Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 11:54 AM EDT

PDB ID	:	4QQV
Title	:	Extracellular domains of mouse IL-3 beta receptor
Authors	:	Jackson, C.J.; Young, I.G.; Murphy, J.M.; Carr, P.D.; Ewens, C.L.; Dai, J.; Ollis, D.L.
Deposited on	:	2014-06-30
Resolution	:	3.45 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

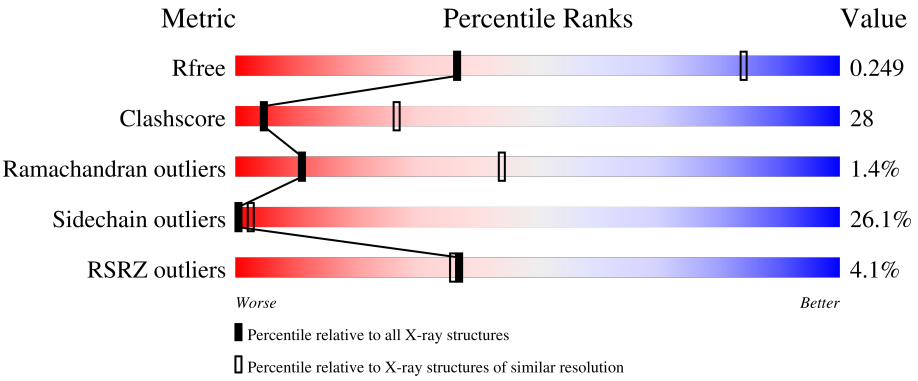
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	A	416	4% 42% 40% 13%
1	B	416	6% 40% 40% 14% 5%
1	C	416	4% 39% 40% 17%
1	D	416	% 33% 33% 10% 24%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12274 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.

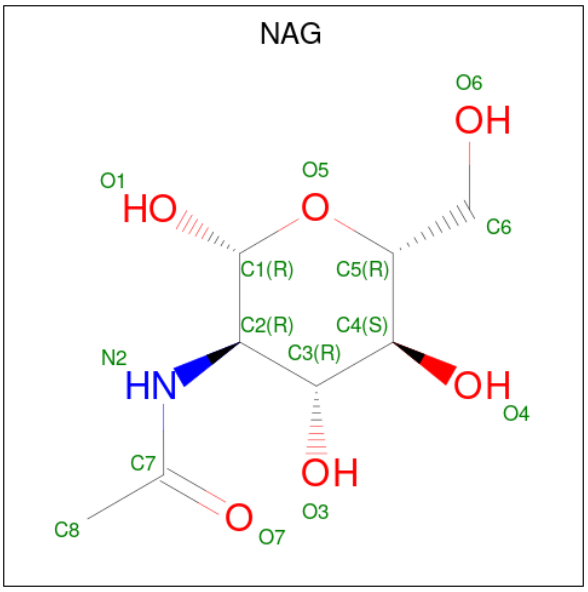
- Molecule 1 is a protein called Interleukin-3 receptor class 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3229	2045	548	619	17			
1	B	395	Total	C	N	O	S	0	0	0
			3195	2023	543	612	17			
1	C	402	Total	C	N	O	S	0	0	0
			3252	2058	552	625	17			
1	D	316	Total	C	N	O	S	0	0	0
			2542	1609	433	485	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	GLN	ASN	engineered mutation	UNP P26954
A	331	ALA	LYS	engineered mutation	UNP P26954
A	333	ALA	ARG	engineered mutation	UNP P26954
A	334	ALA	ASP	engineered mutation	UNP P26954
B	328	GLN	ASN	engineered mutation	UNP P26954
B	331	ALA	LYS	engineered mutation	UNP P26954
B	333	ALA	ARG	engineered mutation	UNP P26954
B	334	ALA	ASP	engineered mutation	UNP P26954
C	328	GLN	ASN	engineered mutation	UNP P26954
C	331	ALA	LYS	engineered mutation	UNP P26954
C	333	ALA	ARG	engineered mutation	UNP P26954
C	334	ALA	ASP	engineered mutation	UNP P26954
D	328	GLN	ASN	engineered mutation	UNP P26954
D	331	ALA	LYS	engineered mutation	UNP P26954
D	333	ALA	ARG	engineered mutation	UNP P26954
D	334	ALA	ASP	engineered mutation	UNP P26954

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



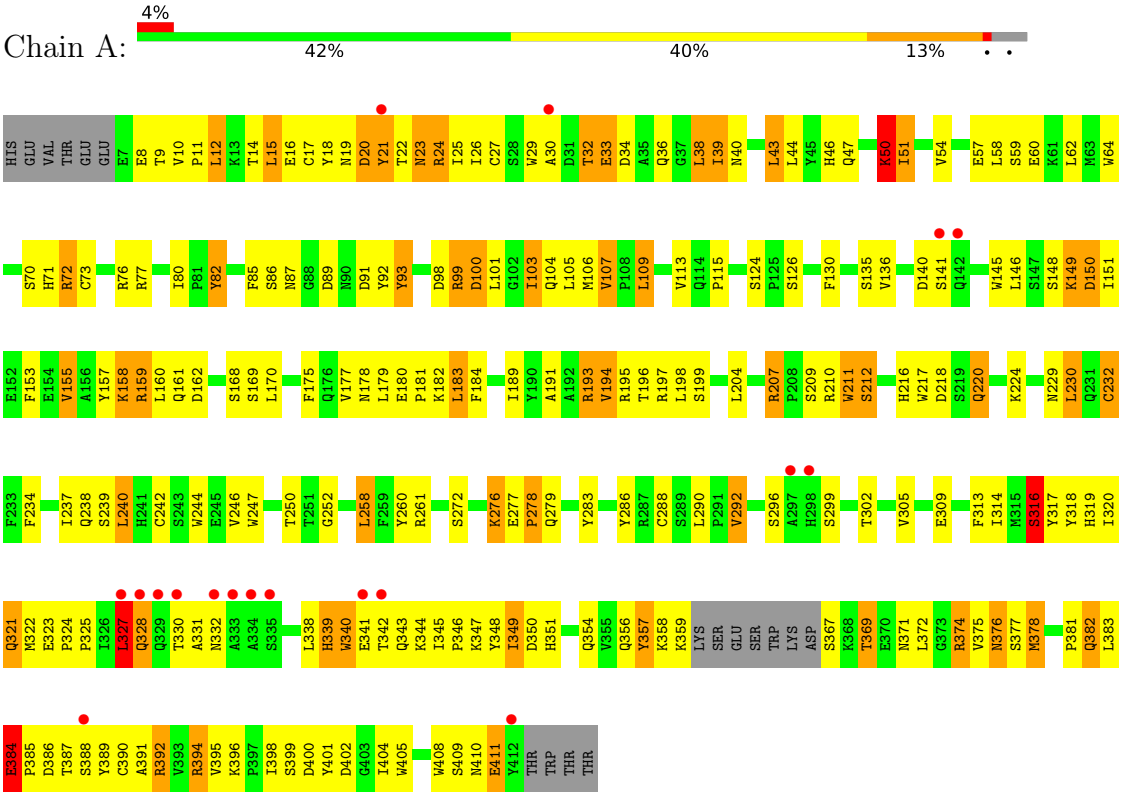
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0

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.

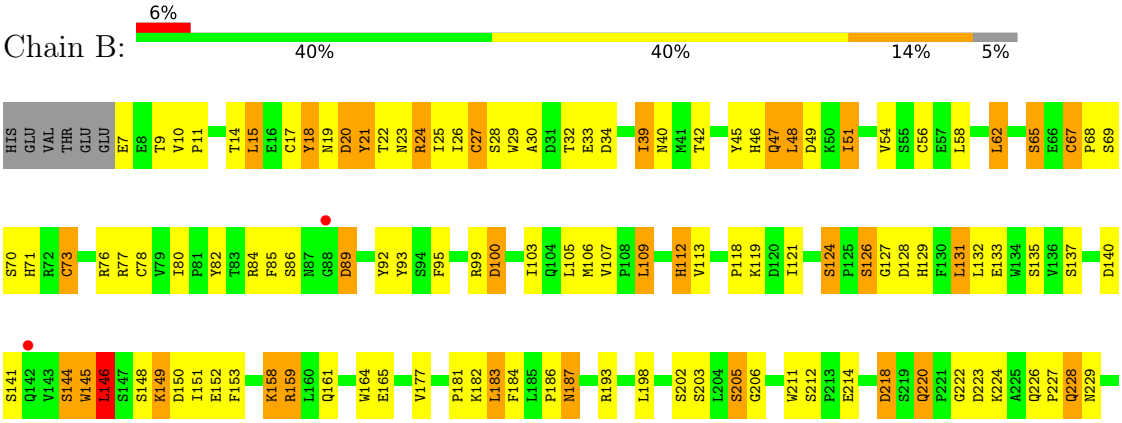
• Molecule 1: Interleukin-3 receptor class 2 subunit beta

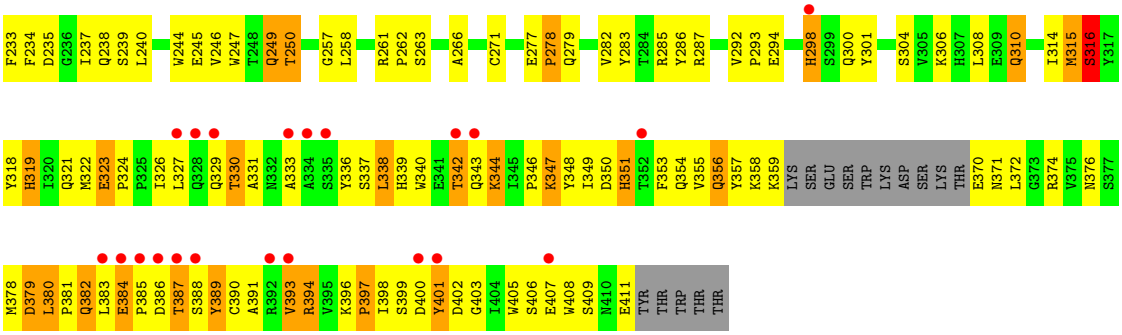
Chain A:



