



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:17 am BST

PDB ID : 4Y3O  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

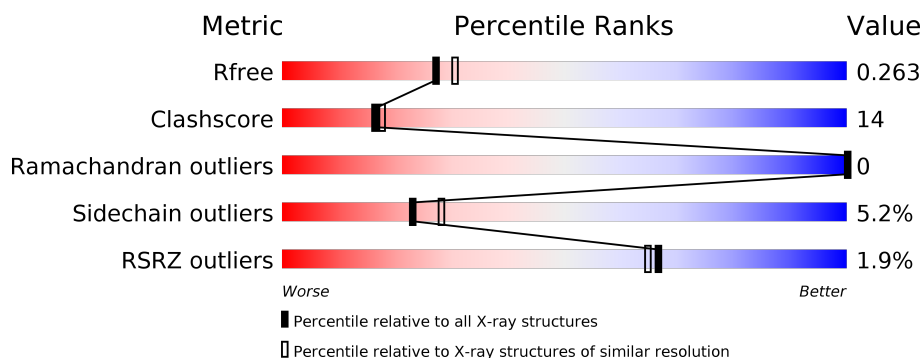
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>• •</div> </div> </div>
1	B	466	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>
2	C	11	<div> <div>9%</div> <div> <div></div> <div>82%</div> <div>18%</div> </div> </div>
2	D	11	<div> <div>18%</div> <div> <div></div> <div>45%</div> <div>55%</div> </div> </div>

## 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			

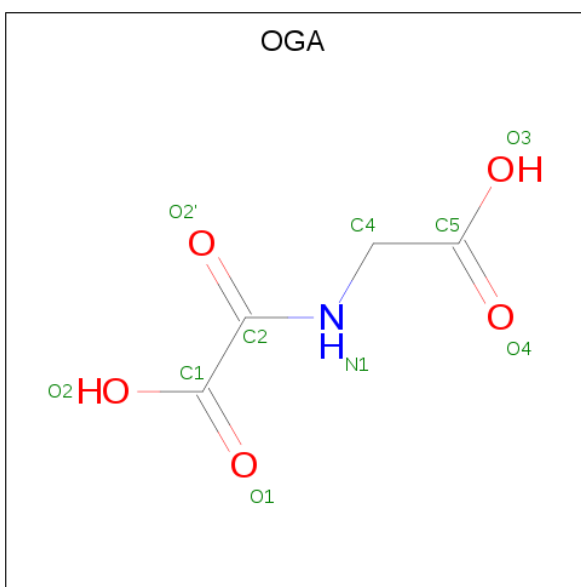
- Molecule 2 is a protein called Rpl8 peptide.

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 (three-letter code: NI) (formula: Ni).

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

- Molecule 4 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: C<sub>4</sub>H<sub>5</sub>NO<sub>5</sub>).



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 (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



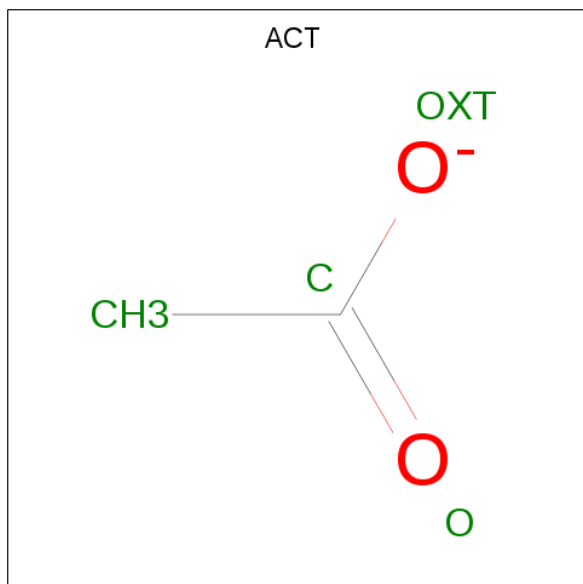
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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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 (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

