Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2022 – 04:49 pm BST

PDB ID	:	7ZXK
Title	:	Human IL-27 in complex with neutralizing SRF388 FAb fragment
Authors	:	Bloch, Y.; Skladanowska, K.; Strand, J.; Welin, M.; Logan, D.; Hill, J.; Savvides, S.N.
Deposited on	:	2022-05-21
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

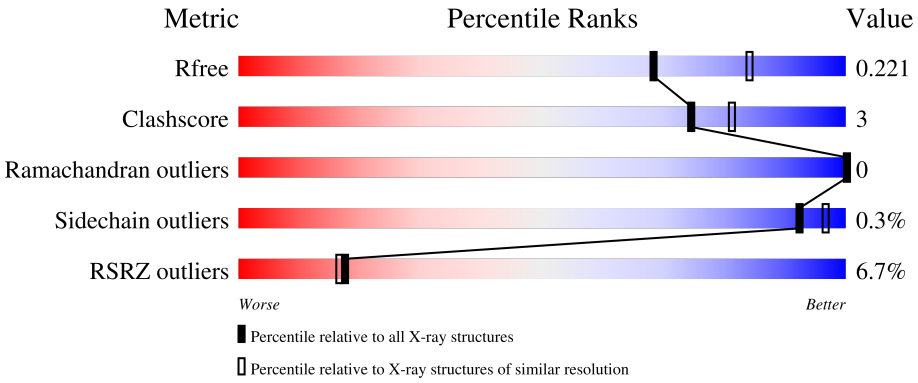
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	215	13% 66% 9% 26%
1	C	215	10% 70% 7% 23%
2	B	209	8% 78% 8% 14%
2	D	209	7% 78% 6% 16%
3	H	229	3% 90% 9% .

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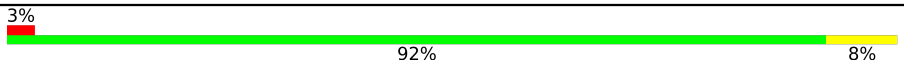
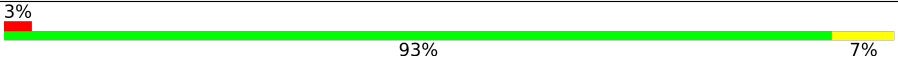
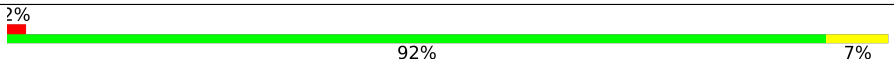
Mol	Chain	Length	Quality of chain
3	J	229	
4	I	220	
4	L	220	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12892 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-27 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1308	837	245	222	4			
1	C	166	Total	C	N	O	S	0	0	0
			1359	871	255	229	4			

- Molecule 2 is a protein called Interleukin-27 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1432	925	246	254	7			
2	D	175	Total	C	N	O	S	0	1	0
			1408	911	241	248	8			

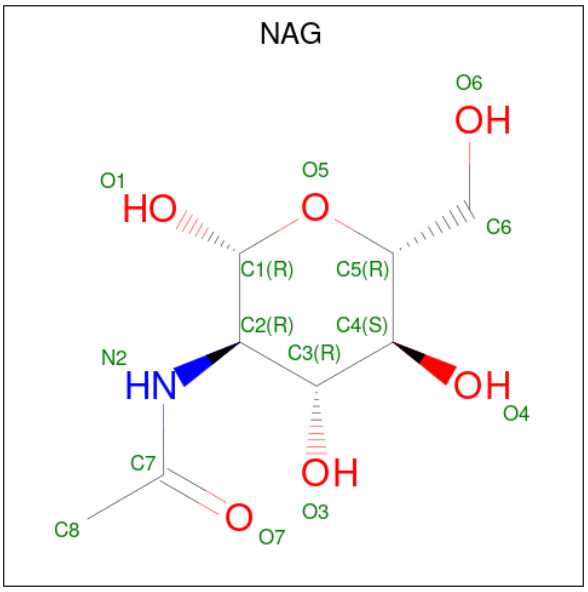
- Molecule 3 is a protein called SRF388 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	226	Total	C	N	O	S	0	3	0
			1696	1068	289	333	6			
3	J	229	Total	C	N	O	S	0	4	0
			1723	1083	294	338	8			