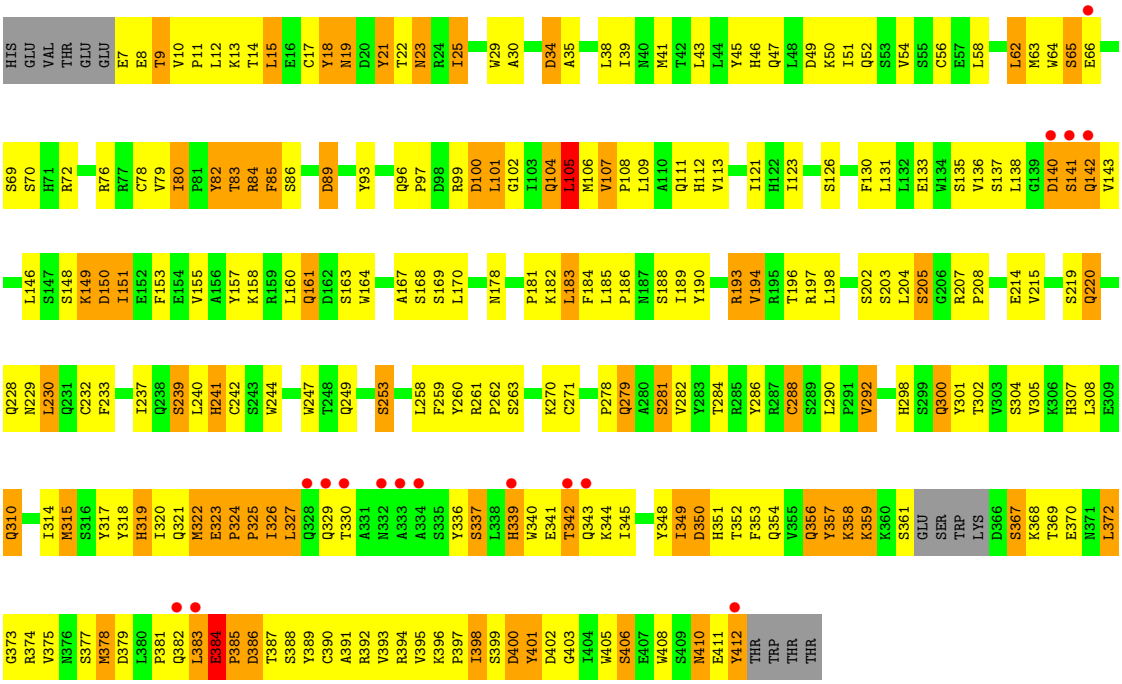
• Molecule 1: Interleukin-3 receptor class 2 subunit beta

Chain B:

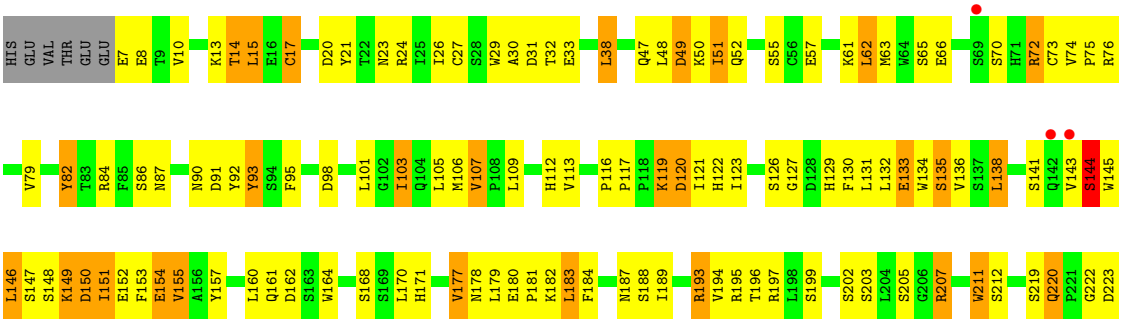


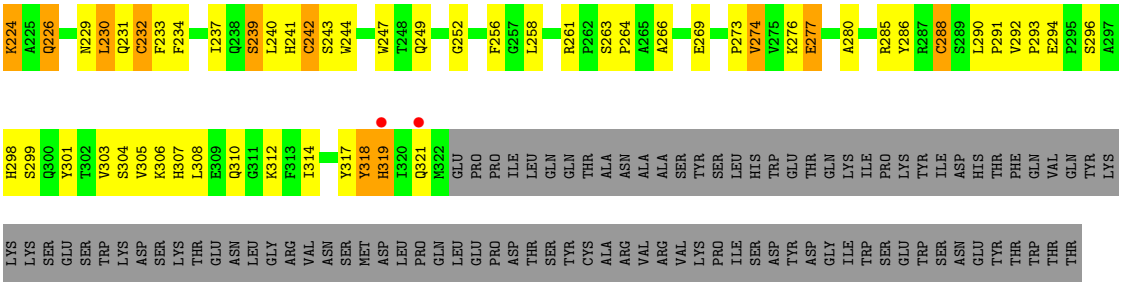


• Molecule 1: Interleukin-3 receptor class 2 subunit beta



• Molecule 1: Interleukin-3 receptor class 2 subunit beta




K224 A225 Q226 M229 L230 Q231 C232 F233 F234 I237 Q238 S239 L240 H241 C242 S243 W244 W247 T248 Q249 G252 F256 G257 L258 R261 P262 S263 P264 A265 A266 E269 P273 V274 V275 K276 E277 A280 R285 Y286 R287 C288 S289 L290 P291 V292 P293 E294 P295 S296 A297
H298 S299 Q300 Y301 T302 V303 S304 V305 K306 H307 L308 E309 Q310 G311 K312 F313 I314 Y317 Y318 H319 I320 Q321 M322 GLU PRO PRO ILE LEU GLN GLN THR ALA ASN ALA ALA SER TYR SER LEU HIS TRP GLU THR GLN LYS ILE PRO LYS TYR ILE ASP HIS THR PHE GLN VAL GLN TYR LYS
LYS LYS SER GLU SER TRP LYS ASP SER LYS THR GLU ASN LEU GLY ARG VAL ASN SER MET ASP LEU PRO GLN LEU GLU PRO ASP THR SER TYR CYS ALA ARG VAL ARG VAL LYS PRO ILE SER ASP TYR ASP GLY ILE TRP SER GLU TRP SER ASN GLU TYR THR TRP THR THR THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	197.15Å 166.46Å 128.00Å 90.00° 122.77° 90.00°	Depositor
Resolution (Å)	19.91 – 3.45 19.91 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.91-3.45) 99.5 (19.91-3.45)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 3.44Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1558)	Depositor
R, R_{free}	0.203 , 0.248 0.208 , 0.249	Depositor DCC
R_{free} test set	2269 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	96.7	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12274	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

5.1 Standard geometry

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

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	0.59	0/3327	0.81	3/4535 (0.1%)
1	B	0.61	2/3292 (0.1%)	0.81	1/4488 (0.0%)
1	C	0.54	0/3350	0.81	3/4565 (0.1%)
1	D	0.55	0/2620	0.74	0/3572
All	All	0.57	2/12589 (0.0%)	0.79	7/17160 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
1	C	0	2
1	D	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	CYS	CB-SG	7.60	1.95	1.82
1	B	67	CYS	CB-SG	6.36	1.93	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	324	PRO	C-N-CD	-8.99	100.83	120.60
1	C	384	GLU	C-N-CD	-8.64	101.58	120.60
1	A	50	LYS	N-CA-C	5.69	126.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	327	LEU	CA-CB-CG	-5.62	102.38	115.30
1	A	22	THR	N-CA-C	-5.60	95.87	111.00
1	B	146	LEU	CA-CB-CG	5.39	127.70	115.30
1	C	105	LEU	CA-CB-CG	5.38	127.67	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	277	GLU	Peptide
1	A	278	PRO	Peptide
1	A	316	SER	Peptide
1	A	384	GLU	Peptide
1	B	278	PRO	Peptide
1	B	316	SER	Peptide
1	B	384	GLU	Peptide
1	C	384	GLU	Peptide
1	C	49	ASP	Peptide
1	D	49	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3229	0	3067	173	0
1	B	3195	0	3035	212	0
1	C	3252	0	3089	211	0
1	D	2542	0	2413	134	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
All	All	12274	0	11656	671	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 28.

