



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:37 PM GMT

PDB ID : 1GHQ  
Title : CR2-C3D COMPLEX STRUCTURE  
Authors : Szakonyi, G.; Guthridge, J.M.; Li, D.; Holers, V.M.; Chen, X.S.  
Deposited on : 2001-01-11  
Resolution : 2.04 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

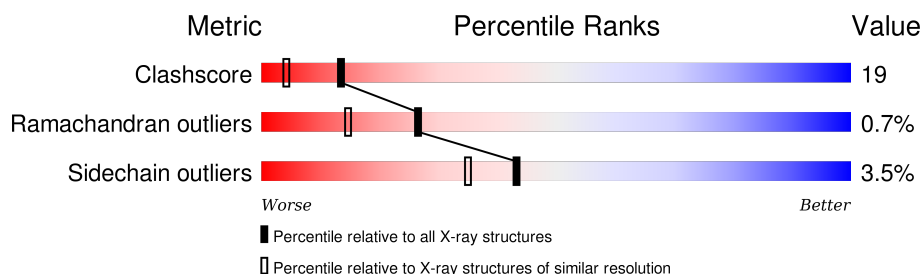
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	308	
2	B	134	
2	C	134	

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	NDG	C	701	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5132 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 COMPLEMENT C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2417	1550	406	452	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP P01024
A	2	LEU	-	CLONING ARTIFACT	UNP P01024
A	17	ALA	CYS	ENGINEERED	UNP P01024
A	295	SER	-	INSERTION	UNP P01024

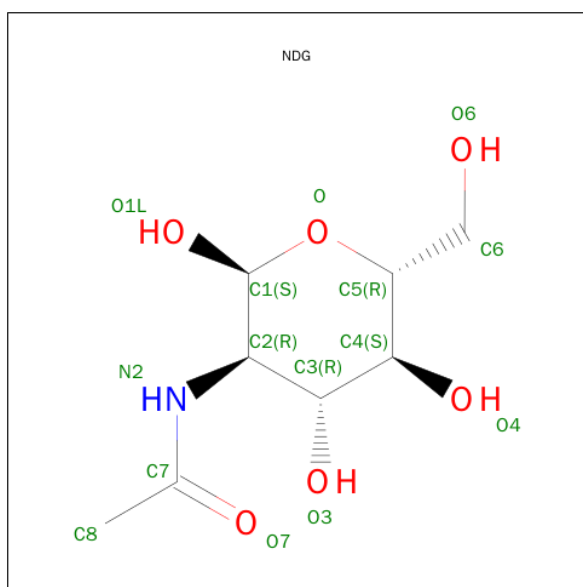
- Molecule 2 is a protein called CR2/CD121/C3D/EPSTEIN-BARR VIRUS RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	129	Total	C	N	O	S	0	0	0
			987	626	169	182	10			
2	C	134	Total	C	N	O	S	1	0	0
			1030	656	174	190	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	CLONING ARTIFACT	UNP P20023
C	1	ALA	-	CLONING ARTIFACT	UNP P20023

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		

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

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

- Molecule 5 is water.

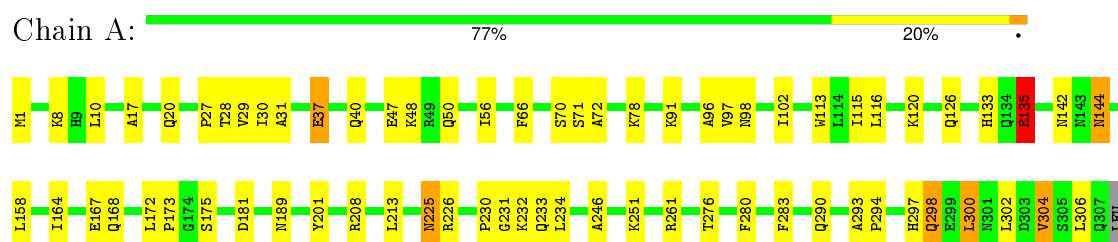
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	372	Total	O	0	0
			372	372		
5	B	170	Total	O	0	0
			170	170		
5	C	124	Total	O	0	0
			124	124		

