



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:19 PM GMT

PDB ID : 1X3Z
Title : Structure of a peptide:N-glycanase-Rad23 complex
Authors : Lee, J.-H.; Choi, J.M.; Lee, C.; Yi, K.J.; Cho, Y.
Deposited on : 2005-05-11
Resolution : 2.80 Å(reported)

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

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

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

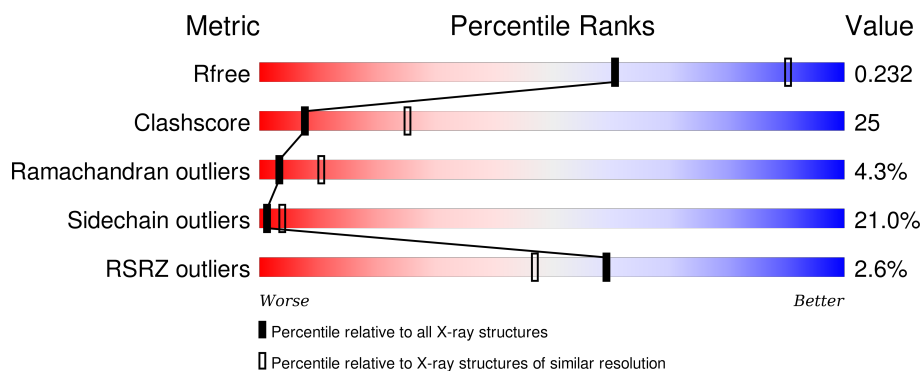
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	335	
2	B	72	
3	I	5	

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
4	SUC	A	1002	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3197 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 peptide: N-glycanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2665	1698	456	494	17			

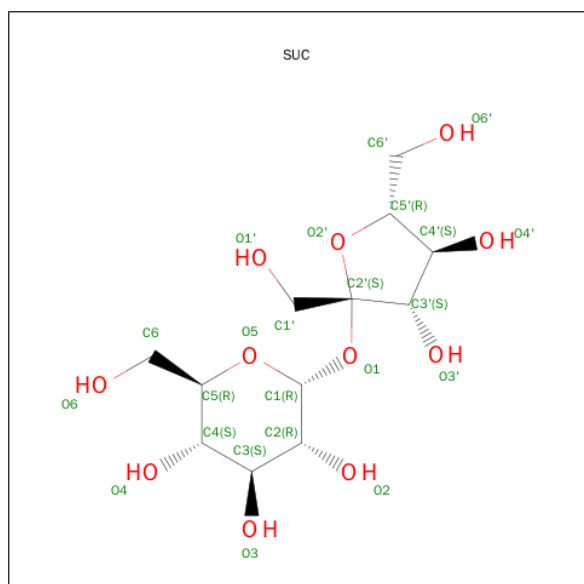
- Molecule 2 is a protein called UV excision repair protein RAD23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	57	Total	C	N	O	S	0	0	0
			435	276	73	84	2			

- Molecule 3 is a protein called peptide PHQ-Val-Ala-Asp-CF0.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	1
			21	13	3	5			

- Molecule 4 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	12	11		
4	A	1	Total	C	O	0	0
			23	12	11		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

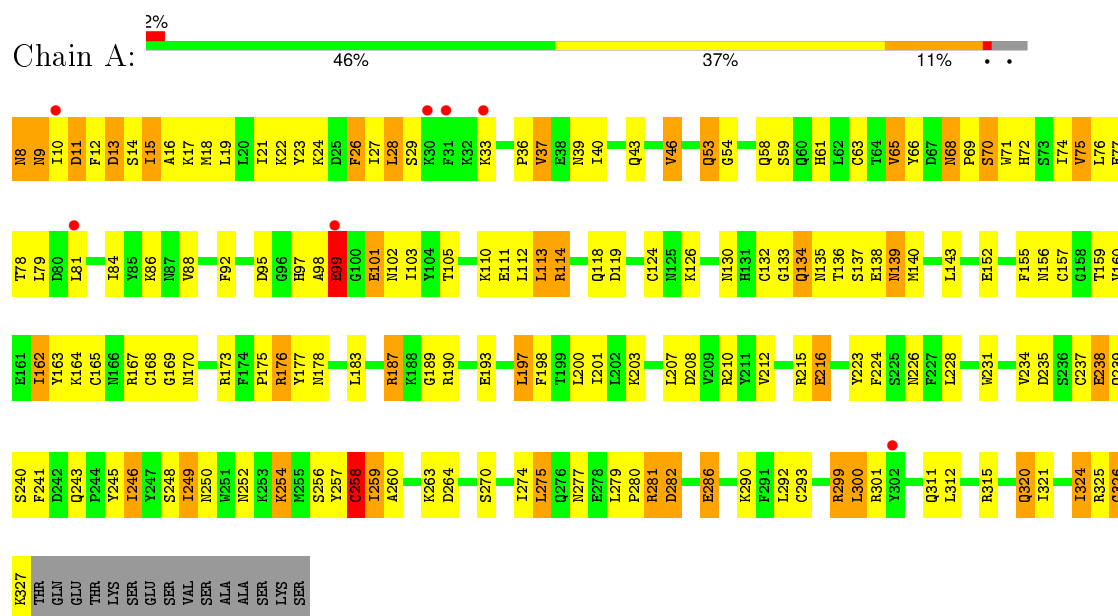
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	26	Total	O	0	0
			26	26		
6	B	3	Total	O	0	0
			3	3		

