



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:37 PM GMT

PDB ID : 1PVH  
Title : Crystal structure of leukemia inhibitory factor in complex with gp130  
Authors : Boulanger, M.J.; Bankovich, A.J.; Kortemme, T.; Baker, D.; Garcia, K.C.  
Deposited on : 2003-06-27  
Resolution : 2.50 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.

---

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

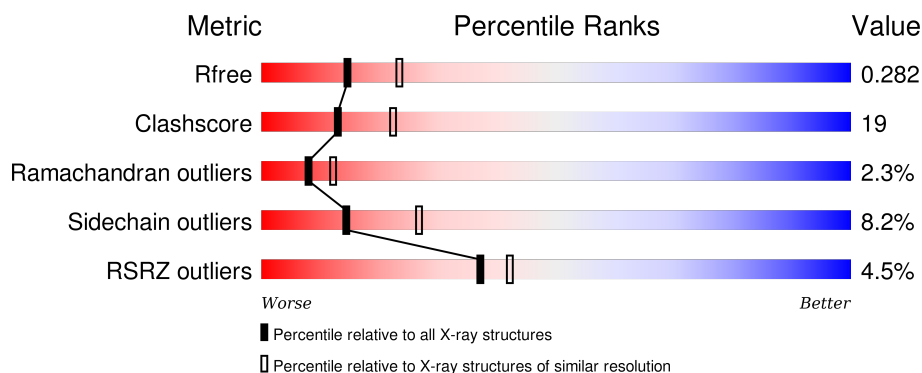
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	201	<div> <div>7%</div> <div>68%</div> <div>29%</div> <div>.</div> </div>
1	C	201	<div> <div>3%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
2	B	169	<div> <div>3%</div> <div>60%</div> <div>31%</div> <div>9%</div> <div>.</div> </div>
2	D	169	<div> <div>4%</div> <div>56%</div> <div>36%</div> <div>8%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6026 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 Interleukin-6 receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1624	1031	269	317	7			
1	C	201	Total	C	N	O	S	0	0	0
			1624	1031	269	317	7			

- Molecule 2 is a protein called Leukemia inhibitory factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	4	0	0
			1292	823	232	230	7			
2	D	169	Total	C	N	O	S	4	0	0
			1292	823	232	230	7			

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	I	0	0
			1	1		
3	D	1	Total	I	0	0
			1	1		

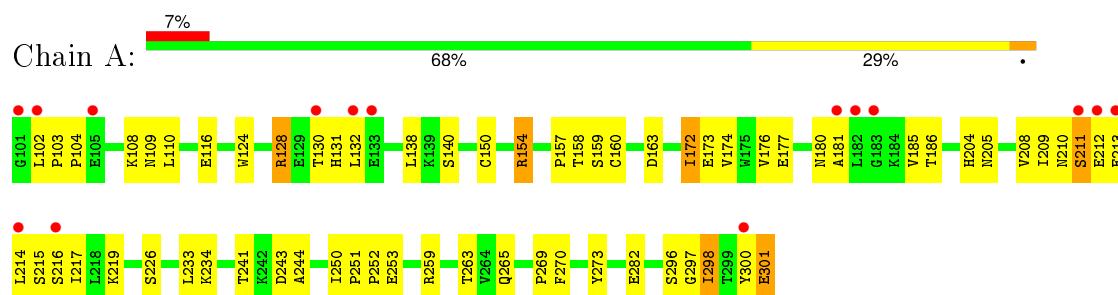
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	33	Total	O	0	0
			33	33		
4	C	61	Total	O	0	0
			61	61		
4	D	27	Total	O	0	0
			27	27		

