Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:55 PM GMT

PDB ID	:	4GL9
Title	:	Crystal structure of inhibitory protein SOCS3 in complex with JAK2 kinase domain and fragment of GP130 intracellular domain
Authors	:	Kershaw, N.J.; Murphy, J.M.; Laktyushin, A.; Nicola, N.A.; Babon, J.J.
Deposited on	:	2012-08-14
Resolution	:	3.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

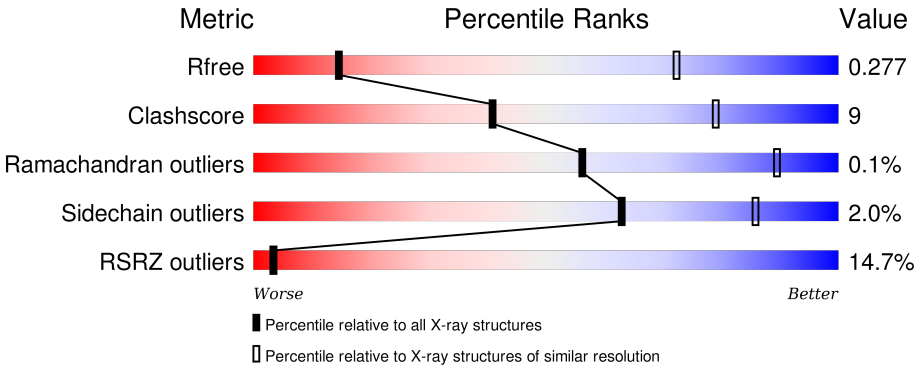
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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 <=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	297	12% 71% 24%
1	B	297	14% 72% 23% 5%
1	C	297	12% 73% 21%
1	D	297	16% 72% 21%
2	I	15	13% 47% 7% 47%

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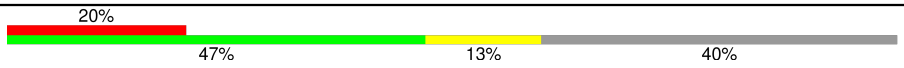
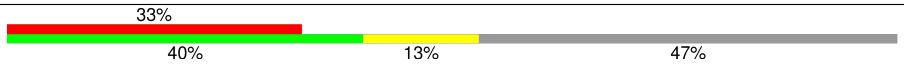
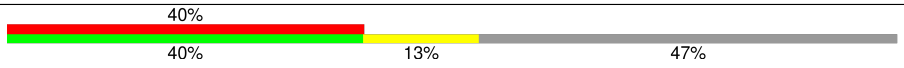
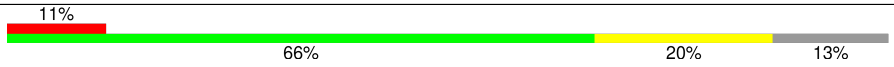
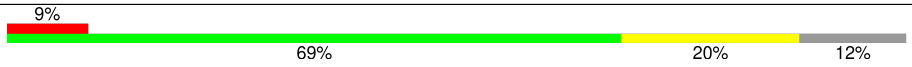
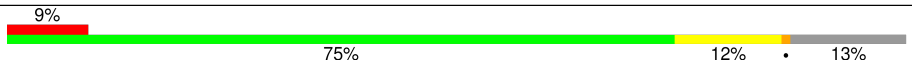
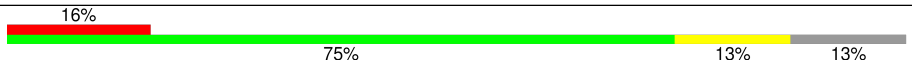
Mol	Chain	Length	Quality of chain
2	J	15	
2	K	15	
2	L	15	
3	E	143	
3	F	143	
3	G	143	
3	H	143	

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
4	IZA	A	2001	-	-	-	X
4	IZA	B	1201	-	-	-	X
4	IZA	C	1201	-	-	-	X
4	IZA	D	1201	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13682 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 Tyrosine-protein kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	P	S	0	0	0
			2355	1497	405	439	2	12			
1	B	282	Total	C	N	O	P	S	0	0	0
			2326	1477	400	435	2	12			
1	C	284	Total	C	N	O	P	S	0	0	0
			2350	1494	403	439	2	12			
1	D	284	Total	C	N	O	P	S	0	0	0
			2351	1494	404	439	2	12			

- Molecule 2 is a protein called Interleukin-6 receptor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	8	Total	C	N	O	P	0	0	0
			69	42	10	16	1			
2	K	8	Total	C	N	O	P	0	0	0
			69	42	10	16	1			
2	J	9	Total	C	N	O	P	0	0	0
			76	46	11	18	1			
2	L	8	Total	C	N	O	P	0	0	0
			69	42	10	16	1			

