



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:18 PM GMT

PDB ID : 1X3W
Title : Structure of a peptide:N-glycanase-Rad23 complex
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Deposited on : 2005-05-11
Resolution : 3.00 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

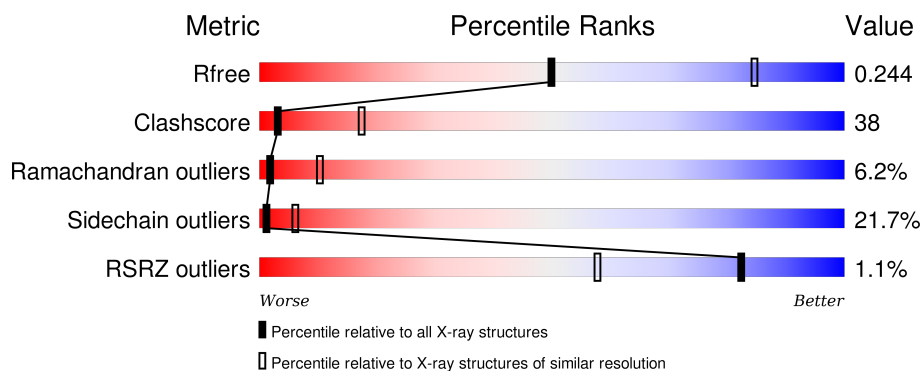
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SUC	A	1001	-	-	-	X
3	SUC	A	1002	-	-	-	X
3	SUC	A	1003	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3187 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	Se	0	0	0
			2665	1698	456	494	14	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MSE	MET	MODIFIED RESIDUE	UNP Q02890
A	140	MSE	MET	MODIFIED RESIDUE	UNP Q02890
A	255	MSE	MET	MODIFIED RESIDUE	UNP Q02890

- 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	Se	0	0	0
			435	276	73	84	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	295	MSE	MET	MODIFIED RESIDUE	UNP P32628
B	304	MSE	MET	MODIFIED RESIDUE	UNP P32628

- Molecule 3 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

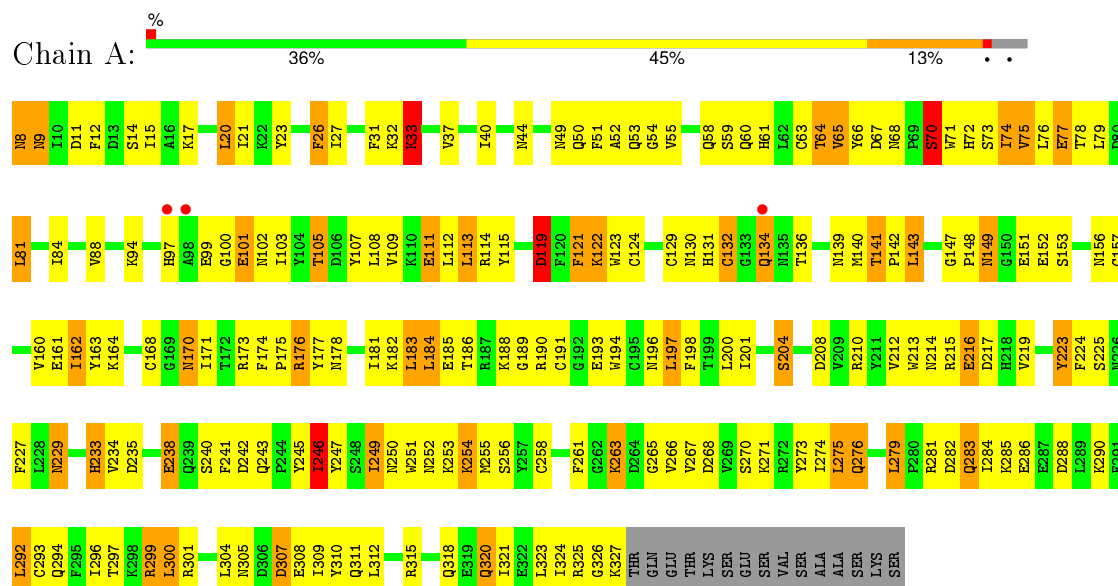
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		

