:HG21	1:P:480:ARG:HG2	1.98	0.44
1:P:361:PHE:CD2	1:P:468:PHE:HB2	2.53	0.44
2:L:89:GLN:HG2	2:L:90:GLN:N	2.31	0.44
1:G:335:LYS:HG3	1:G:414:ILE:HD11	2.00	0.44
1:P:270:ILE:HD12	1:P:344:GLN:HB3	2.00	0.44
2:Q:149:LYS:CE	2:Q:195:GLU:HG3	2.48	0.44
3:R:197:ASN:ND2	3:R:208:ASP:OD1	2.51	0.44
2:L:17:GLU:HG3	2:L:18:ARG:H	1.82	0.44
3:H:168:ALA:HA	3:H:178:LEU:HB3	1.99	0.44
1:G:333:LEU:O	1:G:414:ILE:N	2.45	0.44
2:L:19:ALA:CB	2:L:78:LEU:HD21	2.48	0.43
3:R:54:LEU:O	3:R:56:VAL:HG23	2.18	0.43
3:H:125:ALA:HA	3:H:126:PRO:HD3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:29:VAL:HG11	2:L:90:GLN:HB2	2.00	0.43
3:H:209:LYS:HB2	3:H:209:LYS:HE2	1.81	0.43
2:Q:142:ARG:HB2	2:Q:173:TYR:CE2	2.53	0.43
1:G:259:LEU:HD13	1:G:449:ILE:HD13	2.01	0.43
1:P:270:ILE:HG23	1:P:287:GLN:O	2.18	0.43
1:G:121:LYS:HD2	1:G:426:MET:CE	2.49	0.43
3:H:95:VAL:HG22	3:H:96:TYR:N	2.34	0.43
1:P:93:PHE:CE2	1:P:487:LYS:HB3	2.54	0.43
1:P:234:ASN:C	1:P:234:ASN:OD1	2.56	0.43
1:P:240:THR:HG22	5:P:588:NAG:H3	2.00	0.43
2:L:137:ASN:ND2	2:L:138:ASN:OD1	2.51	0.43
1:P:259:LEU:HD13	1:P:449:ILE:CD1	2.48	0.43
2:Q:110:VAL:HG21	2:Q:199:GLN:NE2	2.33	0.43
1:G:242:VAL:HG22	1:G:243:SER:N	2.32	0.43
1:P:430:VAL:HG21	4:S:1:MPT:HA1	2.00	0.43
2:Q:175:LEU:HD23	2:Q:175:LEU:C	2.39	0.43
3:R:41:PRO:O	3:R:43:GLN:NE2	2.52	0.43
1:G:294:ILE:HG22	1:G:447:SER:O	2.19	0.42
1:G:298:GLY:C	1:G:329:GLY:H	2.22	0.42
2:L:154:LEU:N	2:L:154:LEU:HD22	2.34	0.42
3:H:72:ASP:OD2	3:H:74:SER:HB3	2.19	0.42
1:P:98:ASN:ND2	1:P:98:ASN:C	2.69	0.42
1:P:444:ARG:HH11	1:P:444:ARG:CB	2.30	0.42
2:Q:201:LEU:HD13	2:Q:205:VAL:HG23	2.00	0.42
3:H:68:THR:OG1	3:H:82(A):ARG:NH2	2.31	0.42
3:H:194:TYR:O	3:H:195:ILE:HD13	2.19	0.42
2:L:17:GLU:O	2:L:78:LEU:HD23	2.19	0.42
3:H:213:PRO:O	3:H:214:LYS:C	2.57	0.42
1:G:386:ASN:HB3	1:G:417:PRO:HD2	2.01	0.42
3:H:100:ALA:HA	3:H:100(D):GLU:O	2.19	0.42
3:H:191:THR:HB	7:H:307:HOH:O	2.18	0.42
2:Q:29:VAL:O	2:Q:29:VAL:CG1	2.68	0.42
2:Q:145:LYS:HD3	2:Q:197:THR:HG21	2.00	0.42
3:R:137:ALA:C	3:R:138:LEU:HD12	2.40	0.42
1:P:426:MET:HB2	1:P:429:GLU:O	2.20	0.42
1:G:457:ASP:O	1:G:459:GLY:N	2.52	0.42
2:L:189:HIS:HB2	2:L:192:TYR:OH	2.20	0.42
3:H:40:ALA:HA	3:H:88:ALA:HB2	2.02	0.42
1:P:390:LEU:HG	1:P:416:LEU:HD21	2.01	0.42
3:R:126:PRO:HG3	3:R:138:LEU:CD1	2.50	0.42
