



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:57 AM GMT

PDB ID : 2VE7
Title : CRYSTAL STRUCTURE OF A BONSAI VERSION OF THE HUMAN NDC80 COMPLEX
Authors : Ciferri, C.; Pasqualato, S.; Dos Reis, G.; Screpanti, E.; Maiolica, A.; Polka, J.; De Luca, J.G.; De Wulf, P.; Salek, M.; Rappsilber, J.; Moores, C.A.; Salmon, E.D.; Musacchio, A.
Deposited on : 2007-10-17
Resolution : 2.88 Å(reported)

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

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

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

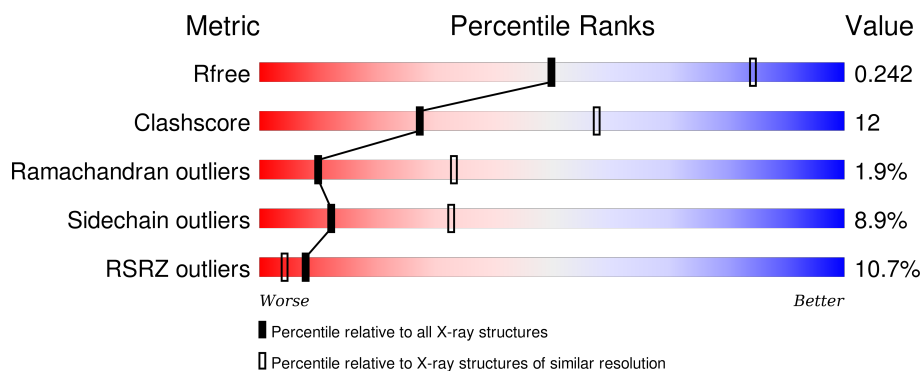
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	315	<div> <div>13%</div> <div>61%13%•22%</div> </div>
1	B	315	<div> <div>7%</div> <div>72%19%••</div> </div>
2	C	250	<div> <div>12%</div> <div>61%21%6%12%</div> </div>
2	D	250	<div> <div>6%</div> <div>69%23%•••</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	2222	-	-	-	X
3	GOL	B	2225	-	-	-	X
4	IPH	D	2198	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8258 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 KINETOCHORE PROTEIN HEC1, KINETOCHORE PROTEIN SPC25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1980	1265	331	373	11			
1	B	303	Total	C	N	O	S	0	0	0
			2447	1566	406	462	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	MET	-	EXPRESSION TAG	UNP Q9HBM1
B	79	MET	-	EXPRESSION TAG	UNP Q9HBM1
A	1224	GLN	ASN	CONFLICT	UNP Q9HBM1
B	1224	GLN	ASN	CONFLICT	UNP Q9HBM1

- Molecule 2 is a protein called KINETOCHORE PROTEIN NUF2, KINETOCHORE PROTEIN SPC24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	219	Total	C	N	O	S	0	0	0
			1800	1168	303	315	14			
2	D	242	Total	C	N	O	S	0	0	0
			1983	1279	333	357	14			

There are 14 discrepancies between the modelled and reference sequences:

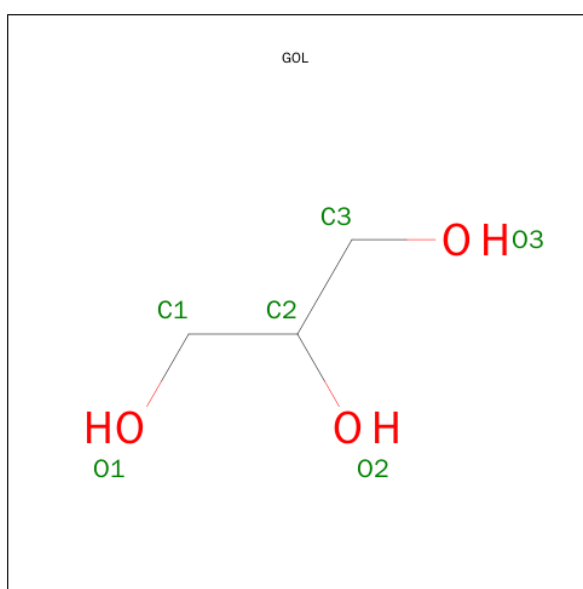
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	EXPRESSION TAG	UNP Q8NBT2
C	-3	PRO	-	EXPRESSION TAG	UNP Q8NBT2
C	-2	LEU	-	EXPRESSION TAG	UNP Q8NBT2
C	-1	GLY	-	EXPRESSION TAG	UNP Q8NBT2
C	0	SER	-	EXPRESSION TAG	UNP Q8NBT2
D	-4	GLY	-	EXPRESSION TAG	UNP Q8NBT2