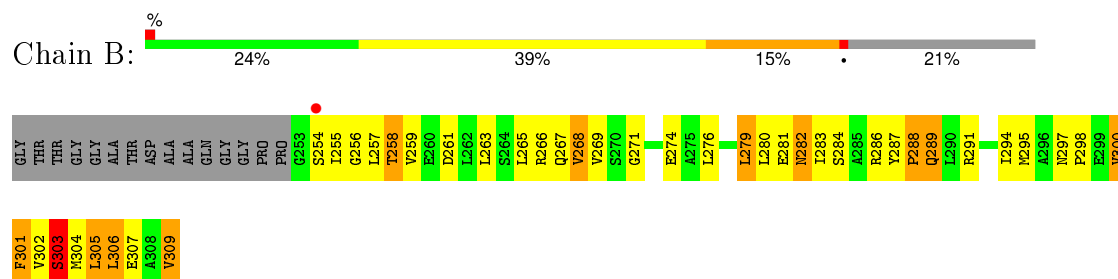
3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.24Å 129.24Å 128.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-3.00) 94.8 (19.86-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.244 , 0.274 0.251 , 0.244	Depositor DCC
R_{free} test set	1210 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.6	EDS
Estimated twinning fraction	0.087 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 25164 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3187	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.76	2/2726 (0.1%)	0.79	1/3674 (0.0%)
2	B	0.80	0/439	0.86	0/593
All	All	0.76	2/3165 (0.1%)	0.80	1/4267 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	GLU	CG-CD	7.10	1.62	1.51
1	A	77	GLU	CG-CD	6.01	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	GLU	N-CA-C	-5.11	97.21	111.00

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	2665	0	2576	188	0
2	B	435	0	446	59	0
3	A	69	0	66	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	17	0	0	2	0
All	All	3187	0	3088	239	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 38.