All (671) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:TYR:HE1	1:B:391:ALA:CB	1.40	1.35
1:B:357:TYR:CE1	1:B:391:ALA:CB	2.16	1.27
1:B:357:TYR:CE1	1:B:391:ALA:HB2	1.79	1.18
1:C:14:THR:HG23	1:C:62:LEU:HD11	1.19	1.12
1:C:169:SER:C	1:C:170:LEU:HD12	1.70	1.11
1:C:14:THR:CG2	1:C:62:LEU:HD11	1.77	1.11
1:C:169:SER:O	1:C:170:LEU:HD12	1.59	1.01
1:B:357:TYR:HE1	1:B:391:ALA:CA	1.74	1.00
1:B:357:TYR:CE1	1:B:391:ALA:HB1	2.02	0.93
1:B:45:TYR:CE2	1:B:47:GLN:NE2	2.35	0.93
1:C:356:GLN:NE2	1:C:368:LYS:O	2.01	0.93
1:C:14:THR:HG22	1:C:29:TRP:HA	1.51	0.92
1:C:325:PRO:O	1:C:410:ASN:ND2	2.07	0.88
1:C:47:GLN:HB2	1:C:50:LYS:HB2	1.59	0.84
1:B:15:LEU:HD23	1:B:29:TRP:HB3	1.61	0.82
1:B:394:ARG:HD2	1:B:408:TRP:HE1	1.45	0.82
1:C:14:THR:HG23	1:C:62:LEU:CD1	2.06	0.81
1:B:357:TYR:CZ	1:B:391:ALA:CB	2.65	0.80
1:B:45:TYR:HE2	1:B:47:GLN:NE2	1.81	0.79
1:A:50:LYS:HE2	1:A:51:ILE:H	1.48	0.79
1:C:352:THR:HA	1:C:373:GLY:HA2	1.65	0.79
1:C:342:THR:HA	1:C:343:GLN:HB2	1.64	0.78
1:C:390:CYS:HB3	1:C:411:GLU:HB3	1.65	0.78
1:D:129:HIS:HA	1:D:181:PRO:HD3	1.66	0.77
1:A:100:ASP:N	1:A:100:ASP:OD1	2.13	0.77
1:C:361:SER:HB3	1:C:367:SER:H	1.50	0.77
1:A:345:ILE:HG22	1:A:347:LYS:HG2	1.67	0.76
1:C:84:ARG:HH11	1:C:84:ARG:HB3	1.50	0.76
1:C:15:LEU:HA	1:C:29:TRP:HB3	1.68	0.75
1:D:207:ARG:HB2	1:D:207:ARG:CZ	2.17	0.74
1:D:230:LEU:HD23	1:D:244:TRP:HB3	1.70	0.74
1:C:54:VAL:HG13	1:C:80:ILE:HG12	1.70	0.74
1:B:357:TYR:CZ	1:B:391:ALA:HB2	2.23	0.73
1:B:227:PRO:HB3	1:B:246:VAL:HG12	1.70	0.73
1:C:108:PRO:HB2	1:C:111:GLN:HG2	1.70	0.73
1:B:331:ALA:HB2	1:B:387:THR:HG23	1.71	0.73
1:D:132:LEU:HB3	1:D:177:VAL:HG12	1.71	0.73
1:A:323:GLU:OE2	1:A:323:GLU:N	2.20	0.72
1:B:351:HIS:HB2	1:B:374:ARG:HG3	1.70	0.72
1:B:10:VAL:HG23	1:B:68:PRO:HG2	1.70	0.72
1:A:46:HIS:HA	1:A:50:LYS:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HG13	1:A:170:LEU:HB2	1.72	0.71
1:C:350:ASP:OD1	1:C:398:ILE:N	2.21	0.71
1:A:305:VAL:HB	1:B:103:ILE:HG22	1.73	0.71
1:B:357:TYR:CZ	1:B:391:ALA:HB1	2.24	0.71
1:B:229:ASN:ND2	1:B:245:GLU:OE2	2.23	0.71
1:C:383:LEU:C	1:C:385:PRO:HD2	2.11	0.71
1:B:218:ASP:OD1	1:B:218:ASP:N	2.24	0.71
1:C:310:GLN:HE21	1:D:8:GLU:HA	1.56	0.71
1:B:327:LEU:HD21	1:B:389:TYR:CZ	2.26	0.71
1:B:338:LEU:HD21	1:B:357:TYR:OH	1.91	0.71
1:C:259:PHE:HE2	1:C:270:LYS:HD2	1.55	0.71
1:B:357:TYR:HE2	1:B:380:LEU:CD2	2.03	0.70
1:C:149:LYS:HD2	1:C:150:ASP:HA	1.72	0.70
1:D:224:LYS:HG3	1:D:247:TRP:CG	2.26	0.70
1:A:399:SER:OG	1:A:400:ASP:N	2.22	0.70
1:D:121:ILE:HD12	1:D:134:TRP:HB3	1.71	0.70
1:B:238:GLN:HA	1:B:292:VAL:HG22	1.73	0.70
1:C:89:ASP:OD1	1:C:89:ASP:N	2.21	0.70
1:B:126:SER:OG	1:B:127:GLY:N	2.24	0.69
1:A:320:ILE:O	1:A:321:GLN:HG2	1.92	0.69
1:B:357:TYR:CE2	1:B:380:LEU:CD2	2.75	0.69
1:C:169:SER:C	1:C:170:LEU:CD1	2.55	0.69
1:C:319:HIS:H	1:C:403:GLY:HA2	1.56	0.69
1:A:230:LEU:HD23	1:A:244:TRP:HB3	1.74	0.69
1:C:400:ASP:N	1:C:400:ASP:OD1	2.26	0.69
1:B:150:ASP:HB3	1:B:202:SER:HB2	1.74	0.68
1:C:230:LEU:HD23	1:C:244:TRP:HB3	1.75	0.68
1:A:384:GLU:HB3	1:A:385:PRO:HD3	1.74	0.68
1:A:30:ALA:HB2	1:A:62:LEU:HD21	1.75	0.68
1:B:357:TYR:HE1	1:B:391:ALA:HA	1.57	0.68
1:B:187:ASN:OD1	1:B:222:GLY:N	2.27	0.68
1:D:229:ASN:O	1:D:244:TRP:HA	1.94	0.68
1:B:398:ILE:HG22	1:B:399:SER:H	1.59	0.67
1:A:328:GLN:H	1:A:328:GLN:HE21	1.41	0.67
1:B:357:TYR:CE2	1:B:380:LEU:HD23	2.29	0.67
1:C:258:LEU:HD23	1:C:288:CYS:SG	2.35	0.67
1:A:19:ASN:N	1:A:19:ASN:OD1	2.27	0.67
1:D:181:PRO:HB3	1:D:220:GLN:HG2	1.75	0.67
1:B:350:ASP:OD2	1:B:398:ILE:N	2.20	0.67
1:C:150:ASP:OD1	1:C:150:ASP:N	2.26	0.67
1:B:357:TYR:OH	1:B:391:ALA:HB1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:CYS:HB2	1:B:411:GLU:HG3	1.77	0.67
1:D:150:ASP:OD1	1:D:150:ASP:N	2.28	0.67
1:A:194:VAL:O	1:A:212:SER:HB3	1.95	0.67
1:C:385:PRO:O	1:C:386:ASP:HB2	1.93	0.66
1:D:179:LEU:HB3	1:D:184:PHE:HZ	1.59	0.66
1:B:357:TYR:OH	1:B:391:ALA:CB	2.44	0.66
1:C:8:GLU:HA	1:D:310:GLN:NE2	2.09	0.66
1:C:202:SER:OG	1:C:204:LEU:HB2	1.96	0.66
1:A:328:GLN:OE1	1:A:339:HIS:NE2	2.26	0.66
1:B:118:PRO:HB2	1:B:212:SER:HB3	1.78	0.66
1:C:140:ASP:N	1:C:140:ASP:OD1	2.28	0.66
1:D:155:VAL:HG13	1:D:170:LEU:HB2	1.77	0.66
1:C:319:HIS:H	1:C:403:GLY:CA	2.09	0.66
1:B:342:THR:HG23	1:B:344:LYS:HD3	1.78	0.65
1:A:325:PRO:HA	1:A:339:HIS:O	1.97	0.65
1:B:358:LYS:HZ3	1:B:370:GLU:N	1.92	0.65
1:A:392:ARG:HB2	1:A:408:TRP:CE3	2.31	0.65
1:B:319:HIS:CD2	1:B:397:PRO:HG3	2.31	0.65
1:B:357:TYR:CE1	1:B:391:ALA:HA	2.32	0.65
1:B:357:TYR:CE1	1:B:391:ALA:CA	2.65	0.65
1:C:185:LEU:HD21	1:C:229:ASN:HB2	1.79	0.64
1:A:58:LEU:HA	1:A:76:ARG:HA	1.78	0.64
1:D:149:LYS:HE2	1:D:150:ASP:HA	1.79	0.64
1:C:21:TYR:CZ	1:C:85:PHE:HB3	2.32	0.64
1:D:144:SER:O	1:D:144:SER:OG	2.13	0.64
1:A:105:LEU:HD22	1:A:106:MET:N	2.13	0.64
1:A:237:ILE:HG22	1:A:238:GLN:HG2	1.78	0.64
1:D:141:SER:O	1:D:144:SER:HB3	1.98	0.64
1:A:372:LEU:HD21	1:A:378:MET:HB2	1.80	0.64
1:C:19:ASN:OD1	1:C:25:ILE:HG22	1.97	0.64
1:A:43:LEU:HD12	1:A:44:LEU:H	1.63	0.63
1:A:278:PRO:HB2	1:A:279:GLN:HA	1.79	0.63
1:C:398:ILE:HG12	1:C:399:SER:N	2.10	0.63
1:A:349:ILE:HG21	1:A:401:TYR:CD2	2.33	0.63
1:C:83:THR:OG1	1:C:84:ARG:NH1	2.28	0.63
1:D:62:LEU:HD12	1:D:62:LEU:H	1.63	0.63
1:C:102:GLY:O	1:D:226:GLN:NE2	2.32	0.63
1:C:9:THR:HB	1:C:11:PRO:HD2	1.81	0.63
1:A:234:PHE:O	1:B:113:VAL:HG23	1.99	0.62
1:C:14:THR:HG21	1:C:30:ALA:N	2.14	0.62
1:B:10:VAL:HG13	1:B:11:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:VAL:HG13	1:C:198:LEU:HD11	1.82	0.62
1:A:47:GLN:H	1:A:50:LYS:CD	2.12	0.62
1:A:99:ARG:NH2	1:B:223:ASP:OD1	2.26	0.62
1:C:327:LEU:H	1:C:327:LEU:HD22	1.64	0.62
1:B:181:PRO:HB3	1:B:220:GLN:HE21	1.64	0.62
1:D:61:LYS:HG3	1:D:62:LEU:N	2.15	0.62
1:A:391:ALA:O	1:A:411:GLU:HG3	1.98	0.62
1:A:89:ASP:OD1	1:A:89:ASP:N	2.33	0.62
1:C:305:VAL:HB	1:D:103:ILE:HG22	1.82	0.61
1:A:276:LYS:HD3	1:A:286:TYR:HE1	1.65	0.61
1:A:86:SER:OG	1:A:89:ASP:N	2.33	0.61
1:D:292:VAL:HG12	1:D:301:TYR:CZ	2.36	0.61
1:D:26:ILE:HG12	1:D:79:VAL:HG12	1.81	0.61
1:C:358:LYS:HE2	1:C:359:LYS:HE2	1.80	0.61
1:B:67:CYS:CB	1:B:73:CYS:SG	2.88	0.61
1:A:314:ILE:HG23	1:A:318:TYR:HD2	1.66	0.61
1:A:330:THR:HB	1:A:387:THR:HB	1.83	0.61
1:B:292:VAL:HG23	1:B:293:PRO:O	2.00	0.61
1:A:351:HIS:HB2	1:A:374:ARG:HG3	1.82	0.61
1:B:330:THR:HG22	1:B:388:SER:H	1.66	0.61
1:C:247:TRP:CD1	1:C:249:GLN:HB2	2.36	0.60
1:A:318:TYR:O	1:B:19:ASN:HB3	2.01	0.60
1:B:357:TYR:HE2	1:B:380:LEU:HD21	1.67	0.60
1:B:402:ASP:OD1	1:B:403:GLY:N	2.34	0.60
1:B:124:SER:HB2	1:B:131:LEU:CD1	2.29	0.60
1:C:8:GLU:HA	1:D:310:GLN:HE21	1.66	0.60
1:C:323:GLU:OE1	1:C:395:VAL:CG2	2.50	0.60
1:A:18:TYR:CD1	1:B:318:TYR:HB3	2.37	0.60
1:A:50:LYS:HE2	1:A:51:ILE:N	2.16	0.60
1:A:314:ILE:HB	1:B:93:TYR:CE1	2.37	0.60
1:C:357:TYR:CE2	1:C:391:ALA:HB2	2.37	0.60
1:B:124:SER:O	1:B:131:LEU:N	2.34	0.59
1:B:132:LEU:HB3	1:B:177:VAL:HG12	1.83	0.59
1:B:229:ASN:HB3	1:B:245:GLU:HG3	1.83	0.59
1:D:10:VAL:O	1:D:14:THR:OG1	2.20	0.59
1:D:47:GLN:HG3	1:D:50:LYS:HD2	1.82	0.59
1:C:375:VAL:HG12	1:C:377:SER:H	1.67	0.59
1:C:399:SER:OG	1:C:400:ASP:OD1	2.20	0.59
1:A:324:PRO:HD2	1:A:342:THR:H	1.67	0.59
1:B:342:THR:C	1:B:344:LYS:HB2	2.23	0.59
1:A:103:ILE:HG22	1:B:227:PRO:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:LEU:O	1:C:99:ARG:NH2	2.33	0.59
1:C:47:GLN:CB	1:C:50:LYS:HB2	2.31	0.59
1:C:390:CYS:HB2	1:C:412:TYR:HB2	1.83	0.59
1:D:277:GLU:OE2	1:D:285:ARG:NH1	2.36	0.59