### 3 Residue-property plots

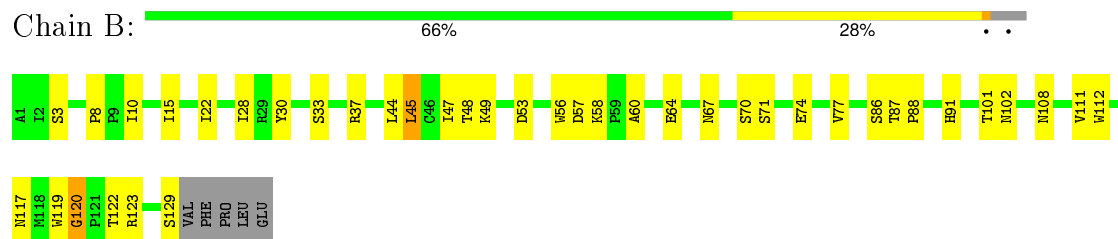
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

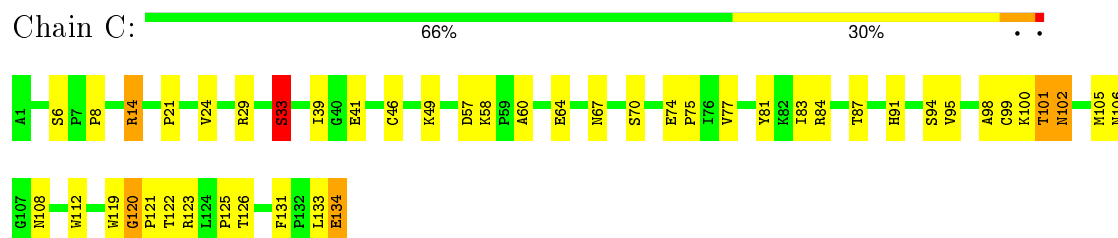
#### • Molecule 1: COMPLEMENT C3



#### • Molecule 2: CR2/CD121/C3D/EPSTEIN-BARR VIRUS RECEPTOR



#### • Molecule 2: CR2/CD121/C3D/EPSTEIN-BARR VIRUS RECEPTOR



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.00Å 170.00Å 174.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.04	Depositor
% Data completeness (in resolution range)	94.1 (25.00-2.04)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.195 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.82	3/2467 (0.1%)	0.80	2/3344 (0.1%)
2	B	0.56	0/1016	0.74	0/1382
2	C	1.19	10/1061 (0.9%)	1.30	13/1443 (0.9%)
All	All	0.87	13/4544 (0.3%)	0.93	15/6169 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	21	PRO	N-CD	-18.03	1.22	1.47
2	C	133	LEU	C-N	-14.21	1.01	1.34
1	A	135	GLU	CB-CG	14.05	1.78	1.52
2	C	134	GLU	C-O	12.87	1.47	1.23
2	C	74	GLU	CB-CG	-11.27	1.30	1.52
2	C	6	SER	CB-OG	-10.39	1.28	1.42
1	A	135	GLU	CG-CD	9.90	1.66	1.51
2	C	134	GLU	C-OXT	-6.81	1.10	1.23
2	C	33	SER	CA-CB	6.79	1.63	1.52
1	A	135	GLU	CD-OE1	-6.32	1.18	1.25
2	C	70	SER	CB-OG	-5.64	1.34	1.42
2	C	102	ASN	C-N	-5.08	1.22	1.34
2	C	102	ASN	C-O	5.06	1.32	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	133	LEU	C-N-CA	20.43	172.77	121.70
2	C	133	LEU	O-C-N	-19.76	91.08	122.70
2	C	133	LEU	CA-C-N	14.02	148.05	117.20
2	C	33	SER	CB-CA-C	10.97	130.94	110.10
1	A	135	GLU	CG-CD-OE2	8.31	134.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	74	GLU	CA-CB-CG	7.42	129.71	113.40
2	C	101	THR	O-C-N	-7.16	111.25	122.70
2	C	134	GLU	CA-C-O	-7.01	105.38	120.10
1	A	135	GLU	CG-CD-OE1	-6.52	105.27	118.30
2	C	100	LYS	O-C-N	6.19	132.60	122.70
2	C	33	SER	N-CA-CB	-5.88	101.68	110.50
2	C	101	THR	CA-C-N	5.67	129.68	117.20
2	C	21	PRO	N-CD-CG	5.50	111.44	103.20
2	C	100	LYS	CA-C-N	-5.14	105.89	117.20
2	C	102	ASN	CA-C-N	5.08	128.38	117.20

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	2417	0	2417	77	0
2	B	987	0	969	45	0
2	C	1030	0	1009	46	0
3	B	15	0	15	3	0
3	C	15	0	15	10	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	372	0	0	17	0
5	B	170	0	0	5	0
5	C	124	0	0	7	1
All	All	5132	0	4425	166	1

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 19.