All (239) 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)
2:B:258:THR:HG22	2:B:287:TYR:OH	1.35	1.24
1:A:176:ARG:HH11	1:A:176:ARG:HG2	1.09	1.08
1:A:214:ASN:ND2	1:A:255:MSE:HG2	1.69	1.06
1:A:143:LEU:CD2	1:A:164:LYS:HB2	1.91	1.00
1:A:8:ASN:HD22	1:A:9:ASN:H	1.07	1.00
1:A:214:ASN:HD21	1:A:255:MSE:CG	1.74	0.99
1:A:214:ASN:HD21	1:A:255:MSE:HG2	0.84	0.97
2:B:258:THR:HG22	2:B:287:TYR:HH	1.30	0.96
1:A:299:ARG:HH11	1:A:299:ARG:HG3	1.28	0.94
1:A:198:PHE:HA	1:A:201:ILE:HD12	1.53	0.89
2:B:301:PHE:CE2	2:B:305:LEU:HD21	2.10	0.87
1:A:176:ARG:HG2	1:A:176:ARG:NH1	1.90	0.86
1:A:225:SER:O	1:A:229:ASN:HA	1.77	0.83
1:A:265:GLY:HA2	1:A:297:THR:HG22	1.61	0.83
1:A:190:ARG:O	1:A:194:TRP:HB2	1.78	0.82
1:A:143:LEU:HD21	1:A:164:LYS:HB2	1.60	0.82
1:A:64:THR:O	1:A:66:TYR:N	2.13	0.81
1:A:246:ILE:HG22	1:A:247:TYR:N	1.95	0.81
1:A:12:PHE:HA	1:A:15:ILE:HG22	1.63	0.80
1:A:168:CYS:SG	1:A:170:ASN:HB2	2.23	0.78
1:A:325:ARG:HH11	2:B:263:LEU:HD23	1.48	0.78
2:B:302:VAL:HA	2:B:305:LEU:HD22	1.64	0.77
1:A:181:ILE:O	1:A:184:LEU:HB2	1.87	0.75
1:A:59:SER:O	1:A:63:CYS:HB2	1.88	0.74
1:A:176:ARG:HH11	1:A:176:ARG:CG	1.94	0.74
1:A:233:HIS:O	1:A:241:PHE:O	2.05	0.73
1:A:8:ASN:HB3	2:B:295:MSE:HE2	1.71	0.73
1:A:55:VAL:HG21	1:A:292:LEU:HD13	1.69	0.73
2:B:297:ASN:HB3	2:B:300:VAL:HG12	1.72	0.71
1:A:74:ILE:O	1:A:78:THR:HG23	1.90	0.71
1:A:183:LEU:HD21	1:A:193:GLU:HB2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASP:O	1:A:238:GLU:O	2.10	0.70
2:B:301:PHE:O	2:B:305:LEU:HD13	1.92	0.69
2:B:258:THR:HG23	2:B:261:ASP:HB2	1.75	0.69
1:A:143:LEU:HD23	1:A:164:LYS:HB2	1.75	0.68
1:A:197:LEU:HD22	1:A:201:ILE:HD11	1.75	0.68
1:A:54:GLY:O	1:A:58:GLN:HG3	1.93	0.68
1:A:320:GLN:HE21	1:A:320:GLN:CA	2.06	0.68
1:A:129:CYS:H	1:A:136:THR:HG23	1.59	0.67
1:A:149:ASN:HB3	1:A:173:ARG:HH12	1.58	0.67
1:A:299:ARG:NH1	1:A:299:ARG:HG3	2.04	0.67
1:A:214:ASN:OD1	1:A:216:GLU:HG2	1.95	0.67
1:A:320:GLN:NE2	1:A:320:GLN:HA	2.08	0.67
1:A:61:HIS:CD2	1:A:65:VAL:HG21	2.30	0.67
1:A:197:LEU:HD22	1:A:201:ILE:CD1	2.26	0.65
1:A:213:TRP:HA	1:A:219:VAL:HG12	1.79	0.65
2:B:301:PHE:CD2	2:B:305:LEU:HD21	2.32	0.65