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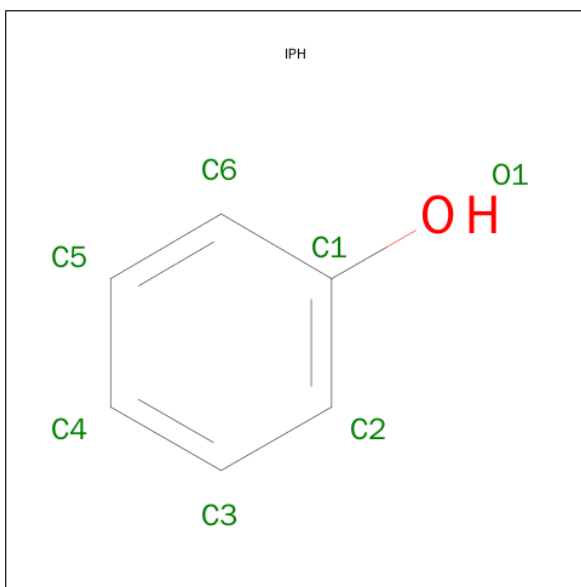
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	PRO	-	EXPRESSION TAG	UNP Q8NBT2
D	-2	LEU	-	EXPRESSION TAG	UNP Q8NBT2
D	-1	GLY	-	EXPRESSION TAG	UNP Q8NBT2
D	0	SER	-	EXPRESSION TAG	UNP Q8NBT2
C	1152	GLU	ASP	CONFLICT	UNP Q8NBT2
D	1152	GLU	ASP	CONFLICT	UNP Q8NBT2
C	72	GLY	GLU	ENGINEERED MUTATION	UNP Q9BZD4
D	72	GLY	GLU	ENGINEERED MUTATION	UNP Q9BZD4

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is PHENOL (three-letter code: IPH) (formula: C₆H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			7	6	1		
4	D	1	Total	C	O	0	0
			7	6	1		

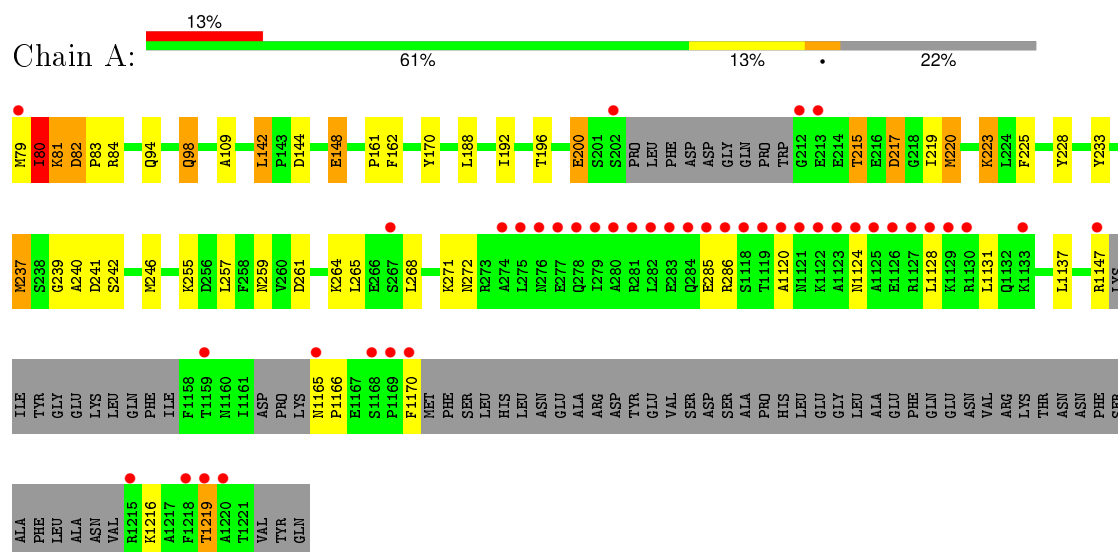
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	10	Total	O	0	0
			10	10		
5	C	3	Total	O	0	0
			3	3		
5	D	4	Total	O	0	0
			4	4		

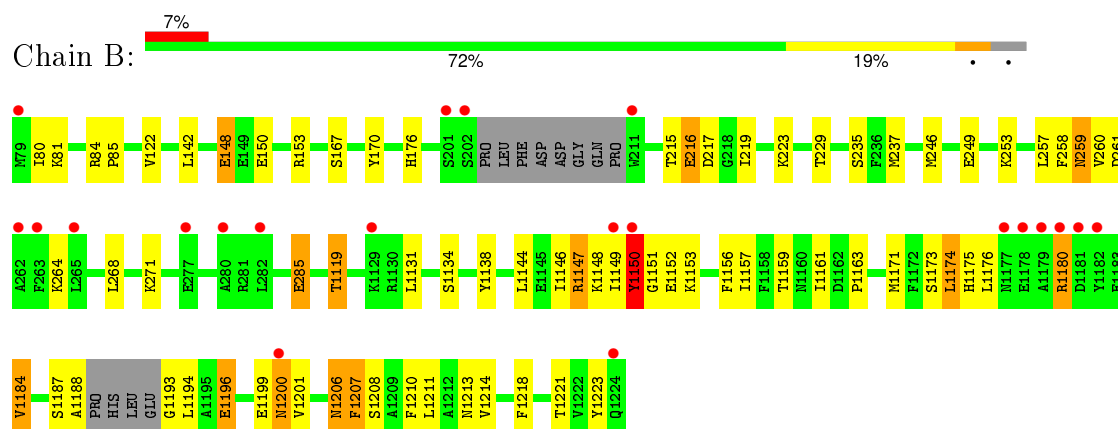
3 Residue-property plots [i](#)

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.

