



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:50 PM UTC

PDB ID : 4Y3O / pdb_00004y3o
Title : Crystal structure of Ribosomal oxygenase NO66 in complex with substrate Rpl8 peptide and Ni(II) and cofactor N-oxalyglycine
Authors : Wang, C.; Zhang, Q.; Zang, J.
Deposited on : 2015-02-10
Resolution : 2.20 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

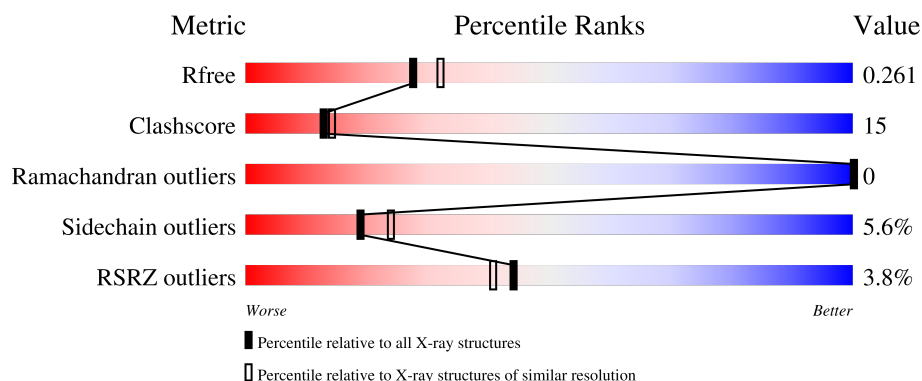
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	466	3% 76% 20% ..
1	B	466	3% 75% 21% ..
2	C	11	45% 82% 18%
2	D	11	36% 45% 55%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8118 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 Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	3	0
			3687	2343	655	674	15			
1	B	461	Total	C	N	O	S	0	0	0
			3670	2334	644	677	15			

- Molecule 2 is a protein called Rpl8 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	0	0
			77	46	18	13			
2	D	11	Total	C	N	O	0	0	0
			77	46	18	13			

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	B	1	Total	Ni	0	0
			1	1		

- Molecule 4 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	4	1	5		
4	B	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		

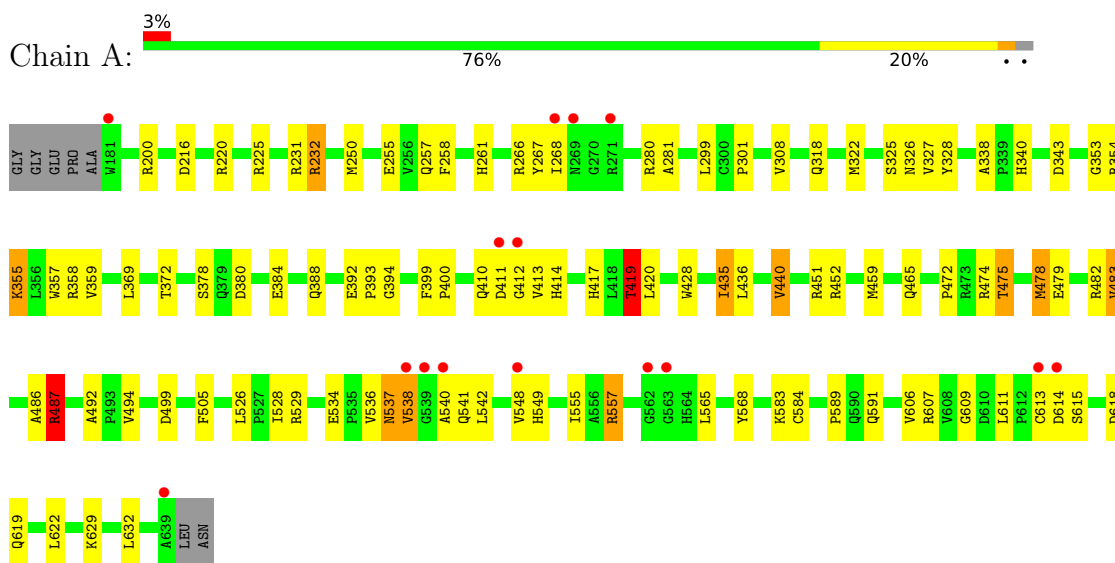
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	264	Total	O	0	0
			264	264		
7	B	289	Total	O	0	0
			289	289		
7	C	4	Total	O	0	0
			4	4		
7	D	6	Total	O	0	0
			6	6		