2:B:294:ILE:HG12	2:B:301:PHE:HD1	1.62	0.64
2:B:258:THR:CG2	2:B:287:TYR:HH	2.09	0.63
1:A:8:ASN:ND2	1:A:9:ASN:H	1.89	0.63
2:B:276:LEU:HD23	2:B:276:LEU:O	1.99	0.63
1:A:66:TYR:HD2	1:A:200:LEU:HB2	1.63	0.63
2:B:301:PHE:HE2	2:B:305:LEU:HD21	1.60	0.63
1:A:67:ASP:HA	1:A:72:HIS:HE2	1.64	0.63
1:A:245:TYR:CD1	1:A:246:ILE:N	2.66	0.63
1:A:268:ASP:OD1	1:A:281:ARG:NH2	2.32	0.62
2:B:281:GLU:O	2:B:284:SER:N	2.27	0.62
1:A:12:PHE:HA	1:A:15:ILE:CG2	2.28	0.61
1:A:156:ASN:O	1:A:178:ASN:N	2.32	0.61
1:A:8:ASN:CB	2:B:295:MSE:HE2	2.29	0.61
1:A:76:LEU:O	1:A:81:LEU:HD11	2.01	0.61
1:A:247:TYR:CB	1:A:255:MSE:HE1	2.30	0.60
1:A:320:GLN:HE21	1:A:320:GLN:HA	1.65	0.60
1:A:99:GLU:O	1:A:101:GLU:HB2	2.02	0.59
1:A:37:VAL:O	1:A:40:ILE:HG13	2.01	0.59
1:A:105:THR:O	1:A:108:LEU:HB3	2.03	0.59
1:A:129:CYS:HB2	1:A:140:MSE:SE	2.53	0.58
1:A:301:ARG:NH2	1:A:312:LEU:HB3	2.18	0.58
1:A:152:GLU:OE1	1:A:160:VAL:HG21	2.04	0.58
1:A:225:SER:O	1:A:229:ASN:CA	2.51	0.58
1:A:266:VAL:H	1:A:297:THR:HG22	1.69	0.58
1:A:307:ASP:O	1:A:308:GLU:C	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:CD2	1:A:164:LYS:CB	2.77	0.57
1:A:103:ILE:HG13	1:A:107:TYR:HE2	1.69	0.57
2:B:298:PRO:O	2:B:301:PHE:HB3	2.04	0.56
2:B:276:LEU:O	2:B:280:LEU:HB2	2.04	0.56
1:A:320:GLN:NE2	1:A:320:GLN:CA	2.67	0.56
1:A:72:HIS:ND1	1:A:204:SER:HA	2.20	0.56
1:A:31:PHE:HB3	1:A:309:ILE:HD11	1.88	0.56
2:B:303:SER:O	2:B:306:LEU:HD12	2.06	0.55
1:A:216:GLU:OE1	1:A:256:SER:N	2.40	0.55
1:A:23:TYR:HA	2:B:306:LEU:HD23	1.87	0.55
1:A:114:ARG:NH2	1:A:119:ASP:OD2	2.39	0.55
1:A:254:LYS:HD3	5:A:1011:HOH:O	2.05	0.55
2:B:301:PHE:C	2:B:301:PHE:HD2	2.10	0.55
2:B:303:SER:O	2:B:305:LEU:N	2.39	0.55
1:A:296:ILE:O	1:A:300:LEU:HB2	2.05	0.55
1:A:224:PHE:CD2	1:A:224:PHE:C	2.80	0.54
2:B:255:ILE:HG23	2:B:256:GLY:N	2.22	0.54
1:A:325:ARG:NH1	2:B:263:LEU:HD23	2.19	0.54
1:A:51:PHE:CB	1:A:283:GLN:HB2	2.38	0.54
1:A:266:VAL:H	1:A:297:THR:CG2	2.21	0.54
1:A:258:CYS:HB2	1:A:270:SER:HA	1.90	0.54
2:B:301:PHE:C	2:B:301:PHE:CD2	2.82	0.53
1:A:265:GLY:CA	1:A:297:THR:HG22	2.35	0.53
1:A:254:LYS:HB3	1:A:279:LEU:HD21	1.91	0.53