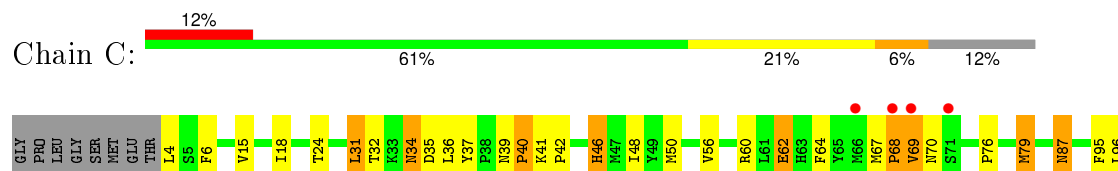
- Molecule 1: KINETOCHORE PROTEIN HEC1, KINETOCHORE PROTEIN SPC25

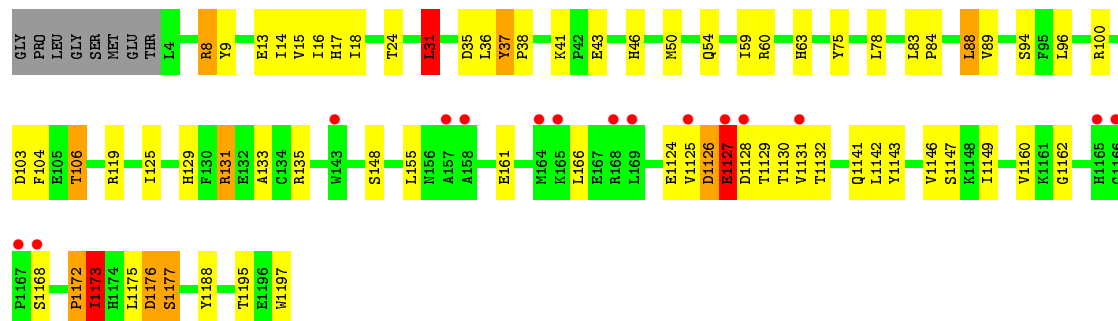


- Molecule 1: KINETOCHORE PROTEIN HEC1, KINETOCHORE PROTEIN SPC25



- Molecule 2: KINETOCHORE PROTEIN NUF2, KINETOCHORE PROTEIN SPC24





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	157.65Å 248.97Å 58.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.88 30.53 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.88) 98.0 (30.53-2.87)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.261 0.245 , 0.242	Depositor DCC
R_{free} test set	2669 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 52709 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8258	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.77	3/2020 (0.1%)	0.78	4/2718 (0.1%)
1	B	0.67	3/2499 (0.1%)	0.68	0/3366
2	C	0.63	1/1848 (0.1%)	0.63	0/2500
2	D	0.67	3/2037 (0.1%)	0.68	1/2763 (0.0%)
All	All	0.69	10/8404 (0.1%)	0.70	5/11347 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1199	GLU	CD-OE2	8.26	1.34	1.25
1	B	1199	GLU	CD-OE1	7.80	1.34	1.25
1	A	286	ARG	CZ-NH1	7.31	1.42	1.33
2	D	161	GLU	CD-OE2	6.59	1.32	1.25
1	A	1170	PHE	CG-CD1	6.40	1.48	1.38
2	D	161	GLU	CD-OE1	6.38	1.32	1.25
2	C	1154	GLU	CD-OE1	6.18	1.32	1.25
1	A	1170	PHE	CE2-CZ	5.73	1.48	1.37
2	D	1127	GLU	C-O	5.30	1.33	1.23
1	B	1193	GLY	N-CA	5.23	1.53	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1147	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	A	1147	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	A	286	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	80	ILE	N-CA-C	-6.11	94.50	111.00
2	D	31	LEU	CA-CB-CG	5.23	127.32	115.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	82	ASP	CA
1	A	237	MET	CA

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	1980	0	1943	57	0
1	B	2447	0	2403	56	0
2	C	1800	0	1792	50	0
2	D	1983	0	1959	52	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	C	7	0	6	3	0
4	D	7	0	6	1	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
5	C	3	0	0	0	0
5	D	4	0	0	0	0
All	All	8258	0	8125	194	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 12.