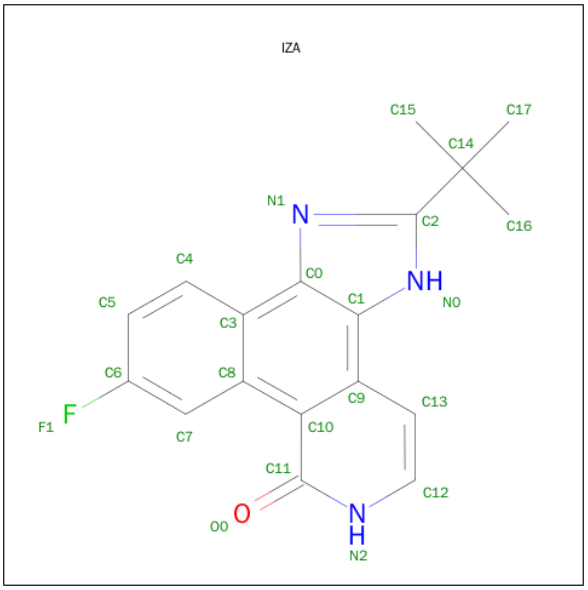
- Molecule 3 is a protein called Suppressor of cytokine signaling 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			976	623	169	181	3			
3	F	126	Total	C	N	O	S	0	0	0
			984	627	171	183	3			
3	G	125	Total	C	N	O	S	0	0	0
			980	625	170	182	3			
3	H	125	Total	C	N	O	S	0	0	0
			980	625	170	182	3			

There are 22 discrepancies between the modelled and reference sequences:

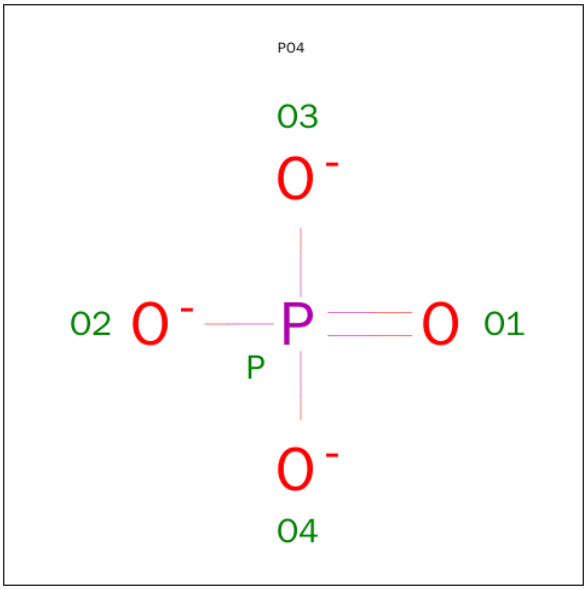
Chain	Residue	Modelled	Actual	Comment	Reference
E	132	GLY	-	LINKER	UNP O35718
E	133	SER	-	LINKER	UNP O35718
E	134	GLY	-	LINKER	UNP O35718
E	135	SER	-	LINKER	UNP O35718
E	136	GLY	-	LINKER	UNP O35718
E	137	SER	-	LINKER	UNP O35718
E	138	GLY	-	LINKER	UNP O35718
E	139	SER	-	LINKER	UNP O35718
G	133	SER	-	LINKER	UNP O35718
G	134	GLY	-	LINKER	UNP O35718
G	135	SER	-	LINKER	UNP O35718
G	136	GLY	-	LINKER	UNP O35718
G	137	SER	-	LINKER	UNP O35718
G	138	GLY	-	LINKER	UNP O35718
G	139	SER	-	LINKER	UNP O35718
H	133	SER	-	LINKER	UNP O35718
H	134	GLY	-	LINKER	UNP O35718
H	135	SER	-	LINKER	UNP O35718
H	136	GLY	-	LINKER	UNP O35718
H	137	SER	-	LINKER	UNP O35718
H	138	GLY	-	LINKER	UNP O35718
H	139	SER	-	LINKER	UNP O35718

- Molecule 4 is 2-TERT-BUTYL-9-FLUORO-3,6-DIHYDRO-7H-BENZ[H]-IMIDAZ[4,5-F]ISOQUINOLINE-7-ONE (three-letter code: IZA) (formula: $C_{18}H_{16}FN_3O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
4	B	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
4	C	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
4	D	1	Total	C	F	N	O	0	0
			23	18	1	3	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



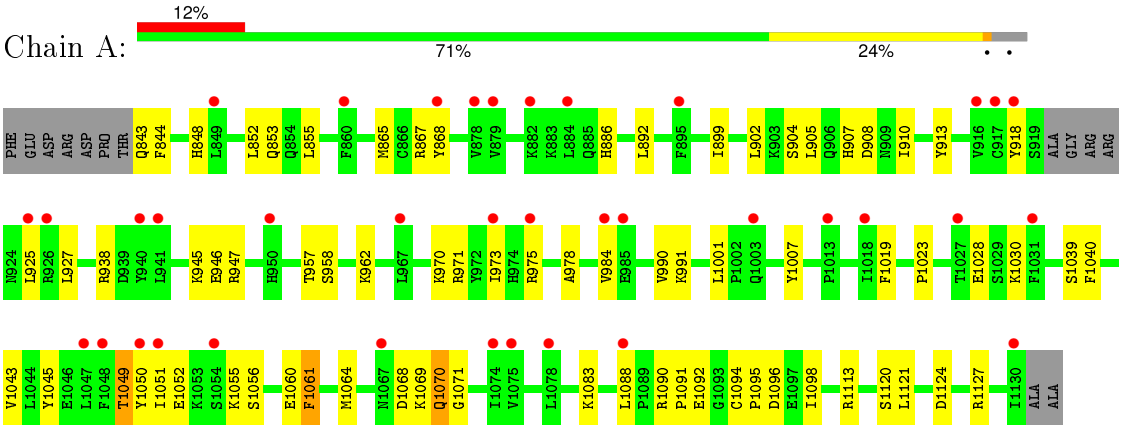
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

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.