- Molecule 4 is a protein called SRF388 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	220	Total	C	N	O	S	0	1	0
			1693	1057	286	344	6			
4	L	219	Total	C	N	O	S	0	0	0
			1679	1050	283	341	5			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

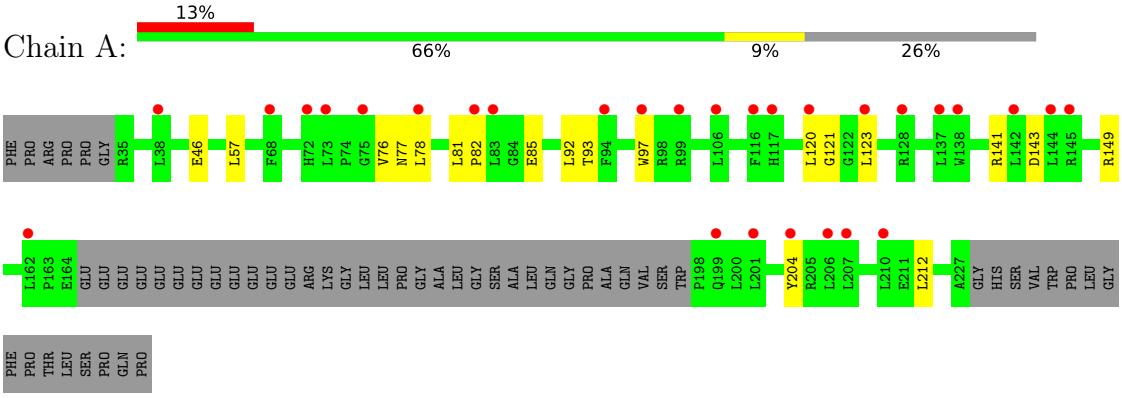
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	12	Total O 12 12	0	0
6	B	54	Total O 54 54	0	0
6	C	25	Total O 25 25	0	0
6	D	62	Total O 62 62	0	0
6	H	107	Total O 107 107	0	0
6	I	89	Total O 89 89	0	0
6	J	108	Total O 108 108	0	0
6	L	109	Total O 109 109	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

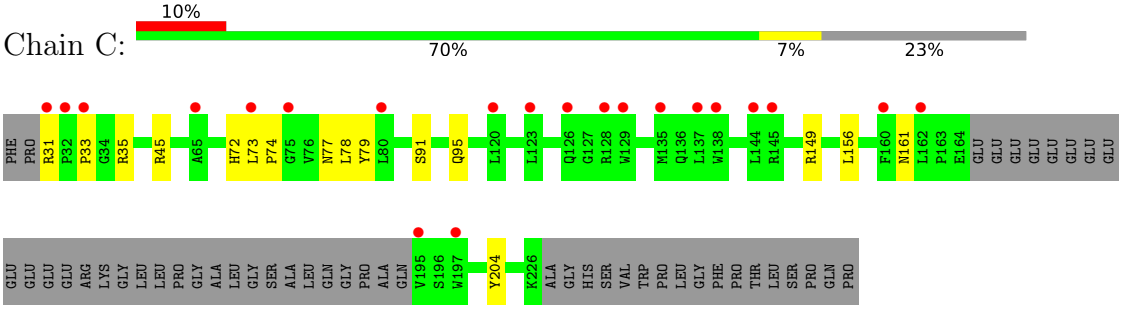
• Molecule 1: Interleukin-27 subunit alpha

Chain A:



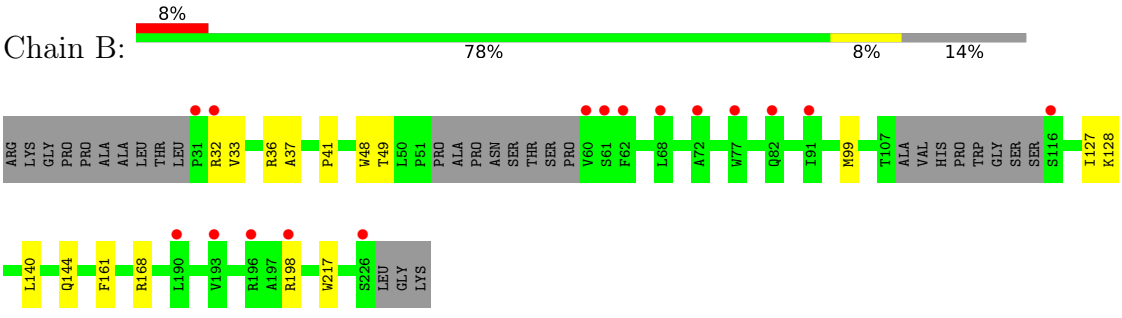
• Molecule 1: Interleukin-27 subunit alpha

Chain C:



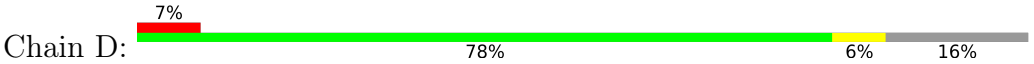
• Molecule 2: Interleukin-27 subunit beta

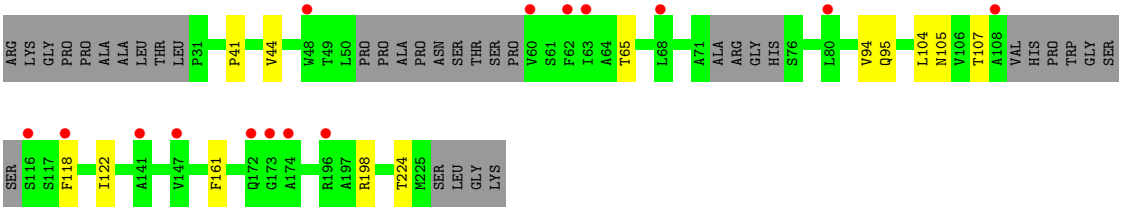
Chain B:



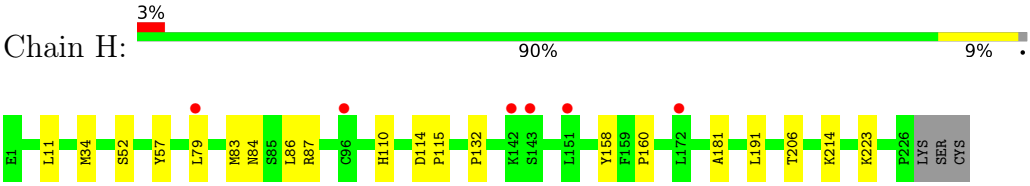
• Molecule 2: Interleukin-27 subunit beta

Chain D:

