



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 10:05 pm GMT

PDB ID : 1W3B
Title : The superhelical TPR domain of O-linked GlcNAc transferase reveals structural similarities to importin alpha.
Authors : Jinek, M.; Rehwinkel, J.; Lazarus, B.D.; Izaurralde, E.; Hanover, J.A.; Conti, E.
Deposited on : 2004-07-14
Resolution : 2.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

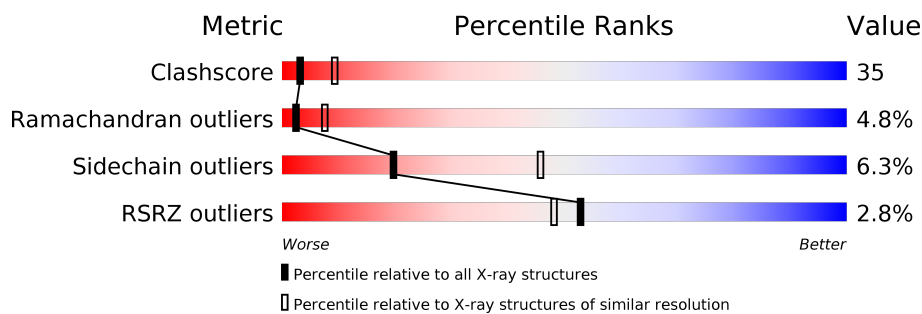
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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))
Clashscore	122126	2976 (2.90-2.82)
Ramachandran outliers	120053	2913 (2.90-2.82)
Sidechain outliers	120020	2916 (2.90-2.82)
RSRZ outliers	108989	2654 (2.90-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 6%, yellow 53%, green 40%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 40% 53% 6% </div> </div>
1	B	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 5%, yellow 38%, green 53%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 4% 53% 38% • 5% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5596 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 UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYL GLUCOSAMINYLTRANSFERASE 110.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			2887	1819	506	548	14			
1	B	368	Total	C	N	O	S	0	0	0
			2681	1692	473	504	12			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

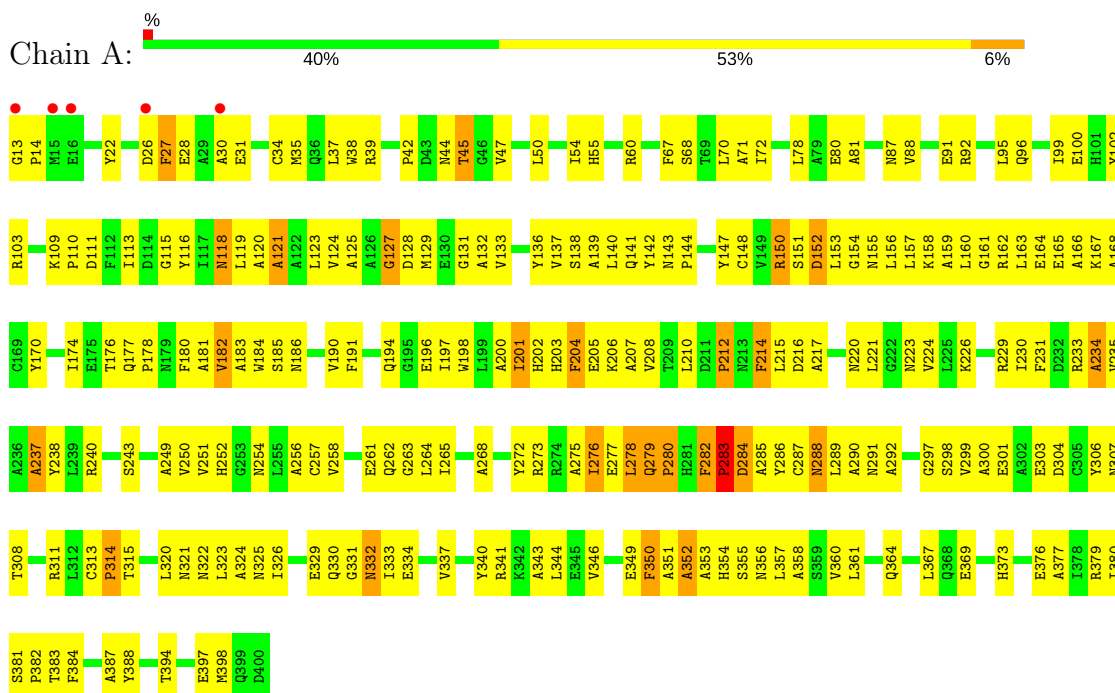
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	7	Total	O	0	0
			7	7		