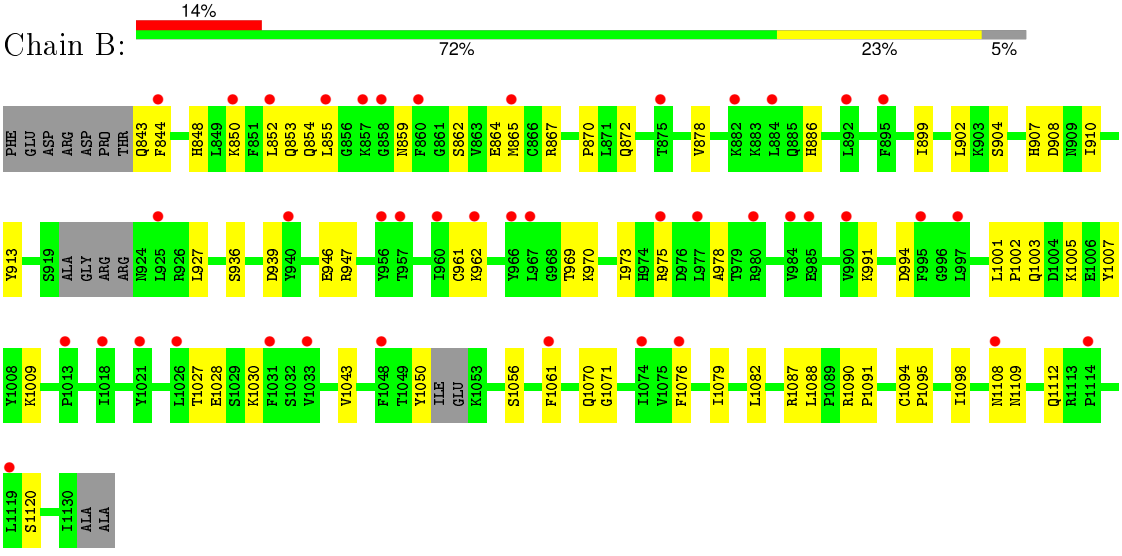
- Molecule 1: Tyrosine-protein kinase

Chain A:



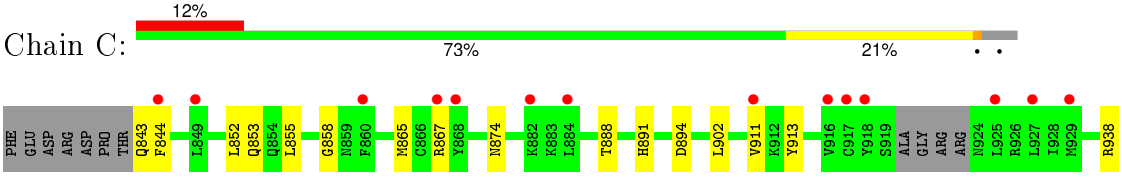
- Molecule 1: Tyrosine-protein kinase

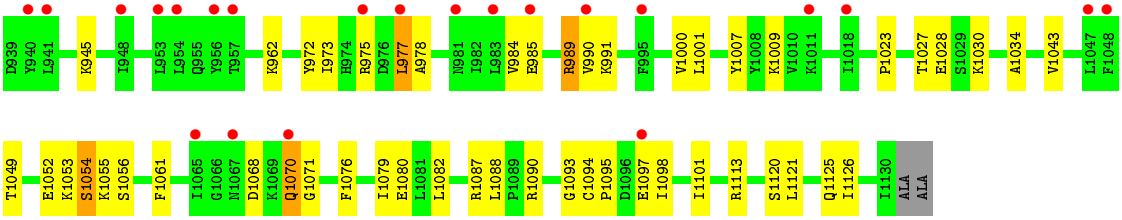
Chain B:



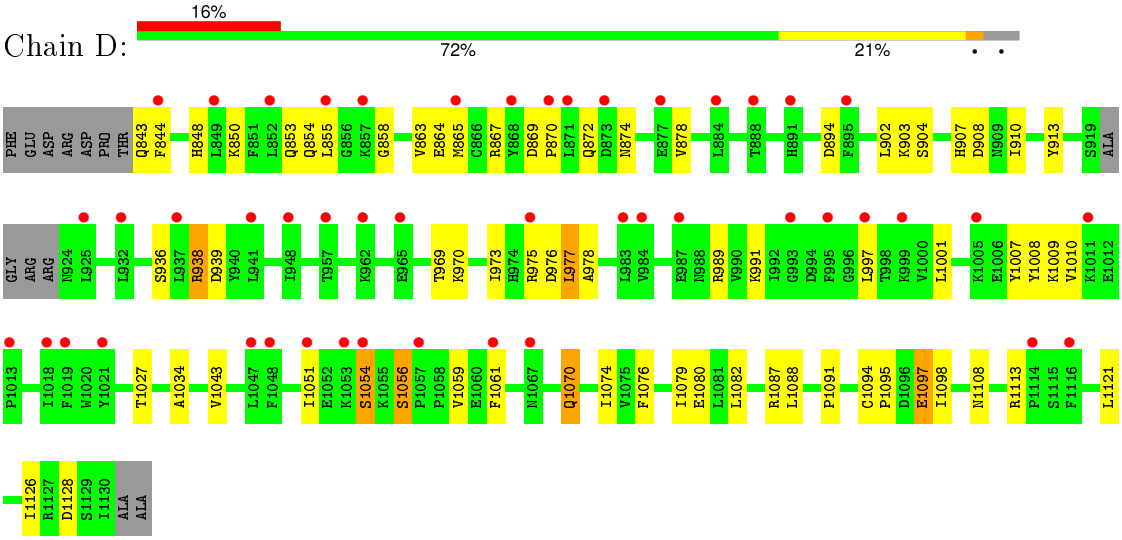
- Molecule 1: Tyrosine-protein kinase

Chain C:

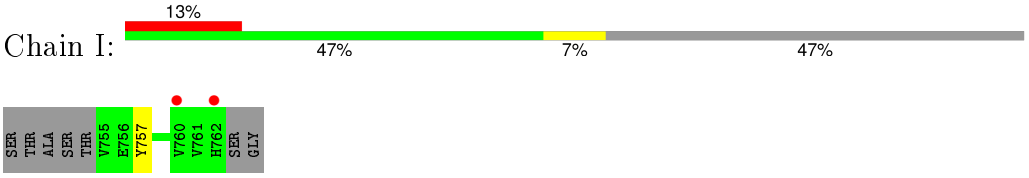




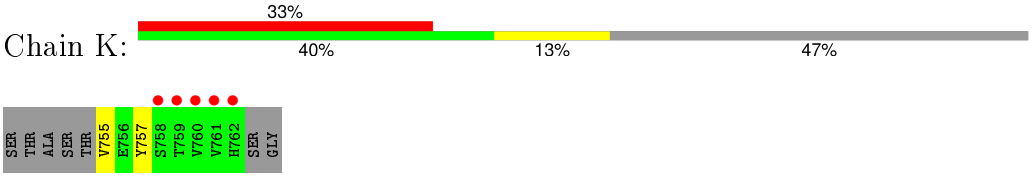
• Molecule 1: Tyrosine-protein kinase



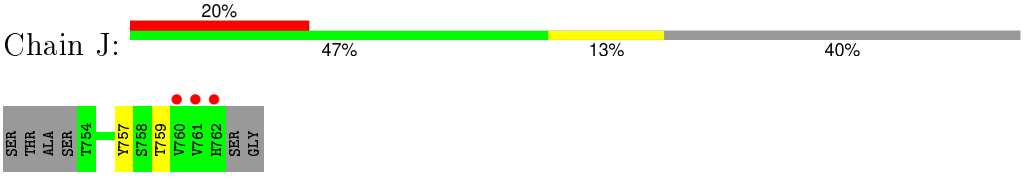
• Molecule 2: Interleukin-6 receptor subunit beta



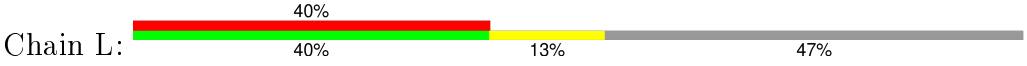
• Molecule 2: Interleukin-6 receptor subunit beta

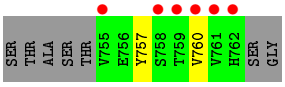


• Molecule 2: Interleukin-6 receptor subunit beta



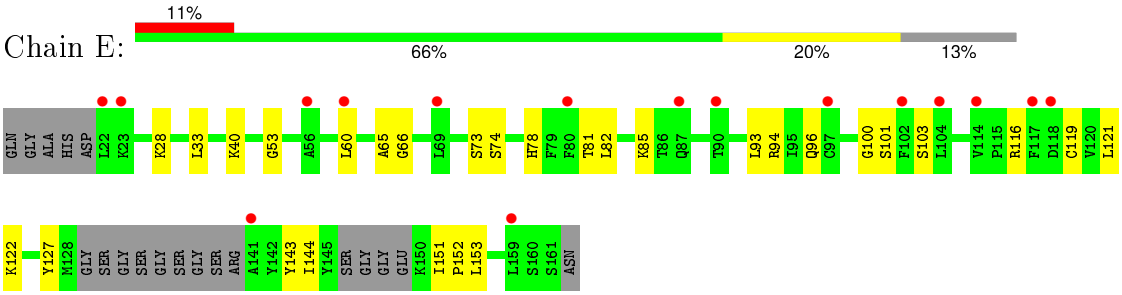
• Molecule 2: Interleukin-6 receptor subunit beta