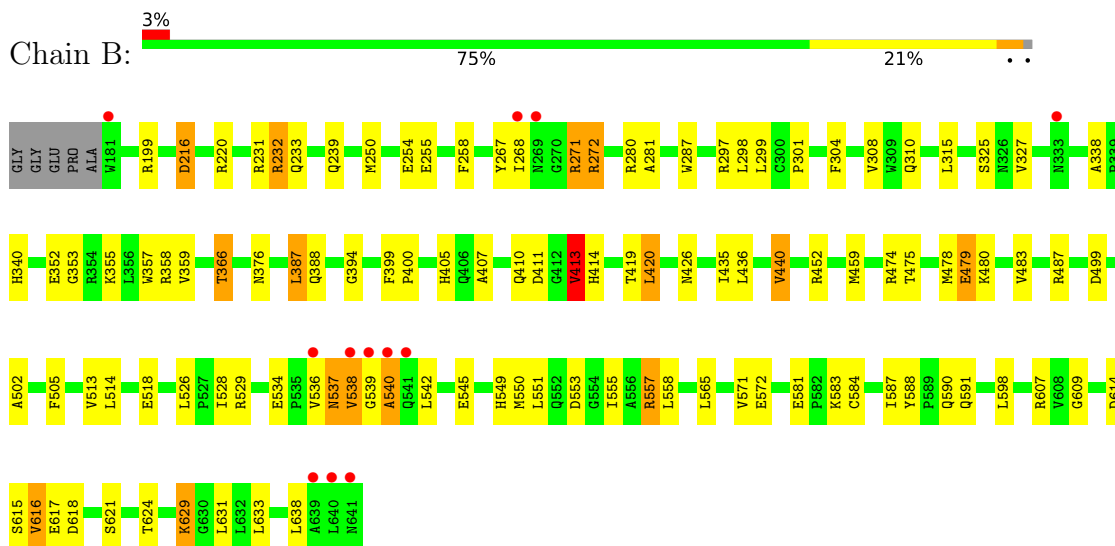
3 Residue-property plots

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.

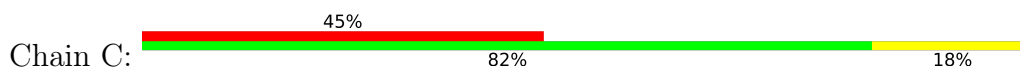
- Molecule 1: Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66

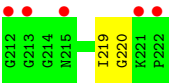


- Molecule 1: Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66



- Molecule 2: Rpl8 peptide





● Molecule 2: Rpl8 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.50Å 202.93Å 85.68Å 90.00° 118.94° 90.00°	Depositor
Resolution (Å)	40.57 – 2.20 40.57 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.9 (40.57-2.20) 97.9 (40.57-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.203 , 0.262 (Not available) , 0.261	Depositor DCC
R_{free} test set	3314 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8118	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0760e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, NI, OGA, ACT

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	1.18	4/3782 (0.1%)	1.19	13/5147 (0.3%)
1	B	1.21	6/3765 (0.2%)	1.22	14/5127 (0.3%)
2	C	0.94	0/79	1.19	0/104
2	D	0.97	0/79	1.24	0/104
All	All	1.19	10/7705 (0.1%)	1.20	27/10482 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	PRO	C-O	6.14	1.30	1.23
1	B	534	GLU	C-N	6.08	1.40	1.33
1	B	359	VAL	N-CA	-6.07	1.39	1.46
1	A	479	GLU	C-O	-5.90	1.17	1.24
1	A	359	VAL	N-CA	-5.64	1.39	1.46
1	A	591	GLN	C-O	-5.57	1.16	1.24
1	B	405	HIS	N-CA	-5.43	1.39	1.45
1	B	591	GLN	C-O	-5.27	1.16	1.24
1	B	479	GLU	C-O	-5.12	1.18	1.24
1	B	609	GLY	C-O	-5.12	1.18	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	539	GLY	N-CA-C	17.44	145.15	113.76
1	B	534	GLU	N-CA-C	8.59	115.95	108.22
1	B	540	ALA	N-CA-C	-8.36	95.11	108.73
1	A	534	GLU	N-CA-C	8.04	115.46	108.22
1	A	483	VAL	N-CA-CB	7.36	121.61	110.58
1	B	537	ASN	N-CA-C	7.09	121.24	112.58
1	A	451	ARG	NE-CZ-NH2	-6.98	112.92	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	537	ASN	CB-CA-C	-6.73	102.85	111.86
1	B	413	VAL	CB-CA-C	-5.96	102.66	111.19
1	B	315	LEU	N-CA-C	5.85	117.66	111.28
1	A	538	VAL	N-CA-CB	5.84	117.96	110.13
1	B	534	GLU	CA-C-N	-5.80	113.58	120.13
1	B	534	GLU	C-N-CA	-5.80	113.58	120.13
1	B	272	ARG	NE-CZ-NH1	-5.73	115.77	121.50
1	A	622	LEU	N-CA-C	-5.61	105.08	111.14
1	A	555	ILE	CB-CA-C	-5.57	104.61	110.62
1	B	555	ILE	CB-CA-C	-5.55	104.82	110.93
1	B	440	VAL	CB-CA-C	-5.44	105.01	111.97
1	B	538	VAL	CB-CA-C	-5.38	102.47	111.29
1	A	541	GLN	N-CA-C	-5.30	102.62	110.46
1	B	536	VAL	CB-CA-C	5.30	118.80	111.38
1	A	487	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	B	614	ASP	N-CA-C	-5.19	105.06	111.40
1	A	399	PHE	CA-C-N	5.18	125.09	119.85
1	A	399	PHE	C-N-CA	5.18	125.09	119.85
1	A	419	THR	CB-CA-C	5.11	118.47	110.19
1	A	440	VAL	CB-CA-C	-5.04	105.27	112.22