1:A:101:GLU:OE1	1:A:102:ASN:N	2.35	0.53
1:A:256:SER:O	1:A:281:ARG:HD2	2.09	0.53
1:A:66:TYR:CD2	1:A:200:LEU:HB2	2.44	0.52
1:A:123:TRP:HA	1:A:194:TRP:CZ3	2.44	0.52
1:A:214:ASN:ND2	1:A:255:MSE:HE2	2.24	0.52
2:B:265:LEU:HA	2:B:279:LEU:HD11	1.92	0.52
1:A:225:SER:HA	5:A:1006:HOH:O	2.09	0.52
2:B:255:ILE:HG23	2:B:256:GLY:H	1.73	0.52
1:A:245:TYR:O	1:A:246:ILE:C	2.46	0.52
1:A:124:CYS:HB2	1:A:188:LYS:HB2	1.91	0.52
2:B:258:THR:HG23	2:B:261:ASP:CB	2.39	0.51
1:A:216:GLU:HG3	1:A:254:LYS:O	2.11	0.51
1:A:122:LYS:O	1:A:188:LYS:HA	2.10	0.51
1:A:103:ILE:HG13	1:A:107:TYR:CE2	2.45	0.51
1:A:246:ILE:CG2	1:A:247:TYR:N	2.66	0.51
1:A:111:GLU:O	1:A:112:LEU:C	2.48	0.50
1:A:250:ASN:HD22	1:A:250:ASN:N	2.07	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:SER:C	2:B:305:LEU:H	2.15	0.50
2:B:281:GLU:HG2	2:B:282:ASN:N	2.27	0.50
2:B:282:ASN:HD21	2:B:286:ARG:HH21	1.58	0.50
1:A:68:ASN:C	1:A:72:HIS:HD2	2.14	0.50
1:A:214:ASN:HD22	1:A:255:MSE:HE2	1.77	0.50
1:A:275:LEU:O	1:A:276:GLN:CB	2.59	0.50
1:A:214:ASN:ND2	1:A:255:MSE:SE	2.95	0.50
1:A:130:ASN:O	1:A:131:HIS:C	2.50	0.50
1:A:160:VAL:HA	1:A:175:PRO:HA	1.93	0.49
1:A:323:LEU:O	1:A:326:GLY:N	2.45	0.49
1:A:32:LYS:HG3	1:A:33:LYS:N	2.27	0.49
1:A:84:ILE:O	1:A:88:VAL:HG23	2.12	0.49
2:B:294:ILE:HG12	2:B:301:PHE:CD1	2.44	0.49
2:B:306:LEU:O	2:B:309:VAL:HB	2.13	0.49
1:A:149:ASN:HB3	1:A:173:ARG:NH1	2.26	0.49
1:A:273:TYR:O	1:A:275:LEU:N	2.45	0.49
2:B:280:LEU:C	2:B:283:ILE:HG22	2.33	0.49
1:A:26:PHE:C	1:A:26:PHE:CD2	2.82	0.48
2:B:287:TYR:HB3	2:B:289:GLN:HE22	1.79	0.48
1:A:8:ASN:HD22	1:A:9:ASN:N	1.92	0.48
1:A:263:LYS:O	1:A:300:LEU:HD22	2.13	0.48
1:A:79:LEU:HD11	1:A:201:ILE:HG23	1.95	0.48
1:A:247:TYR:HB3	1:A:255:MSE:CE	2.43	0.48
1:A:121:PHE:HD1	1:A:194:TRP:CE3	2.32	0.48
1:A:12:PHE:CA	1:A:15:ILE:HG22	2.39	0.48
2:B:279:LEU:O	2:B:283:ILE:HG22	2.14	0.48
1:A:108:LEU:HG	1:A:112:LEU:HD23	1.96	0.48
1:A:109:VAL:HG21	1:A:223:TYR:CE1	2.49	0.48
2:B:284:SER:C	2:B:286:ARG:N	2.67	0.48
1:A:162:ILE:HD12	1:A:163:TYR:N	2.28	0.48
2:B:269:VAL:HG22	2:B:276:LEU:HD12	1.96	0.47
1:A:210:ARG:NH2	1:A:267:VAL:HG11	2.28	0.47