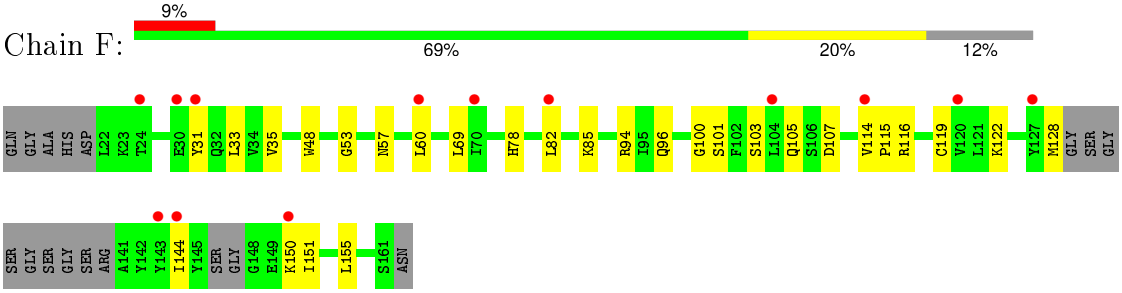
- Molecule 3: Suppressor of cytokine signaling 3

Chain E:



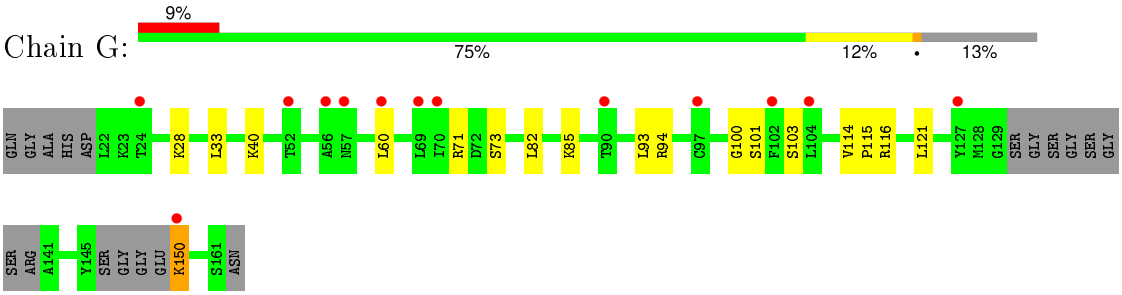
- Molecule 3: Suppressor of cytokine signaling 3

Chain F:



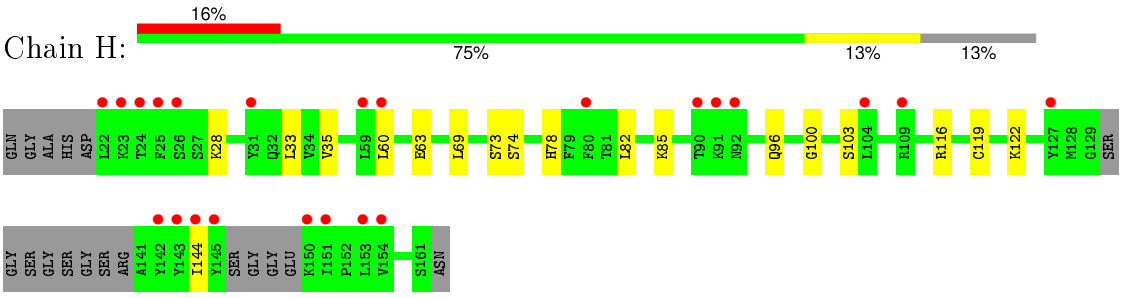
- Molecule 3: Suppressor of cytokine signaling 3

Chain G:



- Molecule 3: Suppressor of cytokine signaling 3

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	139.26Å 139.26Å 316.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.58 – 3.90 95.95 – 3.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.58-3.90) 100.0 (95.95-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 3.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.249 , 0.281 0.254 , 0.277	Depositor DCC
R_{free} test set	1587 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	135.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 192.7	EDS
Estimated twinning fraction	0.186 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 31682 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13682	wwPDB-VP
Average B, all atoms (Å^2)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, 0.375 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: IZA, PO4, PTR

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	0.22	0/2371	0.40	0/3190
1	B	0.22	0/2341	0.39	0/3152
1	C	0.22	0/2366	0.39	0/3185
1	D	0.22	0/2367	0.39	0/3186
2	I	0.18	0/52	0.40	0/69
2	J	0.19	0/59	0.46	0/79
2	K	0.17	0/52	0.39	0/69
2	L	0.19	0/52	0.38	0/69
3	E	0.22	0/996	0.37	0/1344
3	F	0.23	0/1004	0.40	0/1354
3	G	0.22	0/1000	0.37	0/1349
3	H	0.22	0/1000	0.36	0/1349
All	All	0.22	0/13660	0.39	0/18395

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	2355	0	2327	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2326	0	2276	44	0
1	C	2350	0	2311	44	1
1	D	2351	0	2316	47	0
2	I	69	0	58	2	0
2	J	76	0	65	2	0
2	K	69	0	58	4	0
2	L	69	0	58	2	0
3	E	976	0	976	21	0
3	F	984	0	980	18	0
3	G	980	0	979	12	0
3	H	980	0	979	11	1
4	A	23	0	16	1	0
4	B	23	0	16	1	0
4	C	23	0	16	2	0
4	D	23	0	16	2	0
5	B	5	0	0	0	0
All	All	13682	0	13447	232	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 9.