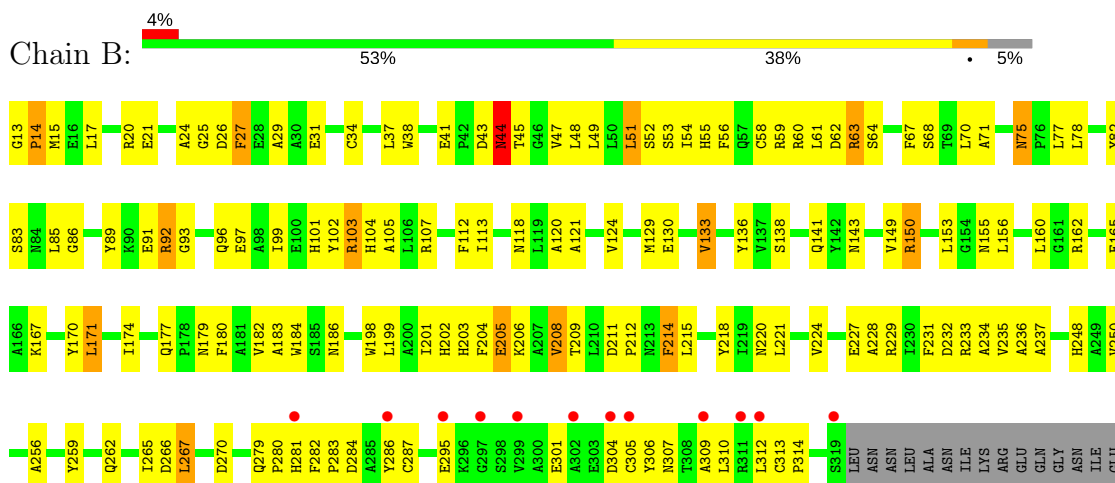
3 Residue-property plots

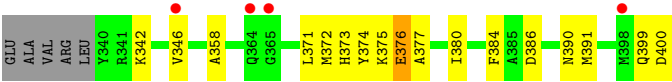
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTRANSFERASE 110



• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYLTRANSFERASE 110





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.32Å 75.51Å 77.67Å 105.08° 105.14° 110.28°	Depositor
Resolution (Å)	200.00 – 2.85 28.74 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.6 (200.00-2.85) 95.8 (28.74-2.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.297 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	87.0	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 94.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5596	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.42	0/2947	0.62	0/4019
1	B	0.40	1/2737 (0.0%)	0.58	0/3737
All	All	0.41	1/5684 (0.0%)	0.60	0/7756

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	376	GLU	CB-CG	-5.19	1.42	1.52

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	A	2887	0	2660	240	0
1	B	2681	0	2423	142	0
2	A	1	0	0	0	0
3	A	20	0	0	7	0
3	B	7	0	0	0	0
All	All	5596	0	5083	377	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 35.