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	3687	0	3588	104	0
1	B	3670	0	3557	121	0
2	C	77	0	70	1	0
2	D	77	0	70	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	3	1	0
4	B	10	0	3	0	0
5	B	18	0	24	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	0	3	0	0
7	A	264	0	0	37	1
7	B	289	0	0	73	1
7	C	4	0	0	0	0
7	D	6	0	0	1	0
All	All	8118	0	7318	224	2

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 15.

All (224) 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:268:ILE:HB	7:A:965:HOH:O	1.58	1.03
1:B:615:SER:C	7:B:987:HOH:O	2.04	0.99
1:B:483:VAL:HB	7:B:1059:HOH:O	1.65	0.97
1:B:271:ARG:HD3	7:B:1067:HOH:O	1.66	0.96
1:B:584:CYS:SG	7:B:1071:HOH:O	1.95	0.95
1:B:514:LEU:HD22	7:B:1075:HOH:O	1.67	0.94
1:B:231:ARG:HG3	7:B:970:HOH:O	1.68	0.93
1:A:384:GLU:OE1	7:A:801:HOH:O	1.87	0.92
1:A:465:GLN:NE2	7:A:997:HOH:O	2.04	0.90
1:B:255:GLU:HG3	7:B:1065:HOH:O	1.75	0.86
1:A:614:ASP:HA	7:A:1059:HOH:O	1.74	0.86
1:B:452:ARG:HG2	7:B:1083:HOH:O	1.77	0.85
1:A:343:ASP:CA	7:A:1037:HOH:O	2.25	0.83
1:B:487:ARG:O	1:B:487:ARG:HD2	1.79	0.81
1:B:358:ARG:NH1	7:B:984:HOH:O	2.12	0.81
1:A:419:THR:HG21	4:A:702:OGA:O1	1.80	0.81
1:B:426:ASN:OD1	5:B:705:GOL:H32	1.80	0.81
1:B:624:THR:CG2	7:B:994:HOH:O	2.28	0.81
1:A:499:ASP:OD1	1:A:557:ARG:NH1	2.12	0.81
1:B:499:ASP:OD1	1:B:557:ARG:NH1	2.14	0.81
1:B:518:GLU:HB3	7:B:1075:HOH:O	1.79	0.81
1:A:343:ASP:CB	7:A:1037:HOH:O	2.30	0.80
1:B:452:ARG:CG	7:B:1083:HOH:O	2.30	0.79
1:B:631:LEU:HG	7:B:973:HOH:O	1.82	0.79
1:A:548:VAL:HG23	1:A:632:LEU:HG	1.67	0.77
1:B:366:THR:HB	7:B:1066:HOH:O	1.86	0.76
1:B:407:ALA:HB1	7:B:1085:HOH:O	1.84	0.76
1:B:571:VAL:HG21	7:B:973:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASP:HA	7:A:1037:HOH:O	1.82	0.76
1:A:343:ASP:HB3	7:A:1037:HOH:O	1.83	0.76
1:B:410:GLN:HG2	7:B:1079:HOH:O	1.85	0.76
1:A:529:ARG:HH12	1:A:537:ASN:HD21	1.30	0.75
1:B:483:VAL:CG2	7:B:1059:HOH:O	2.35	0.75
1:B:407:ALA:CB	7:B:1085:HOH:O	2.34	0.74
1:A:327:VAL:C	7:A:1030:HOH:O	2.31	0.73
1:A:358:ARG:CZ	7:A:971:HOH:O	2.37	0.73
1:A:257:GLN:H	1:A:261:HIS:HD2	1.37	0.71
1:A:487:ARG:HD3	7:A:984:HOH:O	1.91	0.71
1:A:565:LEU:HD23	7:A:1028:HOH:O	1.89	0.71
1:A:231:ARG:HG3	7:A:983:HOH:O	1.90	0.71
1:A:328:TYR:CD2	7:A:1030:HOH:O	2.44	0.70
1:B:475:THR:HG22	7:B:1070:HOH:O	1.91	0.69
1:A:378:SER:HB2	7:A:964:HOH:O	1.92	0.69
1:B:550:MET:O	7:B:1000:HOH:O	2.11	0.69
1:B:616:VAL:HG23	7:B:926:HOH:O	1.91	0.69
1:B:483:VAL:CB	7:B:1059:HOH:O	2.30	0.68
1:A:548:VAL:HG21	1:A:632:LEU:HD21	1.76	0.68
1:B:410:GLN:HB3	7:B:847:HOH:O	1.92	0.68
1:B:618:ASP:N	7:B:987:HOH:O	2.25	0.68