1:A:52:ALA:O	1:A:55:VAL:HG22	2.14	0.47
1:A:225:SER:O	1:A:229:ASN:N	2.47	0.47
1:A:72:HIS:O	1:A:75:VAL:HG13	2.14	0.47
1:A:245:TYR:O	1:A:247:TYR:N	2.47	0.47
1:A:315:ARG:HG2	1:A:315:ARG:O	2.11	0.47
2:B:268:VAL:HG11	2:B:279:LEU:HD12	1.97	0.47
1:A:157:CYS:HB2	1:A:177:TYR:HD1	1.79	0.47
1:A:301:ARG:HG2	1:A:304:LEU:HD12	1.96	0.47
1:A:61:HIS:O	1:A:65:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ILE:HD13	2:B:267:GLN:HB2	1.97	0.46
2:B:297:ASN:OD1	2:B:300:VAL:HB	2.16	0.46
1:A:183:LEU:HD21	1:A:193:GLU:CB	2.42	0.46
1:A:183:LEU:CD2	1:A:193:GLU:HB2	2.42	0.46
2:B:302:VAL:O	2:B:305:LEU:HB2	2.16	0.46
1:A:33:LYS:NZ	1:A:33:LYS:HB2	2.31	0.46
1:A:271:LYS:HE2	1:A:271:LYS:HB3	1.50	0.46
1:A:189:GLY:HA3	1:A:193:GLU:CG	2.46	0.46
1:A:301:ARG:HG2	1:A:304:LEU:CD1	2.45	0.46
2:B:284:SER:C	2:B:286:ARG:H	2.18	0.46
1:A:140:MSE:HE3	1:A:163:TYR:HB3	1.97	0.46
1:A:149:ASN:H	1:A:152:GLU:CG	2.29	0.46
1:A:247:TYR:O	1:A:251:TRP:HB2	2.16	0.46
2:B:276:LEU:HD23	2:B:280:LEU:HB2	1.98	0.46
1:A:59:SER:OG	1:A:60:GLN:N	2.49	0.46
1:A:114:ARG:HG3	1:A:115:TYR:N	2.30	0.46
1:A:250:ASN:ND2	1:A:250:ASN:N	2.64	0.45
1:A:131:HIS:ND1	1:A:131:HIS:C	2.69	0.45
1:A:261:PHE:CD1	1:A:261:PHE:N	2.84	0.45
1:A:249:ILE:CD1	1:A:250:ASN:ND2	2.80	0.45
1:A:68:ASN:HB3	1:A:70:SER:OG	2.16	0.45
1:A:156:ASN:HB3	1:A:178:ASN:HB2	1.98	0.45
2:B:280:LEU:HD11	2:B:301:PHE:CZ	2.51	0.45
1:A:162:ILE:HD13	1:A:171:ILE:HG23	1.98	0.45
1:A:214:ASN:ND2	1:A:255:MSE:CG	2.52	0.45
1:A:72:HIS:O	1:A:76:LEU:HD23	2.16	0.45
1:A:141:THR:HA	1:A:142:PRO:HD2	1.72	0.45
1:A:11:ASP:OD2	1:A:14:SER:HB3	2.15	0.45
2:B:265:LEU:HA	2:B:279:LEU:CD1	2.46	0.45
1:A:266:VAL:O	1:A:293:CYS:HB3	2.18	0.44
1:A:268:ASP:C	1:A:268:ASP:OD2	2.56	0.44
2:B:276:LEU:HD23	2:B:276:LEU:C	2.38	0.44
1:A:162:ILE:CD1	1:A:171:ILE:HG23	2.47	0.44
1:A:198:PHE:CA	1:A:201:ILE:HD12	2.36	0.44
1:A:307:ASP:O	1:A:310:TYR:N	2.50	0.44
1:A:318:GLN:NE2	2:B:271:GLY:HA3	2.32	0.44
2:B:258:THR:CG2	2:B:261:ASP:OD2	2.65	0.44
1:A:143:LEU:HD13	1:A:143:LEU:HA	1.72	0.44
1:A:33:LYS:HB2	1:A:33:LYS:HZ2	1.82	0.44
1:A:123:TRP:HA	1:A:194:TRP:HZ3	1.83	0.43