1:B:124:SER:HB2	1:B:131:LEU:HD13	1.84	0.58
1:A:47:GLN:H	1:A:50:LYS:HD3	1.68	0.58
1:C:324:PRO:HD2	1:C:342:THR:HG23	1.85	0.58
1:C:322:MET:N	1:C:406:SER:OG	2.36	0.58
1:D:240:LEU:HD23	1:D:290:LEU:HD11	1.85	0.58
1:C:300:GLN:OE1	1:D:106:MET:HE2	2.04	0.58
1:D:23:ASN:O	1:D:82:TYR:N	2.25	0.58
1:A:324:PRO:HG2	1:A:341:GLU:HB3	1.85	0.58
1:C:323:GLU:OE1	1:C:395:VAL:HG23	2.03	0.58
1:B:164:TRP:CH2	1:B:193:ARG:HG3	2.38	0.58
1:B:228:GLN:NE2	1:B:283:TYR:OH	2.37	0.58
1:A:386:ASP:OD1	1:A:387:THR:N	2.36	0.57
1:D:17:CYS:SG	1:D:93:TYR:HE2	2.27	0.57
1:C:326:ILE:HG13	1:C:339:HIS:HB3	1.86	0.57
1:C:356:GLN:NE2	1:C:357:TYR:H	2.02	0.57
1:C:23:ASN:O	1:C:82:TYR:N	2.27	0.57
1:C:158:LYS:HE3	1:C:164:TRP:CE2	2.40	0.57
1:A:193:ARG:NH2	1:A:211:TRP:NE1	2.53	0.57
1:B:67:CYS:CB	1:B:73:CYS:HG	2.17	0.57
1:C:323:GLU:OE2	1:C:340:TRP:HB3	2.05	0.57
1:B:396:LYS:HB3	1:B:405:TRP:CE3	2.39	0.57
1:D:119:LYS:HG2	1:D:120:ASP:H	1.69	0.56
1:A:43:LEU:HD12	1:A:44:LEU:N	2.20	0.56
1:D:181:PRO:HA	1:D:220:GLN:HE21	1.69	0.56
1:B:126:SER:HB3	1:B:129:HIS:CD2	2.41	0.56
1:B:316:SER:HA	1:B:318:TYR:H	1.71	0.56
1:C:358:LYS:NZ	1:C:359:LYS:O	2.26	0.56
1:B:394:ARG:HD2	1:B:408:TRP:NE1	2.19	0.56
1:A:159:ARG:NH2	1:A:161:GLN:HE21	2.04	0.56
1:B:82:TYR:OH	1:B:89:ASP:OD2	2.18	0.56
1:A:247:TRP:HE3	1:A:283:TYR:CE1	2.23	0.56
1:A:342:THR:HA	1:A:343:GLN:HB2	1.86	0.56
1:B:357:TYR:CE2	1:B:380:LEU:HD21	2.41	0.56
1:D:187:ASN:ND2	1:D:222:GLY:O	2.39	0.56
1:A:149:LYS:HD2	1:A:150:ASP:HA	1.88	0.55
1:C:249:GLN:NE2	1:D:38:LEU:HD21	2.21	0.55
1:A:47:GLN:O	1:A:50:LYS:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD23	1:A:177:VAL:HG21	1.88	0.55
1:C:160:LEU:HD13	1:C:189:ILE:HG22	1.88	0.55
1:D:15:LEU:HD23	1:D:29:TRP:HB3	1.87	0.55
1:D:151:ILE:HG12	1:D:152:GLU:N	2.21	0.55
1:A:319:HIS:HA	1:B:19:ASN:O	2.06	0.55
1:B:100:ASP:OD1	1:B:100:ASP:N	2.38	0.55
1:B:330:THR:HG23	1:B:388:SER:HB3	1.87	0.55
1:C:321:GLN:HE21	1:C:397:PRO:HD3	1.72	0.55
1:A:196:THR:N	1:A:209:SER:OG	2.29	0.55
1:C:233:PHE:CD2	1:D:207:ARG:NH2	2.74	0.55
1:C:10:VAL:HG23	1:D:252:GLY:O	2.07	0.55
1:C:21:TYR:OH	1:C:85:PHE:HB3	2.07	0.55
1:B:314:ILE:HG22	1:B:315:MET:O	2.07	0.55
1:C:302:THR:HG22	1:D:106:MET:HE3	1.88	0.55
1:B:355:VAL:O	1:B:370:GLU:N	2.40	0.54
1:C:373:GLY:O	1:C:375:VAL:HG23	2.06	0.54
1:D:47:GLN:HB2	1:D:50:LYS:HB2	1.89	0.54
1:A:150:ASP:N	1:A:150:ASP:OD1	2.40	0.54
1:A:342:THR:OG1	1:A:344:LYS:HG2	2.07	0.54
1:B:344:LYS:N	1:B:344:LYS:HD2	2.22	0.54
1:B:346:PRO:HG2	1:B:351:HIS:CE1	2.42	0.54
1:C:340:TRP:CD1	1:C:393:VAL:HG21	2.42	0.54
1:C:259:PHE:CE2	1:C:270:LYS:HD2	2.41	0.54
1:A:160:LEU:HD13	1:A:189:ILE:HB	1.88	0.54
1:B:15:LEU:HG	1:B:95:PHE:CZ	2.42	0.54
1:B:181:PRO:O	1:B:182:LYS:HB2	2.08	0.54
1:C:321:GLN:NE2	1:C:397:PRO:HD3	2.22	0.54
1:B:257:GLY:HA3	1:B:308:LEU:HD21	1.90	0.54
1:C:244:TRP:NE1	1:C:286:TYR:HD2	2.06	0.54
1:C:383:LEU:HD12	1:C:383:LEU:H	1.73	0.54
1:B:396:LYS:HD3	1:B:405:TRP:CE2	2.43	0.54
1:A:313:PHE:CE1	1:B:92:TYR:HB2	2.44	0.53
1:B:396:LYS:HG3	1:B:397:PRO:N	2.23	0.53
1:D:263:SER:HB2	1:D:264:PRO:HD2	1.90	0.53
1:B:10:VAL:HG11	1:B:32:THR:HG23	1.89	0.53
1:B:262:PRO:HB3	1:B:301:TYR:CZ	2.43	0.53
1:C:14:THR:CG2	1:C:29:TRP:HA	2.32	0.53
1:D:121:ILE:HG13	1:D:133:GLU:O	2.07	0.53
1:B:10:VAL:CG1	1:B:11:PRO:HD3	2.37	0.53
1:C:202:SER:O	1:C:203:SER:OG	2.19	0.53
1:C:357:TYR:O	1:C:358:LYS:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ASP:HB3	1:D:93:TYR:HE1	1.74	0.53
1:C:207:ARG:HD2	1:D:233:PHE:CZ	2.43	0.53
1:C:330:THR:HA	1:C:388:SER:HB2	1.90	0.53
1:D:151:ILE:HD11	1:D:196:THR:HG23	1.90	0.53
1:A:130:PHE:N	1:A:179:LEU:O	2.33	0.53
1:A:328:GLN:HE21	1:A:328:GLN:N	2.06	0.53
1:C:317:TYR:HA	1:C:319:HIS:HE1	1.73	0.53
1:A:327:LEU:HD22	1:A:411:GLU:CD	2.28	0.53
1:C:170:LEU:HD12	1:C:170:LEU:N	2.19	0.53
1:B:372:LEU:HD21	1:B:378:MET:HB2	1.91	0.53
1:B:393:VAL:HG12	1:B:394:ARG:H	1.74	0.53
1:B:381:PRO:O	1:B:382:GLN:NE2	2.42	0.53
1:C:261:ARG:HB2	1:C:302:THR:OG1	2.09	0.53
1:A:23:ASN:ND2	1:A:24:ARG:HG2	2.24	0.53
1:B:67:CYS:SG	1:B:68:PRO:HD2	2.48	0.53
1:C:390:CYS:CB	1:C:412:TYR:HB2	2.40	0.52
1:A:43:LEU:HB3	1:A:54:VAL:HB	1.91	0.52
1:B:140:ASP:OD1	1:B:140:ASP:N	2.41	0.52
1:C:350:ASP:C	1:C:351:HIS:HD1	2.13	0.52
1:C:383:LEU:O	1:C:385:PRO:HD2	2.09	0.52
1:D:138:LEU:HD13	1:D:146:LEU:HD13	1.91	0.52
1:C:278:PRO:HB2	1:C:279:GLN:HA	1.91	0.52
1:A:36:GLN:N	1:A:36:GLN:OE1	2.41	0.52
1:B:344:LYS:O	1:B:346:PRO:HD3	2.09	0.52
1:D:61:LYS:HG3	1:D:62:LEU:H	1.72	0.52
1:B:21:TYR:HE1	1:B:85:PHE:CG	2.28	0.52
1:C:325:PRO:HA	1:C:339:HIS:O	2.08	0.52
1:A:252:GLY:O	1:B:10:VAL:HG12	2.10	0.52
1:B:54:VAL:HG13	1:B:80:ILE:CG2	2.40	0.52
1:C:43:LEU:HD11	1:C:93:TYR:HB3	1.91	0.52
1:A:18:TYR:HD1	1:B:318:TYR:HB3	1.74	0.52
1:A:350:ASP:OD2	1:A:398:ILE:HG23	2.10	0.52
1:C:10:VAL:HA	1:C:13:LYS:HE3	1.92	0.52
1:B:323:GLU:OE1	1:B:394:ARG:N	2.43	0.52
1:B:340:TRP:HH2	1:B:372:LEU:HD23	1.75	0.52
1:A:229:ASN:O	1:A:244:TRP:HA	2.10	0.51
1:C:337:SER:HA	1:C:379:ASP:HA	1.93	0.51
1:A:232:CYS:HA	1:A:242:CYS:HA	1.92	0.51
1:A:348:TYR:HB2	1:A:349:ILE:HG23	1.92	0.51
1:A:372:LEU:HD11	1:A:378:MET:HG3	1.90	0.51
1:A:394:ARG:HG3	1:A:405:TRP:CE3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:PRO:HD2	1:B:342:THR:HG22	1.93	0.51
1:C:12:LEU:HD12	1:D:310:GLN:HB3	1.90	0.51
1:A:101:LEU:HB2	1:B:226:GLN:HG2	1.93	0.51
1:C:8:GLU:O	1:C:13:LYS:HE2	2.11	0.51
1:A:113:VAL:HG13	1:A:198:LEU:HD11	1.92	0.51
1:A:207:ARG:HD3	1:B:233:PHE:CE1	2.46	0.51
1:B:46:HIS:HB2	1:B:92:TYR:HB3	1.92	0.51
1:B:319:HIS:NE2	1:B:397:PRO:HG3	2.26	0.51
1:B:113:VAL:HG12	1:B:205:SER:O	2.11	0.51
1:B:329:GLN:NE2	1:B:333:ALA:H	2.08	0.51
1:B:343:GLN:N	1:B:344:LYS:HB2	2.25	0.51
1:C:188:SER:HB2	1:C:190:TYR:HE1	1.74	0.51
1:C:357:TYR:CE1	1:C:388:SER:O	2.63	0.51
1:B:277:GLU:OE2	1:B:285:ARG:NH1	2.44	0.51
1:B:314:ILE:C	1:B:315:MET:HG2	2.31	0.51
1:A:38:LEU:HD11	1:B:249:GLN:HG3	1.92	0.51
1:B:329:GLN:CD	1:B:333:ALA:HB3	2.31	0.51
1:C:247:TRP:HD1	1:C:249:GLN:HB2	1.76	0.51
1:C:372:LEU:HD11	1:C:378:MET:HG3	1.92	0.51
1:C:170:LEU:CD1	1:C:170:LEU:N	2.73	0.51
1:A:193:ARG:NH2	1:A:211:TRP:CE2	2.79	0.50
1:C:15:LEU:HD13	1:D:312:LYS:HE2	1.92	0.50
1:A:10:VAL:HG21	1:A:32:THR:HG23	1.94	0.50
1:A:323:GLU:O	1:A:409:SER:HB3	2.11	0.50
1:A:15:LEU:HD23	1:A:29:TRP:HB3	1.93	0.50
1:B:67:CYS:HG	1:B:73:CYS:CB	2.25	0.50
1:B:350:ASP:HB3	1:B:374:ARG:HH21	1.76	0.50
1:D:62:LEU:H	1:D:62:LEU:CD1	2.24	0.50
1:D:126:SER:HB3	1:D:129:HIS:NE2	2.26	0.50
1:C:109:LEU:HD11	1:D:240:LEU:HD13	1.93	0.50
1:C:244:TRP:HE1	1:C:286:TYR:HD2	1.58	0.50
1:A:318:TYR:HB3	1:B:18:TYR:CD1	2.47	0.50
1:B:394:ARG:HE	1:B:405:TRP:HB3	1.77	0.50
1:A:367:SER:O	1:A:367:SER:OG	2.24	0.50
1:A:354:GLN:NE2	1:A:371:ASN:OD1	2.44	0.50
1:B:140:ASP:HB2	1:B:141:SER:HA	1.94	0.50
1:A:181:PRO:O	1:A:182:LYS:HB2	2.12	0.49
1:B:20:ASP:OD1	1:B:24:ARG:NE	2.44	0.49
1:B:244:TRP:NE1	1:B:286:TYR:HD2	2.09	0.49
1:D:93:TYR:N	1:D:93:TYR:CD1	2.80	0.49
1:D:179:LEU:HB3	1:D:184:PHE:CZ	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:VAL:HG23	1:C:194:VAL:HG22	1.93	0.49
1:D:93:TYR:N	1:D:93:TYR:HD1	2.10	0.49
1:C:9:THR:OG1	1:D:310:GLN:HG3	2.11	0.49
1:C:105:LEU:HD22	1:C:106:MET:N	2.27	0.49
1:B:30:ALA:HB1	1:B:73:CYS:HB2	1.93	0.49
1:B:310:GLN:HA	1:B:310:GLN:HE21	1.77	0.49
1:B:316:SER:HA	1:B:318:TYR:N	2.27	0.49
1:B:357:TYR:CD2	1:B:380:LEU:HD23	2.47	0.49
1:D:130:PHE:HB2	1:D:179:LEU:O	2.11	0.49
1:A:11:PRO:HA	1:A:30:ALA:O	2.13	0.49