1:B:239:GLN:HG3	7:B:888:HOH:O	1.93	0.68
1:A:482:ARG:NH2	7:A:994:HOH:O	2.28	0.67
1:B:357:TRP:CD1	7:B:1085:HOH:O	2.47	0.66
1:A:487:ARG:O	1:A:487:ARG:HD2	1.96	0.66
1:B:413:VAL:HG23	7:B:993:HOH:O	1.95	0.66
1:A:328:TYR:HE2	1:A:419:THR:HG23	1.60	0.66
1:A:369:LEU:HD12	7:B:1083:HOH:O	1.95	0.66
2:D:222:PRO:C	7:D:306:HOH:O	2.38	0.65
1:B:267:TYR:CD2	7:B:1060:HOH:O	2.50	0.64
1:A:565:LEU:CD2	7:A:1028:HOH:O	2.45	0.64
1:B:358:ARG:CZ	7:B:984:HOH:O	2.43	0.63
1:B:255:GLU:CG	7:B:1065:HOH:O	2.41	0.63
1:B:633:LEU:HG	7:B:1000:HOH:O	1.98	0.63
1:A:412:GLY:C	7:A:807:HOH:O	2.41	0.63
1:B:538:VAL:HA	7:B:803:HOH:O	1.98	0.63
1:A:410:GLN:HB3	7:A:845:HOH:O	1.99	0.62
1:A:440:VAL:HG21	1:B:436:LEU:HD12	1.81	0.62
1:B:572:GLU:OE2	1:B:629:LYS:HE2	2.00	0.62
1:A:529:ARG:NH1	1:A:537:ASN:HD21	1.98	0.60
1:A:328:TYR:CE2	1:A:419:THR:HG23	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:ASN:O	2:D:217:GLN:NE2	2.35	0.59
1:A:440:VAL:CG2	1:B:436:LEU:CD1	2.80	0.59
1:B:338:ALA:O	1:B:340:HIS:HD2	1.86	0.59
1:B:621:SER:HB3	7:B:964:HOH:O	2.04	0.58
1:A:557:ARG:CG	1:A:557:ARG:HH11	2.16	0.58
1:B:538:VAL:CA	7:B:803:HOH:O	2.51	0.58
1:B:480:LYS:HA	1:B:483:VAL:HG22	1.85	0.58
1:B:452:ARG:HA	7:B:1083:HOH:O	2.04	0.57
1:B:483:VAL:HG23	7:B:1059:HOH:O	2.03	0.57
1:A:372:THR:C	7:A:1037:HOH:O	2.46	0.57
1:A:436:LEU:CD1	1:B:440:VAL:CG2	2.82	0.57
1:A:436:LEU:HD12	1:B:440:VAL:HG21	1.84	0.57
1:A:436:LEU:HD22	1:B:436:LEU:HD22	1.85	0.57
1:B:267:TYR:CE2	7:B:1060:HOH:O	2.58	0.56
1:A:618:ASP:HB3	7:A:1048:HOH:O	2.05	0.56
1:B:452:ARG:CA	7:B:1083:HOH:O	2.52	0.56
1:B:549:HIS:CE1	7:B:1000:HOH:O	2.58	0.56
1:A:266:ARG:HD2	1:A:268:ILE:HD11	1.87	0.56
1:A:338:ALA:O	1:A:340:HIS:HD2	1.88	0.56
7:A:997:HOH:O	1:B:557:ARG:HD2	2.05	0.55
1:B:551:LEU:HD11	7:B:1075:HOH:O	2.07	0.55
1:A:355[A]:LYS:HE2	1:A:357:TRP:NE1	2.21	0.55
1:A:440:VAL:HG21	1:B:436:LEU:CD1	2.37	0.55
1:B:267:TYR:CG	7:B:1060:HOH:O	2.58	0.55
1:B:588:TYR:HB3	1:B:590:GLN:HE22	1.72	0.55
1:B:607:ARG:CZ	7:B:940:HOH:O	2.55	0.55
1:B:387:LEU:C	1:B:387:LEU:HD12	2.32	0.55
1:A:435:ILE:HD12	1:A:492:ALA:HB1	1.89	0.54
1:B:557:ARG:CG	1:B:557:ARG:HH11	2.20	0.54
1:B:617:GLU:HG3	7:B:964:HOH:O	2.08	0.54
1:B:355:LYS:HE2	7:B:985:HOH:O	2.07	0.54
1:B:436:LEU:O	1:B:440:VAL:HG23	2.08	0.54
1:B:624:THR:CB	7:B:994:HOH:O	2.53	0.54
5:B:703:GOL:H32	7:B:1032:HOH:O	2.07	0.54
1:A:548:VAL:CG2	1:A:632:LEU:HD11	2.37	0.53
1:B:624:THR:HB	7:B:994:HOH:O	2.07	0.53
1:A:257:GLN:H	1:A:261:HIS:CD2	2.24	0.53
1:B:232:ARG:CD	1:B:394:GLY:O	2.56	0.53
1:B:631:LEU:CD2	7:B:973:HOH:O	2.55	0.53