All (194) 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:240:ALA:HB1	1:A:241:ASP:CA	1.49	1.42
1:A:240:ALA:CB	1:A:241:ASP:HA	1.44	1.41
1:A:82:ASP:HB2	1:A:83:PRO:CD	1.69	1.20
1:A:82:ASP:CB	1:A:83:PRO:HD2	1.87	1.04
2:D:35:ASP:HB2	2:D:41:LYS:HD2	1.40	1.03
1:A:82:ASP:HB2	1:A:83:PRO:HD2	1.04	1.02
1:A:82:ASP:CB	1:A:83:PRO:CD	2.36	0.98
1:B:1153:LYS:HD2	1:B:1184:VAL:HG11	1.48	0.95
1:B:1149:ILE:O	1:B:1150:TYR:HD2	1.53	0.91
1:A:109:ALA:H	1:B:176:HIS:HD2	1.15	0.90
1:B:1153:LYS:CD	1:B:1184:VAL:HG11	2.00	0.90
2:D:35:ASP:CB	2:D:41:LYS:HD2	2.05	0.87
1:A:81:LYS:HD3	1:A:81:LYS:H	1.42	0.85
1:A:80:ILE:HG13	1:A:81:LYS:HA	1.57	0.84
2:D:37:TYR:CD2	2:D:37:TYR:C	2.51	0.81
2:D:8:ARG:HG2	2:D:8:ARG:HH11	1.45	0.81
1:A:79:MET:O	1:A:80:ILE:C	2.19	0.81
1:A:81:LYS:O	1:A:83:PRO:HD3	1.82	0.80
1:A:82:ASP:HB3	1:A:162:PHE:CZ	2.19	0.78
1:B:1149:ILE:O	1:B:1150:TYR:CD2	2.37	0.78
2:D:133:ALA:HB1	4:D:2198:IPH:H5	1.68	0.76
1:A:215:THR:HG22	1:A:219:ILE:H	1.51	0.76
2:C:137:THR:HG21	4:C:2194:IPH:C5	2.16	0.74
2:C:1161:LYS:HD3	2:C:1174:HIS:HD2	1.52	0.74
2:C:137:THR:HG21	4:C:2194:IPH:C6	2.19	0.72
2:D:1125:VAL:HG22	2:D:1126:ASP:H	1.55	0.72
1:B:1180:ARG:CG	1:B:1180:ARG:HH11	2.03	0.71
1:A:1165:ASN:N	1:A:1166:PRO:HD3	2.06	0.71
2:C:103:ASP:OD2	2:C:119:ARG:NH2	2.26	0.69
1:B:80:ILE:HG23	1:B:81:LYS:H	1.56	0.68
1:A:81:LYS:H	1:A:81:LYS:CD	2.00	0.68
1:A:148:GLU:HG2	1:A:170:TYR:CZ	2.29	0.68
2:D:103:ASP:OD2	2:D:119:ARG:NH2	2.27	0.68
1:B:1180:ARG:HG3	1:B:1180:ARG:HH11	1.59	0.67
1:A:220:MET:HE2	2:C:142:LEU:HD21	1.75	0.67
1:B:229:THR:HG21	2:D:131:ARG:HB3	1.76	0.67
2:D:37:TYR:HD2	2:D:37:TYR:C	1.97	0.66
2:C:69:VAL:HG23	2:C:70:ASN:H	1.60	0.66
1:B:1153:LYS:HD2	1:B:1184:VAL:CG1	2.24	0.66
1:A:217:ASP:OD2	2:C:131:ARG:NH1	2.28	0.66
2:D:15:VAL:HG13	2:D:31:LEU:HD13	1.77	0.65
1:B:148:GLU:HG2	1:B:170:TYR:CZ	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1179:GLN:O	2:C:1180:LEU:HD13	1.97	0.65
1:A:109:ALA:H	1:B:176:HIS:CD2	2.07	0.64
1:B:1211:LEU:HD22	2:D:1146:VAL:HG11	1.80	0.64
1:A:82:ASP:OD1	1:A:84:ARG:NE	2.29	0.64
1:B:1152:GLU:HG2	1:B:1153:LYS:HG3	1.80	0.63
1:B:1153:LYS:HD3	1:B:1184:VAL:HG11	1.78	0.63
2:D:1127:GLU:O	2:D:1132:THR:HG23	1.98	0.63
1:B:219:ILE:HD11	2:D:135:ARG:HG3	1.82	0.62
1:A:215:THR:HG23	1:A:217:ASP:H	1.65	0.62
1:B:1157:ILE:HG13	1:B:1171:MET:HB3	1.82	0.62
2:D:9:TYR:HB2	2:D:14:ILE:HG13	1.81	0.62
2:C:42:PRO:O	2:C:46:HIS:ND1	2.33	0.61
2:D:35:ASP:HB2	2:D:41:LYS:CD	2.26	0.61
2:C:76:PRO:O	2:C:79:MET:HB2	2.00	0.61
2:C:37:TYR:C	2:C:37:TYR:CD2	2.74	0.61
1:A:82:ASP:OD1	1:A:84:ARG:NH1	2.32	0.61
1:A:80:ILE:CG2	1:A:80:ILE:O	2.48	0.61
2:D:8:ARG:HG2	2:D:8:ARG:NH1	2.09	0.61
1:B:1148:LYS:HD3	1:B:1148:LYS:O	2.01	0.60
1:A:219:ILE:HD11	2:C:135:ARG:HG3	1.84	0.60
1:A:79:MET:N	1:A:161:PRO:HB3	2.16	0.59
2:D:84:PRO:O	2:D:88:LEU:HB2	2.01	0.59
2:D:60:ARG:H	2:D:63:HIS:CD2	2.21	0.58
1:B:1207:PHE:HB3	2:D:1146:VAL:HG22	1.85	0.58