1:B:25:ILE:HB	1:B:80:ILE:HD11	1.94	0.49
1:B:158:LYS:HD3	1:B:159:ARG:O	2.13	0.49
1:C:314:ILE:O	1:C:318:TYR:CE1	2.65	0.49
1:B:34:ASP:OD1	1:D:224:LYS:NZ	2.39	0.49
1:B:67:CYS:HB2	1:B:73:CYS:SG	2.51	0.49
1:A:276:LYS:HD3	1:A:286:TYR:CE1	2.47	0.49
1:B:321:GLN:O	1:B:406:SER:HB2	2.12	0.49
1:A:314:ILE:HG23	1:A:318:TYR:CD2	2.47	0.49
1:D:160:LEU:HD22	1:D:189:ILE:HB	1.94	0.49
1:A:356:GLN:HG3	1:A:369:THR:HG22	1.95	0.49
1:B:357:TYR:HE2	1:B:380:LEU:HD23	1.68	0.49
1:C:25:ILE:HD12	1:C:80:ILE:HD12	1.95	0.49
1:A:314:ILE:HB	1:B:93:TYR:HE1	1.78	0.49
1:D:127:GLY:H	1:D:129:HIS:CD2	2.30	0.49
1:A:292:VAL:HG21	1:B:109:LEU:HD21	1.94	0.48
1:C:34:ASP:HB3	1:D:249:GLN:HB3	1.95	0.48
1:C:47:GLN:N	1:C:50:LYS:HE2	2.28	0.48
1:C:398:ILE:O	1:C:399:SER:OG	2.23	0.48
1:D:150:ASP:HB2	1:D:202:SER:HB2	1.94	0.48
1:D:160:LEU:HD13	1:D:189:ILE:O	2.13	0.48
1:D:232:CYS:HA	1:D:242:CYS:HA	1.94	0.48
1:A:204:LEU:H	1:A:204:LEU:HD12	1.78	0.48
1:C:322:MET:CE	1:C:344:LYS:HE3	2.43	0.48
1:C:317:TYR:OH	1:D:87:ASN:O	2.31	0.48
1:C:385:PRO:O	1:C:386:ASP:CB	2.61	0.48
1:D:180:GLU:O	1:D:183:LEU:HB2	2.13	0.48
1:A:9:THR:HG23	1:A:11:PRO:HD2	1.96	0.48
1:A:195:ARG:HB3	1:A:211:TRP:CE3	2.48	0.48
1:A:189:ILE:HD12	1:D:280:ALA:HB2	1.96	0.48
1:B:21:TYR:HE1	1:B:85:PHE:CD2	2.31	0.48
1:C:14:THR:HG22	1:C:29:TRP:CA	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LEU:HB3	1:C:65:SER:O	2.12	0.48
1:B:330:THR:HG22	1:B:387:THR:HG22	1.95	0.48
1:D:276:LYS:HD2	1:D:286:TYR:HE1	1.77	0.48
1:A:14:THR:HG21	1:A:30:ALA:HB3	1.96	0.48
1:A:39:ILE:HD12	1:A:40:ASN:H	1.79	0.48
1:A:155:VAL:CG1	1:A:170:LEU:HB2	2.42	0.48
1:B:338:LEU:CD2	1:B:357:TYR:OH	2.60	0.48
1:C:314:ILE:HG21	1:D:17:CYS:O	2.14	0.48
1:A:46:HIS:HB2	1:A:92:TYR:HB3	1.95	0.48
1:A:91:ASP:HB3	1:A:93:TYR:HE1	1.78	0.48
1:A:346:PRO:HG2	1:A:351:HIS:HE2	1.77	0.48
1:B:382:GLN:HG2	1:B:383:LEU:N	2.28	0.48
1:C:292:VAL:HG11	1:D:109:LEU:HD21	1.96	0.48
1:B:45:TYR:O	1:B:51:ILE:O	2.32	0.48
1:B:327:LEU:HD21	1:B:389:TYR:CE1	2.48	0.48
1:B:351:HIS:HB3	1:B:353:PHE:CE1	2.49	0.48
1:D:33:GLU:CD	1:D:33:GLU:H	2.16	0.48
1:A:47:GLN:H	1:A:50:LYS:CG	2.27	0.47
1:A:332:ASN:ND2	1:A:332:ASN:O	2.46	0.47
1:B:337:SER:HA	1:B:379:ASP:HA	1.95	0.47
1:D:150:ASP:CB	1:D:202:SER:HB2	2.44	0.47
1:B:354:GLN:NE2	1:B:371:ASN:OD1	2.43	0.47
1:C:148:SER:O	1:C:151:ILE:HG22	2.14	0.47
1:D:38:LEU:HD23	1:D:38:LEU:H	1.79	0.47
1:D:119:LYS:O	1:D:135:SER:OG	2.26	0.47
1:A:46:HIS:HA	1:A:50:LYS:CD	2.44	0.47
1:A:258:LEU:HD22	1:A:288:CYS:HB3	1.95	0.47
1:A:411:GLU:H	1:A:411:GLU:HG2	1.44	0.47
1:B:223:ASP:O	1:B:224:LYS:HB3	2.14	0.47
1:C:14:THR:HG21	1:C:62:LEU:HD11	1.85	0.47
1:C:105:LEU:HB3	1:D:230:LEU:HD12	1.96	0.47
1:B:107:VAL:HG23	1:B:112:HIS:CD2	2.50	0.47
1:B:193:ARG:NH2	1:B:211:TRP:CE2	2.83	0.47
1:B:349:ILE:HG22	1:B:350:ASP:N	2.29	0.47
1:C:21:TYR:O	1:C:85:PHE:CZ	2.66	0.47
1:C:186:PRO:HA	1:C:220:GLN:NE2	2.30	0.47
1:C:259:PHE:HB2	1:C:304:SER:OG	2.15	0.47
1:B:383:LEU:HB3	1:B:385:PRO:HD2	1.96	0.47
1:C:230:LEU:HD23	1:C:230:LEU:HA	1.77	0.47
1:B:54:VAL:HG13	1:B:80:ILE:HG23	1.97	0.47
1:C:46:HIS:C	1:C:50:LYS:HE2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:GLN:OE1	1:C:367:SER:HB3	2.14	0.47
1:A:103:ILE:HG13	1:A:104:GLN:N	2.30	0.47
1:A:325:PRO:O	1:A:410:ASN:ND2	2.47	0.47
1:D:50:LYS:O	1:D:52:GLN:N	2.46	0.47
1:A:9:THR:CG2	1:B:310:GLN:HG2	2.45	0.47
1:A:189:ILE:CD1	1:D:280:ALA:HB2	2.45	0.47
1:A:93:TYR:N	1:A:93:TYR:CD1	2.82	0.47
1:B:21:TYR:CE1	1:B:85:PHE:CG	3.02	0.47
1:C:47:GLN:H	1:C:50:LYS:CB	2.27	0.47
1:C:329:GLN:HG2	1:C:330:THR:H	1.80	0.47
1:D:157:TYR:HE1	1:D:170:LEU:HD13	1.78	0.47
1:B:25:ILE:HD12	1:B:80:ILE:HD11	1.97	0.46
1:B:323:GLU:OE1	1:B:393:VAL:HB	2.15	0.46
1:C:262:PRO:HA	1:C:301:TYR:CE1	2.51	0.46
1:D:231:GLN:O	1:D:242:CYS:HA	2.15	0.46
1:A:357:TYR:HA	1:A:390:CYS:O	2.16	0.46
1:B:396:LYS:HB3	1:B:405:TRP:CZ3	2.50	0.46
1:C:244:TRP:HZ3	1:C:258:LEU:HD22	1.80	0.46
1:B:124:SER:OG	1:B:131:LEU:HB2	2.15	0.46
1:B:340:TRP:CE3	1:B:376:ASN:HA	2.51	0.46
1:C:17:CYS:HB2	1:D:314:ILE:CD1	2.46	0.46
1:C:113:VAL:HG12	1:C:205:SER:O	2.16	0.46
1:A:350:ASP:OD2	1:A:399:SER:HB3	2.16	0.46
1:C:107:VAL:HG22	1:C:107:VAL:O	2.16	0.46
1:C:350:ASP:OD1	1:C:398:ILE:HG23	2.14	0.46
1:D:149:LYS:CE	1:D:150:ASP:HA	2.46	0.46
1:A:320:ILE:HG23	1:A:321:GLN:N	2.30	0.46
1:A:346:PRO:HG2	1:A:351:HIS:NE2	2.30	0.46
1:C:319:HIS:NE2	1:D:21:TYR:CD1	2.83	0.46
1:A:184:PHE:CE2	1:A:217:TRP:HZ2	2.34	0.46
1:B:340:TRP:CZ3	1:B:353:PHE:HB2	2.50	0.46
1:B:394:ARG:HB3	1:B:405:TRP:CZ3	2.51	0.46
1:D:123:ILE:HD12	1:D:131:LEU:O	2.15	0.46
1:C:96:GLN:HB2	1:C:97:PRO:HD2	1.97	0.46
1:C:317:TYR:O	1:C:402:ASP:O	2.33	0.46
1:C:343:GLN:HG2	1:C:345:ILE:HG12	1.98	0.46
1:D:319:HIS:H	1:D:319:HIS:CD2	2.34	0.46
1:A:324:PRO:O	1:A:340:TRP:HA	2.16	0.46
1:D:130:PHE:HB2	1:D:179:LEU:HB2	1.97	0.46
1:A:16:GLU:HB2	1:A:64:TRP:HB2	1.98	0.45
1:A:136:VAL:HG21	1:A:153:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ILE:HD13	1:C:82:TYR:HB2	1.98	0.45
1:C:18:TYR:CE1	1:D:318:TYR:HB3	2.51	0.45
1:C:138:LEU:HA	1:D:237:ILE:HD11	1.98	0.45
1:C:350:ASP:OD2	1:C:398:ILE:HD13	2.15	0.45
1:B:10:VAL:O	1:B:14:THR:OG1	2.28	0.45
1:B:372:LEU:CD2	1:B:378:MET:HB2	2.46	0.45
1:A:158:LYS:HD2	1:A:162:ASP:HB2	1.98	0.45
1:B:244:TRP:CZ3	1:B:258:LEU:HD13	2.51	0.45
1:C:161:GLN:CD	1:C:161:GLN:H	2.19	0.45
1:C:354:GLN:OE1	1:C:394:ARG:NH1	2.49	0.45
1:D:194:VAL:O	1:D:212:SER:OG	2.27	0.45
1:D:224:LYS:HG3	1:D:247:TRP:CD1	2.51	0.45
1:A:349:ILE:HG21	1:A:401:TYR:CE2	2.52	0.45
1:C:315:MET:HE2	1:D:90:ASN:HA	1.98	0.45
1:A:19:ASN:OD1	1:B:318:TYR:O	2.34	0.45
1:A:181:PRO:C	1:A:183:LEU:H	2.20	0.45
1:A:330:THR:HA	1:A:388:SER:HB3	1.98	0.45
1:B:164:TRP:NE1	1:B:214:GLU:OE2	2.48	0.45
1:B:338:LEU:HD12	1:B:378:MET:O	2.17	0.45
1:C:109:LEU:HD12	1:C:109:LEU:HA	1.66	0.45
1:A:107:VAL:HG22	1:A:107:VAL:O	2.17	0.45
1:A:327:LEU:H	1:A:327:LEU:HG	1.36	0.45
1:B:105:LEU:HD22	1:B:106:MET:N	2.32	0.45
1:C:349:ILE:HG21	1:C:401:TYR:CG	2.52	0.45
1:D:74:VAL:HA	1:D:75:PRO:HD3	1.78	0.45
1:D:290:LEU:HA	1:D:291:PRO:HD3	1.83	0.45
1:B:121:ILE:HG13	1:B:133:GLU:O	2.17	0.45
1:B:354:GLN:O	1:B:393:VAL:HA	2.16	0.45
1:B:113:VAL:O	1:B:206:GLY:HA3	2.17	0.45
1:B:152:GLU:HG2	1:B:153:PHE:H	1.81	0.45
1:C:9:THR:O	1:C:13:LYS:HG3	2.16	0.45
1:C:230:LEU:HD12	1:D:105:LEU:HB3	1.99	0.45
1:D:107:VAL:HG23	1:D:112:HIS:CG	2.52	0.45
1:D:119:LYS:HG2	1:D:120:ASP:N	2.32	0.45
1:A:381:PRO:C	1:A:382:GLN:HG3	2.37	0.45
1:A:394:ARG:HD3	1:A:408:TRP:CZ2	2.52	0.45
1:C:383:LEU:O	1:C:385:PRO:CD	2.64	0.45
1:D:92:TYR:C	1:D:93:TYR:HD1	2.20	0.45
1:D:234:PHE:HD1	1:D:239:SER:O	1.99	0.45
1:A:358:LYS:O	1:A:390:CYS:N	2.36	0.44
1:B:15:LEU:HD22	1:B:27:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:PHE:CD1	1:C:395:VAL:HG22	2.51	0.44
1:D:261:ARG:HD3	1:D:266:ALA:O	2.17	0.44
1:D:15:LEU:HG	1:D:95:PHE:CZ	2.53	0.44
1:D:164:TRP:CD2	1:D:193:ARG:NH1	2.86	0.44
1:A:376:ASN:O	1:A:376:ASN:ND2	2.46	0.44
1:B:128:ASP:OD1	1:B:129:HIS:N	2.50	0.44
1:A:351:HIS:HB2	1:A:374:ARG:CG	2.47	0.44
1:B:39:ILE:HD12	1:B:40:ASN:H	1.83	0.44
1:C:136:VAL:HG21	1:C:153:PHE:CZ	2.53	0.44
1:D:136:VAL:HG21	1:D:153:PHE:CE2	2.52	0.44
1:A:191:ALA:HB2	1:A:216:HIS:CE1	2.52	0.44
1:C:157:TYR:HE1	1:C:170:LEU:CD1	2.30	0.44
1:C:386:ASP:HB3	1:C:387:THR:H	1.56	0.44
1:C:315:MET:HA	1:D:91:ASP:HB2	2.00	0.44
1:C:322:MET:O	1:C:323:GLU:HB2	2.18	0.44
1:A:149:LYS:HD2	1:A:149:LYS:HA	1.79	0.44