1:A:232:ARG:CD	1:A:394:GLY:O	2.57	0.53
1:A:548:VAL:HG21	1:A:632:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:ARG:O	1:B:487:ARG:CD	2.56	0.52
1:B:254:GLU:CD	7:B:977:HOH:O	2.53	0.52
1:A:358:ARG:NH2	7:A:971:HOH:O	2.42	0.52
1:B:505:PHE:HB2	5:B:705:GOL:H12	1.92	0.51
1:A:220[B]:ARG:HD2	7:A:936:HOH:O	2.10	0.51
1:B:420:LEU:CD2	1:B:420:LEU:C	2.82	0.51
1:B:502:ALA:HB1	1:B:557:ARG:HG2	1.93	0.51
1:A:232:ARG:HD3	1:A:394:GLY:O	2.11	0.51
1:B:232:ARG:HD3	1:B:394:GLY:O	2.11	0.50
1:A:355[A]:LYS:HE2	1:A:357:TRP:HE1	1.75	0.50
1:A:355[A]:LYS:HZ1	1:A:357:TRP:HE1	1.59	0.50
1:B:233:GLN:HG3	7:B:978:HOH:O	2.11	0.50
1:A:548:VAL:CG2	1:A:632:LEU:CG	2.90	0.50
1:B:540:ALA:HB1	1:B:638:LEU:O	2.12	0.50
1:B:549:HIS:CE1	1:B:633:LEU:HD11	2.47	0.49
1:B:588:TYR:HB3	1:B:590:GLN:NE2	2.26	0.49
1:B:325:SER:HA	1:B:419:THR:O	2.11	0.49
1:B:357:TRP:CG	7:B:1085:HOH:O	2.63	0.49
1:A:322:MET:HE3	7:A:1029:HOH:O	2.12	0.49
1:A:325:SER:HA	1:A:419:THR:O	2.12	0.49
1:A:357:TRP:O	1:A:388:GLN:HA	2.12	0.49
1:A:417:HIS:CD2	1:A:419:THR:HG22	2.47	0.49
1:A:410:GLN:O	1:A:411:ASP:C	2.56	0.49
1:A:369:LEU:CD1	7:B:1083:HOH:O	2.59	0.49
1:A:452:ARG:HD3	7:A:876:HOH:O	2.12	0.48
1:B:413:VAL:O	7:B:993:HOH:O	2.20	0.48
1:A:548:VAL:CG2	1:A:549:HIS:N	2.76	0.48
1:A:326:ASN:HB3	7:A:1030:HOH:O	2.12	0.48
1:B:301:PRO:HB2	1:B:308:VAL:HG11	1.95	0.48
1:A:529:ARG:NH1	1:A:537:ASN:ND2	2.62	0.47
1:A:258:PHE:CE2	1:A:281:ALA:HA	2.50	0.47
1:A:528:ILE:HA	1:A:536:VAL:O	2.13	0.47
1:B:387:LEU:C	1:B:387:LEU:CD1	2.88	0.47
1:A:428:TRP:CZ2	5:B:703:GOL:H11	2.50	0.47
1:B:557:ARG:HH11	1:B:557:ARG:HG3	1.78	0.47
1:A:474:ARG:O	1:A:478:MET:HG2	2.15	0.47
1:A:557:ARG:HH11	1:A:557:ARG:HG3	1.79	0.47
1:B:528:ILE:HA	1:B:537:ASN:HB2	1.97	0.47
2:D:215:ASN:O	2:D:216:HIS:C	2.58	0.47
1:B:233:GLN:CG	7:B:978:HOH:O	2.63	0.47
1:A:472:PRO:HA	1:A:475:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:MET:HE1	5:B:705:GOL:H2	1.96	0.46
1:B:553:ASP:O	5:B:704:GOL:O2	2.19	0.46
1:A:328:TYR:CE2	1:A:419:THR:CG2	2.99	0.46
1:A:548:VAL:CG2	1:A:632:LEU:HG	2.39	0.46
7:B:1082:HOH:O	2:D:216:HIS:HB2	2.15	0.46
1:B:584:CYS:CB	7:B:1071:HOH:O	2.48	0.46
1:A:436:LEU:CD1	1:B:440:VAL:HG21	2.46	0.45
1:B:258:PHE:CE2	1:B:281:ALA:HA	2.51	0.45
1:B:250:MET:HE1	1:B:298:LEU:HD21	1.99	0.45
1:B:615:SER:CA	7:B:987:HOH:O	2.59	0.45
1:B:267:TYR:CD1	7:B:1060:HOH:O	2.70	0.45
1:A:505:PHE:CD2	1:B:459:MET:HE1	2.51	0.45
5:B:704:GOL:H2	7:B:1020:HOH:O	2.15	0.45
1:A:568:TYR:CD1	1:A:584:CYS:HB3	2.53	0.44
1:B:310:GLN:HA	1:B:513:VAL:HG21	1.98	0.44
1:B:542:LEU:HD23	7:B:992:HOH:O	2.17	0.44