1:A:71:TRP:CG	1:A:181:ILE:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:C	1:A:33:LYS:HG3	2.38	0.43
2:B:274:GLU:CD	2:B:274:GLU:H	2.21	0.43
2:B:280:LEU:HA	2:B:283:ILE:CG2	2.49	0.43
1:A:247:TYR:HB3	1:A:255:MSE:HE1	2.00	0.43
1:A:321:ILE:HA	1:A:324:ILE:HG22	2.01	0.43
2:B:289:GLN:CD	2:B:289:GLN:H	2.21	0.43
1:A:76:LEU:CD1	1:A:81:LEU:HD21	2.49	0.43
2:B:269:VAL:HG22	2:B:276:LEU:CD1	2.49	0.43
1:A:176:ARG:NH1	1:A:176:ARG:CG	2.61	0.43
1:A:251:TRP:O	1:A:252:ASN:HB2	2.18	0.43
1:A:301:ARG:NH2	1:A:312:LEU:CB	2.82	0.43
1:A:32:LYS:HG3	1:A:33:LYS:H	1.84	0.43
1:A:49:ASN:OD1	1:A:51:PHE:N	2.51	0.43
1:A:143:LEU:HD21	1:A:164:LYS:CB	2.41	0.42
1:A:281:ARG:HG2	1:A:286:GLU:OE2	2.19	0.42
1:A:305:ASN:OD1	1:A:305:ASN:C	2.58	0.42
1:A:134:GLN:O	1:A:136:THR:HG22	2.19	0.42
2:B:301:PHE:O	2:B:305:LEU:CD1	2.66	0.42
1:A:71:TRP:CD1	1:A:181:ILE:HD11	2.54	0.42
1:A:241:PHE:CD2	1:A:242:ASP:HB2	2.54	0.42
1:A:216:GLU:HB2	1:A:253:LYS:HE2	2.02	0.42
1:A:49:ASN:OD1	1:A:50:GLN:N	2.53	0.41
1:A:161:GLU:OE2	1:A:190:ARG:NH2	2.40	0.41
1:A:182:LYS:C	1:A:184:LEU:H	2.24	0.41
2:B:255:ILE:CG2	2:B:256:GLY:H	2.34	0.41
1:A:249:ILE:HD11	1:A:250:ASN:ND2	2.36	0.41
1:A:113:LEU:HD13	1:A:113:LEU:HA	1.62	0.41
2:B:297:ASN:HA	2:B:298:PRO:HD2	1.83	0.41
1:A:174:PHE:CZ	1:A:176:ARG:NH1	2.88	0.41
1:A:12:PHE:CZ	2:B:281:GLU:HA	2.56	0.41
1:A:147:GLY:HA2	1:A:148:PRO:HD3	1.85	0.41
1:A:215:ARG:HB3	1:A:216:GLU:OE2	2.20	0.41
1:A:178:ASN:ND2	3:A:1003:SUC:H5	2.35	0.41
1:A:285:LYS:HB2	1:A:288:ASP:OD2	2.21	0.41
2:B:306:LEU:HD12	2:B:306:LEU:H	1.85	0.40
1:A:50:GLN:O	1:A:53:GLN:HB2	2.20	0.40
1:A:77:GLU:OE1	1:A:77:GLU:HA	2.21	0.40
1:A:189:GLY:O	1:A:194:TRP:CE3	2.74	0.40
1:A:309:ILE:HG23	1:A:310:TYR:N	2.35	0.40
1:A:17:LYS:O	1:A:21:ILE:HD12	2.21	0.40
1:A:216:GLU:OE2	1:A:216:GLU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:HB	1:A:227:PHE:CD1	2.57	0.40
2:B:287:TYR:O	2:B:288:PRO:C	2.58	0.40
1:A:266:VAL:N	1:A:297:THR:HG22	2.36	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%)	241 (76%)	60 (19%)	17 (5%)	2	14
2	B	55/72 (76%)	27 (49%)	22 (40%)	6 (11%)	0	2
All	All	373/407 (92%)	268 (72%)	82 (22%)	23 (6%)	2	10