1:A:57:GLU:O	1:A:77:ARG:N	2.45	0.44
1:C:101:LEU:HD13	1:D:256:PHE:CZ	2.52	0.44
1:C:342:THR:OG1	1:C:344:LYS:HG2	2.17	0.44
1:C:351:HIS:HB3	1:C:353:PHE:CE1	2.53	0.44
1:D:154:GLU:HB3	1:D:197:ARG:HD3	2.00	0.44
1:D:306:LYS:HA	1:D:306:LYS:HD3	1.61	0.44
1:A:140:ASP:N	1:A:140:ASP:OD1	2.51	0.43
1:B:9:THR:HB	1:B:11:PRO:HD2	2.00	0.43
1:B:278:PRO:HG2	1:B:279:GLN:HA	2.00	0.43
1:B:337:SER:HA	1:B:378:MET:O	2.18	0.43
1:C:323:GLU:OE1	1:C:395:VAL:HG21	2.18	0.43
1:D:231:GLN:N	1:D:243:SER:O	2.47	0.43
1:C:35:ALA:HB1	1:C:39:ILE:HG22	2.00	0.43
1:C:183:LEU:HB3	1:C:184:PHE:CE1	2.53	0.43
1:D:256:PHE:HD2	1:D:305:VAL:HG12	1.82	0.43
1:A:157:TYR:CZ	1:A:168:SER:HB2	2.53	0.43
1:B:29:TRP:CH2	1:B:76:ARG:HG3	2.53	0.43
1:B:340:TRP:CH2	1:B:372:LEU:HD23	2.54	0.43
1:C:164:TRP:CH2	1:C:193:ARG:HG3	2.54	0.43
1:B:20:ASP:CG	1:B:24:ARG:HE	2.20	0.43
1:B:149:LYS:HE3	1:B:149:LYS:HB2	1.92	0.43
1:B:234:PHE:HD1	1:B:239:SER:O	2.01	0.43
1:B:383:LEU:CB	1:B:385:PRO:HD2	2.49	0.43
1:D:144:SER:O	1:D:145:TRP:HB2	2.18	0.43
1:D:14:THR:HG21	1:D:30:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LEU:HD23	1:D:38:LEU:N	2.33	0.43
1:D:256:PHE:C	1:D:308:LEU:HD13	2.39	0.43
1:B:400:ASP:HB3	1:B:401:TYR:HD1	1.83	0.43
1:C:17:CYS:HB2	1:D:314:ILE:HD13	2.01	0.43
1:D:72:ARG:HG3	1:D:73:CYS:N	2.33	0.43
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.78	0.43
1:B:277:GLU:OE2	1:B:287:ARG:HD3	2.19	0.43
1:C:184:PHE:CD1	1:C:184:PHE:N	2.86	0.43
1:D:154:GLU:OE1	1:D:195:ARG:NH2	2.50	0.43
1:C:351:HIS:HB2	1:C:374:ARG:HA	1.99	0.43
1:A:23:ASN:O	1:A:82:TYR:HB3	2.18	0.43
1:A:136:VAL:HG21	1:A:153:PHE:HZ	1.84	0.43
1:B:347:LYS:HE2	1:B:347:LYS:HB3	1.92	0.43
1:C:109:LEU:HG	1:D:234:PHE:CD2	2.54	0.43
1:C:353:PHE:CD1	1:C:353:PHE:N	2.86	0.43
1:A:91:ASP:HB2	1:B:315:MET:H	1.84	0.42
1:A:325:PRO:HD2	1:A:410:ASN:CG	2.40	0.42
1:A:340:TRP:CZ3	1:A:375:VAL:O	2.72	0.42
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.76	0.42
1:B:20:ASP:OD2	1:B:24:ARG:NH2	2.52	0.42
1:C:185:LEU:HD21	1:C:229:ASN:CB	2.47	0.42
1:C:396:LYS:HB2	1:C:405:TRP:CE3	2.54	0.42
1:A:50:LYS:HD2	1:A:51:ILE:N	2.33	0.42
1:B:400:ASP:HB3	1:B:401:TYR:CD1	2.54	0.42
1:B:7:GLU:N	1:B:7:GLU:OE2	2.51	0.42
1:B:261:ARG:HG2	1:B:266:ALA:O	2.19	0.42
1:B:382:GLN:HG2	1:B:383:LEU:H	1.84	0.42
1:C:22:THR:OG1	1:C:23:ASN:N	2.52	0.42
1:C:278:PRO:CB	1:C:279:GLN:HA	2.49	0.42
1:C:369:THR:OG1	1:C:370:GLU:N	2.51	0.42
1:A:240:LEU:HD22	1:A:290:LEU:HD11	2.00	0.42
1:A:320:ILE:HG23	1:A:321:GLN:H	1.83	0.42
1:A:394:ARG:NH2	1:A:405:TRP:CD1	2.87	0.42
1:B:339:HIS:O	1:B:340:TRP:HD1	2.03	0.42
1:C:12:LEU:CD1	1:D:310:GLN:HB3	2.48	0.42
1:D:258:LEU:HD11	1:D:303:VAL:HG12	2.02	0.42
1:A:20:ASP:O	1:A:21:TYR:CB	2.67	0.42
1:A:105:LEU:HD22	1:A:106:MET:H	1.82	0.42
1:A:159:ARG:HG3	1:A:162:ASP:OD2	2.18	0.42
1:B:198:LEU:HD23	1:B:198:LEU:HA	1.84	0.42
1:C:260:TYR:CD2	1:C:290:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ASP:OD1	1:C:100:ASP:N	2.49	0.42
1:C:391:ALA:O	1:C:411:GLU:HB2	2.19	0.42
1:C:197:ARG:HG2	1:C:208:PRO:HB3	2.00	0.42
1:A:59:SER:OG	1:A:60:GLU:N	2.53	0.42
1:C:29:TRP:CH2	1:C:76:ARG:HG3	2.54	0.42
1:C:63:MET:HB2	1:C:64:TRP:CE3	2.54	0.42
1:C:99:ARG:NE	1:D:223:ASP:OD2	2.53	0.42
1:C:247:TRP:HE1	1:C:249:GLN:NE2	2.18	0.42
1:C:353:PHE:N	1:C:353:PHE:HD1	2.17	0.42
1:D:293:PRO:HG2	1:D:294:GLU:H	1.84	0.42
1:A:109:LEU:HD12	1:A:109:LEU:HA	1.72	0.42
1:A:396:LYS:HB2	1:A:405:TRP:CD2	2.55	0.42
1:B:22:THR:OG1	1:B:23:ASN:N	2.52	0.42
1:B:70:SER:OG	1:B:71:HIS:ND1	2.52	0.42
1:C:140:ASP:HA	1:C:141:SER:HA	1.54	0.42
1:A:33:GLU:OE2	1:A:72:ARG:HG2	2.20	0.42
1:A:244:TRP:CZ3	1:A:258:LEU:HD13	2.55	0.42
1:A:317:TYR:O	1:A:318:TYR:CD1	2.72	0.42
1:B:86:SER:OG	1:B:89:ASP:N	2.53	0.42
1:B:353:PHE:CD1	1:B:353:PHE:N	2.88	0.42
1:C:21:TYR:O	1:C:85:PHE:CE1	2.73	0.42
1:D:273:PRO:O	1:D:288:CYS:HB2	2.20	0.41
1:B:356:GLN:O	1:B:356:GLN:HG2	2.21	0.41
1:C:239:SER:HB2	1:C:241:HIS:HE1	1.85	0.41
1:D:116:PRO:HA	1:D:117:PRO:HD2	1.94	0.41
1:B:342:THR:CG2	1:B:344:LYS:HD3	2.46	0.41
1:B:383:LEU:C	1:B:385:PRO:HD2	2.40	0.41
1:A:136:VAL:H	1:A:175:PHE:HE2	1.68	0.41
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.79	0.41
1:A:247:TRP:CE3	1:A:283:TYR:CE1	3.07	0.41
1:A:318:TYR:HB3	1:B:18:TYR:HD1	1.85	0.41
1:B:62:LEU:HD12	1:B:65:SER:H	1.86	0.41
1:B:319:HIS:CD2	1:B:397:PRO:CG	3.02	0.41
1:C:244:TRP:CE2	1:C:286:TYR:HB2	2.55	0.41
1:C:136:VAL:HG21	1:C:153:PHE:HZ	1.85	0.41
1:A:140:ASP:HB2	1:A:141:SER:HA	2.01	0.41
1:B:379:ASP:OD1	1:B:379:ASP:N	2.54	0.41
1:C:184:PHE:HD2	1:C:190:TYR:CE2	2.39	0.41
1:C:262:PRO:O	1:C:263:SER:HB3	2.20	0.41
1:D:8:GLU:O	1:D:13:LYS:HE2	2.20	0.41
1:D:180:GLU:H	1:D:183:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLN:HB3	1:A:392:ARG:HG3	2.01	0.41
1:B:18:TYR:HD1	1:B:18:TYR:HA	1.66	0.41
1:C:188:SER:HB2	1:C:190:TYR:CE1	2.55	0.41
1:C:281:SER:OG	1:C:282:VAL:N	2.54	0.41
1:D:149:LYS:NZ	1:D:199:SER:HB3	2.35	0.41
1:A:181:PRO:HG3	1:A:220:GLN:HG2	2.03	0.41
1:B:183:LEU:HB3	1:B:184:PHE:CE1	2.56	0.41
1:B:382:GLN:O	1:B:383:LEU:HD13	2.21	0.41
1:C:47:GLN:N	1:C:50:LYS:HB2	2.36	0.41
1:C:123:ILE:HG22	1:C:215:VAL:HG22	2.03	0.41
1:C:184:PHE:HD2	1:C:190:TYR:CD2	2.38	0.41
1:D:193:ARG:HD3	1:D:211:TRP:CD1	2.56	0.41
1:D:232:CYS:HA	1:D:241:HIS:O	2.21	0.41
1:D:274:VAL:HA	1:D:288:CYS:HB2	2.03	0.41
1:A:8:GLU:HB3	1:A:12:LEU:CD2	2.51	0.41
1:A:98:ASP:OD1	1:A:98:ASP:N	2.42	0.41
1:A:389:TYR:HA	1:A:390:CYS:HA	1.71	0.41
1:B:150:ASP:HB3	1:B:202:SER:CB	2.46	0.41
1:B:235:ASP:C	1:B:237:ILE:H	2.24	0.41
1:B:244:TRP:NE1	1:B:286:TYR:CD2	2.88	0.41
1:B:350:ASP:HA	1:B:374:ARG:HE	1.86	0.41
1:C:47:GLN:HB2	1:C:50:LYS:HD3	2.03	0.41
1:C:104:GLN:HG3	1:D:304:SER:HB3	2.02	0.41
1:C:123:ILE:HD12	1:C:131:LEU:O	2.21	0.41
1:D:74:VAL:HG12	1:D:76:ARG:NH1	2.36	0.41
1:D:154:GLU:OE1	1:D:195:ARG:NE	2.46	0.41
1:D:258:LEU:HD11	1:D:303:VAL:CG1	2.51	0.41
1:A:260:TYR:CD1	1:A:290:LEU:HD22	2.56	0.41
1:A:343:GLN:N	1:A:344:LYS:HB2	2.35	0.41
1:B:247:TRP:O	1:B:250:THR:HB	2.20	0.41
1:C:39:ILE:HD12	1:C:39:ILE:HA	1.89	0.41
1:C:45:TYR:CG	1:C:50:LYS:HE3	2.56	0.41
1:C:158:LYS:HB3	1:C:167:ALA:HB2	2.02	0.41
1:C:181:PRO:O	1:C:182:LYS:HB2	2.21	0.41
1:A:115:PRO:HG3	1:A:198:LEU:HD21	2.03	0.40
1:A:161:GLN:OE1	1:A:161:GLN:N	2.48	0.40
1:B:39:ILE:HD13	1:B:99:ARG:NH2	2.36	0.40
1:C:47:GLN:H	1:C:50:LYS:HB3	1.86	0.40
1:C:142:GLN:HG3	1:C:143:VAL:HG23	2.03	0.40
1:A:17:CYS:SG	1:A:25:ILE:HG22	2.61	0.40
1:A:150:ASP:O	1:A:199:SER:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:HB3	1:B:49:ASP:H	1.53	0.40
1:B:144:SER:O	1:B:146:LEU:N	2.40	0.40
1:B:181:PRO:C	1:B:183:LEU:H	2.24	0.40
1:C:93:TYR:HE1	1:D:314:ILE:HB	1.86	0.40
1:A:157:TYR:HA	1:A:191:ALA:O	2.22	0.40
1:A:357:TYR:HB2	1:A:358:LYS:H	1.64	0.40
1:C:253:SER:OG	1:D:31:ASP:OD1	2.35	0.40
1:C:389:TYR:N	1:C:389:TYR:CD1	2.90	0.40
1:D:49:ASP:O	1:D:51:ILE:HG12	2.22	0.40
1:A:394:ARG:NH2	1:A:405:TRP:CG	2.89	0.40
1:B:278:PRO:CB	1:B:279:GLN:HA	2.52	0.40
1:C:149:LYS:HA	1:C:150:ASP:HA	1.83	0.40
1:B:70:SER:OG	1:B:71:HIS:N	2.54	0.40
1:B:298:HIS:O	1:B:300:GLN:HG2	2.21	0.40
1:C:130:PHE:O	1:C:178:ASN:HA	2.22	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	395/416 (95%)	354 (90%)	36 (9%)	5 (1%)	12	46
1	B	391/416 (94%)	353 (90%)	33 (8%)	5 (1%)	12	46
1	C	398/416 (96%)	355 (89%)	35 (9%)	8 (2%)	7	37
1	D	314/416 (76%)	291 (93%)	20 (6%)	3 (1%)	15	52
All	All	1498/1664 (90%)	1353 (90%)	124 (8%)	21 (1%)	11	44