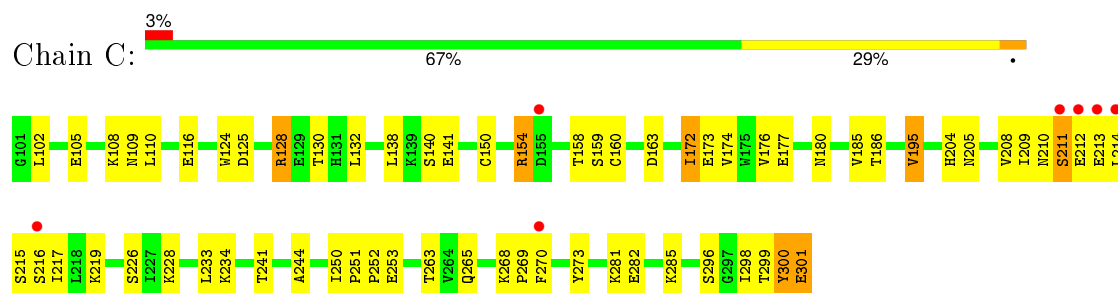
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

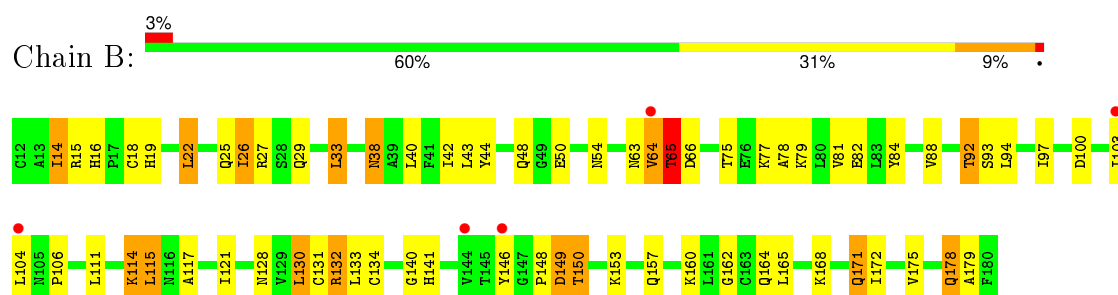
- Molecule 1: Interleukin-6 receptor beta chain



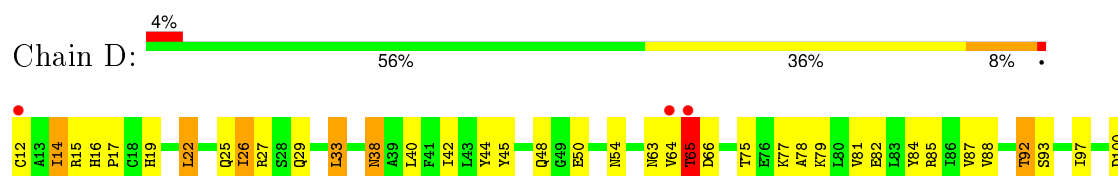
- Molecule 1: Interleukin-6 receptor beta chain

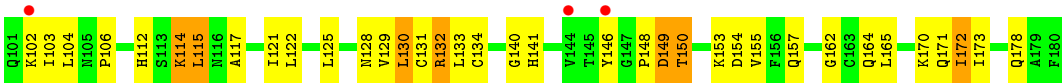


- Molecule 2: Leukemia inhibitory factor



- Molecule 2: Leukemia inhibitory factor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.71Å 86.70Å 146.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.86 – 2.50 39.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.8 (39.86-2.50) 90.9 (39.85-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.248 , 0.289 0.243 , 0.282	Depositor DCC
$R_{free}$ test set	2616 reflections (8.73%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.9	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 32572 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6026	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.54	0/1668	0.74	0/2267
1	C	0.54	0/1668	0.75	0/2267
2	B	0.50	0/1318	0.71	0/1783
2	D	0.51	0/1318	0.69	0/1783
All	All	0.53	0/5972	0.72	0/8100

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
2	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	45	TYR	Sidechain

### 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	1624	0	1571	60	0
1	C	1624	0	1571	68	0
2	B	1292	0	1304	46	0
2	D	1292	0	1304	50	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	71	0	0	5	0
4	B	33	0	0	0	0
4	C	61	0	0	2	0
4	D	27	0	0	4	0
All	All	6026	0	5750	221	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 19.