All (377) 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:45:THR:CG2	1:B:78:LEU:HD11	1.91	0.98
1:B:55:HIS:CD2	1:B:63:ARG:HB3	1.99	0.96
1:A:140:LEU:HD21	1:A:150:ARG:NE	1.82	0.94
1:A:197:ILE:O	1:A:201:ILE:HG22	1.65	0.93
1:A:133:VAL:O	1:A:137:VAL:HG23	1.67	0.93
1:A:150:ARG:HH11	1:A:150:ARG:HG3	1.34	0.90
1:B:55:HIS:HD2	1:B:63:ARG:HB3	1.34	0.89
1:A:231:PHE:O	1:A:235:VAL:HG23	1.79	0.83
1:B:45:THR:HG21	1:B:78:LEU:HD11	1.59	0.83
1:A:191:PHE:HE1	1:A:203:HIS:HE2	1.25	0.82
1:A:341:ARG:HH12	1:A:357:LEU:HD21	1.41	0.82
1:A:140:LEU:HD21	1:A:150:ARG:CZ	2.10	0.82
1:B:45:THR:HG23	1:B:78:LEU:HD11	1.61	0.80
1:A:13:GLY:N	1:A:14:PRO:HD3	1.97	0.79
1:A:303:GLU:HG3	1:A:323:LEU:HD11	1.64	0.79
1:B:17:LEU:HD23	1:B:20:ARG:NH1	1.99	0.77
1:A:325:ASN:O	1:A:329:GLU:HG3	1.86	0.76
1:A:291:ASN:HD21	1:A:322:ASN:HD22	1.34	0.75
1:A:124:VAL:HG13	1:A:129:MET:HE1	1.66	0.75
1:A:28:GLU:N	3:A:2002:HOH:O	2.22	0.73
1:A:350:PHE:HE2	1:A:352:ALA:HB3	1.53	0.72
1:A:35:MET:O	1:A:39:ARG:HG3	1.89	0.72
1:A:129:MET:O	1:A:133:VAL:HG23	1.88	0.72
1:B:162:ARG:HD3	1:B:165:GLU:OE2	1.89	0.72
1:B:376:GLU:O	1:B:380:ILE:HG13	1.89	0.71
1:B:85:LEU:O	1:B:89:TYR:HD1	1.74	0.71
1:A:384:PHE:HD2	1:A:387:ALA:H	1.38	0.71
1:A:341:ARG:HH11	1:A:341:ARG:HG3	1.56	0.70
1:A:164:GLU:OE1	1:A:164:GLU:HA	1.90	0.70
1:A:170:TYR:CE2	1:A:186:ASN:HB3	2.26	0.70
1:A:350:PHE:CE2	1:A:352:ALA:HB3	2.27	0.70
1:B:75:ASN:HD22	1:B:75:ASN:C	1.95	0.69
1:B:342:LYS:O	1:B:346:VAL:HG23	1.93	0.69
1:A:99:ILE:O	1:A:103:ARG:HG3	1.93	0.69
1:A:291:ASN:ND2	1:A:306:TYR:OH	2.27	0.68
1:A:258:VAL:O	1:A:262:GLN:HG2	1.93	0.68
1:A:315:THR:O	1:A:315:THR:HG22	1.94	0.68
1:A:234:ALA:O	1:A:238:TYR:HD1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ARG:HD3	1:B:231:PHE:CZ	2.30	0.67
1:B:91:GLU:C	1:B:93:GLY:H	1.97	0.67
1:A:354:HIS:HB3	1:A:377:ALA:HB2	1.77	0.67
1:A:326:ILE:O	1:A:330:GLN:HG3	1.95	0.66
1:A:325:ASN:ND2	1:A:340:TYR:OH	2.29	0.66
1:A:290:ALA:HB1	1:A:306:TYR:CE1	2.30	0.65
1:A:358:ALA:HB2	1:A:373:HIS:HB2	1.78	0.65
1:A:190:VAL:O	1:A:194:GLN:HG3	1.96	0.65
1:A:297:GLY:O	1:A:299:VAL:HG23	1.96	0.65
1:A:321:ASN:ND2	1:A:353:ALA:HA	2.11	0.65
1:A:360:VAL:O	1:A:364:GLN:HG3	1.95	0.65
1:B:129:MET:O	1:B:133:VAL:HG12	1.95	0.65
1:A:180:PHE:CD1	1:A:183:ALA:HB2	2.31	0.65
1:A:45:THR:CG2	1:A:78:LEU:HD11	2.27	0.65
1:A:273:ARG:O	1:A:276:ILE:HG22	1.96	0.64
1:A:147:TYR:CD1	1:A:148:CYS:N	2.65	0.64
1:A:226:LYS:HD2	1:A:258:VAL:CG2	2.27	0.64
1:A:297:GLY:O	1:A:299:VAL:N	2.31	0.64
1:A:210:LEU:O	1:A:212:PRO:HD3	1.98	0.64
1:A:150:ARG:HG3	1:A:150:ARG:NH1	2.11	0.64
1:A:334:GLU:N	3:A:2019:HOH:O	2.30	0.64
1:B:155:ASN:ND2	1:B:170:TYR:OH	2.28	0.64
1:B:82:TYR:HB2	1:B:105:ALA:HB2	1.80	0.64
1:B:227:GLU:OE1	1:B:227:GLU:HA	1.99	0.63
1:B:228:ALA:O	1:B:229:ARG:HB2	1.98	0.63
1:A:34:CYS:SG	1:A:47:VAL:HG13	2.39	0.63
1:A:268:ALA:O	1:A:272:TYR:HD1	1.82	0.63
1:A:272:TYR:CE2	1:A:288:ASN:HB3	2.34	0.62
1:A:341:ARG:NH1	1:A:357:LEU:HD21	2.12	0.62
1:A:68:SER:O	1:A:72:ILE:HG13	2.00	0.62
1:A:256:ALA:HB1	1:A:272:TYR:CE1	2.35	0.62
1:A:204:PHE:O	1:A:208:VAL:HG22	1.99	0.61
1:A:394:THR:O	1:A:398:MET:HG3	2.00	0.61
1:A:226:LYS:HD2	1:A:258:VAL:HG23	1.81	0.61
1:B:301:GLU:HG2	1:B:301:GLU:O	2.01	0.61
1:A:150:ARG:HH11	1:A:150:ARG:CG	2.10	0.60
1:A:180:PHE:O	1:A:183:ALA:HB3	2.01	0.60
1:B:75:ASN:ND2	1:B:77:LEU:H	1.99	0.60
1:B:182:VAL:HG12	1:B:186:ASN:HD21	1.66	0.60
1:A:140:LEU:HD21	1:A:150:ARG:HE	1.62	0.60
1:B:358:ALA:HB2	1:B:373:HIS:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:TYR:CD2	1:A:177:GLN:HB2	2.37	0.60
1:A:278:LEU:O	1:A:279:GLN:HB2	2.02	0.59
1:A:150:ARG:O	1:A:153:LEU:HB3	2.02	0.59
1:B:13:GLY:C	1:B:15:MET:H	2.05	0.59
1:B:97:GLU:O	1:B:101:HIS:HD2	1.85	0.59
1:B:180:PHE:HD2	1:B:183:ALA:HB2	1.68	0.59
1:B:51:LEU:HD13	1:B:67:PHE:CE2	2.38	0.59
1:A:276:ILE:HD11	1:A:286:TYR:OH	2.03	0.58
1:A:38:TRP:CD1	1:A:42:PRO:HA	2.39	0.58
1:A:367:LEU:CD1	1:A:398:MET:HG2	2.33	0.58
1:A:324:ALA:HB3	1:A:340:TYR:CE2	2.39	0.58
1:A:208:VAL:HG13	1:A:217:ALA:HB1	1.86	0.58
1:A:240:ARG:HG3	1:A:240:ARG:HH11	1.68	0.57
1:A:50:LEU:O	1:A:54:ILE:HG13	2.04	0.57