2:D:1175:LEU:HD11	2:D:1188:TYR:CD1	2.39	0.58
1:A:79:MET:C	1:A:80:ILE:O	2.36	0.58
2:C:96:LEU:HD13	2:C:104:PHE:CD1	2.39	0.58
2:C:69:VAL:HG23	2:C:70:ASN:N	2.18	0.57
2:D:46:HIS:HD2	2:D:50:MET:CE	2.17	0.57
2:D:1173:ILE:O	2:D:1173:ILE:HG12	2.03	0.57
1:B:1153:LYS:HG2	1:B:1175:HIS:HB3	1.85	0.57
1:A:237:MET:HE3	2:C:4:LEU:HB3	1.87	0.57
1:A:268:LEU:HA	1:A:271:LYS:HB3	1.87	0.57
2:C:39:ASN:O	2:C:40:PRO:C	2.41	0.57
1:A:80:ILE:O	1:A:80:ILE:HG23	2.03	0.57
1:A:219:ILE:HD13	1:A:225:PHE:CE2	2.39	0.57
2:C:1156:GLU:HB3	2:C:1157:PRO:CD	2.34	0.56
1:A:215:THR:HG21	1:A:219:ILE:HD12	1.87	0.56
2:C:64:PHE:HA	2:C:87:ASN:HD22	1.71	0.56
2:C:1190:TRP:O	2:C:1193:VAL:HG12	2.05	0.56
2:D:37:TYR:CD2	2:D:38:PRO:N	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ASP:HB2	1:A:264:LYS:H	1.70	0.56
1:A:81:LYS:N	1:A:81:LYS:CD	2.69	0.55
2:C:1161:LYS:HD3	2:C:1174:HIS:CD2	2.36	0.55
1:B:150:GLU:OE2	1:B:153:ARG:NH1	2.39	0.55
1:B:216:GLU:HG2	1:B:216:GLU:O	2.07	0.55
2:D:1130:THR:HG23	2:D:1131:VAL:HG23	1.88	0.54
2:C:1160:VAL:HG22	2:C:1175:LEU:HB2	1.90	0.54
2:D:18:ILE:HG13	2:D:125:ILE:HD11	1.90	0.54
1:B:1148:LYS:CD	1:B:1148:LYS:O	2.56	0.54
1:A:94:GLN:O	1:A:98:GLN:HG2	2.07	0.54
1:A:1165:ASN:N	1:A:1166:PRO:CD	2.71	0.54
1:A:200:GLU:OE2	1:B:122:VAL:N	2.37	0.53
1:B:1180:ARG:NH1	1:B:1180:ARG:HG3	2.24	0.53
1:B:259:ASN:HB3	1:B:264:LYS:HE2	1.91	0.52
1:B:285:GLU:HA	1:B:1119:THR:HG22	1.92	0.52
2:D:46:HIS:CD2	2:D:50:MET:CE	2.92	0.52
2:D:75:TYR:CB	2:D:78:LEU:HD12	2.39	0.52
1:B:1146:ILE:HG22	1:B:1156:PHE:CD1	2.45	0.52
2:C:103:ASP:CG	2:C:119:ARG:HH22	2.13	0.51
2:C:1133:ILE:C	2:C:1135:SER:H	2.14	0.51
1:B:1146:ILE:HG12	2:D:1143:TYR:CZ	2.45	0.51
2:C:39:ASN:O	2:C:40:PRO:O	2.29	0.50
1:A:265:LEU:HD21	2:C:151:LYS:HD2	1.94	0.50
2:C:6:PHE:HB2	2:C:126:ASN:ND2	2.27	0.50
1:B:1173:SER:HB2	1:B:1184:VAL:HG13	1.94	0.50
1:B:80:ILE:HG23	1:B:81:LYS:HG2	1.94	0.50
2:D:46:HIS:HD2	2:D:50:MET:HE3	1.76	0.49
1:A:109:ALA:N	1:B:176:HIS:HD2	1.97	0.49
1:A:228:TYR:OH	4:C:2194:IPH:H4	2.13	0.49
1:B:1156:PHE:CD1	1:B:1211:LEU:HD21	2.48	0.49
1:B:1206:ASN:HD21	1:B:1208:SER:HB2	1.77	0.49
1:A:1120:ALA:O	1:A:1124:ASN:ND2	2.45	0.49
1:A:237:MET:CE	2:C:4:LEU:HB3	2.42	0.49
1:B:268:LEU:HD12	1:B:271:LYS:HD3	1.95	0.48
1:B:258:PHE:O	1:B:260:VAL:N	2.46	0.48
2:D:1128:ASP:HB3	2:D:1132:THR:OG1	2.14	0.48
2:C:35:ASP:HA	2:C:41:LYS:HG3	1.95	0.48
2:D:1176:ASP:O	2:D:1177:SER:CB	2.62	0.47
1:B:215:THR:HG22	1:B:217:ASP:H	1.79	0.47
2:D:37:TYR:CG	2:D:38:PRO:HA	2.49	0.47
1:A:240:ALA:CB	1:A:241:ASP:CA	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:ILE:HD13	2:C:48:ILE:HD13	1.96	0.47
2:C:99:CYS:O	2:C:100:ARG:HB2	2.15	0.46
1:A:81:LYS:N	1:A:81:LYS:HD3	2.22	0.46
1:B:1210:PHE:O	1:B:1214:VAL:HG23	2.16	0.46
1:B:237:MET:HG2	2:D:100:ARG:HD2	1.97	0.46
2:D:1128:ASP:CB	2:D:1132:THR:OG1	2.64	0.46
2:C:139:MET:O	2:C:143:TRP:CD1	2.69	0.46
2:D:1125:VAL:HG22	2:D:1126:ASP:N	2.27	0.46
2:C:1179:GLN:CG	2:C:1179:GLN:O	2.64	0.46