1:P:246:GLN:HA	1:P:246:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:386:ASN:CG	5:P:886:NAG:H82	2.40	0.42
1:P:391:PHE:CD1	1:P:470:PRO:HG3	2.55	0.42
3:R:87:THR:O	3:R:88:ALA:HB2	2.20	0.42
1:G:122:LEU:HA	1:G:199:SER:O	2.21	0.41
1:P:227:LYS:HA	1:P:485:LYS:O	2.20	0.41
1:G:456:ARG:HA	1:G:467:ILE:O	2.20	0.41
1:P:212:PRO:HG2	5:P:762:NAG:H4	2.02	0.41
1:P:239:CYS:HB3	1:P:242:VAL:HG12	2.03	0.41
1:P:292:VAL:HB	1:P:449:ILE:HB	2.03	0.41
2:L:29:VAL:O	2:L:29:VAL:CG1	2.67	0.41
2:Q:50:GLY:O	2:Q:51:ALA:HB3	2.21	0.41
1:G:439:ILE:CG1	1:G:440:ARG:N	2.81	0.41
1:P:347:ILE:O	1:P:350:LYS:HG3	2.20	0.41
1:G:334:SER:CB	1:G:337:GLN:HB2	2.51	0.41
1:P:105:HIS:HB2	1:P:479:TRP:CD1	2.56	0.41
1:G:456:ARG:HD3	1:G:468:PHE:CE2	2.56	0.41
2:L:95(B):ARG:HD2	3:H:61:PRO:HD3	2.02	0.41
1:P:269:GLU:HA	5:P:789:NAG:C1	2.51	0.41
1:P:351:GLU:O	1:P:351:GLU:HG2	2.20	0.41
2:Q:100:GLN:HG2	2:Q:101:GLY:N	2.36	0.41
3:R:23:LYS:HE3	3:R:75:THR:O	2.21	0.41
2:L:32:ASP:OD2	2:L:92:ASN:ND2	2.42	0.41
2:Q:29:VAL:HG13	2:Q:92:ASN:CB	2.51	0.41
1:P:335:LYS:HB2	1:P:414:ILE:HG13	2.03	0.40
3:H:116:THR:HB	3:R:203:SER:HA	2.03	0.40
1:P:222:GLY:O	1:P:491:ILE:HG12	2.21	0.40
1:P:257:THR:O	1:P:259:LEU:N	2.54	0.40
1:P:341:THR:HG22	1:P:345:ILE:CD1	2.51	0.40
1:P:351:GLU:OE2	1:P:352:GLN:HG2	2.21	0.40
1:P:375:SER:O	1:P:376:PHE:HB3	2.21	0.40
1:P:480:ARG:C	1:P:482:GLU:N	2.75	0.40
2:Q:78:LEU:HD21	2:Q:104:LEU:HD21	2.03	0.40
2:L:207:LYS:HA	2:L:207:LYS:HD3	1.92	0.40
1:G:463:ASN:HB2	1:G:465:THR:CG2	2.51	0.40
5:G:795:NAG:O3	5:G:795:NAG:H83	2.22	0.40
2:L:11:LEU:HD23	2:L:104:LEU:HD11	2.04	0.40
3:H:82(A):ARG:O	3:H:82(B):ASN:C	2.59	0.40
3:H:195:ILE:CD1	3:H:210:LYS:HA	2.51	0.40
1:P:100:MET:HE1	1:P:486:TYR:HB3	2.02	0.40
1:P:270:ILE:HG22	1:P:271:VAL:N	2.37	0.40
1:P:416:LEU:HA	1:P:417:PRO:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:40:ALA:HB1	3:R:41:PRO:HD2	2.02	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	G	297/313 (95%)	279 (94%)	12 (4%)	6 (2%)	7	9
1	P	296/313 (95%)	266 (90%)	25 (8%)	5 (2%)	9	11
2	L	212/214 (99%)	200 (94%)	11 (5%)	1 (0%)	29	41
2	Q	212/214 (99%)	194 (92%)	15 (7%)	3 (1%)	11	15
3	H	217/229 (95%)	203 (94%)	11 (5%)	3 (1%)	11	15
3	R	218/229 (95%)	203 (93%)	12 (6%)	3 (1%)	11	15
4	M	24/27 (89%)	23 (96%)	1 (4%)	0	100	100
4	S	24/27 (89%)	23 (96%)	1 (4%)	0	100	100
All	All	1500/1566 (96%)	1391 (93%)	88 (6%)	21 (1%)	11	15