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	PRO
1	C	323	GLU
1	C	385	PRO
1	A	384	GLU
1	B	51	ILE
1	C	386	ASP
1	D	51	ILE
1	D	143	VAL
1	D	144	SER
1	A	51	ILE
1	C	51	ILE
1	A	331	ALA
1	B	145	TRP
1	A	316	SER
1	A	321	GLN
1	C	281	SER
1	C	337	SER
1	C	325	PRO
1	B	263	SER
1	B	397	PRO
1	C	381	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	A	368/385 (96%)	274 (74%)	94 (26%)	0 2
1	B	364/385 (94%)	277 (76%)	87 (24%)	0 3
1	C	371/385 (96%)	264 (71%)	107 (29%)	0 2
1	D	291/385 (76%)	215 (74%)	76 (26%)	0 2
All	All	1394/1540 (90%)	1030 (74%)	364 (26%)	0 2

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU

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Mol	Chain	Res	Type
1	A	15	LEU
1	A	20	ASP
1	A	21	TYR
1	A	23	ASN
1	A	24	ARG
1	A	26	ILE
1	A	27	CYS
1	A	32	THR
1	A	33	GLU
1	A	34	ASP
1	A	38	LEU
1	A	39	ILE
1	A	43	LEU
1	A	50	LYS
1	A	70	SER
1	A	71	HIS
1	A	72	ARG
1	A	73	CYS
1	A	80	ILE
1	A	82	TYR
1	A	85	PHE
1	A	87	ASN
1	A	93	TYR
1	A	99	ARG
1	A	100	ASP
1	A	103	ILE
1	A	107	VAL
1	A	109	LEU
1	A	124	SER
1	A	126	SER
1	A	135	SER
1	A	145	TRP
1	A	146	LEU
1	A	148	SER
1	A	149	LYS
1	A	150	ASP
1	A	151	ILE
1	A	155	VAL
1	A	158	LYS
1	A	159	ARG
1	A	169	SER
1	A	178	ASN

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Mol	Chain	Res	Type
1	A	180	GLU
1	A	183	LEU
1	A	193	ARG
1	A	194	VAL
1	A	197	ARG
1	A	207	ARG
1	A	210	ARG
1	A	211	TRP
1	A	212	SER
1	A	218	ASP
1	A	220	GLN
1	A	224	LYS
1	A	230	LEU
1	A	232	CYS
1	A	239	SER
1	A	240	LEU
1	A	246	VAL
1	A	250	THR
1	A	258	LEU
1	A	261	ARG
1	A	272	SER
1	A	276	LYS
1	A	292	VAL
1	A	296	SER
1	A	299	SER
1	A	302	THR
1	A	309	GLU
1	A	316	SER
1	A	322	MET
1	A	327	LEU
1	A	328	GLN
1	A	338	LEU
1	A	339	HIS
1	A	340	TRP
1	A	349	ILE
1	A	357	TYR
1	A	359	LYS
1	A	369	THR
1	A	374	ARG
1	A	376	ASN
1	A	377	SER
1	A	378	MET