1:B:232:ARG:HD2	1:B:394:GLY:O	2.17	0.44
1:A:232:ARG:HD2	1:A:394:GLY:O	2.18	0.44
1:A:613:CYS:HB3	7:A:1048:HOH:O	2.16	0.44
1:A:486:ALA:HB3	7:A:1050:HOH:O	2.16	0.44
1:B:558:LEU:HD11	1:B:587:ILE:HG13	2.00	0.44
1:A:353:GLY:O	1:A:393:PRO:HD3	2.18	0.44
1:A:548:VAL:HG23	1:A:632:LEU:CG	2.42	0.44
1:B:411:ASP:HB2	7:B:941:HOH:O	2.18	0.44
1:B:420:LEU:C	1:B:420:LEU:HD22	2.42	0.44
1:B:299:LEU:O	2:D:220:GLY:HA2	2.17	0.44
1:B:297:ARG:HA	1:B:327:VAL:O	2.18	0.43
1:A:613:CYS:CB	7:A:1048:HOH:O	2.66	0.43
1:B:355:LYS:CE	7:B:985:HOH:O	2.65	0.43
1:B:551:LEU:CD1	7:B:1075:HOH:O	2.65	0.43
1:A:615:SER:C	7:A:1009:HOH:O	2.61	0.43
1:A:299:LEU:O	2:C:220:GLY:HA2	2.18	0.43
1:B:250:MET:HE3	1:B:304:PHE:CG	2.53	0.43
1:A:435:ILE:HD11	1:A:494:VAL:HA	2.01	0.43
1:A:538:VAL:HG22	7:A:819:HOH:O	2.17	0.43
1:A:609:GLY:HA2	1:A:619:GLN:OE1	2.19	0.43
1:A:548:VAL:HG21	1:A:632:LEU:CD2	2.47	0.43
1:A:548:VAL:HG22	1:A:549:HIS:N	2.32	0.43
1:B:615:SER:OG	7:B:987:HOH:O	2.21	0.42
1:B:615:SER:CB	7:B:987:HOH:O	2.66	0.42
1:A:354:ARG:HH11	1:A:354:ARG:HG3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ARG:CZ	7:B:1010:HOH:O	2.66	0.42
1:B:353:GLY:HA3	1:B:414:HIS:O	2.19	0.42
1:B:474:ARG:O	1:B:478:MET:HG2	2.20	0.42
1:B:352:GLU:OE1	1:B:414:HIS:HE1	2.03	0.42
1:A:268:ILE:HD12	1:A:268:ILE:N	2.35	0.42
1:A:301:PRO:HG3	1:A:327:VAL:HG23	2.01	0.42
1:B:621:SER:CB	7:B:964:HOH:O	2.64	0.42
1:B:216:ASP:OD1	1:B:220:ARG:NH2	2.53	0.42
1:A:355[A]:LYS:NZ	1:A:357:TRP:HE1	2.17	0.42
1:A:267:TYR:CE2	7:A:978:HOH:O	2.72	0.41
1:B:357:TRP:O	1:B:388:GLN:HA	2.21	0.41
1:A:392:GLU:O	1:A:393:PRO:C	2.63	0.41
1:A:548:VAL:HG12	1:A:606:VAL:O	2.20	0.41
1:A:540:ALA:HB2	7:A:1019:HOH:O	2.20	0.41
1:A:589:PRO:N	7:A:1028:HOH:O	2.54	0.41
1:B:502:ALA:CB	1:B:557:ARG:HG2	2.51	0.41
1:B:271:ARG:CD	7:B:1067:HOH:O	2.45	0.41
1:B:287:TRP:HA	1:B:287:TRP:CE3	2.56	0.41
1:A:353:GLY:HA3	1:A:414:HIS:O	2.21	0.41
1:A:413:VAL:N	7:A:807:HOH:O	2.52	0.41
7:A:1021:HOH:O	1:B:459:MET:HE2	2.21	0.41
1:B:301:PRO:HG3	1:B:327:VAL:HG23	2.03	0.41
1:B:550:MET:HE3	1:B:598:LEU:HB3	2.03	0.41
1:B:399:PHE:HA	1:B:400:PRO:HD3	1.87	0.41
1:A:250:MET:HE3	1:A:250:MET:HB2	1.92	0.40
1:A:301:PRO:HB2	1:A:308:VAL:HG11	2.03	0.40
1:A:611:LEU:O	1:A:613:CYS:N	2.54	0.40
1:B:376:ASN:ND2	7:B:1035:HOH:O	2.53	0.40
1:A:355[A]:LYS:CE	1:A:357:TRP:HE1	2.33	0.40
1:A:548:VAL:CG2	1:A:632:LEU:CD1	2.99	0.40
1:B:538:VAL:N	7:B:803:HOH:O	2.55	0.40
7:B:932:HOH:O	2:D:219:ILE:HG21	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:827:HOH:O	7:A:834:HOH:O[2_655]	2.03	0.17
7:B:835:HOH:O	7:B:836:HOH:O[2_656]	2.05	0.15