All (232) 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:B:902:LEU:HG	1:B:913:TYR:HB2	1.66	0.77
1:A:904:SER:O	1:A:970:LYS:NZ	2.21	0.72
1:D:908:ASP:O	1:D:991:LYS:NZ	2.25	0.69
3:E:101:SER:O	3:E:116:ARG:NH1	2.26	0.68
1:B:904:SER:O	1:B:970:LYS:NZ	2.26	0.68
1:D:977:LEU:HD12	1:D:1043:VAL:HG21	1.77	0.66
1:A:905:LEU:HB3	1:A:910:ILE:HG21	1.77	0.66
1:C:852:LEU:HD11	1:C:867:ARG:HB2	1.77	0.65
1:C:1090:ARG:HD2	1:C:1094:CYS:HB3	1.80	0.64
1:C:1125:GLN:NE2	1:D:1128:ASP:OD2	2.30	0.64
1:A:1049:THR:HG23	1:A:1091:PRO:HB3	1.80	0.64
3:E:82:LEU:O	3:E:93:LEU:N	2.31	0.63
1:D:907:HIS:HB3	1:D:910:ILE:HB	1.80	0.63
1:B:899:ILE:HG12	1:B:927:LEU:HD22	1.81	0.63
3:F:103:SER:HB3	3:F:116:ARG:HD3	1.81	0.62
1:A:946:GLU:HG2	1:A:947:ARG:HG3	1.79	0.61
1:A:971:ARG:HB3	1:A:1001:LEU:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:853:GLN:HE22	1:C:867:ARG:HH22	1.47	0.61
1:B:853:GLN:HG2	1:B:865:MET:HB3	1.81	0.61
1:B:853:GLN:OE1	1:C:874:ASN:ND2	2.34	0.60
1:D:908:ASP:HB3	1:D:989:ARG:NH1	2.15	0.60
1:D:904:SER:O	1:D:970:LYS:NZ	2.35	0.60
1:D:902:LEU:HG	1:D:913:TYR:HB2	1.83	0.59
1:C:1054:SER:OG	1:C:1054:SER:O	2.20	0.59
1:C:1095:PRO:HB2	1:C:1098:ILE:HG12	1.84	0.59
1:B:1087:ARG:NH2	1:B:1108:ASN:OD1	2.36	0.58
1:D:936:SER:OG	1:D:939:ASP:OD2	2.21	0.58
3:E:82:LEU:HD23	3:E:93:LEU:HD12	1.86	0.57
1:C:853:GLN:HG2	1:C:865:MET:HB3	1.85	0.57
1:C:973:ILE:HG22	1:C:975:ARG:HG3	1.86	0.57
1:D:973:ILE:HG22	1:D:975:ARG:HG3	1.86	0.57
1:A:902:LEU:HG	1:A:913:TYR:HB2	1.85	0.57
2:K:757:PTR:HE2	3:E:81:THR:HG21	1.86	0.57
1:B:867:ARG:NH1	1:C:852:LEU:O	2.38	0.57
2:I:757:PTR:O2P	3:G:94:ARG:NE	2.37	0.57
1:B:850:LYS:NZ	1:B:872:GLN:OE1	2.37	0.56
1:C:985:GLU:OE1	1:C:989:ARG:NE	2.36	0.56
1:D:1097:GLU:HG3	1:D:1126:ILE:HD13	1.88	0.56
3:H:33:LEU:HD22	3:H:100:GLY:HA2	1.88	0.55
1:D:908:ASP:HB3	1:D:989:ARG:HH12	1.70	0.55
1:B:1109:ASN:HD22	1:B:1112:GLN:HG3	1.71	0.55
1:D:1007:PTR:HE1	1:D:1009:LYS:HD3	1.89	0.55
1:B:973:ILE:HG22	1:B:975:ARG:HG3	1.88	0.55
3:G:33:LEU:HD22	3:G:100:GLY:HA2	1.89	0.55
1:D:1008:PTR:HE2	1:D:1010:VAL:HG22	1.89	0.54
1:A:852:LEU:HD11	1:A:867:ARG:HB2	1.90	0.54
1:B:1091:PRO:HB2	1:B:1094:CYS:HB2	1.90	0.54
1:D:858:GLY:HA3	4:D:1201:IZA:H161	1.90	0.54
2:J:757:PTR:O2P	3:F:94:ARG:NE	2.41	0.54
1:C:977:LEU:HD22	1:C:1043:VAL:HG21	1.89	0.54
1:B:1090:ARG:NH1	1:B:1094:CYS:O	2.42	0.53
1:B:854:GLN:HG3	1:B:864:GLU:HG2	1.90	0.53
1:B:852:LEU:HD11	1:B:867:ARG:HB2	1.90	0.53
2:L:760:VAL:HA	3:H:144:ILE:HG22	1.91	0.53
1:D:1054:SER:OG	1:D:1054:SER:O	2.24	0.53
2:K:757:PTR:O2P	3:E:94:ARG:NE	2.42	0.52