All (166) 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:135:GLU:CG	1:A:135:GLU:CB	1.78	1.60
2:C:102:ASN:ND2	3:C:701:NDG:H1	1.41	1.35
2:C:102:ASN:HD21	3:C:701:NDG:C1	1.49	1.23
1:A:302:LEU:HD11	1:A:304:VAL:HG12	1.13	1.12
2:B:102:ASN:HD21	3:B:702:NDG:H1	0.97	1.10
2:C:134:GLU:HG2	5:C:797:HOH:O	1.52	1.07
1:A:40:GLN:OE1	1:A:304:VAL:HG22	1.57	1.05
2:B:102:ASN:ND2	3:B:702:NDG:H1	1.71	1.04
2:C:102:ASN:CG	3:C:701:NDG:H1	1.82	0.99
2:C:102:ASN:HD21	3:C:701:NDG:H1	0.89	0.97
1:A:47:GLU:HG3	5:A:980:HOH:O	1.67	0.93
1:A:298:GLN:HE21	1:A:298:GLN:H	1.15	0.93
2:C:102:ASN:HD21	3:C:701:NDG:C2	1.82	0.92
1:A:133:HIS:ND1	1:A:135:GLU:OE2	2.01	0.92
1:A:302:LEU:HD11	1:A:304:VAL:CG1	1.99	0.91
2:B:111:VAL:HG21	2:B:119:TRP:HB3	1.53	0.91
1:A:304:VAL:HG21	5:A:846:HOH:O	1.76	0.85
1:A:8:LYS:HE2	1:A:48:LYS:HE2	1.58	0.84
2:B:111:VAL:HG23	2:B:120:GLY:HA3	1.59	0.84
1:A:276:THR:HG23	5:A:963:HOH:O	1.78	0.84
1:A:300:LEU:HD12	1:A:300:LEU:H	1.43	0.82
2:C:106:ASN:HB3	2:C:126:THR:HG22	1.62	0.81
1:A:225:ASN:HD21	1:A:226:ARG:HH11	1.26	0.81
1:A:302:LEU:CD1	1:A:304:VAL:HG12	2.05	0.80
1:A:234:LEU:HD23	1:A:234:LEU:H	1.47	0.80
2:C:112:TRP:H	2:C:120:GLY:HA2	1.49	0.78
2:B:87:THR:HG22	2:B:88:PRO:HA	1.66	0.78
2:C:83:ILE:HG22	2:C:84:ARG:HG3	1.67	0.77
2:C:122:THR:HG22	2:C:123:ARG:H	1.49	0.76
2:C:106:ASN:HB3	2:C:126:THR:CG2	2.16	0.75
2:C:122:THR:HG22	2:C:123:ARG:N	2.02	0.74
2:C:102:ASN:OD1	3:C:701:NDG:H1	1.87	0.74
1:A:115:ILE:HD12	1:A:175:SER:OG	1.88	0.74
2:B:102:ASN:HD21	3:B:702:NDG:C1	1.89	0.73
2:C:75:PRO:HG3	2:C:95:VAL:HG21	1.70	0.73
2:B:8:PRO:HG2	2:B:60:ALA:HB2	1.69	0.73
2:C:14:ARG:NH2	2:C:33:SER:HB3	2.03	0.73
1:A:30:ILE:HD12	1:A:31:ALA:N	2.04	0.72
2:B:87:THR:CG2	2:B:88:PRO:HA	2.20	0.72
1:A:30:ILE:HG21	1:A:280:PHE:HA	1.72	0.71
2:C:122:THR:HG23	5:C:778:HOH:O	1.88	0.71
2:B:67:ASN:H	2:B:91:HIS:HD2	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ILE:HG22	2:B:48:THR:N	2.07	0.69
2:C:102:ASN:ND2	3:C:701:NDG:C1	2.23	0.67
1:A:37:GLU:HG2	5:A:892:HOH:O	1.93	0.67
2:B:111:VAL:CG2	2:B:119:TRP:HB3	2.24	0.66
1:A:298:GLN:H	1:A:298:GLN:NE2	1.89	0.65
1:A:20:GLN:HG3	5:A:808:HOH:O	1.97	0.65
2:B:45:LEU:HD13	2:B:47:ILE:HD11	1.79	0.64
1:A:302:LEU:HD12	1:A:304:VAL:H	1.62	0.64
1:A:8:LYS:CE	1:A:48:LYS:HE2	2.28	0.64
2:B:111:VAL:HG23	2:B:120:GLY:CA	2.27	0.64
1:A:29:VAL:HG22	1:A:56:ILE:HD12	1.80	0.64
1:A:133:HIS:HD1	1:A:135:GLU:CD	2.02	0.62