1:B:184:TRP:HE3	1:B:203:HIS:HD1	1.50	0.57
1:A:333:ILE:O	1:A:337:VAL:HG23	2.05	0.57
1:B:221:LEU:O	1:B:221:LEU:HD12	2.05	0.57
1:A:331:GLY:O	1:A:333:ILE:N	2.38	0.57
1:B:377:ALA:HA	1:B:380:ILE:HD12	1.87	0.57
1:A:95:LEU:O	1:A:99:ILE:HG13	2.05	0.57
1:B:118:ASN:O	1:B:121:ALA:HB3	2.05	0.57
1:B:286:TYR:CB	1:B:309:ALA:HB2	2.35	0.56
1:B:51:LEU:O	1:B:52:SER:C	2.43	0.56
1:B:180:PHE:CD2	1:B:183:ALA:HB2	2.40	0.56
1:A:155:ASN:N	1:A:155:ASN:HD22	2.04	0.56
1:A:118:ASN:HD22	1:A:118:ASN:H	1.53	0.56
1:A:204:PHE:CZ	1:A:220:ASN:HB3	2.40	0.56
1:A:116:TYR:CB	1:A:139:ALA:HB2	2.35	0.56
1:B:91:GLU:C	1:B:93:GLY:N	2.60	0.56
1:A:231:PHE:CZ	1:A:261:GLU:HG2	2.41	0.55
1:B:279:GLN:C	1:B:281:HIS:H	2.10	0.55
1:A:99:ILE:HD13	1:A:123:LEU:HD23	1.87	0.55
1:A:257:CYS:HG	1:A:272:TYR:HH	1.54	0.55
1:B:374:TYR:HB2	1:B:391:MET:HE2	1.87	0.55
1:A:273:ARG:O	1:A:276:ILE:CG2	2.54	0.55
1:A:116:TYR:O	1:A:119:LEU:HB3	2.06	0.55
1:A:204:PHE:CE2	1:A:220:ASN:HB3	2.41	0.55
1:B:13:GLY:O	1:B:15:MET:N	2.40	0.55
1:B:167:LYS:O	1:B:171:LEU:HD12	2.07	0.55
1:A:191:PHE:CE1	1:A:203:HIS:NE2	2.71	0.54
1:A:221:LEU:O	1:A:224:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ASP:O	1:B:390:ASN:ND2	2.40	0.54
1:B:75:ASN:ND2	1:B:75:ASN:C	2.59	0.54
1:A:315:THR:HG23	1:A:346:VAL:CG2	2.37	0.54
1:A:367:LEU:HD13	1:A:398:MET:HG2	1.88	0.54
1:A:118:ASN:HD22	1:A:118:ASN:N	2.06	0.54
1:B:13:GLY:C	1:B:15:MET:N	2.60	0.54
1:B:63:ARG:NE	1:B:63:ARG:HA	2.22	0.54
1:A:320:LEU:HD12	1:A:343:ALA:HA	1.90	0.54
1:B:130:GLU:O	1:B:133:VAL:HG13	2.08	0.54
1:A:87:ASN:ND2	1:A:102:TYR:OH	2.32	0.54
1:A:354:HIS:O	1:A:373:HIS:HB3	2.07	0.54
1:B:62:ASP:OD1	1:B:92:ARG:NH2	2.41	0.53
1:A:381:SER:O	1:A:383:THR:N	2.41	0.53
1:B:25:GLY:O	1:B:27:PHE:CD1	2.62	0.53
1:A:151:SER:O	1:A:154:GLY:N	2.41	0.53
1:A:249:ALA:O	1:A:252:HIS:N	2.38	0.53
1:B:21:GLU:HA	1:B:21:GLU:OE2	2.09	0.53
1:A:202:HIS:CD2	1:B:199:LEU:HG	2.44	0.53
1:A:313:CYS:O	1:A:315:THR:N	2.42	0.53
1:A:116:TYR:HE1	1:A:142:TYR:CE1	2.27	0.53
1:B:97:GLU:O	1:B:101:HIS:CD2	2.62	0.53
1:A:116:TYR:HE1	1:A:142:TYR:CD1	2.27	0.52
1:B:374:TYR:CB	1:B:391:MET:HE2	2.39	0.52
1:A:238:TYR:HD2	1:A:251:VAL:HG13	1.74	0.52
1:A:304:ASP:O	1:A:307:ASN:HB2	2.10	0.52
1:A:128:ASP:OD1	1:A:131:GLY:N	2.39	0.52
1:B:138:SER:O	1:B:141:GLN:HB2	2.10	0.52
1:B:17:LEU:HD23	1:B:20:ARG:HH12	1.70	0.52
1:A:140:LEU:HD21	1:A:150:ARG:NH2	2.25	0.52
1:B:58:CYS:O	1:B:60:ARG:N	2.42	0.52
1:A:341:ARG:NH1	1:A:341:ARG:HG3	2.25	0.52
1:B:279:GLN:O	1:B:281:HIS:N	2.41	0.52
1:A:140:LEU:HD11	1:A:150:ARG:HG2	1.92	0.52
1:A:150:ARG:CG	1:A:150:ARG:NH1	2.70	0.52
1:A:263:GLY:O	1:A:265:ILE:N	2.42	0.52
1:A:88:VAL:O	1:A:92:ARG:HG2	2.10	0.52
1:A:256:ALA:HB1	1:A:272:TYR:CD1	2.45	0.51
1:A:286:TYR:O	1:A:288:ASN:N	2.44	0.51
1:A:34:CYS:O	1:A:37:LEU:N	2.43	0.51
1:A:337:VAL:HG12	1:A:341:ARG:HD2	1.92	0.51
1:B:211:ASP:O	1:B:214:PHE:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:THR:O	1:A:311:ARG:HB2	2.10	0.51
1:A:237:ALA:O	1:A:240:ARG:N	2.43	0.51
1:A:333:ILE:HG21	1:A:364:GLN:NE2	2.26	0.51
1:B:75:ASN:HD22	1:B:77:LEU:H	1.59	0.51
1:A:315:THR:HG23	1:A:346:VAL:HG22	1.93	0.51
1:A:208:VAL:HG13	1:A:217:ALA:CB	2.41	0.50
1:A:96:GLN:O	1:A:100:GLU:HG2	2.11	0.50
1:A:230:ILE:O	1:A:230:ILE:HG22	2.10	0.50
1:A:283:PRO:O	1:A:286:TYR:N	2.44	0.50
1:B:37:LEU:HD23	1:B:47:VAL:CG2	2.41	0.50
1:A:201:ILE:HG13	1:A:221:LEU:HD11	1.93	0.50
1:B:208:VAL:HG12	1:B:209:THR:N	2.27	0.50
1:B:371:LEU:HD12	1:B:391:MET:HG3	1.94	0.50
1:A:200:ALA:O	1:A:204:PHE:CD1	2.65	0.50
1:A:268:ALA:HB1	1:A:272:TYR:HE1	1.76	0.50
1:A:361:LEU:CD1	1:A:369:GLU:HG2	2.42	0.50
1:B:58:CYS:C	1:B:60:ARG:H	2.14	0.50
1:A:210:LEU:C	1:A:212:PRO:HD3	2.32	0.50
1:A:321:ASN:HD21	1:A:353:ALA:HA	1.76	0.50
1:B:235:VAL:HG21	1:B:262:GLN:HE22	1.76	0.49
1:A:157:LEU:HD13	1:A:165:GLU:HB3	1.94	0.49
1:A:214:PHE:O	1:A:217:ALA:HB3	2.12	0.49
1:A:273:ARG:C	1:A:276:ILE:HG22	2.33	0.49
1:A:277:GLU:O	1:A:280:PRO:HD3	2.12	0.49
1:A:384:PHE:O	1:A:388:TYR:HD1	1.95	0.49
1:B:304:ASP:HA	1:B:307:ASN:HD22	1.77	0.49
1:A:170:TYR:O	1:A:174:ILE:HG13	2.12	0.49
1:B:283:PRO:HG2	1:B:284:ASP:H	1.77	0.49