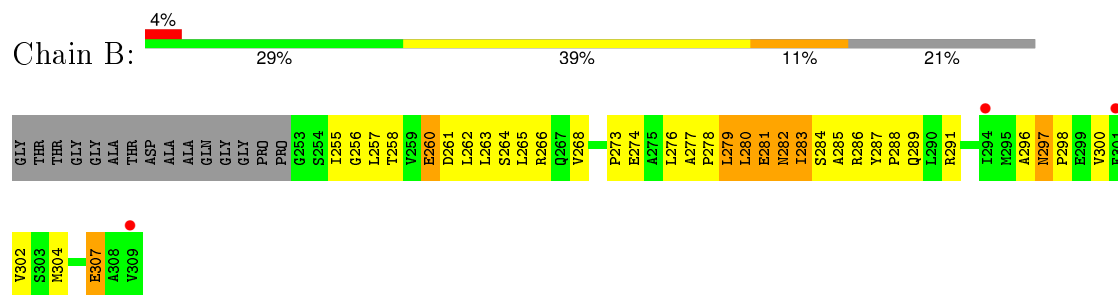
3 Residue-property plots

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

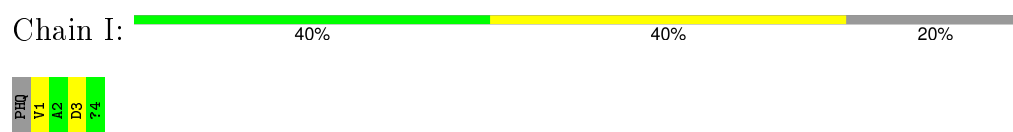
- Molecule 1: peptide: N-glycanase



- Molecule 2: UV excision repair protein RAD23



- Molecule 3: peptide PHQ-Val-Ala-Asp-CF0



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.80Å 128.80Å 128.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.80) 97.5 (19.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.236 , 0.270 0.238 , 0.232	Depositor DCC
R_{free} test set	1492 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.6	EDS
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 30635 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3197	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SUC, CF0

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	0.72	2/2729 (0.1%)	0.81	0/3683
2	B	0.72	0/441	0.70	0/599
3	I	0.89	0/19	0.51	0/25
All	All	0.72	2/3189 (0.1%)	0.80	0/4307

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	CYS	CB-SG	-7.47	1.69	1.82
1	A	293	CYS	CB-SG	-5.33	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2665	0	2575	125	0
2	B	435	0	446	34	0
3	I	21	0	20	3	0
4	A	46	0	44	1	0
5	A	1	0	0	0	0
6	A	26	0	0	2	0
6	B	3	0	0	0	0
All	All	3197	0	3085	157	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 25.