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	62	HIS
1	P	114	GLN
2	Q	138	ASN
3	R	62	HIS
3	R	64	GLN
1	G	129	ALA
1	G	268	GLU
1	P	462	THR
1	P	113	ASP

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Mol	Chain	Res	Type
3	R	61	PRO
1	G	128	GLY
1	G	299	ALA
2	Q	199	GLN
1	G	276	ASN
3	H	61	PRO
1	P	268	GLU
2	Q	2	ILE
1	G	463	ASN
2	L	59	PRO
1	P	212	PRO
3	H	147	PRO

5.3.2 Protein sidechains (i)

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	G	266/276 (96%)	259 (97%)	7 (3%)	46	66
1	P	265/276 (96%)	250 (94%)	15 (6%)	20	33
2	L	184/184 (100%)	179 (97%)	5 (3%)	44	65
2	Q	184/184 (100%)	170 (92%)	14 (8%)	13	20
3	H	186/193 (96%)	174 (94%)	12 (6%)	17	27
3	R	187/193 (97%)	176 (94%)	11 (6%)	19	32
4	M	20/20 (100%)	19 (95%)	1 (5%)	24	40
4	S	20/20 (100%)	19 (95%)	1 (5%)	24	40
All	All	1312/1346 (98%)	1246 (95%)	66 (5%)	24	40

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	111	LEU
1	G	216	HIS
1	G	337	GLN

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Mol	Chain	Res	Type
1	G	352	GLN
1	G	358	THR
1	G	424	ILE
1	G	478	ASN
2	L	13	VAL
2	L	105	GLU
2	L	125	LEU
2	L	135	LEU
2	L	160	GLN
3	H	38	ARG
3	H	43	GLN
3	H	54	LEU
3	H	82	LEU
3	H	83	ARG
3	H	100(D)	GLU
3	H	124	LEU
3	H	147	PRO
3	H	149	PRO
3	H	179	SER
3	H	191	THR
3	H	197	ASN
4	M	18	ARG
1	P	98	ASN
1	P	111	LEU
1	P	113	ASP
1	P	114	GLN
1	P	216	HIS
1	P	226	LEU
1	P	283	THR
1	P	333	LEU
1	P	350	LYS
1	P	351	GLU
1	P	355	ASN
1	P	374	HIS
1	P	412	ARG
1	P	418	CYS
1	P	478	ASN
2	Q	31	SER
2	Q	46	LEU
2	Q	73	LEU
2	Q	81	GLU
2	Q	90	GLN