1:A:147:TYR:HE1	1:A:148:CYS:HG	1.57	0.49
1:A:191:PHE:HE1	1:A:203:HIS:NE2	2.04	0.49
1:A:27:PHE:N	1:A:27:PHE:CD2	2.80	0.49
1:A:111:ASP:OD1	1:A:111:ASP:O	2.30	0.49
1:A:233:ARG:O	1:A:235:VAL:N	2.45	0.49
1:B:306:TYR:O	1:B:310:LEU:HG	2.12	0.49
1:A:147:TYR:O	1:A:150:ARG:HB2	2.12	0.49
1:A:176:THR:O	1:A:178:PRO:HD3	2.13	0.49
1:B:212:PRO:O	1:B:218:TYR:HE1	1.96	0.49
1:B:21:GLU:HG3	1:B:29:ALA:CB	2.43	0.49
1:A:376:GLU:OE2	1:A:379:ARG:NH2	2.46	0.49
1:B:31:GLU:CD	1:B:55:HIS:HE1	2.16	0.49
1:B:61:LEU:O	1:B:64:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLU:O	1:A:168:ALA:N	2.45	0.48
1:A:191:PHE:HD1	1:A:203:HIS:CD2	2.30	0.48
1:B:48:LEU:HD13	1:B:70:LEU:HB3	1.94	0.48
1:B:104:HIS:O	1:B:107:ARG:N	2.43	0.48
1:A:34:CYS:HB3	1:A:47:VAL:HG13	1.94	0.48
1:B:174:ILE:HG13	1:B:183:ALA:HB1	1.96	0.48
1:B:89:TYR:CD2	1:B:97:GLU:CB	2.97	0.48
1:A:233:ARG:HG2	1:A:233:ARG:HH11	1.78	0.48
1:A:203:HIS:O	1:A:205:GLU:N	2.46	0.48
1:A:313:CYS:C	1:A:315:THR:H	2.17	0.48
1:A:344:LEU:HD22	1:A:354:HIS:CD2	2.49	0.48
1:B:37:LEU:HD23	1:B:47:VAL:HG21	1.96	0.48
1:A:120:ALA:HB1	1:A:136:TYR:CE1	2.48	0.48
1:A:234:ALA:O	1:A:238:TYR:CD1	2.63	0.48
1:B:150:ARG:O	1:B:153:LEU:HB3	2.14	0.48
1:A:233:ARG:C	1:A:235:VAL:H	2.17	0.48
1:A:273:ARG:HA	1:A:276:ILE:HG22	1.96	0.48
1:A:158:LYS:O	1:A:160:LEU:N	2.47	0.48
1:A:158:LYS:C	1:A:160:LEU:H	2.17	0.48
1:B:51:LEU:O	1:B:54:ILE:N	2.47	0.48
1:A:181:ALA:O	1:A:182:VAL:C	2.50	0.47
1:A:201:ILE:HD13	1:B:198:TRP:CE3	2.49	0.47
1:A:286:TYR:C	1:A:288:ASN:H	2.18	0.47
1:B:120:ALA:O	1:B:124:VAL:HG23	2.14	0.47
1:B:304:ASP:CG	1:B:305:CYS:N	2.68	0.47
1:B:113:ILE:CD1	1:B:143:ASN:HB2	2.44	0.47
1:A:161:GLY:O	1:A:163:LEU:N	2.48	0.47
1:A:45:THR:HG23	1:A:78:LEU:HD11	1.97	0.47
1:A:198:TRP:NE1	1:B:205:GLU:OE2	2.48	0.47
1:B:124:VAL:HG13	1:B:129:MET:SD	2.55	0.47
1:B:17:LEU:HD23	1:B:20:ARG:HH11	1.77	0.47
1:A:184:TRP:O	1:A:185:SER:C	2.53	0.47
1:A:268:ALA:O	1:A:272:TYR:CD1	2.65	0.47
1:A:299:VAL:O	1:A:299:VAL:HG12	2.15	0.47
1:A:26:ASP:C	3:A:2002:HOH:O	2.53	0.46
1:A:28:GLU:HA	1:A:31:GLU:HB3	1.97	0.46
1:B:184:TRP:CE3	1:B:206:LYS:HG2	2.50	0.46
1:A:283:PRO:O	1:A:285:ALA:N	2.47	0.46
1:B:45:THR:O	1:B:49:LEU:HB2	2.15	0.46
1:B:48:LEU:HD12	1:B:71:ALA:HA	1.97	0.46
1:A:166:ALA:O	1:A:170:TYR:CD1	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:HIS:O	1:A:205:GLU:HB2	2.15	0.46
1:B:136:TYR:CD2	1:B:149:VAL:HG13	2.51	0.46
1:B:156:LEU:O	1:B:160:LEU:HG	2.16	0.46
1:B:399:GLN:O	1:B:400:ASP:C	2.54	0.46
1:B:374:TYR:CZ	1:B:390:ASN:HB3	2.51	0.46
1:A:182:VAL:CG1	1:A:186:ASN:ND2	2.78	0.46
1:B:89:TYR:CD2	1:B:97:GLU:HB2	2.50	0.46
1:A:181:ALA:O	1:A:183:ALA:N	2.49	0.46
1:A:147:TYR:CE2	1:A:177:GLN:HB2	2.51	0.46
1:B:182:VAL:HG12	1:B:186:ASN:ND2	2.31	0.46
1:A:300:ALA:HB3	3:A:2017:HOH:O	2.16	0.46
1:A:44:ASN:CB	1:A:47:VAL:HB	2.46	0.46
1:B:53:SER:O	1:B:56:PHE:HB3	2.16	0.46
1:A:332:ASN:C	3:A:2019:HOH:O	2.54	0.45
1:A:333:ILE:HG21	1:A:364:GLN:HE21	1.79	0.45
1:B:58:CYS:C	1:B:60:ARG:N	2.70	0.45
1:A:116:TYR:HB2	1:A:139:ALA:HB2	1.98	0.45
1:A:123:LEU:HB2	1:A:132:ALA:HB2	1.98	0.45
1:A:147:TYR:HD1	1:A:148:CYS:N	2.12	0.45
1:A:164:GLU:OE1	1:A:167:LYS:NZ	2.46	0.45
1:A:252:HIS:HB3	1:A:275:ALA:HB2	1.98	0.45
1:B:184:TRP:CZ3	1:B:206:LYS:HG2	2.52	0.45
1:A:13:GLY:N	1:A:14:PRO:CD	2.76	0.45
1:A:206:LYS:O	1:A:208:VAL:N	2.49	0.45
1:A:22:TYR:HA	1:A:30:ALA:HB2	1.99	0.45
1:A:340:TYR:CZ	1:A:356:ASN:HB3	2.52	0.45
1:B:231:PHE:HA	1:B:234:ALA:HB3	1.98	0.45
1:B:281:HIS:O	1:B:283:PRO:HD3	2.17	0.45
1:A:78:LEU:O	1:A:81:ALA:HB3	2.17	0.45
1:A:341:ARG:HH12	1:A:357:LEU:CD2	2.21	0.45
1:B:281:HIS:O	1:B:283:PRO:N	2.50	0.45
1:B:301:GLU:CG	1:B:301:GLU:O	2.65	0.45
1:B:63:ARG:HE	1:B:63:ARG:HA	1.80	0.45
1:A:229:ARG:HA	1:A:231:PHE:CE2	2.52	0.45
1:B:47:VAL:C	1:B:49:LEU:N	2.69	0.45
1:A:263:GLY:O	1:A:265:ILE:HG13	2.16	0.45
1:A:129:MET:SD	1:A:156:LEU:HD11	2.57	0.44
1:A:333:ILE:N	3:A:2019:HOH:O	2.50	0.44
1:A:113:ILE:C	1:A:115:GLY:N	2.70	0.44
1:A:138:SER:C	1:A:140:LEU:N	2.71	0.44
1:A:283:PRO:O	1:A:284:ASP:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:HIS:O	1:A:206:LYS:N	2.51	0.44