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	460/466 (99%)	448 (97%)	12 (3%)	0	100	100
1	B	459/466 (98%)	446 (97%)	13 (3%)	0	100	100
2	C	9/11 (82%)	6 (67%)	3 (33%)	0	100	100
2	D	9/11 (82%)	6 (67%)	3 (33%)	0	100	100
All	All	937/954 (98%)	906 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	388/397 (98%)	365 (94%)	23 (6%)	18	22
1	B	386/397 (97%)	365 (95%)	21 (5%)	20	25
2	C	7/7 (100%)	6 (86%)	1 (14%)	3	3
2	D	7/7 (100%)	7 (100%)	0	100	100
All	All	788/808 (98%)	743 (94%)	45 (6%)	19	23

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	216	ASP

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Mol	Chain	Res	Type
1	A	225	ARG
1	A	232	ARG
1	A	255	GLU
1	A	280	ARG
1	A	318	GLN
1	A	355[A]	LYS
1	A	355[B]	LYS
1	A	380	ASP
1	A	419	THR
1	A	420	LEU
1	A	435	ILE
1	A	475	THR
1	A	478	MET
1	A	483	VAL
1	A	487	ARG
1	A	526	LEU
1	A	542	LEU
1	A	557	ARG
1	A	583	LYS
1	A	607	ARG
1	A	629	LYS
1	B	216	ASP
1	B	232	ARG
1	B	268	ILE
1	B	271	ARG
1	B	272	ARG
1	B	280	ARG
1	B	366	THR
1	B	387	LEU
1	B	413	VAL
1	B	420	LEU
1	B	435	ILE
1	B	479	GLU
1	B	526	LEU
1	B	529	ARG
1	B	545	GLU
1	B	557	ARG
1	B	565	LEU
1	B	581	GLU
1	B	583	LYS
1	B	616	VAL
1	B	629	LYS

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Mol	Chain	Res	Type
2	C	219	ILE