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Mol	Chain	Res	Type
2	Q	95(B)	ARG
2	Q	105	GLU
2	Q	125	LEU
2	Q	135	LEU
2	Q	151	ASP
2	Q	154	LEU
2	Q	180	THR
2	Q	195	GLU
2	Q	197	THR
3	R	10	GLU
3	R	30	ILE
3	R	38	ARG
3	R	43	GLN
3	R	64	GLN
3	R	100(D)	GLU
3	R	124	LEU
3	R	143	LYS
3	R	147	PRO
3	R	149	PRO
3	R	150	VAL
4	S	4	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	197	ASN
1	G	203	GLN
1	G	216	HIS
1	G	337	GLN
1	G	352	GLN
1	G	355	ASN
1	G	413	ASN
1	G	478	ASN
2	L	79	GLN
2	L	166	GLN
2	L	199	GLN
2	L	210	ASN
3	H	171	GLN
3	H	199	ASN
4	M	2	ASN
1	P	98	ASN
1	P	99	ASN

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Mol	Chain	Res	Type
1	P	203	GLN
1	P	216	HIS
1	P	246	GLN
1	P	340	ASN
1	P	355	ASN
1	P	356	ASN
1	P	362	ASN
1	P	389	GLN
1	P	442	GLN
1	P	478	ASN
2	Q	90	GLN
2	Q	147	GLN
2	Q	160	GLN
2	Q	199	GLN
2	Q	210	ASN
3	R	43	GLN
3	R	64	GLN
3	R	192	GLN
3	R	199	ASN
4	S	2	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	VLM	S	27	4	6,7,7	1.30	1 (16%)	7,9,9	0.63	0
4	VLM	M	27	4	6,7,7	1.55	1 (16%)	7,9,9	0.66	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
4	VLM	S	27	4	-	0/7/8/8	-
4	VLM	M	27	4	-	0/7/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	27	VLM	C-NT	-3.78	1.23	1.32
4	S	27	VLM	C-NT	-3.03	1.25	1.32

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	27	VLM	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
5	NAG	G	588	1	14,14,15	0.55	0	17,19,21	0.67	1 (5%)
5	NAG	P	776	1	14,14,15	0.55	0	17,19,21	0.67	1 (5%)
6	IPA	P	502	-	3,3,3	0.61	0	3,3,3	0.35	0
5	NAG	P	789	1	14,14,15	0.65	0	17,19,21	0.83	1 (5%)
6	IPA	G	501	-	3,3,3	0.65	0	3,3,3	0.31	0
5	NAG	P	588	1	14,14,15	0.65	0	17,19,21	0.68	0
5	NAG	G	776	1	14,14,15	0.51	0	17,19,21	0.77	0
5	NAG	P	886	1	14,14,15	0.54	0	17,19,21	0.75	1 (5%)
5	NAG	P	762	1	14,14,15	0.51	0	17,19,21	0.71	0
5	NAG	P	741	1	14,14,15	0.65	0	17,19,21	0.72	0
5	NAG	G	734	1	14,14,15	0.53	0	17,19,21	0.68	0
5	NAG	P	795	1	14,14,15	0.58	0	17,19,21	0.81	1 (5%)
5	NAG	G	795	1	14,14,15	0.57	0	17,19,21	0.81	1 (5%)
5	NAG	G	789	1	14,14,15	0.45	0	17,19,21	0.72	0
5	NAG	G	762	1	14,14,15	0.50	0	17,19,21	0.76	0
5	NAG	P	734	1	14,14,15	0.63	0	17,19,21	0.67	0
5	NAG	G	886	1	14,14,15	0.89	1 (7%)	17,19,21	0.83	0
5	NAG	G	741	1	14,14,15	0.55	0	17,19,21	0.70	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
5	NAG	G	588	1	-	4/6/23/26	0/1/1/1
5	NAG	P	776	1	-	4/6/23/26	0/1/1/1
5	NAG	P	789	1	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	P	588	1	-	3/6/23/26	0/1/1/1
5	NAG	G	776	1	-	4/6/23/26	0/1/1/1
5	NAG	P	886	1	-	4/6/23/26	0/1/1/1
5	NAG	P	762	1	-	2/6/23/26	0/1/1/1
5	NAG	P	741	1	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	G	734	1	-	5/6/23/26	0/1/1/1
5	NAG	P	795	1	-	4/6/23/26	0/1/1/1
5	NAG	G	795	1	-	4/6/23/26	0/1/1/1
5	NAG	G	789	1	-	0/6/23/26	0/1/1/1
5	NAG	G	762	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	P	734	1	1/1/5/7	6/6/23/26	0/1/1/1
5	NAG	G	886	1	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	G	741	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	886	NAG	C1-C2	2.83	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	795	NAG	C2-N2-C7	-2.40	119.48	122.90
5	P	795	NAG	C2-N2-C7	-2.39	119.50	122.90
5	P	789	NAG	C2-N2-C7	-2.29	119.64	122.90
5	P	886	NAG	C2-N2-C7	-2.08	119.94	122.90
5	P	776	NAG	C2-N2-C7	-2.07	119.96	122.90
5	G	588	NAG	C2-N2-C7	-2.00	120.05	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	886	NAG	C1
5	P	734	NAG	C1
5	P	741	NAG	C1
5	P	789	NAG	C1