1:B:91:GLU:O	1:B:93:GLY:N	2.51	0.44
1:A:138:SER:O	1:A:140:LEU:N	2.51	0.44
1:A:158:LYS:C	1:A:160:LEU:N	2.71	0.44
1:A:203:HIS:C	1:A:205:GLU:N	2.71	0.44
1:A:349:GLU:HA	1:A:380:ILE:HD13	2.00	0.44
1:A:367:LEU:HD11	1:A:397:GLU:HG3	2.00	0.44
1:A:34:CYS:CB	1:A:47:VAL:HG13	2.48	0.44
1:B:83:SER:HB2	1:B:112:PHE:HE1	1.82	0.44
1:A:182:VAL:HG13	1:A:186:ASN:ND2	2.33	0.44
1:A:22:TYR:CB	1:A:50:LEU:HD21	2.48	0.44
1:A:233:ARG:C	1:A:235:VAL:N	2.71	0.44
1:B:167:LYS:HG2	1:B:171:LEU:HD12	2.00	0.44
1:A:268:ALA:HB1	1:A:272:TYR:CE1	2.52	0.43
1:A:351:ALA:O	1:A:354:HIS:HB2	2.17	0.43
1:B:113:ILE:HD11	1:B:143:ASN:HB2	2.00	0.43
1:B:399:GLN:HA	1:B:399:GLN:OE1	2.18	0.43
1:B:256:ALA:O	1:B:259:TYR:HB2	2.18	0.43
1:B:14:PRO:HD2	1:B:37:LEU:HD13	2.00	0.43
1:B:99:ILE:O	1:B:103:ARG:HG3	2.17	0.43
1:A:341:ARG:NH1	1:A:357:LEU:CD2	2.81	0.43
1:B:63:ARG:O	1:B:67:PHE:HD1	2.02	0.43
1:A:321:ASN:ND2	1:A:353:ALA:CA	2.81	0.43
1:B:177:GLN:HE21	1:B:179:ASN:H	1.67	0.43
1:B:266:ASP:CG	1:B:267:LEU:N	2.72	0.43
1:B:96:GLN:OE1	1:B:96:GLN:HA	2.19	0.43
1:B:89:TYR:CD2	1:B:97:GLU:HB3	2.54	0.43
1:B:177:GLN:HG3	1:B:180:PHE:HB2	2.01	0.43
1:A:45:THR:HG21	1:A:78:LEU:HD11	2.01	0.43
1:B:102:TYR:CZ	1:B:118:ASN:HB3	2.54	0.43
1:B:83:SER:O	1:B:86:GLY:N	2.52	0.43
1:A:380:ILE:O	1:A:380:ILE:HG22	2.18	0.43
1:B:232:ASP:CG	1:B:233:ARG:N	2.73	0.43
1:B:270:ASP:C	1:B:270:ASP:OD1	2.57	0.43
1:B:24:ALA:C	1:B:26:ASP:H	2.22	0.42
1:A:138:SER:O	1:A:141:GLN:N	2.48	0.42
1:B:221:LEU:O	1:B:224:VAL:HG22	2.19	0.42
1:A:191:PHE:CD1	1:A:203:HIS:CD2	3.07	0.42
1:A:198:TRP:O	1:A:201:ILE:HG23	2.20	0.42
1:A:279:GLN:O	1:A:282:PHE:HB2	2.19	0.42
1:A:352:ALA:O	1:A:353:ALA:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:SER:HA	1:A:358:ALA:HB3	2.01	0.42
1:A:330:GLN:HB2	1:A:332:ASN:HD22	1.84	0.42
1:B:54:ILE:C	1:B:56:PHE:N	2.70	0.42
1:A:279:GLN:O	1:A:280:PRO:C	2.57	0.42
1:A:286:TYR:CE1	1:A:308:THR:HG21	2.55	0.42
1:B:235:VAL:O	1:B:237:ALA:N	2.53	0.42
1:B:34:CYS:CB	1:B:51:LEU:HD21	2.50	0.42
1:B:89:TYR:CE2	1:B:97:GLU:HB3	2.54	0.42
1:A:177:GLN:HB3	1:A:180:PHE:HB2	2.01	0.42
1:A:286:TYR:CZ	1:A:308:THR:HG21	2.55	0.42
1:A:369:GLU:O	1:A:373:HIS:HD2	2.01	0.42
1:A:381:SER:C	1:A:383:THR:H	2.23	0.42
1:B:204:PHE:CZ	1:B:220:ASN:HB3	2.55	0.42
1:A:240:ARG:O	1:A:243:SER:N	2.52	0.42
1:B:41:GLU:OE1	1:B:44:ASN:ND2	2.52	0.41
1:A:27:PHE:HB3	1:A:54:ILE:HG23	2.02	0.41
1:A:124:VAL:HG22	1:A:129:MET:HE1	2.02	0.41
1:A:164:GLU:HB2	3:A:2007:HOH:O	2.20	0.41
1:A:354:HIS:CB	1:A:377:ALA:HB2	2.48	0.41
1:B:43:ASP:O	1:B:45:THR:N	2.53	0.41
1:A:301:GLU:O	1:A:304:ASP:N	2.53	0.41
1:A:34:CYS:O	1:A:35:MET:C	2.58	0.41
1:B:313:CYS:HA	1:B:314:PRO:HD3	1.68	0.41
1:B:375:LYS:N	1:B:391:MET:HE1	2.35	0.41
1:A:289:LEU:O	1:A:292:ALA:HB3	2.21	0.41
1:B:58:CYS:CB	1:B:60:ARG:HH21	2.32	0.41
1:A:127:GLY:O	1:A:129:MET:HG2	2.18	0.41
1:A:198:TRP:CE3	1:B:201:ILE:HG21	2.56	0.41
1:B:21:GLU:HG3	1:B:29:ALA:HB3	2.01	0.41
1:A:196:GLU:OE1	1:B:202:HIS:HE1	2.04	0.41
1:A:286:TYR:C	1:A:288:ASN:N	2.74	0.41
1:A:55:HIS:CB	1:A:60:ARG:HB2	2.51	0.41
1:B:248:HIS:CE1	1:B:250:VAL:HB	2.55	0.41
1:B:38:TRP:CD1	1:B:48:LEU:HD21	2.56	0.41
1:B:49:LEU:HA	1:B:49:LEU:HD12	1.79	0.41
1:A:143:ASN:HA	1:A:144:PRO:HD2	1.89	0.41
1:A:67:PHE:O	1:A:70:LEU:HB2	2.21	0.41
1:B:265:ILE:HD13	1:B:295:GLU:CB	2.50	0.41
1:B:97:GLU:OE1	1:B:97:GLU:HA	2.21	0.41
1:A:116:TYR:HB3	1:A:139:ALA:HB2	2.02	0.41
1:B:281:HIS:HA	1:B:312:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ILE:O	1:B:56:PHE:N	2.54	0.41
1:A:100:GLU:H	1:A:100:GLU:HG2	1.68	0.40
1:B:375:LYS:N	1:B:391:MET:CE	2.85	0.40
1:A:165:GLU:O	1:A:166:ALA:C	2.59	0.40
1:A:71:ALA:O	1:A:78:LEU:HD12	2.21	0.40
1:A:80:GLU:OE2	1:A:109:LYS:NZ	2.53	0.40
1:A:123:LEU:CB	1:A:132:ALA:HB2	2.52	0.40
1:A:120:ALA:O	1:A:121:ALA:C	2.59	0.40
1:A:87:ASN:HA	1:A:102:TYR:OH	2.21	0.40
1:B:372:MET:O	1:B:376:GLU:CG	2.70	0.40
1:B:54:ILE:C	1:B:56:PHE:H	2.25	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	386/388 (100%)	303 (78%)	57 (15%)	26 (7%)	1	3
1	B	364/388 (94%)	309 (85%)	45 (12%)	10 (3%)	5	19
All	All	750/776 (97%)	612 (82%)	102 (14%)	36 (5%)	2	7