3:H:103:SER:HB3	3:H:116:ARG:HD3	1.92	0.52
1:A:899:ILE:HG12	1:A:927:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:902:LEU:HG	1:C:913:TYR:HB2	1.92	0.52
1:D:976:ASP:HB2	1:D:997:LEU:HB2	1.91	0.52
3:G:60:LEU:HB3	3:G:85:LYS:HB2	1.90	0.52
1:B:848:HIS:ND1	1:B:870:PRO:HA	2.24	0.52
1:D:1027:THR:HG22	1:D:1079:ILE:HD13	1.91	0.52
1:C:1034:ALA:HB1	1:C:1113:ARG:HD2	1.92	0.51
1:B:907:HIS:HB3	1:B:910:ILE:HB	1.92	0.51
1:D:854:GLN:HG3	1:D:864:GLU:HG2	1.92	0.51
1:B:1088:LEU:HD12	1:B:1088:LEU:H	1.76	0.51
1:A:1055:LYS:HE2	1:A:1092:GLU:HG3	1.93	0.51
1:B:1095:PRO:HB2	1:B:1098:ILE:HG12	1.93	0.51
1:B:1002:PRO:HG2	1:B:1005:LYS:HB2	1.93	0.51
3:G:101:SER:O	3:G:116:ARG:NH1	2.44	0.51
4:A:2001:IZA:H7	4:A:2001:IZA:O0	2.10	0.51
3:H:60:LEU:HB3	3:H:85:LYS:HB2	1.92	0.51
2:K:755:VAL:HG12	3:E:53:GLY:HA3	1.91	0.51
2:I:757:PTR:OH	3:G:71:ARG:NH2	2.40	0.51
1:A:946:GLU:HG3	1:C:1093:GLY:HA3	1.93	0.51
2:J:759:THR:OG1	3:F:107:ASP:OD2	2.20	0.51
3:E:60:LEU:HB3	3:E:85:LYS:HB2	1.92	0.50
1:A:1083:LYS:O	1:B:1003:GLN:NE2	2.44	0.50
3:F:53:GLY:O	3:F:57:ASN:ND2	2.45	0.50
1:B:946:GLU:HG2	1:B:947:ARG:HG3	1.92	0.50
1:A:867:ARG:NH2	1:D:853:GLN:OE1	2.44	0.50
4:D:1201:IZA:O0	4:D:1201:IZA:H7	2.12	0.50
1:A:984:VAL:HG22	1:A:990:VAL:HG12	1.94	0.50
1:B:859:ASN:ND2	1:B:994:ASP:OD2	2.44	0.50
1:D:850:LYS:NZ	1:D:869:ASP:HB3	2.27	0.50
1:C:984:VAL:HG22	1:C:990:VAL:HG12	1.93	0.50
3:E:66:GLY:N	3:E:85:LYS:O	2.43	0.49
1:A:1095:PRO:HB2	1:A:1098:ILE:HG12	1.94	0.49
1:B:853:GLN:HE21	1:B:855:LEU:HD23	1.76	0.49
1:A:908:ASP:O	1:A:991:LYS:NZ	2.37	0.49
4:C:1201:IZA:H7	4:C:1201:IZA:O0	2.12	0.49
3:F:119:CYS:HB3	3:F:122:LYS:HG3	1.94	0.49
4:B:1201:IZA:O0	4:B:1201:IZA:H7	2.12	0.49
1:A:945:LYS:NZ	1:A:1052:GLU:HB3	2.28	0.49
1:B:1082:LEU:HA	1:B:1087:ARG:HH12	1.78	0.49
1:A:945:LYS:HZ3	1:A:1050:TYR:HB2	1.77	0.49
2:L:757:PTR:O1P	3:H:74:SER:N	2.39	0.49
1:A:853:GLN:HG2	1:A:865:MET:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1088:LEU:H	1:A:1088:LEU:HD12	1.78	0.49
3:F:101:SER:O	3:F:116:ARG:NH1	2.46	0.48
1:C:858:GLY:HA3	4:C:1201:IZA:H161	1.96	0.48
1:A:843:GLN:HB3	1:A:844:PHE:H	1.56	0.48
1:B:1027:THR:HG22	1:B:1079:ILE:HD13	1.96	0.48
1:D:1088:LEU:HD12	1:D:1088:LEU:H	1.77	0.48
3:E:33:LEU:HD22	3:E:100:GLY:HA2	1.95	0.48
1:D:848:HIS:ND1	1:D:870:PRO:HA	2.28	0.48
1:B:936:SER:OG	1:B:939:ASP:OD2	2.32	0.48
1:C:972:TYR:CE1	1:C:1000:VAL:HG22	2.49	0.47
3:E:103:SER:HB3	3:E:116:ARG:HD3	1.97	0.47
1:A:1071:GLY:HA3	3:E:73:SER:O	2.15	0.47
1:A:1028:GLU:HG2	3:E:28:LYS:HB2	1.97	0.47
1:B:865:MET:HE3	1:B:878:VAL:HG11	1.96	0.47