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	588	NAG	C8-C7-N2-C2
5	G	588	NAG	O7-C7-N2-C2
5	G	734	NAG	C8-C7-N2-C2
5	G	734	NAG	O7-C7-N2-C2
5	G	762	NAG	C8-C7-N2-C2
5	G	762	NAG	O7-C7-N2-C2
5	G	776	NAG	C8-C7-N2-C2
5	G	776	NAG	O7-C7-N2-C2
5	G	795	NAG	C8-C7-N2-C2
5	G	795	NAG	O7-C7-N2-C2
5	G	886	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	G	886	NAG	O7-C7-N2-C2
5	P	734	NAG	C8-C7-N2-C2
5	P	734	NAG	O7-C7-N2-C2
5	P	741	NAG	C8-C7-N2-C2
5	P	741	NAG	O7-C7-N2-C2
5	P	762	NAG	C8-C7-N2-C2
5	P	762	NAG	O7-C7-N2-C2
5	P	776	NAG	C8-C7-N2-C2
5	P	776	NAG	O7-C7-N2-C2
5	P	789	NAG	C8-C7-N2-C2
5	P	789	NAG	O7-C7-N2-C2
5	P	795	NAG	C8-C7-N2-C2
5	P	795	NAG	O7-C7-N2-C2
5	P	886	NAG	C8-C7-N2-C2
5	P	886	NAG	O7-C7-N2-C2
5	P	734	NAG	O5-C5-C6-O6
5	G	762	NAG	C4-C5-C6-O6
5	P	776	NAG	O5-C5-C6-O6
5	P	886	NAG	O5-C5-C6-O6
5	G	734	NAG	O5-C5-C6-O6
5	P	734	NAG	C4-C5-C6-O6
5	P	886	NAG	C4-C5-C6-O6
5	P	795	NAG	O5-C5-C6-O6
5	P	741	NAG	C4-C5-C6-O6
5	G	734	NAG	C4-C5-C6-O6
5	P	795	NAG	C4-C5-C6-O6
5	P	776	NAG	C4-C5-C6-O6
5	P	588	NAG	C8-C7-N2-C2
5	G	762	NAG	O5-C5-C6-O6
5	P	741	NAG	O5-C5-C6-O6
5	G	795	NAG	O5-C5-C6-O6
5	P	588	NAG	O7-C7-N2-C2
5	G	886	NAG	C1-C2-N2-C7
5	G	734	NAG	C3-C2-N2-C7
5	G	795	NAG	C4-C5-C6-O6
5	G	776	NAG	C4-C5-C6-O6
5	G	588	NAG	C4-C5-C6-O6
5	P	789	NAG	O5-C5-C6-O6
5	G	588	NAG	O5-C5-C6-O6
5	P	734	NAG	C3-C2-N2-C7
5	P	588	NAG	O5-C5-C6-O6
5	G	776	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	P	734	NAG	C1-C2-N2-C7