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	65	VAL
1	A	97	HIS
1	A	246	ILE
1	A	276	GLN
2	B	254	SER
1	A	132	CYS
2	B	259	VAL
2	B	303	SER
2	B	304	MSE
1	A	9	ASN
1	A	119	ASP
1	A	274	ILE
1	A	282	ASP
2	B	307	GLU

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Mol	Chain	Res	Type
1	A	94	LYS
1	A	196	ASN
1	A	229	ASN
1	A	20	LEU
1	A	70	SER
2	B	288	PRO
1	A	100	GLY
1	A	284	ILE

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	296/306 (97%)	235 (79%)	61 (21%)	1	7
2	B	49/54 (91%)	35 (71%)	14 (29%)	0	2
All	All	345/360 (96%)	270 (78%)	75 (22%)	1	6

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	20	LEU
1	A	26	PHE
1	A	27	ILE
1	A	33	LYS
1	A	44	ASN
1	A	64	THR
1	A	70	SER
1	A	73	SER
1	A	74	ILE
1	A	75	VAL
1	A	81	LEU
1	A	101	GLU
1	A	105	THR
1	A	111	GLU

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Mol	Chain	Res	Type
1	A	113	LEU
1	A	119	ASP
1	A	121	PHE
1	A	122	LYS
1	A	132	CYS
1	A	134	GLN
1	A	139	ASN
1	A	141	THR
1	A	143	LEU
1	A	149	ASN
1	A	151	GLU
1	A	153	SER
1	A	162	ILE
1	A	170	ASN
1	A	176	ARG
1	A	183	LEU
1	A	184	LEU
1	A	186	THR
1	A	191	CYS
1	A	197	LEU
1	A	204	SER
1	A	208	ASP
1	A	212	VAL
1	A	216	GLU
1	A	217	ASP
1	A	223	TYR
1	A	233	HIS
1	A	234	VAL
1	A	240	SER
1	A	243	GLN
1	A	246	ILE
1	A	249	ILE
1	A	254	LYS
1	A	263	LYS
1	A	275	LEU
1	A	279	LEU
1	A	283	GLN
1	A	290	LYS
1	A	292	LEU
1	A	294	GLN
1	A	299	ARG
1	A	300	LEU

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Mol	Chain	Res	Type
1	A	307	ASP
1	A	311	GLN
1	A	320	GLN
1	A	327	LYS
2	B	257	LEU
2	B	258	THR
2	B	266	ARG
2	B	268	VAL
2	B	279	LEU
2	B	282	ASN
2	B	289	GLN
2	B	291	ARG
2	B	300	VAL
2	B	301	PHE
2	B	303	SER
2	B	305	LEU
2	B	306	LEU
2	B	309	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	61	HIS
1	A	87	ASN
1	A	97	HIS
1	A	102	ASN
1	A	134	GLN
1	A	146	GLN
1	A	178	ASN
1	A	218	HIS
1	A	250	ASN
1	A	318	GLN
1	A	320	GLN

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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$
3	SUC	A	1001	-	24,24,24	0.69	0	36,36,36	0.95	1 (2%)
3	SUC	A	1002	-	24,24,24	0.56	0	36,36,36	0.83	1 (2%)
3	SUC	A	1003	-	24,24,24	0.46	0	36,36,36	1.01	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SUC	A	1001	-	-	0/12/51/51	0/2/2/2
3	SUC	A	1002	-	-	0/12/51/51	0/2/2/2
3	SUC	A	1003	-	-	0/12/51/51	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	SUC	C2'-O1-C1	-2.07	112.08	117.53
3	A	1003	SUC	C3-C4-C5	-2.07	106.60	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	SUC	O3-C3-C4	2.37	115.67	110.34
3	A	1002	SUC	C1-O5-C5	2.74	119.07	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
3	A	1003	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	317/335 (94%)	-0.48	3 (0%) 85 64	41, 69, 110, 116	0
2	B	55/72 (76%)	-0.45	1 (1%) 71 43	56, 79, 115, 116	0
All	All	372/407 (91%)	-0.48	4 (1%) 82 58	41, 71, 113, 116	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	GLN	2.7
2	B	254	SER	2.2
1	A	97	HIS	2.1
1	A	98	ALA	2.1

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(\AA^2)	Q<0.9
3	SUC	A	1002	23/23	0.82	0.48	9.44	113,115,115,116	23
3	SUC	A	1003	23/23	0.84	0.32	6.03	104,111,113,117	23
3	SUC	A	1001	23/23	0.79	0.26	2.14	81,88,90,93	23
4	ZN	A	999	1/1	0.72	0.11	-1.08	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.