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

Mol	Chain	Res	Type
1	A	291	GLN
1	A	333	ASN
1	A	340	HIS
1	A	388	GLN
1	A	410	GLN
1	A	414	HIS
1	A	537	ASN
1	B	340	HIS
1	B	376	ASN
1	B	414	HIS
1	B	537	ASN
1	B	590	GLN
2	C	215	ASN
2	C	217	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
5	GOL	B	703	-	5,5,5	0.39	0	5,5,5	0.87	0
5	GOL	B	705	-	5,5,5	0.60	0	5,5,5	1.35	1 (20%)
4	OGA	A	702	3	9,9,9	1.68	1 (11%)	8,11,11	1.52	2 (25%)
5	GOL	B	704	-	5,5,5	1.17	0	5,5,5	1.63	1 (20%)
4	OGA	B	702	3	9,9,9	1.74	2 (22%)	8,11,11	1.78	2 (25%)
6	ACT	B	706	-	3,3,3	1.02	0	3,3,3	1.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	703	-	-	1/4/4/4	-
5	GOL	B	705	-	-	4/4/4/4	-
4	OGA	A	702	3	-	2/8/9/9	-
5	GOL	B	704	-	-	2/4/4/4	-
4	OGA	B	702	3	-	0/8/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	OGA	C2-C1	-4.37	1.49	1.54
4	A	702	OGA	C2-C1	-3.85	1.49	1.54
4	B	702	OGA	O1-C1	2.22	1.28	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	702	OGA	O2'-C2-N1	-3.34	117.32	123.35
4	B	702	OGA	C4-N1-C2	-2.89	116.83	121.29
5	B	704	GOL	O2-C2-C3	2.39	119.08	109.18
4	A	702	OGA	C4-N1-C2	2.28	124.81	121.29
4	A	702	OGA	O2-C1-O1	-2.16	118.76	123.90
5	B	705	GOL	O3-C3-C2	2.07	119.67	110.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	704	GOL	O1-C1-C2-C3
5	B	705	GOL	C1-C2-C3-O3
4	A	702	OGA	N1-C4-C5-O4
5	B	705	GOL	O2-C2-C3-O3
5	B	705	GOL	O1-C1-C2-C3
4	A	702	OGA	N1-C4-C5-O3
5	B	703	GOL	O2-C2-C3-O3
5	B	704	GOL	O1-C1-C2-O2
5	B	705	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	703	GOL	2	0
5	B	705	GOL	3	0
4	A	702	OGA	1	0
5	B	704	GOL	2	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

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	459/466 (98%)	0.11	15 (3%) 49 46	8, 22, 41, 58	4 (0%)
1	B	461/466 (98%)	0.04	12 (2%) 57 54	11, 21, 41, 78	1 (0%)
2	C	11/11 (100%)	1.73	5 (45%) 0 0	26, 34, 56, 58	0
2	D	11/11 (100%)	1.66	4 (36%) 1 0	25, 33, 59, 65	0
All	All	942/954 (98%)	0.11	36 (3%) 44 41	8, 22, 43, 78	5 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	540	ALA	6.2
1	B	641	ASN	5.5
1	B	539	GLY	5.2
2	D	212	GLY	5.1
1	A	181	TRP	4.9
1	A	538	VAL	4.8
2	D	222	PRO	4.4
1	B	640	LEU	4.0
2	C	212	GLY	3.9
1	B	268	ILE	3.8
2	C	222	PRO	3.5
1	A	613	CYS	3.1
1	A	540	ALA	3.1
1	A	539	GLY	2.9
1	B	639	ALA	2.9
2	D	213	GLY	2.9
1	A	548	VAL	2.9
1	A	269	ASN	2.9
1	B	269	ASN	2.8
2	C	213	GLY	2.7
1	B	536	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	538	VAL	2.6
1	A	412	GLY	2.6
1	A	614	ASP	2.5
2	C	221	LYS	2.5
2	D	215	ASN	2.4
2	C	215	ASN	2.4
1	B	181	TRP	2.4
1	A	562	GLY	2.3
1	B	541	GLN	2.3
1	A	411	ASP	2.2
1	A	268	ILE	2.2
1	A	271[A]	ARG	2.2
1	A	563	GLY	2.1
1	A	639	ALA	2.1
1	B	333	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ACT	B	706	4/4	0.59	0.18	33,35,37,38	0
5	GOL	B	704	6/6	0.77	0.18	27,29,32,35	0
5	GOL	B	703	6/6	0.88	0.12	29,30,33,35	0
4	OGA	B	702	10/10	0.90	0.10	29,36,41,44	0
5	GOL	B	705	6/6	0.90	0.14	26,28,32,34	0
4	OGA	A	702	10/10	0.90	0.09	30,33,36,37	0
3	NI	A	701	1/1	0.99	0.06	34,34,34,34	0
3	NI	B	701	1/1	0.99	0.05	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.