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	776	NAG	1	0
6	P	502	IPA	2	0
5	P	789	NAG	3	0
5	P	588	NAG	2	0
5	G	776	NAG	1	0
5	P	886	NAG	3	0
5	P	762	NAG	1	0
5	P	795	NAG	1	0
5	G	795	NAG	1	0
5	G	762	NAG	1	0
5	P	734	NAG	1	0
5	G	886	NAG	3	0
5	G	741	NAG	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	G	301/313 (96%)	-0.13	5 (1%) 70 68	17, 35, 65, 76	0
1	P	300/313 (95%)	0.17	14 (4%) 31 30	28, 48, 73, 87	0
2	L	214/214 (100%)	-0.53	0 100 100	14, 29, 42, 48	0
2	Q	214/214 (100%)	-0.24	4 (1%) 66 64	19, 36, 59, 68	0
3	H	221/229 (96%)	-0.52	0 100 100	15, 25, 40, 73	0
3	R	222/229 (96%)	-0.41	2 (0%) 84 82	15, 33, 48, 75	0
4	M	24/27 (88%)	0.04	0 100 100	27, 40, 51, 59	0
4	S	24/27 (88%)	-0.25	0 100 100	32, 38, 47, 58	0
All	All	1520/1566 (97%)	-0.24	25 (1%) 72 70	14, 35, 64, 87	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	459	GLY	7.0
1	P	462	THR	5.1
1	P	441	GLY	4.9
1	P	458	GLY	4.3
1	P	129	ALA	4.2
2	Q	150	VAL	4.0
1	P	460	LYS	3.7
1	P	444	ARG	3.1
3	R	214	LYS	3.0
3	R	1	GLU	2.7
1	G	459	GLY	2.7
1	P	355	ASN	2.4
1	G	129	ALA	2.4
1	G	462	THR	2.4
1	P	196	CYS	2.4
2	Q	146	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	Q	129	THR	2.3
1	P	492	GLU	2.3
1	G	126	CYS	2.2
1	G	460	LYS	2.2
2	Q	126	LYS	2.2
1	P	359	ILE	2.2
1	P	127	VAL	2.2
1	P	268	GLU	2.1
1	P	350	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	VLM	M	27	8/8	0.85	0.19	35,36,38,39	0
4	DPR	S	21	7/8	0.93	0.14	31,32,34,35	0
4	VLM	S	27	8/8	0.93	0.15	40,41,43,44	0
4	DPR	M	21	7/8	0.96	0.12	26,27,28,30	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	P	741	14/15	0.38	0.53	77,80,80,81	0
5	NAG	P	795	14/15	0.56	0.33	71,74,75,77	0
5	NAG	P	588	14/15	0.62	0.23	61,65,65,66	0
5	NAG	P	734	14/15	0.68	0.29	81,83,84,84	0
5	NAG	P	776	14/15	0.71	0.26	63,65,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	G	886	14/15	0.78	0.17	49,52,56,56	0
5	NAG	G	741	14/15	0.78	0.28	65,67,70,70	0
5	NAG	G	795	14/15	0.78	0.20	52,54,55,55	0
5	NAG	P	886	14/15	0.79	0.23	63,67,69,71	0
5	NAG	G	734	14/15	0.82	0.17	66,67,69,69	0
5	NAG	P	789	14/15	0.84	0.22	65,69,74,75	0
5	NAG	G	588	14/15	0.88	0.18	66,67,69,70	0
6	IPA	G	501	4/4	0.90	0.28	44,47,48,48	0
5	NAG	G	762	14/15	0.91	0.18	32,34,38,39	0
5	NAG	G	776	14/15	0.91	0.13	42,44,47,48	0
5	NAG	G	789	14/15	0.92	0.11	40,42,44,45	0
5	NAG	P	762	14/15	0.94	0.13	40,42,45,46	0
6	IPA	P	502	4/4	0.94	0.31	46,47,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.