All (221) 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:177:GLU:HG3	1:A:186:THR:HG22	1.46	0.96
1:C:177:GLU:HG3	1:C:186:THR:HG22	1.49	0.92
2:D:40:LEU:HD11	2:D:115:LEU:HD13	1.58	0.83
1:A:130:THR:HG21	1:A:180:ASN:ND2	1.94	0.83
2:B:38:ASN:O	2:B:42:ILE:HG12	1.80	0.81
1:A:219:LYS:HG3	1:A:263:THR:HG22	1.64	0.80
1:C:130:THR:HG21	1:C:180:ASN:ND2	2.00	0.76
1:A:102:LEU:HD22	1:A:103:PRO:HD2	1.66	0.76
2:B:40:LEU:HD11	2:B:115:LEU:HD13	1.67	0.75
2:D:114:LYS:HA	2:D:114:LYS:HE3	1.68	0.75
2:D:38:ASN:O	2:D:42:ILE:HG12	1.85	0.75
1:C:219:LYS:HG3	1:C:263:THR:HG22	1.69	0.75
1:A:177:GLU:CG	1:A:186:THR:HG22	2.19	0.72
2:D:93:SER:O	2:D:97:ILE:HG12	1.89	0.72
2:B:14:ILE:HD11	2:B:18:CYS:SG	2.29	0.72
1:C:130:THR:HG22	1:C:132:LEU:H	1.55	0.71
2:B:114:LYS:HA	2:B:114:LYS:HE3	1.73	0.71
2:B:93:SER:O	2:B:97:ILE:HG12	1.90	0.70
1:C:215:SER:HB3	1:C:301:GLU:N	2.06	0.70
2:B:75:THR:O	2:B:79:LYS:HG3	1.94	0.68
1:A:128:ARG:HD2	1:A:128:ARG:O	1.93	0.68
2:B:26:ILE:HA	2:B:29:GLN:HE21	1.59	0.67
1:C:298:ILE:N	1:C:298:ILE:HD12	2.10	0.66
1:C:177:GLU:CG	1:C:186:THR:HG22	2.23	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:THR:O	2:D:79:LYS:HG3	1.96	0.65
1:C:215:SER:HB3	1:C:301:GLU:C	2.17	0.65
2:D:77:LYS:O	2:D:81:VAL:HG23	1.97	0.65
2:B:26:ILE:HG13	2:B:27:ARG:N	2.12	0.64
2:D:25:GLN:O	2:D:29:GLN:HG3	1.98	0.64
2:D:100:ASP:O	2:D:104:LEU:HG	1.97	0.64
2:D:26:ILE:HA	2:D:29:GLN:HE21	1.62	0.64
1:C:141:GLU:OE2	2:D:15:ARG:NH1	2.30	0.64
1:A:102:LEU:CD2	1:A:103:PRO:HD2	2.27	0.63
1:C:102:LEU:O	1:C:130:THR:HG23	1.98	0.63
1:C:241:THR:OG1	1:C:244:ALA:HB2	1.98	0.63
1:A:138:LEU:HB3	1:A:150:CYS:HB3	1.80	0.62
1:C:253:GLU:CD	1:C:253:GLU:H	2.03	0.62
1:A:217:ILE:HD13	1:A:265:GLN:HB3	1.82	0.61
1:C:252:PRO:HD2	1:C:253:GLU:OE2	1.99	0.61
2:D:84:TYR:O	2:D:88:VAL:HG23	2.00	0.61
1:A:102:LEU:O	1:A:130:THR:HG23	2.01	0.60
2:D:26:ILE:HG13	2:D:27:ARG:N	2.16	0.60
1:A:241:THR:HG23	4:A:341:HOH:O	2.01	0.60
2:D:63:ASN:OD1	2:D:63:ASN:O	2.20	0.59
1:A:234:LYS:HB2	1:A:282:GLU:HA	1.85	0.59
1:A:140:SER:HB2	1:A:172:ILE:HD11	1.85	0.59
1:C:209:ILE:HG22	1:C:211:SER:H	1.68	0.59
2:B:92:THR:HG21	2:B:146:TYR:CD2	2.38	0.59
1:A:253:GLU:CD	1:A:253:GLU:H	2.05	0.58
1:C:154:ARG:H	1:C:154:ARG:CD	2.17	0.58
1:A:130:THR:HG22	1:A:132:LEU:H	1.68	0.58
2:B:77:LYS:O	2:B:81:VAL:HG23	2.02	0.58
2:B:84:TYR:O	2:B:88:VAL:HG23	2.04	0.58
1:C:116:GLU:OE2	1:C:226:SER:HB2	2.04	0.58
1:A:130:THR:HG22	1:A:132:LEU:HB2	1.86	0.57
2:D:87:VAL:HG13	2:D:122:LEU:HD22	1.87	0.56