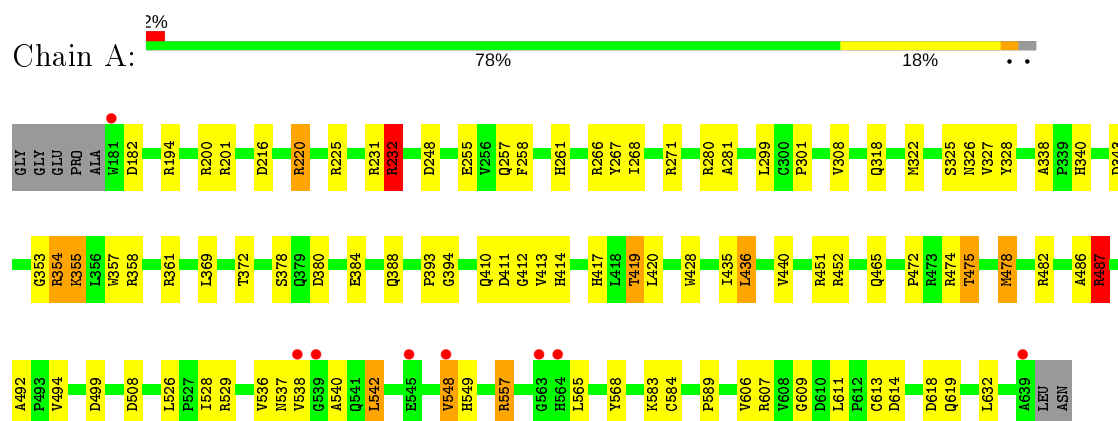
- Molecule 7 is water.

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		

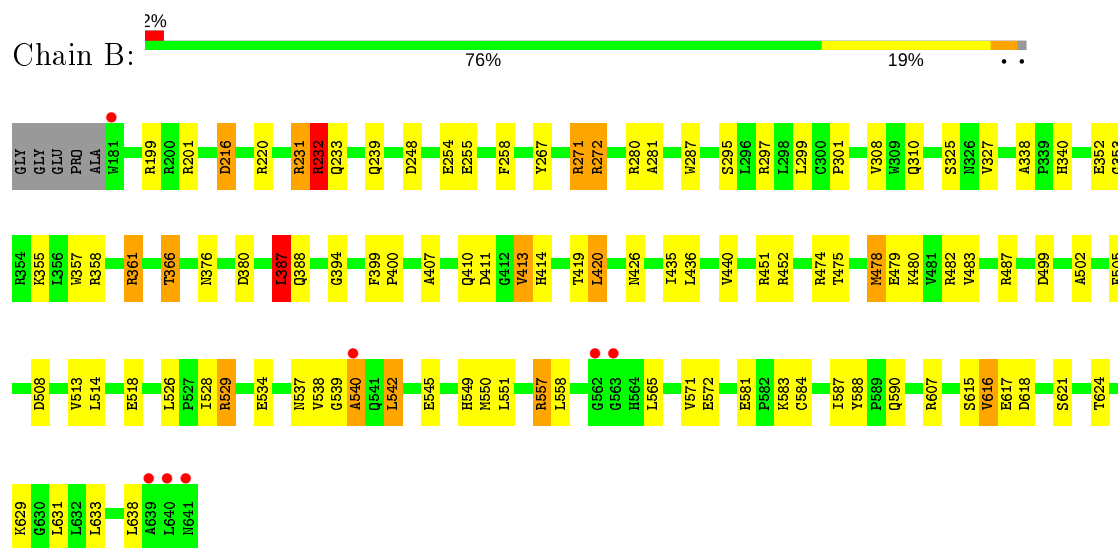
### 3 Residue-property plots

These plots are drawn for all protein, RNA 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.

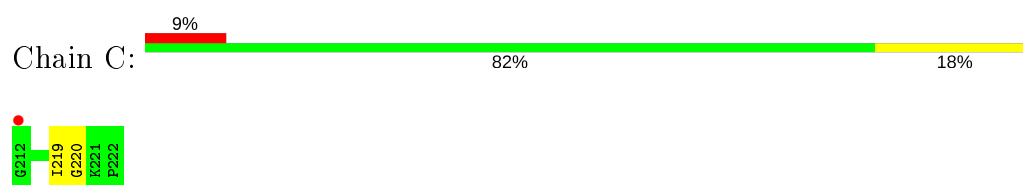
- Molecule 1: Bifunctional lysine-specific demethylase and histidyl-hydroxylase NO66



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



- Molecule 2: Rpl8 peptide



- Molecule 2: Rpl8 peptide

Chain D:  18% 45% 55%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.50Å 202.93Å 85.68Å 90.00° 118.94° 90.00°	Depositor
Resolution (Å)	40.57 – 2.20 38.72 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.9 (40.57-2.20) 97.9 (38.72-2.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.203 , 0.262 0.209 , 0.263	Depositor DCC
$R_{free}$ test set	3314 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, OGA, NI

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	0.89	0/3782	1.07	21/5147 (0.4%)
1	B	0.91	1/3765 (0.0%)	1.06	22/5127 (0.4%)
2	C	0.70	0/79	0.80	0/104
2	D	0.77	0/79	0.88	0/104
All	All	0.90	1/7705 (0.0%)	1.06	43/10482 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	295	SER	CB-OG	5.35	1.49	1.42