2:D:50:MET:O	2:D:54:GLN:HG3	2.16	0.45
2:D:35:ASP:HB3	2:D:41:LYS:HD2	1.95	0.45
1:B:1206:ASN:ND2	1:B:1208:SER:HB2	2.31	0.45
1:A:82:ASP:OD1	1:A:84:ARG:CZ	2.64	0.45
1:A:188:LEU:O	1:A:192:ILE:HG13	2.16	0.45
1:B:1187:SER:O	1:B:1188:ALA:HB3	2.16	0.45
2:C:50:MET:HG2	2:C:64:PHE:CD2	2.51	0.45
2:C:32:THR:O	2:C:35:ASP:OD1	2.35	0.45
2:C:67:MET:HA	2:C:68:PRO:HD2	1.80	0.45
1:A:268:LEU:HB3	2:C:155:LEU:HD12	1.99	0.45
1:B:249:GLU:HG2	1:B:253:LYS:HE3	1.99	0.45
2:D:9:TYR:HB3	2:D:13:GLU:HB2	1.99	0.45
1:B:148:GLU:HG2	1:B:170:TYR:CE2	2.51	0.44
1:A:255:LYS:HG3	2:C:145:TYR:CE1	2.52	0.44
2:C:164:MET:HA	2:C:164:MET:CE	2.47	0.44
1:A:81:LYS:O	1:A:83:PRO:CD	2.61	0.44
2:D:35:ASP:HB3	2:D:41:LYS:NZ	2.33	0.44
2:D:1176:ASP:O	2:D:1177:SER:HB3	2.18	0.44
1:B:1153:LYS:HB2	1:B:1153:LYS:HZ2	1.83	0.43
1:B:215:THR:HB	1:B:219:ILE:HB	2.00	0.43
2:C:62:GLU:CD	2:C:62:GLU:H	2.21	0.43
1:A:1137:LEU:HD23	2:C:1151:TRP:CD1	2.53	0.43
1:B:1156:PHE:HE2	1:B:1174:LEU:HD22	1.82	0.43
2:C:15:VAL:HG13	2:C:31:LEU:HD13	1.99	0.43
2:C:1133:ILE:N	2:C:1134:PRO:HD2	2.34	0.43
1:B:1200:ASN:N	1:B:1200:ASN:OD1	2.51	0.43
2:D:103:ASP:CG	2:D:119:ARG:HH22	2.22	0.43
1:B:1161:ILE:O	1:B:1163:PRO:HD3	2.19	0.43
2:D:1147:SER:O	2:D:1149:ILE:HG23	2.18	0.43
2:C:34:ASN:OD1	2:C:34:ASN:N	2.51	0.43
1:B:258:PHE:O	1:B:259:ASN:C	2.56	0.43
2:D:1162:GLY:O	2:D:1172:PRO:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1149:ILE:HG23	2:C:1164:HIS:HD2	1.84	0.43
1:A:219:ILE:HD13	1:A:225:PHE:CD2	2.54	0.42
2:D:96:LEU:CD1	2:D:104:PHE:CD1	3.02	0.42
2:C:151:LYS:O	2:C:155:LEU:HB2	2.19	0.42
1:B:1218:PHE:O	1:B:1221:THR:HB	2.18	0.42
1:A:142:LEU:CD2	1:A:142:LEU:H	2.33	0.42
2:D:1124:GLU:HG2	2:D:1125:VAL:O	2.20	0.42
2:D:96:LEU:HD23	2:D:96:LEU:HA	1.89	0.42
1:A:1128:LEU:HA	1:A:1131:LEU:HG	2.02	0.42
2:D:75:TYR:HB3	2:D:78:LEU:HD12	2.01	0.42
1:A:223:LYS:C	1:A:223:LYS:HD3	2.40	0.42
2:C:96:LEU:HD13	2:C:104:PHE:CG	2.54	0.42
1:B:1176:LEU:HB2	1:B:1180:ARG:HA	2.01	0.42
2:C:87:ASN:OD1	2:C:87:ASN:N	2.52	0.42
1:B:1213:ASN:OD1	2:D:1195:THR:HG23	2.19	0.42
2:C:56:VAL:HG21	2:C:95:PHE:CE1	2.54	0.42
1:A:80:ILE:HA	1:A:162:PHE:HE1	1.85	0.42
1:A:259:ASN:O	1:A:264:LYS:HD3	2.20	0.42
2:D:89:VAL:HG21	2:D:106:THR:HG22	2.01	0.41
1:B:1147:ARG:H	1:B:1147:ARG:HG2	1.73	0.41
2:D:17:HIS:ND1	2:D:129:HIS:HE1	2.19	0.41
2:C:105:GLU:HG2	2:C:108:ASP:OD2	2.19	0.41
2:D:8:ARG:CG	2:D:8:ARG:HH11	2.25	0.41
2:C:142:LEU:O	2:C:142:LEU:HG	2.20	0.41
1:A:1216:LYS:HA	1:A:1219:THR:HG22	2.01	0.41
1:B:1134:SER:O	1:B:1138:TYR:HD1	2.04	0.41
1:B:260:VAL:HG21	2:D:148:SER:HB3	2.03	0.41
1:B:84:ARG:HA	1:B:85:PRO:HD3	1.78	0.41
1:A:98:GLN:H	1:A:98:GLN:HG2	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	236/315 (75%)	228 (97%)	7 (3%)	1 (0%)	39	73
1	B	297/315 (94%)	269 (91%)	21 (7%)	7 (2%)	7	27
2	C	213/250 (85%)	188 (88%)	21 (10%)	4 (2%)	10	33
2	D	240/250 (96%)	221 (92%)	12 (5%)	7 (3%)	6	21
All	All	986/1130 (87%)	906 (92%)	61 (6%)	19 (2%)	10	33