2:C:108:ASN:O	2:C:125:PRO:HB3	2.00	0.62
2:B:53:ASP:HB2	5:C:716:HOH:O	1.99	0.61
2:B:44:LEU:HD22	2:B:58:LYS:HG3	1.82	0.61
2:B:47:ILE:CG2	2:B:48:THR:N	2.63	0.61
1:A:120:LYS:NZ	1:A:126:GLN:NE2	2.49	0.61
2:C:131:PHE:O	2:C:134:GLU:HA	2.01	0.60
2:C:67:ASN:H	2:C:91:HIS:HD2	1.50	0.60
1:A:167:GLU:HB2	5:A:1059:HOH:O	2.01	0.60
2:B:64:GLU:OE1	2:B:91:HIS:HE1	1.84	0.60
1:A:276:THR:HG22	5:A:813:HOH:O	2.01	0.59
2:C:108:ASN:HB3	5:C:764:HOH:O	2.01	0.59
2:B:71:SER:H	2:B:117:ASN:HD22	1.51	0.59
1:A:96:ALA:HB3	1:A:102:ILE:HD11	1.84	0.59
2:B:111:VAL:CG2	2:B:120:GLY:N	2.66	0.58
1:A:120:LYS:HZ1	1:A:126:GLN:NE2	2.01	0.58
1:A:300:LEU:H	1:A:300:LEU:CD1	2.15	0.58
2:C:112:TRP:H	2:C:120:GLY:CA	2.17	0.57
1:A:29:VAL:CG2	1:A:56:ILE:HD12	2.34	0.57
1:A:225:ASN:HD22	1:A:226:ARG:N	2.02	0.57
2:C:24:VAL:HA	2:C:46:CYS:SG	2.44	0.57
2:C:64:GLU:OE1	2:C:91:HIS:HE1	1.88	0.56
2:B:87:THR:HG22	2:B:88:PRO:CA	2.34	0.56
1:A:298:GLN:HE21	1:A:298:GLN:N	1.97	0.54
2:B:108:ASN:ND2	2:B:122:THR:HG21	2.22	0.54
1:A:1:MET:N	5:A:1162:HOH:O	2.35	0.54
2:B:67:ASN:H	2:B:91:HIS:CD2	2.21	0.54
1:A:91:LYS:NZ	5:A:1079:HOH:O	2.40	0.54
2:B:102:ASN:O	2:B:129:SER:HA	2.08	0.53
1:A:225:ASN:HD21	1:A:226:ARG:NH1	2.01	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:THR:CG2	2:C:123:ARG:N	2.71	0.53
2:C:101:THR:O	2:C:102:ASN:HB2	2.08	0.53
1:A:17:ALA:HA	1:A:66:PHE:CZ	2.44	0.53
2:B:71:SER:H	2:B:117:ASN:ND2	2.07	0.53
1:A:225:ASN:HD22	1:A:225:ASN:C	2.11	0.52
2:B:112:TRP:O	2:B:120:GLY:N	2.42	0.52
2:C:112:TRP:O	2:C:120:GLY:N	2.43	0.52
2:C:122:THR:CG2	2:C:123:ARG:H	2.19	0.52
1:A:30:ILE:C	1:A:30:ILE:HD12	2.30	0.52
1:A:172:LEU:HB3	1:A:173:PRO:HD3	1.91	0.52
2:C:99:CYS:SG	2:C:105:MET:HB2	2.50	0.51
1:A:78:LYS:HG3	5:A:827:HOH:O	2.09	0.51
2:C:39:ILE:HG22	2:C:121:PRO:HG3	1.92	0.51
2:C:102:ASN:ND2	3:C:701:NDG:C2	2.63	0.51
1:A:70:SER:O	1:A:71:SER:HB2	2.09	0.51
1:A:133:HIS:HB3	1:A:135:GLU:HG3	1.93	0.50
1:A:213:LEU:N	1:A:213:LEU:HD12	2.27	0.50
2:B:111:VAL:HG23	2:B:120:GLY:N	2.27	0.50
1:A:231:GLY:O	1:A:232:LYS:HB2	2.11	0.50
2:B:111:VAL:HG22	2:B:119:TRP:HE3	1.77	0.49
1:A:116:LEU:HD12	2:B:86:SER:HB3	1.92	0.49
2:C:8:PRO:HB2	2:C:60:ALA:HB2	1.93	0.49
1:A:232:LYS:O	1:A:234:LEU:HD23	2.12	0.49
1:A:300:LEU:HD11	5:A:1044:HOH:O	2.12	0.49
2:C:58:LYS:HG2	5:C:787:HOH:O	2.12	0.49
1:A:115:ILE:HD11	1:A:158:LEU:CD1	2.43	0.49
2:B:77:VAL:HG13	5:B:877:HOH:O	2.13	0.49
2:C:81:TYR:CE1	2:C:83:ILE:HD11	2.47	0.48