1:C:215:SER:HB3	1:C:301:GLU:CA	2.35	0.56
2:B:29:GLN:NE2	2:B:128:ASN:HD22	2.04	0.56
1:C:217:ILE:HD13	1:C:265:GLN:HB3	1.87	0.56
2:D:44:TYR:O	2:D:48:GLN:HG2	2.05	0.55
1:C:210:ASN:O	1:C:212:GLU:N	2.38	0.55
2:B:63:ASN:O	2:B:63:ASN:OD1	2.24	0.55
1:A:250:ILE:HG23	1:A:251:PRO:HD2	1.89	0.54
2:B:100:ASP:O	2:B:104:LEU:HG	2.07	0.54
2:B:140:GLY:O	2:B:141:HIS:HB3	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PRO:HD3	1:A:180:ASN:OD1	2.07	0.54
1:A:241:THR:OG1	1:A:244:ALA:HB2	2.07	0.54
1:A:104:PRO:HD3	1:A:180:ASN:CG	2.29	0.53
1:A:108:LYS:HD2	4:A:371:HOH:O	2.08	0.53
2:D:22:LEU:O	2:D:26:ILE:HG23	2.08	0.53
1:A:273:TYR:O	1:A:296:SER:HA	2.09	0.53
1:A:298:ILE:N	1:A:298:ILE:HD13	2.23	0.53
1:A:130:THR:CG2	1:A:132:LEU:HB2	2.39	0.52
2:D:33:LEU:HD13	2:D:121:ILE:HG21	1.90	0.52
1:C:215:SER:HA	1:C:300:TYR:HB2	1.90	0.52
1:C:269:PRO:HB3	1:C:301:GLU:HA	1.90	0.52
2:D:29:GLN:NE2	2:D:128:ASN:HD22	2.07	0.52
2:D:14:ILE:HG23	2:D:16:HIS:H	1.75	0.52
2:D:92:THR:HG21	2:D:146:TYR:CD2	2.44	0.52
1:C:270:PHE:CD2	1:C:270:PHE:O	2.63	0.52
2:D:66:ASP:N	2:D:66:ASP:OD2	2.42	0.52
2:D:63:ASN:ND2	2:D:164:GLN:HB3	2.24	0.52
2:B:22:LEU:O	2:B:26:ILE:HG23	2.10	0.52
2:B:63:ASN:ND2	2:B:164:GLN:HB3	2.25	0.51
1:C:273:TYR:O	1:C:296:SER:HA	2.10	0.51
1:A:210:ASN:O	1:A:212:GLU:N	2.40	0.51
1:C:234:LYS:HB2	1:C:282:GLU:HA	1.91	0.51
1:A:116:GLU:OE2	1:A:226:SER:HB2	2.11	0.51
1:C:128:ARG:HH11	1:C:128:ARG:HG2	1.75	0.51
1:A:208:VAL:C	1:A:209:ILE:HD12	2.30	0.51
1:C:130:THR:HG21	1:C:180:ASN:HD22	1.74	0.51
1:C:130:THR:HG22	1:C:132:LEU:N	2.24	0.51
1:C:105:GLU:HG3	1:C:128:ARG:HG3	1.93	0.51
1:A:124:TRP:O	1:A:158:THR:HB	2.11	0.51
1:A:270:PHE:CD2	1:A:270:PHE:O	2.64	0.51
2:D:132:ARG:CD	4:D:224:HOH:O	2.59	0.50
1:A:154:ARG:H	1:A:154:ARG:CD	2.24	0.50
1:A:259:ARG:NH1	4:A:319:HOH:O	2.35	0.50
1:C:250:ILE:HG23	1:C:251:PRO:HD2	1.93	0.50
1:A:209:ILE:HG22	1:A:211:SER:H	1.76	0.50
2:B:44:TYR:O	2:B:48:GLN:HG2	2.12	0.50
1:A:110:LEU:HD22	1:A:176:VAL:HG23	1.93	0.50
2:B:103:ILE:O	2:B:106:PRO:HD3	2.11	0.50
1:C:138:LEU:HB3	1:C:150:CYS:HB3	1.93	0.50
1:A:252:PRO:HD2	1:A:253:GLU:OE2	2.11	0.50
1:A:215:SER:HA	1:A:300:TYR:HB2	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:THR:CG2	1:C:132:LEU:HB2	2.42	0.49
1:C:141:GLU:HG3	2:D:16:HIS:CE1	2.47	0.49
1:C:138:LEU:HD11	1:C:174:VAL:CG1	2.42	0.49
2:B:22:LEU:HD23	2:B:132:ARG:HH11	1.77	0.49
2:B:25:GLN:O	2:B:29:GLN:HG3	2.12	0.49
1:C:208:VAL:C	1:C:209:ILE:HD12	2.33	0.49