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	SER
1	A	332	ASN
1	B	59	ARG
1	A	162	ARG
1	A	204	PHE
1	A	207	ALA
1	A	264	LEU

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Mol	Chain	Res	Type
1	A	284	ASP
1	A	287	CYS
1	A	382	PRO
1	B	215	LEU
1	A	121	ALA
1	A	152	ASP
1	A	159	ALA
1	A	234	ALA
1	A	237	ALA
1	A	283	PRO
1	A	314	PRO
1	B	27	PHE
1	B	280	PRO
1	A	216	ASP
1	A	278	LEU
1	A	352	ALA
1	B	236	ALA
1	A	125	ALA
1	A	250	VAL
1	B	44	ASN
1	B	51	LEU
1	B	92	ARG
1	B	282	PHE
1	A	212	PRO
1	A	215	LEU
1	A	279	GLN
1	B	14	PRO
1	A	127	GLY
1	A	182	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/314 (86%)	252 (93%)	18 (7%)	18	42
1	B	238/314 (76%)	224 (94%)	14 (6%)	21	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	508/628 (81%)	476 (94%)	32 (6%)	20	46

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	PHE
1	A	45	THR
1	A	91	GLU
1	A	110	PRO
1	A	118	ASN
1	A	150	ARG
1	A	152	ASP
1	A	201	ILE
1	A	214	PHE
1	A	223	ASN
1	A	254	ASN
1	A	276	ILE
1	A	280	PRO
1	A	282	PHE
1	A	283	PRO
1	A	288	ASN
1	A	314	PRO
1	A	350	PHE
1	B	44	ASN
1	B	63	ARG
1	B	68	SER
1	B	75	ASN
1	B	103	ARG
1	B	133	VAL
1	B	150	ARG
1	B	171	LEU
1	B	205	GLU
1	B	208	VAL
1	B	214	PHE
1	B	267	LEU
1	B	287	CYS
1	B	384	PHE