2:B:47:ILE:HD12	2:B:57:ASP:HB3	1.96	0.48
1:A:97:VAL:HG11	1:A:164:ILE:HD11	1.95	0.48
2:C:134:GLU:OE2	5:C:813:HOH:O	2.20	0.48
1:A:142:ASN:OD1	1:A:144:ASN:HB2	2.13	0.48
1:A:261:ARG:NH2	5:A:1018:HOH:O	2.47	0.47
1:A:30:ILE:HD13	1:A:283:PHE:CG	2.49	0.47
1:A:120:LYS:HZ3	1:A:126:GLN:CD	2.17	0.47
2:C:94:SER:HB3	2:C:112:TRP:CD1	2.50	0.47
2:C:67:ASN:H	2:C:91:HIS:CD2	2.29	0.47
1:A:302:LEU:CD1	1:A:304:VAL:CG1	2.78	0.46
1:A:304:VAL:HG23	5:A:823:HOH:O	2.15	0.46
1:A:10:LEU:O	1:A:27:PRO:HB2	2.15	0.46
1:A:28:THR:HG22	1:A:56:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LYS:HE2	5:A:1167:HOH:O	2.15	0.46
1:A:302:LEU:C	1:A:302:LEU:HD12	2.35	0.45
1:A:290:GLN:OE1	1:A:304:VAL:HG23	2.16	0.45
2:B:101:THR:O	2:B:102:ASN:HB2	2.15	0.45
2:B:22:ILE:HD13	2:B:56:TRP:HZ2	1.81	0.45
2:C:119:TRP:O	2:C:120:GLY:O	2.34	0.45
1:A:97:VAL:HG21	1:A:164:ILE:CD1	2.47	0.45
1:A:230:PRO:HG2	5:A:1008:HOH:O	2.16	0.45
1:A:72:ALA:HB2	1:A:113:TRP:CD2	2.52	0.45
1:A:40:GLN:OE1	1:A:304:VAL:CG2	2.45	0.45
1:A:234:LEU:H	1:A:234:LEU:CD2	2.24	0.45
2:B:45:LEU:HD13	2:B:47:ILE:CG1	2.47	0.45
2:C:83:ILE:HD11	2:C:98:ALA:HB3	1.99	0.44
2:B:70:SER:HA	2:B:117:ASN:HD21	1.81	0.44
2:B:123:ARG:HG3	5:B:966:HOH:O	2.17	0.44
2:B:47:ILE:HG23	5:B:862:HOH:O	2.17	0.44
1:A:120:LYS:HZ1	1:A:126:GLN:HE22	1.64	0.44
2:B:15:ILE:HG23	2:B:28:ILE:HG23	1.99	0.44
2:B:30:TYR:CE1	2:B:44:LEU:HG	2.53	0.43
2:B:45:LEU:HD13	2:B:47:ILE:CD1	2.47	0.43
2:B:37:ARG:HA	2:B:37:ARG:HD3	1.88	0.43
1:A:115:ILE:HD11	1:A:158:LEU:HD11	2.00	0.43
1:A:120:LYS:NZ	1:A:126:GLN:CD	2.71	0.43
1:A:181:ASP:HA	1:A:208:ARG:NH2	2.34	0.43
1:A:293:ALA:HB3	1:A:294:PRO:HD3	2.01	0.43
1:A:98:ASN:HB2	5:A:997:HOH:O	2.19	0.42
1:A:135:GLU:CG	1:A:135:GLU:H	2.33	0.42
2:B:49:LYS:HD2	2:C:49:LYS:HD2	2.01	0.42
2:C:102:ASN:OD1	3:C:701:NDG:C1	2.64	0.42
2:C:101:THR:HB	3:C:701:NDG:H8C3	2.02	0.42
1:A:304:VAL:O	1:A:306:LEU:HD22	2.20	0.42
1:A:30:ILE:HD13	1:A:283:PHE:CB	2.50	0.42
2:C:134:GLU:HA	2:C:134:GLU:OE1	2.20	0.41
2:C:57:ASP:CG	2:C:58:LYS:HD3	2.41	0.41
2:B:15:ILE:HD12	5:B:906:HOH:O	2.20	0.41
2:C:77:VAL:HG13	5:C:754:HOH:O	2.21	0.41
1:A:300:LEU:CD1	5:A:1044:HOH:O	2.68	0.41
2:B:10:ILE:O	2:B:10:ILE:HG23	2.21	0.41
1:A:201:TYR:HA	1:A:246:ALA:HB2	2.02	0.40
2:C:41:GLU:HG2	2:C:58:LYS:HE3	2.03	0.40
2:B:22:ILE:HG21	2:B:56:TRP:CZ2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:SER:HB3	5:B:944:HOH:O	2.21	0.40