1:C:141:GLU:HG3	2:D:16:HIS:HE1	1.78	0.49
1:C:140:SER:HB2	1:C:172:ILE:HD11	1.95	0.49
1:C:298:ILE:HG22	1:C:299:THR:N	2.27	0.49
1:A:130:THR:HG21	1:A:180:ASN:HD22	1.73	0.48
2:B:19:HIS:O	2:B:22:LEU:HD22	2.13	0.48
2:D:78:ALA:O	2:D:82:GLU:HG3	2.13	0.48
1:A:209:ILE:HG22	1:A:210:ASN:N	2.28	0.48
1:C:212:GLU:HG2	1:C:217:ILE:HG13	1.95	0.48
2:D:103:ILE:O	2:D:106:PRO:HD3	2.12	0.48
2:B:64:VAL:HG22	2:B:168:LYS:NZ	2.28	0.48
2:D:140:GLY:O	2:D:141:HIS:HB3	2.13	0.48
2:D:130:LEU:HD22	2:D:134:CYS:SG	2.53	0.48
2:D:22:LEU:HD23	2:D:132:ARG:HH11	1.78	0.48
1:C:105:GLU:CD	1:C:128:ARG:HG3	2.34	0.47
1:C:270:PHE:HB2	1:C:301:GLU:OE2	2.14	0.47
1:C:130:THR:HG22	1:C:132:LEU:HB2	1.96	0.47
1:C:154:ARG:H	1:C:154:ARG:HD2	1.78	0.47
1:A:301:GLU:N	1:A:301:GLU:CD	2.68	0.47
1:C:215:SER:C	1:C:217:ILE:H	2.17	0.47
1:A:128:ARG:HH11	1:A:128:ARG:HG2	1.78	0.47
2:B:78:ALA:O	2:B:82:GLU:HG3	2.15	0.47
2:B:14:ILE:HG23	2:B:16:HIS:H	1.80	0.47
1:A:212:GLU:HG2	1:A:217:ILE:HG13	1.97	0.47
2:B:160:LYS:O	2:B:164:GLN:HG3	2.15	0.46
1:A:213:GLU:O	1:A:214:LEU:HD23	2.15	0.46
1:C:215:SER:CB	1:C:301:GLU:C	2.82	0.46
1:C:209:ILE:HG22	1:C:211:SER:N	2.30	0.46
2:B:130:LEU:HD22	2:B:134:CYS:SG	2.55	0.46
2:B:148:PRO:O	2:B:149:ASP:C	2.54	0.46
1:C:270:PHE:HB2	1:C:301:GLU:OE1	2.16	0.46
2:B:50:GLU:OE2	2:B:54:ASN:ND2	2.49	0.46
1:C:172:ILE:HD13	1:C:173:GLU:N	2.30	0.46
1:C:209:ILE:HG22	1:C:210:ASN:N	2.31	0.46
1:C:213:GLU:O	1:C:214:LEU:HD23	2.15	0.46
1:C:215:SER:O	1:C:217:ILE:N	2.42	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ARG:O	1:C:128:ARG:HD2	2.16	0.46
1:C:110:LEU:HD22	1:C:176:VAL:HG23	1.98	0.46
1:A:259:ARG:HD2	4:A:319:HOH:O	2.16	0.45
1:A:138:LEU:HD11	1:A:174:VAL:CG1	2.47	0.45
2:B:33:LEU:HD13	2:B:121:ILE:HG21	1.98	0.45
2:D:148:PRO:O	2:D:149:ASP:C	2.55	0.45
2:D:149:ASP:O	2:D:150:THR:O	2.34	0.45
1:C:270:PHE:HB2	1:C:301:GLU:CD	2.38	0.45
2:B:79:LYS:HE3	2:B:179:ALA:O	2.16	0.45
2:D:63:ASN:HD21	2:D:164:GLN:HB3	1.81	0.45
2:D:170:LYS:O	2:D:173:ILE:HG22	2.17	0.45
2:B:93:SER:HB3	2:B:165:LEU:CD2	2.47	0.44
2:B:175:VAL:O	2:B:178:GLN:OE1	2.36	0.44
1:C:108:LYS:O	1:C:109:ASN:HB2	2.17	0.44
1:C:285:LYS:HE2	4:C:350:HOH:O	2.17	0.44
1:A:185:VAL:HG22	1:A:186:THR:N	2.32	0.44
1:C:140:SER:HA	1:C:173:GLU:O	2.18	0.44
1:A:130:THR:HG22	1:A:132:LEU:CB	2.47	0.44
2:D:132:ARG:HD3	4:D:224:HOH:O	2.15	0.44
1:A:104:PRO:HD3	1:A:180:ASN:ND2	2.33	0.44
2:D:117:ALA:O	2:D:121:ILE:HG13	2.18	0.44
2:D:65:THR:HB	2:D:66:ASP:OD2	2.17	0.44