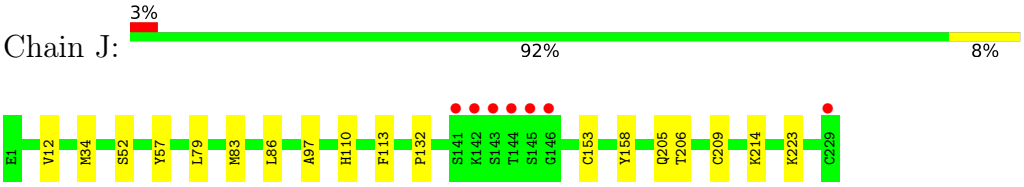




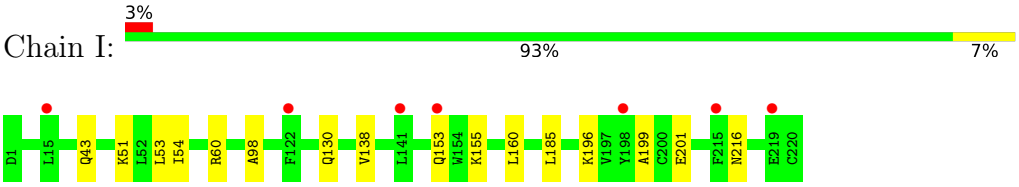
• Molecule 3: SRF388 Heavy Chain



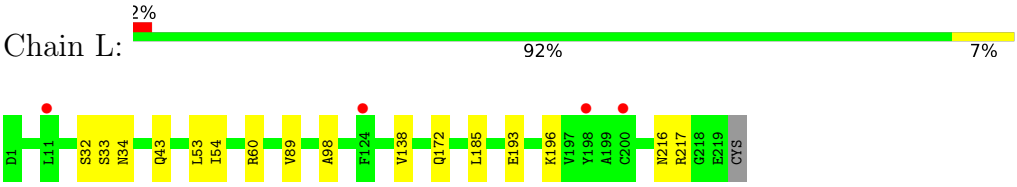
• Molecule 3: SRF388 Heavy Chain



• Molecule 4: SRF388 Light Chain



• Molecule 4: SRF388 Light Chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.81Å 104.62Å 121.75Å 90.00° 98.65° 90.00°	Depositor
Resolution (Å)	60.18 – 2.20 120.37 – 2.20	Depositor EDS
% Data completeness (in resolution range)	80.0 (60.18-2.20) 99.8 (120.37-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.20Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.184 , 0.221 0.194 , 0.221	Depositor DCC
R_{free} test set	5446 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	59.3	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12892	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG

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	0.29	0/1335	0.54	0/1804
1	C	0.29	0/1390	0.52	0/1882
2	B	0.28	0/1477	0.52	0/2020
2	D	0.29	0/1454	0.52	0/1986
3	H	0.25	0/1748	0.51	0/2380
3	J	0.26	0/1775	0.50	0/2415
4	I	0.25	0/1730	0.48	0/2351
4	L	0.25	0/1716	0.48	0/2332
All	All	0.27	0/12625	0.51	0/17170

There are no bond length outliers.

There are no bond angle outliers.

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	1308	0	1352	14	0
1	C	1359	0	1400	13	0
2	B	1432	0	1403	8	0
2	D	1408	0	1387	9	0
3	H	1696	0	1656	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1723	0	1682	13	0
4	I	1693	0	1637	10	0
4	L	1679	0	1628	10	0
5	B	14	0	13	0	0
5	D	14	0	13	1	0
6	A	12	0	0	0	0
6	B	54	0	0	0	0
6	C	25	0	0	1	0
6	D	62	0	0	0	0
6	H	107	0	0	3	0
6	I	89	0	0	2	0
6	J	108	0	0	2	0
6	L	109	0	0	0	0
All	All	12892	0	12171	79	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 3.