All (1) 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)
5:C:757:HOH:O	5:C:757:HOH:O[4_555]	1.41	0.79

## 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	305/308 (99%)	298 (98%)	7 (2%)	0	100	100
2	B	127/134 (95%)	123 (97%)	2 (2%)	2 (2%)	12	3
2	C	132/134 (98%)	128 (97%)	2 (2%)	2 (2%)	13	3
All	All	564/576 (98%)	549 (97%)	11 (2%)	4 (1%)	26	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	120	GLY
2	C	120	GLY
2	B	33	SER
2	C	33	SER

### 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	255/257 (99%)	243 (95%)	12 (5%)	32	23
2	B	112/117 (96%)	110 (98%)	2 (2%)	66	62
2	C	117/117 (100%)	114 (97%)	3 (3%)	54	47
All	All	484/491 (99%)	467 (96%)	17 (4%)	43	35

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	50	GLN
1	A	135	GLU
1	A	144	ASN
1	A	168	GLN
1	A	189	ASN
1	A	225	ASN
1	A	233	GLN
1	A	297	HIS
1	A	298	GLN
1	A	300	LEU
1	A	304	VAL
2	B	45	LEU
2	B	74	GLU
2	C	14	ARG
2	C	29	ARG
2	C	87	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	168	GLN
1	A	225	ASN
1	A	264	ASN
1	A	288	GLN
1	A	298	GLN
2	B	91	HIS
2	B	102	ASN
2	B	108	ASN

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Mol	Chain	Res	Type
2	B	117	ASN
2	C	91	HIS
2	C	102	ASN
2	C	114	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 4 ligands modelled in this entry, 2 are 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	$\# Z  > 2$
3	NDG	B	702	-	15,15,15	0.57	0	17,21,21	0.78	1 (5%)
3	NDG	C	701	-	15,15,15	0.67	0	17,21,21	0.81	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
3	NDG	B	702	-	-	0/6/26/26	0/1/1/1
3	NDG	C	701	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	B	702	NDG	C4-C3-C2	2.06	113.29	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	NDG	3	0
3	C	701	NDG	10	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

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.