All (157) 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:A:187:ARG:HH11	1:A:187:ARG:HG2	1.08	1.13
1:A:176:ARG:HG2	1:A:176:ARG:HH11	1.09	1.10
1:A:189:GLY:HA3	1:A:193:GLU:HG3	1.33	1.09
1:A:281:ARG:HG2	1:A:281:ARG:HH11	1.18	1.04
1:A:70:SER:O	1:A:74:ILE:HD13	1.58	1.01
1:A:254:LYS:HB3	1:A:279:LEU:HD21	1.48	0.95
1:A:299:ARG:HH11	1:A:299:ARG:HG3	1.33	0.92
1:A:216:GLU:OE1	1:A:256:SER:N	2.03	0.91
1:A:176:ARG:NH1	1:A:176:ARG:HG2	1.82	0.91
1:A:189:GLY:HA3	1:A:193:GLU:CG	2.03	0.88
1:A:281:ARG:HG2	1:A:281:ARG:NH1	1.85	0.86
1:A:176:ARG:HB3	3:I:1:VAL:HG11	1.56	0.86
1:A:249:ILE:HG13	1:A:250:ASN:HD22	1.45	0.77
1:A:187:ARG:HH11	1:A:187:ARG:CG	1.92	0.76
1:A:176:ARG:HB3	3:I:1:VAL:CG1	2.16	0.75
1:A:299:ARG:HH11	1:A:299:ARG:CG	1.98	0.75
1:A:19:LEU:HD13	2:B:302:VAL:HG23	1.67	0.74
1:A:187:ARG:HG2	1:A:187:ARG:NH1	1.88	0.73
1:A:274:ILE:HG22	1:A:274:ILE:O	1.88	0.72
1:A:157:CYS:HB2	1:A:177:TYR:HD1	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:PHE:HA	1:A:15:ILE:HG23	1.71	0.71
2:B:268:VAL:HG11	2:B:279:LEU:HD12	1.73	0.70
1:A:36:PRO:HA	1:A:39:ASN:HB2	1.72	0.69
1:A:254:LYS:HB3	1:A:279:LEU:CD2	2.21	0.69
2:B:255:ILE:HG23	2:B:256:GLY:N	2.09	0.68
2:B:264:SER:O	2:B:268:VAL:HG12	1.93	0.68
1:A:98:ALA:O	1:A:101:GLU:HB2	1.94	0.66
1:A:138:GLU:C	1:A:140:MET:H	1.96	0.66
1:A:68:ASN:O	1:A:72:HIS:HD2	1.79	0.66
1:A:157:CYS:HB2	1:A:177:TYR:CD1	2.31	0.65
2:B:258:THR:HG23	2:B:261:ASP:H	1.62	0.65
1:A:301:ARG:NH2	1:A:312:LEU:HB3	2.12	0.65
2:B:260:GLU:N	2:B:260:GLU:OE2	2.30	0.64
1:A:68:ASN:C	1:A:68:ASN:ND2	2.50	0.64
1:A:239:GLN:N	4:A:1002:SUC:O4'	2.32	0.63
2:B:296:ALA:O	2:B:297:ASN:HB2	1.99	0.63
1:A:68:ASN:C	1:A:68:ASN:HD22	2.02	0.62
1:A:249:ILE:HG13	1:A:250:ASN:ND2	2.14	0.62
2:B:258:THR:HG22	2:B:261:ASP:HB2	1.81	0.62
1:A:176:ARG:CG	1:A:176:ARG:HH11	1.96	0.61
1:A:99:GLU:HB2	6:A:1006:HOH:O	2.01	0.61
1:A:26:PHE:O	1:A:29:SER:OG	2.14	0.60
1:A:299:ARG:NH1	1:A:299:ARG:HG3	2.07	0.60
1:A:156:ASN:HB3	1:A:178:ASN:HB2	1.84	0.60
1:A:263:LYS:O	1:A:300:LEU:HD22	2.02	0.59
1:A:70:SER:O	1:A:74:ILE:CD1	2.42	0.59
2:B:296:ALA:O	2:B:297:ASN:CB	2.49	0.59
1:A:46:VAL:O	1:A:53:GLN:HG2	2.02	0.59
2:B:255:ILE:HG23	2:B:256:GLY:H	1.68	0.59
1:A:61:HIS:HE1	6:A:1003:HOH:O	1.85	0.58
1:A:13:ASP:OD1	1:A:13:ASP:N	2.34	0.58
1:A:264:ASP:O	1:A:301:ARG:HD2	2.04	0.58
1:A:84:ILE:O	1:A:88:VAL:HG23	2.05	0.57