All (79) 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:76:VAL:HG12	1:A:77:ASN:H	1.59	0.65
3:J:132:PRO:HB3	3:J:158:TYR:HB3	1.79	0.64
3:H:132:PRO:HB3	3:H:158:TYR:HB3	1.84	0.60
3:J:83:MET:HE2	3:J:86:LEU:HD21	1.84	0.58
1:A:120:LEU:HD13	1:A:123:LEU:HD12	1.84	0.58
3:J:214:LYS:NZ	6:J:302:HOH:O	2.36	0.57
4:L:43:GLN:HB2	4:L:53:LEU:HD11	1.86	0.57
3:J:34:MET:HB3	3:J:79:LEU:HD22	1.86	0.57
1:A:76:VAL:HG12	1:A:77:ASN:N	2.20	0.56
1:A:78:LEU:HD13	1:A:204:TYR:CZ	2.40	0.56
2:B:33:VAL:HG22	2:B:48:TRP:HB3	1.87	0.56
3:H:83:MET:HE2	3:H:86:LEU:HD21	1.88	0.56
4:I:43:GLN:HB2	4:I:53:LEU:HD11	1.86	0.56
3:H:84:ASN:ND2	6:H:301:HOH:O	2.37	0.55
3:H:214:LYS:NZ	6:H:305:HOH:O	2.40	0.55
4:I:153:GLN:HE21	4:I:160:LEU:HD13	1.71	0.55
3:J:97:ALA:HB1	3:J:113:PHE:HB3	1.89	0.55
1:A:92:LEU:HD11	1:A:97:TRP:HB2	1.87	0.55
4:L:196:LYS:HE2	4:L:216:ASN:HB3	1.89	0.55
1:A:81:LEU:HD12	1:A:82:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:138:VAL:HG13	4:I:185:LEU:HB3	1.89	0.52
1:A:92:LEU:CD1	1:A:93:THR:O	2.57	0.52
3:H:52:SER:HB3	3:H:57:TYR:HB2	1.92	0.52
2:B:36:ARG:HD3	2:B:128:LYS:HD3	1.93	0.51
1:A:82:PRO:HB2	1:A:85:GLU:HG2	1.91	0.51
1:A:92:LEU:HD12	1:A:93:THR:O	2.10	0.50
4:I:130:GLN:NE2	6:I:304:HOH:O	2.43	0.50
1:C:79:TYR:HE1	2:D:122:ILE:HG13	1.76	0.50
3:J:52:SER:HB3	3:J:57:TYR:HB2	1.94	0.50
4:L:193:GLU:OE1	4:L:217:ARG:NH1	2.46	0.49
1:C:73:LEU:N	1:C:74:PRO:HD3	2.28	0.49
1:A:212:LEU:HD12	2:B:99:MET:HG2	1.95	0.49
3:H:87:ARG:NH1	6:H:308:HOH:O	2.45	0.49
1:A:57:LEU:HD21	1:A:143:ASP:HB2	1.95	0.49
3:J:205:GLN:NE2	6:J:301:HOH:O	2.31	0.47
2:D:44:VAL:HG23	2:D:94:VAL:HG11	1.96	0.47
1:C:161:ASN:ND2	4:L:33:SER:O	2.46	0.47
3:H:34:MET:HB3	3:H:79:LEU:HD22	1.96	0.47
1:C:78:LEU:HD13	1:C:204:TYR:OH	2.15	0.47
4:L:89:VAL:HG11	4:L:172:GLN:HB3	1.97	0.47
4:I:155:LYS:NZ	4:I:201:GLU:OE1	2.48	0.46
2:B:41:PRO:HG3	2:B:161:PHE:CE1	2.50	0.46
3:J:12:VAL:HG11	3:J:86:LEU:HD13	1.98	0.46
1:C:77:ASN:HD21	1:C:79:TYR:HB2	1.80	0.46
2:B:140:LEU:HB2	2:B:144:GLN:HB2	1.98	0.46
1:C:79:TYR:CE1	2:D:122:ILE:HG13	2.51	0.46
4:L:54:ILE:HD13	4:L:60:ARG:HA	1.98	0.46
2:B:32:ARG:HB2	2:B:49:THR:HG23	1.99	0.45
1:C:72:HIS:C	1:C:74:PRO:HD3	2.36	0.45
1:C:45:ARG:NH1	6:C:304:HOH:O	2.49	0.45
1:C:77:ASN:ND2	1:C:79:TYR:HB2	2.31	0.45
4:I:51:LYS:NZ	6:I:307:HOH:O	2.49	0.45
2:D:107:THR:HG21	5:D:301:NAG:H5	1.97	0.45
1:C:31:ARG:HD3	1:C:35:ARG:HB3	2.00	0.44
3:H:110[B]:HIS:HD2	4:L:98:ALA:O	2.00	0.44
2:D:41:PRO:HG3	2:D:161:PHE:CE1	2.53	0.44
3:H:206:THR:HG23	3:H:223:LYS:HE3	1.99	0.44
2:D:65:THR:HG23	2:D:105:ASN:HB3	2.00	0.44
4:I:54:ILE:HD13	4:I:60:ARG:HA	2.00	0.44
2:D:198:ARG:NH1	2:D:224:THR:OG1	2.51	0.43
4:I:98:ALA:O	3:J:110[B]:HIS:HD2	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLY:HA2	1:A:141:ARG:NH1	2.34	0.42
3:H:11:LEU:HB2	3:H:160:PRO:HG3	2.01	0.42
4:I:196:LYS:HE3	4:I:216:ASN:HB3	2.01	0.42
2:D:104:LEU:O	2:D:118:PHE:HA	2.19	0.42
1:C:91:SER:OG	2:D:95:GLN:HG3	2.19	0.42
3:J:206:THR:HG23	3:J:223:LYS:HE3	2.00	0.42
1:C:156:LEU:HD21	4:L:34:ASN:ND2	2.35	0.42
3:H:114:ASP:HA	3:H:115:PRO:HA	1.78	0.41
1:A:46:GLU:OE2	3:J:110[B]:HIS:HE1	2.03	0.41
2:B:168:ARG:HD3	2:B:217:TRP:CE2	2.56	0.41
3:J:153[B]:CYS:HB3	3:J:209:CYS:SG	2.61	0.41
2:B:37:ALA:HB3	2:B:127:ILE:HA	2.01	0.41
3:H:181:ALA:HA	3:H:191:LEU:HB3	2.03	0.41