1:A:130:THR:O	1:A:131:HIS:HB2	2.18	0.44
2:B:97:ILE:CD1	2:B:162:GLY:HA2	2.47	0.44
1:A:172:ILE:HD13	1:A:173:GLU:N	2.33	0.44
1:A:108:LYS:O	1:A:109:ASN:HB2	2.18	0.43
1:C:195:VAL:HG13	1:C:281:LYS:HE3	2.00	0.43
2:B:97:ILE:HD12	2:B:162:GLY:HA2	1.99	0.43
1:A:297:GLY:C	1:A:298:ILE:HD13	2.38	0.43
2:B:92:THR:HG21	2:B:146:TYR:HD2	1.82	0.43
2:D:154:ASP:O	2:D:155:VAL:C	2.57	0.43
1:A:154:ARG:O	1:A:157:PRO:HD3	2.18	0.43
2:B:171:GLN:O	2:B:175:VAL:HG23	2.19	0.43
1:C:185:VAL:HG22	1:C:186:THR:N	2.33	0.43
2:B:93:SER:HB3	2:B:165:LEU:HD22	2.01	0.43
2:D:50:GLU:OE2	2:D:54:ASN:ND2	2.52	0.43
2:B:22:LEU:HD12	2:B:22:LEU:HA	1.85	0.43
1:A:215:SER:O	1:A:217:ILE:N	2.45	0.42
2:D:19:HIS:HB3	2:D:22:LEU:HD13	2.01	0.42
1:A:204:HIS:O	1:A:205:ASN:HB2	2.19	0.42
1:C:215:SER:HB3	1:C:301:GLU:O	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:ALA:O	2:B:121:ILE:HG13	2.19	0.42
2:B:65:THR:HB	2:B:66:ASP:OD2	2.19	0.42
2:D:93:SER:HB3	2:D:165:LEU:CD2	2.49	0.42
1:A:243:ASP:HB2	4:A:337:HOH:O	2.19	0.42
1:C:125:ASP:HB3	4:C:328:HOH:O	2.19	0.42
2:B:15:ARG:O	2:B:16:HIS:HB3	2.19	0.41
1:C:226:SER:C	1:C:228:LYS:H	2.23	0.41
2:B:66:ASP:OD2	2:B:66:ASP:N	2.37	0.41
2:D:102:LYS:HA	2:D:112:HIS:CE1	2.54	0.41
2:D:93:SER:HB3	2:D:165:LEU:HD22	2.02	0.41
1:C:212:GLU:CB	1:C:217:ILE:HG21	2.51	0.41
2:D:85:ARG:NH1	4:D:223:HOH:O	2.53	0.41
1:C:204:HIS:O	1:C:205:ASN:HB2	2.20	0.41
1:A:215:SER:C	1:A:217:ILE:H	2.22	0.41
1:A:140:SER:HA	1:A:173:GLU:O	2.19	0.41
2:B:149:ASP:O	2:B:150:THR:O	2.38	0.41
2:D:12:CYS:HB2	4:D:207:HOH:O	2.19	0.41
1:A:130:THR:HG22	1:A:132:LEU:N	2.35	0.41
1:C:251:PRO:HA	1:C:252:PRO:HD3	1.88	0.41
1:A:251:PRO:HA	1:A:252:PRO:HD3	1.87	0.41
2:B:63:ASN:HD21	2:B:164:GLN:HB3	1.84	0.41
1:C:105:GLU:CG	1:C:128:ARG:HG3	2.50	0.41
1:A:154:ARG:H	1:A:154:ARG:HD2	1.86	0.41
2:D:172:ILE:CG2	2:D:173:ILE:N	2.84	0.41
1:C:124:TRP:O	1:C:158:THR:HB	2.21	0.41
1:C:268:LYS:HA	1:C:269:PRO:HD3	1.87	0.41
2:B:43:LEU:HD13	2:B:111:LEU:HA	2.03	0.41
2:D:40:LEU:HD11	2:D:115:LEU:CD1	2.42	0.40
2:D:97:ILE:HD12	2:D:162:GLY:HA2	2.03	0.40
1:C:212:GLU:HB2	1:C:217:ILE:HG21	2.02	0.40
2:D:65:THR:HB	2:D:66:ASP:H	1.51	0.40
1:A:269:PRO:HB3	1:A:301:GLU:HA	2.04	0.40
2:D:125:LEU:O	2:D:129:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	13	22
1	C	199/201 (99%)	188 (94%)	8 (4%)	3 (2%)	13	22
2	B	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	5	7
2	D	167/169 (99%)	151 (90%)	10 (6%)	6 (4%)	4	5
All	All	732/740 (99%)	678 (93%)	37 (5%)	17 (2%)	8	12