1:A:113:LEU:HD13	1:A:198:PHE:CZ	2.40	0.56
1:A:259:ILE:HD12	1:A:260:ALA:N	2.19	0.56
1:A:249:ILE:HG13	1:A:250:ASN:N	2.21	0.56
1:A:71:TRP:O	1:A:75:VAL:HG12	2.06	0.55
1:A:250:ASN:N	1:A:250:ASN:HD22	2.04	0.55
1:A:274:ILE:O	1:A:274:ILE:CG2	2.55	0.54
1:A:126:LYS:NZ	1:A:138:GLU:HA	2.22	0.54
2:B:300:VAL:O	2:B:304:MET:HG3	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:CD1	1:A:155:PHE:N	2.77	0.53
1:A:76:LEU:HD22	1:A:81:LEU:HD21	1.91	0.53
1:A:235:ASP:O	1:A:238:GLU:O	2.26	0.52
1:A:215:ARG:NH1	1:A:256:SER:OG	2.42	0.52
1:A:12:PHE:O	1:A:16:ALA:N	2.29	0.52
1:A:54:GLY:O	1:A:58:GLN:HG3	2.10	0.52
1:A:12:PHE:HA	1:A:15:ILE:CG2	2.37	0.52
1:A:101:GLU:CD	1:A:102:ASN:H	2.13	0.52
1:A:257:TYR:CZ	1:A:281:ARG:HG3	2.44	0.52
1:A:138:GLU:C	1:A:140:MET:N	2.64	0.52
1:A:39:ASN:O	1:A:43:GLN:HB2	2.10	0.51
1:A:75:VAL:HG11	1:A:200:LEU:HD21	1.92	0.51
1:A:16:ALA:O	1:A:19:LEU:HB3	2.10	0.51
1:A:26:PHE:CD2	1:A:26:PHE:C	2.82	0.51
1:A:168:CYS:SG	1:A:170:ASN:HB2	2.51	0.51
1:A:110:LYS:HE2	1:A:241:PHE:CD2	2.46	0.51
2:B:255:ILE:HG12	2:B:257:LEU:HD12	1.94	0.50
1:A:61:HIS:O	1:A:65:VAL:CG2	2.60	0.50
1:A:165:CYS:O	1:A:169:GLY:HA2	2.11	0.50
1:A:79:LEU:HD11	1:A:201:ILE:HG23	1.93	0.50
1:A:8:ASN:HD22	1:A:9:ASN:H	1.58	0.50
2:B:268:VAL:CG1	2:B:279:LEU:HD12	2.41	0.50
1:A:143:LEU:CD2	1:A:164:LYS:HB2	2.42	0.49
1:A:139:ASN:N	1:A:139:ASN:OD1	2.34	0.49
1:A:248:SER:HB3	1:A:275:LEU:HD12	1.95	0.49
2:B:304:MET:O	2:B:307:GLU:HB2	2.12	0.49
2:B:261:ASP:OD2	2:B:286:ARG:NH1	2.42	0.49
1:A:75:VAL:HG11	1:A:200:LEU:CD2	2.43	0.48
1:A:66:TYR:HB3	1:A:203:LYS:HD3	1.95	0.48
1:A:61:HIS:O	1:A:65:VAL:HG22	2.14	0.48
1:A:258:CYS:HB2	1:A:270:SER:HA	1.95	0.48
1:A:13:ASP:HA	1:A:16:ALA:HB3	1.94	0.48
2:B:255:ILE:CG2	2:B:256:GLY:N	2.76	0.48
1:A:320:GLN:O	1:A:324:ILE:HG23	2.14	0.48
1:A:245:TYR:CD1	1:A:246:ILE:N	2.81	0.48
1:A:26:PHE:O	1:A:26:PHE:HD2	1.96	0.48
1:A:24:LYS:O	1:A:28:LEU:HD12	2.13	0.48
1:A:111:GLU:OE2	1:A:114:ARG:NH1	2.47	0.47
2:B:263:LEU:O	2:B:266:ARG:HG2	2.15	0.47
2:B:277:ALA:HB3	2:B:278:PRO:CD	2.45	0.47
1:A:95:ASP:OD2	1:A:97:HIS:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLU:O	1:A:157:CYS:HB3	2.15	0.47
2:B:258:THR:HG22	2:B:261:ASP:CB	2.45	0.47
2:B:257:LEU:HD23	2:B:287:TYR:CZ	2.50	0.47
1:A:143:LEU:HD21	1:A:164:LYS:HB2	1.96	0.46
1:A:190:ARG:HD2	3:I:3:ASP:OD2	2.15	0.46
2:B:265:LEU:HA	2:B:279:LEU:HD11	1.98	0.46