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Mol	Chain	Res	Type
1	A	382	GLN
1	A	383	LEU
1	A	384	GLU
1	A	392	ARG
1	A	394	ARG
1	A	395	VAL
1	A	402	ASP
1	A	404	ILE
1	A	411	GLU
1	B	15	LEU
1	B	17	CYS
1	B	18	TYR
1	B	20	ASP
1	B	21	TYR
1	B	24	ARG
1	B	26	ILE
1	B	27	CYS
1	B	28	SER
1	B	33	GLU
1	B	39	ILE
1	B	42	THR
1	B	47	GLN
1	B	48	LEU
1	B	56	CYS
1	B	58	LEU
1	B	62	LEU
1	B	65	SER
1	B	69	SER
1	B	77	ARG
1	B	78	CYS
1	B	84	ARG
1	B	89	ASP
1	B	100	ASP
1	B	109	LEU
1	B	112	HIS
1	B	119	LYS
1	B	124	SER
1	B	126	SER
1	B	131	LEU
1	B	135	SER
1	B	137	SER
1	B	144	SER

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Mol	Chain	Res	Type
1	B	145	TRP
1	B	146	LEU
1	B	148	SER
1	B	149	LYS
1	B	151	ILE
1	B	158	LYS
1	B	159	ARG
1	B	161	GLN
1	B	165	GLU
1	B	183	LEU
1	B	187	ASN
1	B	203	SER
1	B	205	SER
1	B	218	ASP
1	B	220	GLN
1	B	228	GLN
1	B	240	LEU
1	B	249	GLN
1	B	250	THR
1	B	271	CYS
1	B	282	VAL
1	B	294	GLU
1	B	298	HIS
1	B	304	SER
1	B	306	LYS
1	B	310	GLN
1	B	315	MET
1	B	316	SER
1	B	319	HIS
1	B	322	MET
1	B	323	GLU
1	B	326	ILE
1	B	330	THR
1	B	336	TYR
1	B	338	LEU
1	B	342	THR
1	B	344	LYS
1	B	347	LYS
1	B	348	TYR
1	B	351	HIS
1	B	356	GLN
1	B	359	LYS

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Mol	Chain	Res	Type
1	B	379	ASP
1	B	380	LEU
1	B	382	GLN
1	B	384	GLU
1	B	386	ASP
1	B	387	THR
1	B	389	TYR
1	B	393	VAL
1	B	394	ARG
1	B	401	TYR
1	B	407	GLU
1	B	409	SER
1	C	7	GLU
1	C	9	THR
1	C	15	LEU
1	C	18	TYR
1	C	19	ASN
1	C	21	TYR
1	C	23	ASN
1	C	25	ILE
1	C	34	ASP
1	C	41	MET
1	C	52	GLN
1	C	56	CYS
1	C	58	LEU
1	C	62	LEU
1	C	65	SER
1	C	66	GLU
1	C	69	SER
1	C	70	SER
1	C	72	ARG
1	C	78	CYS
1	C	79	VAL
1	C	80	ILE
1	C	82	TYR
1	C	83	THR
1	C	84	ARG
1	C	85	PHE
1	C	86	SER
1	C	89	ASP
1	C	100	ASP
1	C	101	LEU

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Mol	Chain	Res	Type
1	C	104	GLN
1	C	105	LEU
1	C	107	VAL
1	C	112	HIS
1	C	121	ILE
1	C	126	SER
1	C	133	GLU
1	C	135	SER
1	C	137	SER
1	C	140	ASP
1	C	141	SER
1	C	142	GLN
1	C	146	LEU
1	C	149	LYS
1	C	150	ASP
1	C	151	ILE
1	C	161	GLN
1	C	163	SER
1	C	168	SER
1	C	183	LEU
1	C	193	ARG
1	C	194	VAL
1	C	196	THR
1	C	205	SER
1	C	214	GLU
1	C	219	SER
1	C	220	GLN
1	C	228	GLN
1	C	230	LEU
1	C	232	CYS
1	C	237	ILE
1	C	239	SER
1	C	240	LEU
1	C	241	HIS
1	C	242	CYS
1	C	253	SER
1	C	271	CYS
1	C	279	GLN
1	C	284	THR
1	C	288	CYS
1	C	292	VAL
1	C	298	HIS

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Mol	Chain	Res	Type
1	C	300	GLN
1	C	307	HIS
1	C	308	LEU
1	C	310	GLN
1	C	315	MET
1	C	319	HIS
1	C	320	ILE
1	C	322	MET
1	C	326	ILE
1	C	327	LEU
1	C	336	TYR
1	C	339	HIS
1	C	341	GLU
1	C	342	THR
1	C	348	TYR
1	C	349	ILE
1	C	350	ASP
1	C	356	GLN
1	C	357	TYR
1	C	358	LYS
1	C	359	LYS
1	C	367	SER
1	C	372	LEU
1	C	378	MET
1	C	382	GLN
1	C	383	LEU
1	C	384	GLU
1	C	392	ARG
1	C	398	ILE
1	C	400	ASP
1	C	401	TYR
1	C	406	SER
1	C	408	TRP
1	C	410	ASN
1	C	412	TYR
1	D	7	GLU
1	D	14	THR
1	D	15	LEU
1	D	17	CYS
1	D	20	ASP
1	D	24	ARG
1	D	27	CYS

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Mol	Chain	Res	Type
1	D	32	THR
1	D	38	LEU
1	D	48	LEU
1	D	55	SER
1	D	57	GLU
1	D	62	LEU
1	D	63	MET
1	D	65	SER
1	D	66	GLU
1	D	70	SER
1	D	72	ARG
1	D	82	TYR
1	D	84	ARG
1	D	86	SER
1	D	93	TYR
1	D	98	ASP
1	D	101	LEU
1	D	103	ILE
1	D	107	VAL
1	D	113	VAL
1	D	119	LYS
1	D	120	ASP
1	D	122	HIS
1	D	133	GLU
1	D	135	SER
1	D	138	LEU
1	D	144	SER
1	D	146	LEU
1	D	147	SER
1	D	148	SER
1	D	149	LYS
1	D	150	ASP
1	D	151	ILE
1	D	154	GLU
1	D	155	VAL
1	D	161	GLN
1	D	162	ASP
1	D	168	SER
1	D	171	HIS
1	D	177	VAL
1	D	178	ASN
1	D	182	LYS

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Mol	Chain	Res	Type
1	D	183	LEU
1	D	188	SER
1	D	193	ARG
1	D	203	SER
1	D	205	SER
1	D	207	ARG
1	D	211	TRP
1	D	219	SER
1	D	220	GLN
1	D	224	LYS
1	D	226	GLN
1	D	230	LEU
1	D	232	CYS
1	D	239	SER
1	D	242	CYS
1	D	269	GLU
1	D	274	VAL
1	D	277	GLU
1	D	288	CYS
1	D	296	SER
1	D	298	HIS
1	D	299	SER
1	D	307	HIS
1	D	317	TYR
1	D	318	TYR
1	D	319	HIS
1	D	321	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	220	GLN
1	A	228	GLN
1	A	354	GLN
1	B	178	ASN
1	B	228	GLN
1	B	328	GLN
1	B	329	GLN
1	B	382	GLN
1	C	249	GLN
1	C	321	GLN

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Mol	Chain	Res	Type
1	C	328	GLN
1	C	356	GLN
1	C	410	ASN
1	D	112	HIS
1	D	178	ASN
1	D	220	GLN
1	D	310	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	501	1	14,14,15	0.66	0	17,19,21	0.58	1 (5%)
2	NAG	D	501	1	14,14,15	0.50	0	17,19,21	0.37	0
2	NAG	C	501	1	14,14,15	0.66	0	17,19,21	0.56	0
2	NAG	B	501	1	14,14,15	1.13	1 (7%)	17,19,21	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
2	NAG	A	501	1	-	2/6/23/26	0/1/1/1
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	501	1	-	2/6/23/26	0/1/1/1
2	NAG	B	501	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAG	C1-C2	3.72	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NAG	C1-O5-C5	2.12	115.07	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	NAG	O5-C5-C6-O6
2	C	501	NAG	C4-C5-C6-O6
2	C	501	NAG	O5-C5-C6-O6
2	A	501	NAG	O5-C5-C6-O6
2	A	501	NAG	C4-C5-C6-O6
2	B	501	NAG	C1-C2-N2-C7
2	B	501	NAG	C4-C5-C6-O6
2	B	501	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	399/416 (95%)	-0.01	18 (4%)	33	32	59, 121, 191, 245	0
1	B	395/416 (94%)	0.04	23 (5%)	23	23	54, 100, 229, 299	0
1	C	402/416 (96%)	-0.05	16 (3%)	38	36	58, 113, 195, 262	0
1	D	316/416 (75%)	-0.32	5 (1%)	72	69	62, 99, 153, 240	0
All	All	1512/1664 (90%)	-0.07	62 (4%)	37	36	54, 107, 200, 299	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	GLN	14.2
1	A	334	ALA	9.9
1	B	342	THR	8.4
1	B	387	THR	6.2
1	C	334	ALA	6.2
1	B	329	GLN	5.9
1	A	333	ALA	5.6
1	A	142	GLN	5.4
1	C	412	TYR	4.8
1	C	329	GLN	4.7
1	B	333	ALA	4.6
1	B	386	ASP	4.3
1	A	328	GLN	4.3
1	C	330	THR	3.9
1	B	343	GLN	3.9
1	C	333	ALA	3.8
1	C	343	GLN	3.8
1	C	328	GLN	3.7
1	B	334	ALA	3.5
1	B	388	SER	3.4
1	B	407	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	412	TYR	3.3
1	B	401	TYR	3.2
1	B	400	ASP	3.2
1	C	66	GLU	3.1
1	C	382	GLN	3.1
1	C	342	THR	3.0
1	A	30	ALA	3.0
1	B	385	PRO	2.9
1	A	330	THR	2.9
1	C	332	ASN	2.8
1	B	327	LEU	2.8
1	B	328	GLN	2.6
1	B	298	HIS	2.6
1	B	384	GLU	2.6
1	D	142	GLN	2.5
1	A	335	SER	2.5
1	B	352	THR	2.5
1	C	339	HIS	2.5
1	B	393	VAL	2.4
1	C	140	ASP	2.3
1	D	143	VAL	2.3
1	A	341	GLU	2.3
1	A	21	TYR	2.2
1	A	297	ALA	2.2
1	C	142	GLN	2.2
1	A	298	HIS	2.2
1	B	142	GLN	2.2
1	A	327	LEU	2.2
1	A	388	SER	2.1
1	A	332	ASN	2.1
1	D	319	HIS	2.1
1	B	335	SER	2.1
1	D	321	GLN	2.1
1	D	69	SER	2.1
1	A	342	THR	2.1
1	B	392	ARG	2.0
1	A	141	SER	2.0
1	B	88	GLY	2.0
1	B	383	LEU	2.0
1	C	141	SER	2.0
1	C	383	LEU	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 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, 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	B-factors(Å^2)	Q<0.9
2	NAG	D	501	14/15	0.81	0.30	141,157,168,168	0
2	NAG	B	501	14/15	0.82	0.20	125,145,155,157	0
2	NAG	A	501	14/15	0.82	0.23	136,149,152,153	0
2	NAG	C	501	14/15	0.88	0.29	134,148,158,160	0

6.5 Other polymers (i)

There are no such residues in this entry.