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	ARG	NE-CZ-NH2	-14.77	112.92	120.30
1	B	539	GLY	N-CA-C	12.82	145.15	113.10
1	A	451	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	A	354	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	A	232	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	B	232	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	B	272	ARG	NE-CZ-NH1	-9.06	115.77	120.30
1	B	451	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	A	487	ARG	NE-CZ-NH1	-8.13	116.23	120.30
1	A	542	LEU	CA-CB-CG	7.97	133.62	115.30
1	A	232	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	542	LEU	CA-CB-CG	7.12	131.68	115.30
1	B	232	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	B	361	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	220[A]	ARG	NE-CZ-NH1	-6.79	116.90	120.30
1	A	220[B]	ARG	NE-CZ-NH1	-6.79	116.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	451	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	194	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	482	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	482	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	272	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	A	361	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	231	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	548	VAL	CG1-CB-CG2	-6.07	101.19	110.90
1	B	361	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	529	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	540	ALA	N-CA-C	-5.89	95.11	111.00
1	B	478	MET	CG-SD-CE	-5.84	90.86	100.20
1	B	231	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	534	GLU	C-N-CD	5.68	140.33	128.40
1	A	248	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	436	LEU	CB-CG-CD1	-5.64	101.42	111.00
1	B	201	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	201	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	248	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	355[A]	LYS	CD-CE-NZ	5.31	123.92	111.70
1	A	355[B]	LYS	CD-CE-NZ	5.31	123.92	111.70
1	B	508	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	508	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	182	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	322	MET	CG-SD-CE	-5.13	91.98	100.20
1	B	387	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	508	ASP	CB-CG-OD2	-5.04	113.76	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3687	0	3588	98	0
1	B	3670	0	3557	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	0
6	B	4	0	3	0	0
7	A	264	0	0	34	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	212	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 14.

All (212) 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: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:615:SER:C	7:B:987:HOH:O	2.04	0.94
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:HD2	1:B:487:ARG:O	1.79	0.81
1:B:358:ARG:NH1	7:B:984:HOH:O	2.12	0.81
1:B:426:ASN:OD1	5:B:705:GOL:H32	1.80	0.81
1:A:419:THR:HG21	4:A:702:OGA:O1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:327:VAL:C	7:A:1030:HOH:O	2.31	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:369:LEU:HD12	7:B:1083:HOH:O	1.95	0.66
1:A:328:TYR:HE2	1:A:419:THR:HG23	1.60	0.66
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:B:538:VAL:HA	7:B:803:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:222:PRO:C	7:D:306:HOH:O	2.38	0.61
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
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:A:412:GLY:C	7:A:807:HOH:O	2.41	0.58
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:A:355[A]:LYS:HZ3	1:A:357:TRP:HE1	1.51	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: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:B:267:TYR:CG	7:B:1060:HOH:O	2.58	0.55
1:A:440:VAL:HG21	1:B:436:LEU:CD1	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:372:THR:C	7:A:1037:HOH:O	2.46	0.53
1:A:548:VAL:HG21	1:A:632:LEU:HD11	1.91	0.52
1:B:487:ARG:CD	1:B:487:ARG:O	2.56	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: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: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:387:LEU:C	1:B:387:LEU:HD12	2.32	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:357:TRP:CG	7:B:1085:HOH:O	2.63	0.49
1:B:325:SER:HA	1:B:419:THR:O	2.11	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: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:A:428:TRP:CZ2	5:B:703:GOL:H11	2.50	0.47
1:B:254:GLU:CD	7:B:977:HOH:O	2.53	0.47
1:B:557:ARG:HG3	1:B:557:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:LEU:CD2	1:B:420:LEU:C	2.82	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
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:B:258:PHE:CE2	1:B:281:ALA:HA	2.51	0.45
1:A:436:LEU:CD1	1:B:440:VAL:HG21	2.46	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
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:A:410:GLN:O	1:A:411:ASP:C	2.56	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: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:299:LEU:O	2:C:220:GLY:HA2	2.18	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:387:LEU:C	1:B:387:LEU:CD1	2.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:215:ASN:O	2:D:216:HIS:C	2.58	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: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:CE3	1:B:287:TRP:HA	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
1:B:301:PRO:HG3	1:B:327:VAL:HG23	2.03	0.41
1:B:399:PHE:HA	1:B:400:PRO:HD3	1.87	0.41
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%)	368 (95%)	20 (5%)	23	28
1	B	386/397 (97%)	365 (95%)	21 (5%)	22	26
2	C	7/7 (100%)	6 (86%)	1 (14%)	3	2
2	D	7/7 (100%)	7 (100%)	0	100	100
All	All	788/808 (98%)	746 (95%)	42 (5%)	23	27