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

Mol	Chain	Res	Type
1	A	84	ASN
1	A	87	ASN
1	A	118	ASN
1	A	155	ASN
1	A	186	ASN
1	A	223	ASN
1	A	254	ASN
1	A	288	ASN
1	A	291	ASN
1	A	307	ASN
1	A	316	HIS
1	A	321	ASN
1	A	325	ASN
1	A	332	ASN
1	A	354	HIS
1	A	356	ASN
1	A	362	GLN
1	A	364	GLN
1	A	373	HIS
1	A	390	ASN
1	B	19	HIS
1	B	33	HIS
1	B	55	HIS
1	B	75	ASN
1	B	84	ASN
1	B	101	HIS
1	B	118	ASN
1	B	155	ASN
1	B	177	GLN
1	B	186	ASN
1	B	202	HIS
1	B	223	ASN
1	B	252	HIS
1	B	254	ASN
1	B	262	GLN
1	B	307	ASN
1	B	390	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/388 (100%)	-0.23	5 (1%) 77 75	41, 87, 134, 150	0
1	B	368/388 (94%)	-0.07	16 (4%) 35 30	37, 86, 146, 156	0
All	All	756/776 (97%)	-0.15	21 (2%) 53 48	37, 87, 145, 156	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	GLY	6.8
1	B	297	GLY	4.6
1	A	15	MET	4.3
1	B	364	GLN	3.8
1	B	311	ARG	3.6
1	B	309	ALA	3.5
1	B	299	VAL	3.0
1	B	319	SER	2.9
1	B	286	TYR	2.8
1	B	346	VAL	2.8
1	A	26	ASP	2.6
1	A	16	GLU	2.6
1	B	312	LEU	2.5
1	B	365	GLY	2.4
1	B	305	CYS	2.3
1	B	302	ALA	2.3
1	B	295	GLU	2.3
1	B	304	ASP	2.2
1	A	30	ALA	2.2
1	B	398	MET	2.1
1	B	281	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
2	CA	A	1001	1/1	0.97	0.13	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.