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1150	TYR
1	B	1223	TYR
1	B	259	ASN
1	B	1151	GLY
2	D	1176	ASP
2	C	69	VAL
2	C	1156	GLU
2	D	1127	GLU
2	D	1129	THR
2	D	1168	SER
1	A	239	GLY
1	B	261	ASP
1	B	1196	GLU
2	D	1177	SER
2	C	40	PRO
2	C	68	PRO
2	D	1172	PRO
2	D	1173	ILE
1	B	1184	VAL

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	215/279 (77%)	194 (90%)	21 (10%)	10	27
1	B	266/279 (95%)	243 (91%)	23 (9%)	13	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	199/226 (88%)	184 (92%)	15 (8%)	17	42
2	D	220/226 (97%)	199 (90%)	21 (10%)	11	29
All	All	900/1010 (89%)	820 (91%)	80 (9%)	12	33

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ILE
1	A	81	LYS
1	A	82	ASP
1	A	98	GLN
1	A	142	LEU
1	A	144	ASP
1	A	148	GLU
1	A	196	THR
1	A	200	GLU
1	A	215	THR
1	A	217	ASP
1	A	220	MET
1	A	223	LYS
1	A	233	TYR
1	A	237	MET
1	A	242	SER
1	A	246	MET
1	A	257	LEU
1	A	272	ASN
1	A	285	GLU
1	A	1219	THR
1	B	142	LEU
1	B	148	GLU
1	B	167	SER
1	B	216	GLU
1	B	223	LYS
1	B	235	SER
1	B	246	MET
1	B	257	LEU
1	B	285	GLU
1	B	1119	THR
1	B	1131	LEU
1	B	1144	LEU
1	B	1147	ARG

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Mol	Chain	Res	Type
1	B	1150	TYR
1	B	1159	THR
1	B	1174	LEU
1	B	1180	ARG
1	B	1194	LEU
1	B	1196	GLU
1	B	1200	ASN
1	B	1201	VAL
1	B	1206	ASN
1	B	1207	PHE
2	C	24	THR
2	C	31	LEU
2	C	34	ASN
2	C	36	LEU
2	C	46	HIS
2	C	60	ARG
2	C	62	GLU
2	C	79	MET
2	C	87	ASN
2	C	131	ARG
2	C	137	THR
2	C	146	LYS
2	C	155	LEU
2	C	164	MET
2	C	1180	LEU
2	D	8	ARG
2	D	16	ILE
2	D	24	THR
2	D	31	LEU
2	D	36	LEU
2	D	37	TYR
2	D	43	GLU
2	D	59	ILE
2	D	83	LEU
2	D	88	LEU
2	D	94	SER
2	D	106	THR
2	D	131	ARG
2	D	155	LEU
2	D	166	LEU
2	D	1126	ASP
2	D	1141	GLN