1:A:68:ASN:H	1:A:72:HIS:HE2	1.64	0.46
1:A:245:TYR:O	1:A:246:ILE:C	2.54	0.46
1:A:68:ASN:O	1:A:72:HIS:CD2	2.66	0.46
1:A:114:ARG:NH2	1:A:119:ASP:OD1	2.48	0.46
1:A:26:PHE:HD2	1:A:26:PHE:C	2.19	0.46
1:A:197:LEU:O	1:A:201:ILE:HG12	2.16	0.45
1:A:160:VAL:HG22	1:A:175:PRO:HB3	1.98	0.45
1:A:325:ARG:NH1	2:B:263:LEU:HD23	2.31	0.45
2:B:273:PRO:HD2	2:B:274:GLU:OE2	2.17	0.45
1:A:92:PHE:HE2	1:A:103:ILE:HG23	1.82	0.45
1:A:281:ARG:O	1:A:282:ASP:HB3	2.16	0.45
2:B:257:LEU:HD21	2:B:283:ILE:HD11	1.98	0.44
1:A:126:LYS:HZ2	1:A:138:GLU:HA	1.82	0.44
1:A:69:PRO:HA	1:A:72:HIS:CD2	2.53	0.44
2:B:297:ASN:HA	2:B:298:PRO:HD2	1.85	0.44
1:A:8:ASN:ND2	1:A:9:ASN:H	2.16	0.44
1:A:134:GLN:HE21	1:A:135:ASN:N	2.14	0.44
1:A:248:SER:HB3	1:A:275:LEU:CD1	2.48	0.44
1:A:17:LYS:O	1:A:21:ILE:HD12	2.18	0.44
2:B:276:LEU:HG	2:B:276:LEU:O	2.17	0.43
2:B:280:LEU:HA	2:B:280:LEU:HD13	1.74	0.43
2:B:255:ILE:CG2	2:B:256:GLY:H	2.30	0.43
2:B:284:SER:C	2:B:286:ARG:H	2.21	0.43
1:A:59:SER:O	1:A:63:CYS:HB2	2.18	0.43
2:B:280:LEU:C	2:B:283:ILE:HG22	2.39	0.42
1:A:162:ILE:HD12	1:A:163:TYR:N	2.35	0.42
1:A:281:ARG:NH1	1:A:286:GLU:OE2	2.53	0.41
2:B:282:ASN:C	2:B:282:ASN:OD1	2.58	0.41
1:A:72:HIS:O	1:A:75:VAL:HG13	2.20	0.41
1:A:224:PHE:CD2	1:A:224:PHE:C	2.94	0.41
2:B:278:PRO:O	2:B:281:GLU:HB3	2.21	0.41
1:A:152:GLU:OE1	1:A:160:VAL:HG21	2.21	0.41
1:A:101:GLU:OE2	1:A:102:ASN:N	2.48	0.41
1:A:324:ILE:HG13	1:A:325:ARG:N	2.31	0.41
1:A:37:VAL:O	1:A:40:ILE:HG13	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TYR:CD2	1:A:200:LEU:HB2	2.56	0.41
1:A:259:ILE:HD12	1:A:259:ILE:C	2.41	0.41
1:A:18:MET:CG	1:A:22:LYS:NZ	2.84	0.41
2:B:276:LEU:HD21	2:B:280:LEU:HD23	2.03	0.41
1:A:301:ARG:NH2	1:A:312:LEU:CB	2.82	0.41
1:A:210:ARG:NH2	1:A:231:TRP:NE1	2.69	0.41
1:A:23:TYR:CZ	1:A:27:ILE:HD11	2.56	0.41
1:A:237:CYS:HB2	1:A:238:GLU:H	1.67	0.41
1:A:325:ARG:O	1:A:326:GLY:C	2.59	0.41
2:B:276:LEU:CD2	2:B:280:LEU:HD23	2.52	0.40
1:A:279:LEU:HB3	1:A:280:PRO:CD	2.50	0.40
1:A:12:PHE:O	1:A:15:ILE:HG23	2.21	0.40
1:A:254:LYS:HA	1:A:277:ASN:HB3	2.02	0.40
1:A:68:ASN:HA	1:A:69:PRO:HD3	1.90	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	318/335 (95%)	257 (81%)	50 (16%)	11 (4%)	4	15
2	B	55/72 (76%)	39 (71%)	11 (20%)	5 (9%)	1	2
3	I	1/5 (20%)	1 (100%)	0	0	100	100
All	All	374/412 (91%)	297 (79%)	61 (16%)	16 (4%)	3	10