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	65	THR
2	B	150	THR
2	B	153	LYS
1	C	211	SER
1	C	300	TYR
2	D	65	THR
2	D	150	THR
2	D	153	LYS
1	A	211	SER
1	A	216	SER
2	B	64	VAL
1	C	216	SER
2	D	64	VAL
2	B	149	ASP
2	D	149	ASP
1	A	181	ALA
2	D	17	PRO

### 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	185/185 (100%)	176 (95%)	9 (5%)	31	55
1	C	185/185 (100%)	176 (95%)	9 (5%)	31	55
2	B	139/144 (96%)	121 (87%)	18 (13%)	5	10
2	D	139/144 (96%)	122 (88%)	17 (12%)	6	11
All	All	648/658 (98%)	595 (92%)	53 (8%)	14	27

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ARG
1	A	154	ARG
1	A	159	SER
1	A	160	CYS
1	A	163	ASP
1	A	172	ILE
1	A	233	LEU
1	A	298	ILE
1	A	301	GLU
2	B	14	ILE
2	B	22	LEU
2	B	26	ILE
2	B	33	LEU
2	B	38	ASN
2	B	65	THR
2	B	92	THR
2	B	94	LEU
2	B	114	LYS
2	B	115	LEU
2	B	130	LEU
2	B	131	CYS
2	B	132	ARG
2	B	133	LEU
2	B	157	GLN
2	B	171	GLN
2	B	172	ILE
2	B	178	GLN
1	C	128	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	154	ARG
1	C	159	SER
1	C	160	CYS
1	C	163	ASP
1	C	172	ILE
1	C	195	VAL
1	C	233	LEU
1	C	301	GLU
2	D	14	ILE
2	D	22	LEU
2	D	26	ILE
2	D	33	LEU
2	D	38	ASN
2	D	65	THR
2	D	92	THR
2	D	114	LYS
2	D	115	LEU
2	D	130	LEU
2	D	131	CYS
2	D	132	ARG
2	D	133	LEU
2	D	157	GLN
2	D	171	GLN
2	D	172	ILE
2	D	178	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
2	B	29	GLN
2	B	32	GLN
2	B	34	ASN
2	B	54	ASN
2	B	63	ASN
2	B	112	HIS
2	B	157	GLN
2	D	29	GLN
2	D	32	GLN
2	D	34	ASN
2	D	54	ASN
2	D	63	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	D	112	HIS
2	D	157	GLN
2	D	178	GLN