4:I:155:LYS:HB2	4:I:199:ALA:HB3	2.02	0.41
4:L:138:VAL:HG13	4:L:185:LEU:HB3	2.03	0.41
1:A:92:LEU:CD1	1:A:97:TRP:HB2	2.51	0.41
3:J:83:MET:HB3	3:J:86:LEU:HD21	2.03	0.40
1:C:33:PRO:HG3	4:L:32:SER:HB3	2.02	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	156/215 (73%)	151 (97%)	5 (3%)	0	100	100
1	C	162/215 (75%)	159 (98%)	3 (2%)	0	100	100
2	B	174/209 (83%)	171 (98%)	3 (2%)	0	100	100
2	D	168/209 (80%)	163 (97%)	5 (3%)	0	100	100
3	H	227/229 (99%)	224 (99%)	3 (1%)	0	100	100
3	J	231/229 (101%)	226 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	219/220 (100%)	211 (96%)	8 (4%)	0	100	100
4	L	217/220 (99%)	211 (97%)	6 (3%)	0	100	100
All	All	1554/1746 (89%)	1516 (98%)	38 (2%)	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	142/187 (76%)	141 (99%)	1 (1%)	84	91
1	C	148/187 (79%)	146 (99%)	2 (1%)	67	80
2	B	155/179 (87%)	154 (99%)	1 (1%)	86	93
2	D	154/179 (86%)	154 (100%)	0	100	100
3	H	189/189 (100%)	189 (100%)	0	100	100
3	J	193/189 (102%)	193 (100%)	0	100	100
4	I	193/192 (100%)	193 (100%)	0	100	100
4	L	191/192 (100%)	191 (100%)	0	100	100
All	All	1365/1494 (91%)	1361 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ARG
2	B	198	ARG
1	C	95	GLN
1	C	149	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	136	GLN
4	I	153	GLN
4	L	216	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
5	NAG	D	301	2	14,14,15	0.32	0	17,19,21	0.58	0
5	NAG	B	301	2	14,14,15	0.30	0	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	301	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	301	2	-	0/6/23/26	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	301	NAG	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^{th} 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	160/215 (74%)	1.05	29 (18%) 1 1	39, 72, 135, 155	0
1	C	166/215 (77%)	1.03	21 (12%) 3 3	34, 61, 119, 154	0
2	B	180/209 (86%)	0.91	16 (8%) 9 8	39, 69, 118, 142	0
2	D	175/209 (83%)	0.96	15 (8%) 10 9	36, 61, 121, 130	0
3	H	226/229 (98%)	0.61	6 (2%) 54 52	32, 49, 68, 108	0
3	J	229/229 (100%)	0.69	7 (3%) 49 47	34, 46, 73, 175	0
4	I	220/220 (100%)	0.51	7 (3%) 47 45	37, 53, 81, 149	0
4	L	219/220 (99%)	0.55	4 (1%) 68 66	33, 55, 91, 127	0
All	All	1575/1746 (90%)	0.76	105 (6%) 17 16	32, 54, 114, 175	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	60	VAL	8.0
1	C	123	LEU	6.3
3	J	145	SER	6.0
2	B	196	ARG	5.9
1	C	138	TRP	5.8
3	J	143	SER	5.8
1	C	126	GLN	5.7
2	D	63	ILE	5.5
1	C	33	PRO	5.4
1	A	123	LEU	5.3
1	A	201	LEU	5.3
1	C	195	VAL	5.2
1	A	138	TRP	5.2
1	C	197	TRP	5.1
2	B	68	LEU	4.9
1	C	31	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
2	D	60	VAL	4.6
1	A	199	GLN	4.5
1	C	129	TRP	4.4
3	J	142	LYS	4.1
2	D	108	ALA	4.1
1	A	120	LEU	4.0
3	J	141	SER	3.8
2	B	32	ARG	3.7
4	I	219	GLU	3.3
1	C	32	PRO	3.3
1	C	162	LEU	3.3
1	A	83	LEU	3.2
2	D	172	GLN	3.1
1	A	204	TYR	3.1
1	C	65	ALA	3.0
1	A	82	PRO	3.0
1	C	137	LEU	3.0
2	B	62	PHE	2.9
1	C	160	PHE	2.9
1	A	78	LEU	2.9
1	A	162	LEU	2.8
1	A	38	LEU	2.8
1	A	73	LEU	2.8
2	B	61	SER	2.7
2	D	174	ALA	2.7
2	D	62	PHE	2.7
1	A	106	LEU	2.7
2	B	72	ALA	2.7
2	D	173	GLY	2.7
3	J	229	CYS	2.5
1	A	99	ARG	2.5
1	A	72	HIS	2.5
2	D	68	LEU	2.5
1	A	117	HIS	2.5
2	D	196	ARG	2.5
1	C	120	LEU	2.5
2	D	80	LEU	2.5
2	B	116	SER	2.4
1	A	137	LEU	2.4
1	A	116	PHE	2.4
2	D	147	VAL	2.4
1	C	135	MET	2.4