All (42) 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	271[A]	ARG
1	A	271[B]	ARG
1	A	280	ARG
1	A	318	GLN
1	A	380	ASP
1	A	419	THR
1	A	420	LEU
1	A	475	THR
1	A	478	MET
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	B	216	ASP
1	B	232	ARG
1	B	271	ARG
1	B	272	ARG
1	B	280	ARG
1	B	361	ARG
1	B	366	THR
1	B	380	ASP
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
2	C	219	ILE

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	261	HIS
1	A	333	ASN
1	A	340	HIS
1	A	410	GLN
1	A	414	HIS
1	A	537	ASN
1	B	340	HIS
1	B	376	ASN
1	B	410	GLN
1	B	414	HIS
1	B	537	ASN
1	B	590	GLN
2	C	217	GLN
2	D	215	ASN

### 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 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	704	-	5,5,5	1.14	0	5,5,5	1.54	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	OGA	B	702	3	3,9,9	0.49	0	4,11,11	4.01	4 (100%)
5	GOL	B	703	-	5,5,5	0.37	0	5,5,5	0.82	0
6	ACT	B	706	-	1,3,3	2.23	1 (100%)	0,3,3	0.00	-
5	GOL	B	705	-	5,5,5	0.59	0	5,5,5	1.27	0
4	OGA	A	702	3	3,9,9	0.56	0	4,11,11	2.59	2 (50%)

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	704	-	-	3/4/4/4	-
4	OGA	B	702	3	-	0/3/9/9	-
5	GOL	B	703	-	-	1/4/4/4	-
5	GOL	B	705	-	-	4/4/4/4	-
4	OGA	A	702	3	-	0/3/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	706	ACT	CH3-C	2.23	1.51	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	702	OGA	C1-C2-N1	6.89	122.45	115.60
4	A	702	OGA	C1-C2-N1	3.84	119.42	115.60
4	A	702	OGA	C5-C4-N1	3.14	116.47	110.43
4	B	702	OGA	O2'-C2-N1	-2.65	117.32	122.61
4	B	702	OGA	C5-C4-N1	2.29	114.85	110.43
5	B	704	GOL	O2-C2-C3	2.26	119.08	109.12
4	B	702	OGA	C4-N1-C2	-2.10	116.83	121.81

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	705	GOL	C1-C2-C3-O3
5	B	704	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	B	705	GOL	O1-C1-C2-C3
5	B	705	GOL	O2-C2-C3-O3
5	B	704	GOL	O1-C1-C2-O2
5	B	703	GOL	O2-C2-C3-O3
5	B	705	GOL	O1-C1-C2-O2
5	B	704	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	459/466 (98%)	-0.25	8 (1%) 70 68	12, 22, 42, 58	1 (0%)
1	B	461/466 (98%)	-0.28	7 (1%) 73 72	11, 21, 41, 78	1 (0%)
2	C	11/11 (100%)	0.60	1 (9%) 9 8	26, 34, 56, 58	0
2	D	11/11 (100%)	0.64	2 (18%) 1 1	25, 33, 59, 65	0
All	All	942/954 (98%)	-0.24	18 (1%) 66 65	11, 22, 43, 78	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	641	ASN	8.0
1	B	640	LEU	4.4
1	A	538	VAL	3.9
1	A	639	ALA	3.2
1	A	181	TRP	3.1
1	A	539	GLY	3.1
1	B	540	ALA	2.5
1	A	564	HIS	2.5
2	D	212	GLY	2.5
2	D	222	PRO	2.3
1	B	563	GLY	2.2
1	B	181	TRP	2.2
2	C	212	GLY	2.1
1	B	562	GLY	2.1
1	A	548	VAL	2.1
1	A	563	GLY	2.1
1	B	639	ALA	2.0
1	A	545	GLU	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
6	ACT	B	706	4/4	0.62	0.27	33,35,37,38	0
5	GOL	B	704	6/6	0.76	0.22	27,29,32,35	0
4	OGA	B	702	10/10	0.88	0.18	29,36,41,44	0
5	GOL	B	703	6/6	0.90	0.20	29,30,33,35	0
5	GOL	B	705	6/6	0.91	0.19	26,28,32,34	0
4	OGA	A	702	10/10	0.94	0.14	30,33,36,37	0
3	NI	A	701	1/1	0.99	0.03	34,34,34,34	0
3	NI	B	701	1/1	0.99	0.03	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.