### 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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

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	201/201 (100%)	0.27	15 (7%) 17 19	29, 48, 78, 97	0
1	C	201/201 (100%)	0.12	7 (3%) 48 53	32, 47, 79, 98	0
2	B	169/169 (100%)	0.21	5 (2%) 54 59	34, 54, 87, 98	1 (0%)
2	D	169/169 (100%)	0.28	6 (3%) 46 51	36, 55, 87, 99	1 (0%)
All	All	740/740 (100%)	0.22	33 (4%) 37 42	29, 51, 82, 99	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	211	SER	7.1
1	C	212	GLU	6.9
2	B	64	VAL	6.3
1	C	213	GLU	5.9
1	A	212	GLU	5.1
1	A	182	LEU	4.7
1	A	211	SER	4.7
1	C	270	PHE	4.5
2	D	64	VAL	4.3
1	A	130	THR	4.2
1	A	102	LEU	3.7
1	C	214	LEU	3.7
1	A	213	GLU	3.5
2	D	146	TYR	3.5
1	A	181	ALA	3.1
1	A	300	TYR	2.9
1	A	132	LEU	2.8
2	D	12	CYS	2.8
1	C	155	ASP	2.7
1	A	214	LEU	2.7
2	D	144	VAL	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	146	TYR	2.6
1	A	105	GLU	2.5
1	A	101	GLY	2.5
1	A	133	GLU	2.4
2	B	144	VAL	2.4
2	B	103	ILE	2.3
2	D	65	THR	2.2
2	D	102	LYS	2.1
1	A	183	GLY	2.1
2	B	104	LEU	2.1
1	A	216	SER	2.1
1	C	216	SER	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	IOD	A	302	1/1	1.00	0.14	-0.87	44,44,44,44	0
3	IOD	D	202	1/1	1.00	0.14	-1.22	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.