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Mol	Chain	Res	Type	RSRZ
4	L	11	LEU	2.4
2	B	31	PRO	2.4
4	I	15	LEU	2.4
3	J	144	THR	2.4
2	B	82	GLN	2.4
2	D	48	TRP	2.3
4	I	215	PHE	2.3
3	H	96	CYS	2.3
4	I	198	TYR	2.3
1	A	68	PHE	2.3
1	C	73	LEU	2.3
2	B	198	ARG	2.3
1	A	210	LEU	2.3
4	L	198	TYR	2.3
2	D	141	ALA	2.3
4	L	124	PHE	2.3
1	A	207	LEU	2.2
2	B	190	LEU	2.2
4	L	200	CYS	2.2
2	D	118	PHE	2.2
2	B	226	SER	2.2
2	D	116	SER	2.2
3	H	143	SER	2.2
3	J	146	GLY	2.2
1	C	128	ARG	2.2
2	B	77	TRP	2.2
1	C	75	GLY	2.2
1	A	206	LEU	2.1
1	A	97	TRP	2.1
1	A	128	ARG	2.1
4	I	141	LEU	2.1
1	A	144	LEU	2.1
3	H	79	LEU	2.1
3	H	151	LEU	2.1
1	A	145	ARG	2.1
4	I	122	PHE	2.1
1	C	145	ARG	2.1
3	H	142	LYS	2.1
1	C	80	LEU	2.1
4	I	153	GLN	2.1
1	A	75	GLY	2.1
2	B	193	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	144	LEU	2.0
2	B	91	ILE	2.0
1	A	94	PHE	2.0
1	A	142	LEU	2.0
3	H	172	LEU	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 monosaccharides 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	D	301	14/15	0.81	0.19	101,108,115,120	0
5	NAG	B	301	14/15	0.82	0.23	98,106,117,118	0

6.5 Other polymers (i)

There are no such residues in this entry.