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Mol	Chain	Res	Type
2	D	1142	LEU
2	D	1160	VAL
2	D	1173	ILE
2	D	1197	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	110	HIS
1	A	1160	ASN
1	B	98	GLN
1	B	106	ASN
1	B	176	HIS
1	B	1206	ASN
2	C	17	HIS
2	C	39	ASN
2	C	63	HIS
2	C	126	ASN
2	C	129	HIS
2	C	1144	HIS
2	C	1164	HIS
2	C	1174	HIS
2	D	46	HIS
2	D	63	HIS
2	D	129	HIS
2	D	144	GLN
2	D	153	GLN
2	D	154	GLN
2	D	1144	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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	GOL	A	2222	-	5,5,5	0.22	0	5,5,5	0.37	0
3	GOL	B	2225	-	5,5,5	0.23	0	5,5,5	0.42	0
4	IPH	C	2194	-	7,7,7	0.50	0	8,8,8	0.34	0
4	IPH	D	2198	-	7,7,7	0.58	0	8,8,8	0.64	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	GOL	A	2222	-	-	0/4/4/4	0/0/0/0
3	GOL	B	2225	-	-	0/4/4/4	0/0/0/0
4	IPH	C	2194	-	-	0/0/0/0	0/1/1/1
4	IPH	D	2198	-	-	0/0/0/0	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2194	IPH	3	0
4	D	2198	IPH	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, 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	246/315 (78%)	0.65	42 (17%) 2 1	10, 52, 153, 176	0
1	B	303/315 (96%)	0.34	21 (6%) 20 15	12, 56, 131, 162	0
2	C	219/250 (87%)	0.64	30 (13%) 4 2	19, 48, 164, 233	0
2	D	242/250 (96%)	0.33	15 (6%) 24 18	17, 50, 125, 155	0
All	All	1010/1130 (89%)	0.48	108 (10%) 8 4	10, 52, 143, 233	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1125	ALA	7.8
1	A	1128	LEU	7.6
2	C	1155	CYS	7.4
1	A	1129	LYS	7.0
1	A	1169	PRO	6.5
1	A	1126	GLU	6.4
2	C	1157	PRO	6.3
1	A	1124	ASN	6.2
2	C	1133	ILE	5.9
1	B	202	SER	5.4
1	A	277	GLU	5.4
1	A	1123	ALA	4.9
2	C	161	GLU	4.9
1	B	79	MET	4.8
2	C	164	MET	4.8
2	C	157	ALA	4.8
1	B	263	PHE	4.7
2	C	163	LEU	4.7
1	A	1119	THR	4.6
1	B	1177	ASN	4.6
1	B	1180	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	1181	ASP	4.4
2	C	1193	VAL	4.4
1	A	1120	ALA	4.3
2	C	158	ALA	4.3
1	A	1219	THR	4.2
1	A	285	GLU	4.1
1	A	278	GLN	4.1
1	B	1224	GLN	4.1
2	C	159	HIS	4.1
2	C	1179	GLN	4.0
2	D	1125	VAL	4.0
1	A	1121	ASN	4.0
1	A	1127	ARG	4.0
1	B	1178	GLU	3.9
2	C	1171	GLN	3.9
1	A	286	ARG	3.9
1	A	282	LEU	3.8
1	B	211	TRP	3.7
2	C	1138	TYR	3.7
1	B	265	LEU	3.7
1	A	276	ASN	3.6
1	A	1168	SER	3.6
2	D	1168	SER	3.5
1	A	1130	ARG	3.5
2	C	143	TRP	3.4
1	A	274	ALA	3.4
2	C	162	ALA	3.4
1	B	262	ALA	3.3
2	C	1143	TYR	3.2
1	A	212	GLY	3.2
2	D	1165	HIS	3.2
1	B	280	ALA	3.2
2	D	143	TRP	3.2
1	A	281	ARG	3.2
1	A	1133	LYS	3.1
2	C	1156	GLU	3.0
1	A	213	GLU	3.0
2	D	165	LYS	3.0
2	D	1166	GLY	2.9
2	C	160	GLN	2.9
2	C	154	GLN	2.9
2	C	1134	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	201	SER	2.9
1	B	282	LEU	2.9
2	D	1127	GLU	2.8
1	A	279	ILE	2.8
2	D	164	MET	2.8
1	A	1170	PHE	2.8
1	B	1182	TYR	2.7
1	A	1215	ARG	2.7
2	C	1146	VAL	2.7
1	A	1218	PHE	2.7
1	A	1118	SER	2.6
2	C	1137	VAL	2.6
1	A	284	GLN	2.6
1	B	1179	ALA	2.6
1	A	283	GLU	2.6
1	A	1122	LYS	2.5
1	B	277	GLU	2.5
1	A	202	SER	2.4
2	C	66	MET	2.4
2	C	165	LYS	2.4
1	A	79	MET	2.4
2	C	1163	ILE	2.4
2	D	1128	ASP	2.4
1	A	1159	THR	2.4
2	C	167	GLU	2.4
1	A	267	SER	2.3
1	B	1200	ASN	2.3
2	C	166	LEU	2.3
2	C	69	VAL	2.3
1	A	280	ALA	2.3
1	A	1165	ASN	2.2
2	D	157	ALA	2.2
2	D	1167	PRO	2.2
1	B	1150	TYR	2.2
1	A	275	LEU	2.1
1	B	1149	ILE	2.1
1	A	1220	ALA	2.1
2	C	71	SER	2.1
1	B	1129	LYS	2.1
2	D	169	LEU	2.1
2	D	158	ALA	2.1
2	D	168	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1147	ARG	2.0
2	D	1131	VAL	2.0
2	C	68	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	A	2222	6/6	0.88	0.27	4.33	63,66,66,67	0
4	IPH	D	2198	7/7	0.93	0.26	2.62	54,56,57,57	0
3	GOL	B	2225	6/6	0.88	0.27	2.56	68,70,70,71	0
4	IPH	C	2194	7/7	0.94	0.22	0.91	44,45,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.