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	10	ILE
1	A	11	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	99	GLU
1	A	282	ASP
2	B	297	ASN
1	A	33	LYS
1	A	246	ILE
2	B	291	ARG
1	A	132	CYS
1	A	133	GLY
2	B	262	LEU
1	A	290	LYS
2	B	285	ALA
2	B	288	PRO
1	A	326	GLY

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	296/309 (96%)	231 (78%)	65 (22%)	1	3
2	B	49/56 (88%)	41 (84%)	8 (16%)	3	8
3	I	2/2 (100%)	2 (100%)	0	100	100
All	All	347/367 (95%)	274 (79%)	73 (21%)	1	4

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	13	ASP
1	A	14	SER
1	A	15	ILE
1	A	26	PHE
1	A	28	LEU
1	A	37	VAL
1	A	46	VAL
1	A	53	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	65	VAL
1	A	68	ASN
1	A	70	SER
1	A	75	VAL
1	A	77	GLU
1	A	78	THR
1	A	86	LYS
1	A	99	GLU
1	A	101	GLU
1	A	105	THR
1	A	112	LEU
1	A	113	LEU
1	A	114	ARG
1	A	118	GLN
1	A	124	CYS
1	A	130	ASN
1	A	134	GLN
1	A	136	THR
1	A	137	SER
1	A	139	ASN
1	A	159	THR
1	A	162	ILE
1	A	167	ARG
1	A	173	ARG
1	A	176	ARG
1	A	183	LEU
1	A	187	ARG
1	A	197	LEU
1	A	207	LEU
1	A	208	ASP
1	A	212	VAL
1	A	216	GLU
1	A	223	TYR
1	A	226	ASN
1	A	228	LEU
1	A	234	VAL
1	A	238	GLU
1	A	240	SER
1	A	243	GLN
1	A	249	ILE
1	A	252	ASN
1	A	254	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	258	CYS
1	A	259	ILE
1	A	275	LEU
1	A	281	ARG
1	A	286	GLU
1	A	292	LEU
1	A	299	ARG
1	A	300	LEU
1	A	311	GLN
1	A	315	ARG
1	A	320	GLN
1	A	321	ILE
1	A	324	ILE
1	A	327	LYS
2	B	260	GLU
2	B	279	LEU
2	B	280	LEU
2	B	281	GLU
2	B	282	ASN
2	B	283	ILE
2	B	289	GLN
2	B	307	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	60	GLN
1	A	61	HIS
1	A	68	ASN
1	A	72	HIS
1	A	131	HIS
1	A	134	GLN
1	A	178	ASN
1	A	250	ASN
1	A	252	ASN
1	A	277	ASN
1	A	318	GLN
1	A	320	GLN
2	B	267	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	SUC	A	1001	-	24,24,24	0.34	0	36,36,36	1.08	1 (2%)
4	SUC	A	1002	-	24,24,24	0.94	2 (8%)	36,36,36	1.16	4 (11%)

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	SUC	A	1001	-	-	0/12/51/51	0/2/2/2
4	SUC	A	1002	-	-	0/12/51/51	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	SUC	O5-C5	2.15	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	SUC	O5-C1	2.84	1.49	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	SUC	C6-C5-C4	-2.47	106.93	113.02
4	A	1002	SUC	O5-C1-C2	2.35	115.10	110.28
4	A	1002	SUC	O5-C5-C4	2.51	114.40	109.68
4	A	1002	SUC	O5-C5-C6	2.96	113.85	106.36
4	A	1001	SUC	C1-O5-C5	3.57	120.68	113.75

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	A	1002	SUC	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	A	320/335 (95%)	0.49	7 (2%) 65 54	30, 57, 93, 110	0
2	B	57/72 (79%)	0.63	3 (5%) 30 20	49, 70, 106, 109	0
3	I	3/5 (60%)	0.24	0 100 100	50, 50, 51, 54	0
All	All	380/412 (92%)	0.51	10 (2%) 59 47	30, 58, 102, 110	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	309	VAL	2.8
1	A	33	LYS	2.7
1	A	31	PHE	2.7
2	B	301	PHE	2.6
1	A	10	ILE	2.3
1	A	99	GLU	2.2
1	A	302	TYR	2.2
1	A	30	LYS	2.1
1	A	81	LEU	2.0
2	B	294	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
4	SUC	A	1002	23/23	0.68	0.58	8.94	107,110,110,110	23
4	SUC	A	1001	23/23	0.91	0.28	1.17	66,70,74,74	23
5	ZN	A	999	1/1	0.98	0.22	0.17	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.