3:F:144:ILE:HG13	3:F:151:ILE:HG13	1.97	0.47
1:A:962:LYS:NZ	1:A:1120:SER:HB2	2.30	0.47
3:F:33:LEU:HD22	3:F:100:GLY:HA2	1.97	0.47
1:A:973:ILE:HG22	1:A:975:ARG:HG3	1.97	0.47
3:F:114:VAL:HA	3:F:115:PRO:HD3	1.82	0.47
1:B:843:GLN:HB3	1:B:844:PHE:H	1.54	0.46
1:C:1070:GLN:HE21	1:C:1070:GLN:H	1.63	0.46
1:B:1028:GLU:HG2	3:H:28:LYS:HB2	1.97	0.46
1:C:1088:LEU:HD12	1:C:1088:LEU:H	1.80	0.46
1:A:907:HIS:HB3	1:A:910:ILE:HB	1.97	0.46
1:D:1070:GLN:HA	1:D:1074:ILE:HD11	1.98	0.46
3:G:114:VAL:HA	3:G:115:PRO:HD3	1.83	0.46
3:E:127:TYR:HB3	3:E:153:LEU:HD21	1.97	0.46
1:D:867:ARG:HD2	1:D:869:ASP:HB2	1.97	0.46
1:B:854:GLN:OE1	1:B:862:SER:OG	2.33	0.46
1:A:853:GLN:HB3	1:D:878:VAL:HG23	1.97	0.46
1:C:1090:ARG:NH1	1:C:1094:CYS:O	2.49	0.46
1:A:867:ARG:HH22	1:D:853:GLN:HE22	1.63	0.45
1:A:1096:ASP:HB3	1:B:907:HIS:NE2	2.31	0.45
3:F:69:LEU:O	3:F:82:LEU:HD12	2.15	0.45
1:C:978:ALA:HA	1:C:1043:VAL:HG22	1.98	0.45
1:C:1068:ASP:O	1:C:1070:GLN:HG3	2.16	0.45
1:D:1095:PRO:HB2	1:D:1098:ILE:HG12	1.97	0.45
1:A:945:LYS:HZ2	1:A:1052:GLU:HB3	1.81	0.45
1:A:938:ARG:NE	1:A:1051:ILE:HD12	2.32	0.45
1:D:1087:ARG:NH2	1:D:1108:ASN:OD1	2.48	0.45
3:F:48:TRP:CD1	3:F:69:LEU:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:ALA:HA	1:A:1043:VAL:HG22	1.97	0.45
1:A:945:LYS:NZ	1:A:1050:TYR:HB2	2.32	0.45
3:E:119:CYS:HB3	3:E:122:LYS:HG3	1.99	0.45
1:A:918:TYR:CE2	1:A:925:LEU:HD22	2.51	0.45
1:B:848:HIS:HA	1:B:872:GLN:NE2	2.31	0.45
2:K:757:PTR:O1P	3:E:74:SER:N	2.49	0.45
1:B:848:HIS:CG	1:B:870:PRO:HA	2.52	0.45
3:F:128:MET:HG2	3:F:155:LEU:HB3	1.98	0.45
1:B:961:CYS:HB3	1:B:1120:SER:HB3	1.99	0.45
1:D:1034:ALA:HB1	1:D:1113:ARG:HD2	1.98	0.45
3:F:150:LYS:HD2	3:F:150:LYS:HA	1.80	0.45
1:D:978:ALA:HA	1:D:1043:VAL:HG22	1.99	0.45
1:C:1027:THR:HG22	1:C:1079:ILE:HD13	1.99	0.44
1:B:1007:PTR:HE2	1:B:1009:LYS:HD3	1.99	0.44
1:B:1076:PHE:HE1	3:H:35:VAL:HG22	1.82	0.44
1:D:938:ARG:HG2	1:D:1051:ILE:HD12	1.98	0.44
1:D:855:LEU:HD12	1:D:863:VAL:HG12	2.00	0.44
1:D:1076:PHE:HE1	3:F:35:VAL:HG22	1.83	0.44
1:A:1070:GLN:HE21	1:A:1070:GLN:H	1.64	0.44
1:C:1049:THR:HB	1:C:1055:LYS:HB3	1.99	0.44
1:B:962:LYS:NZ	1:B:1120:SER:HB2	2.33	0.44
1:B:1071:GLY:HA3	3:H:73:SER:O	2.18	0.44
1:C:843:GLN:HB3	1:C:844:PHE:H	1.53	0.44
1:C:855:LEU:HD21	1:C:865:MET:HB2	1.99	0.44
3:E:143:TYR:HA	3:E:152:PRO:HA	2.00	0.44
1:D:973:ILE:HD11	1:D:1001:LEU:HD11	2.00	0.44
1:C:1023:PRO:HD2	1:C:1113:ARG:NH2	2.33	0.44
1:B:853:GLN:NE2	1:C:867:ARG:HH22	2.15	0.43
1:A:1045:TYR:O	1:A:1049:THR:OG1	2.36	0.43
3:E:78:HIS:ND1	3:E:94:ARG:HD2	2.33	0.43
1:C:962:LYS:NZ	1:C:1120:SER:HB2	2.32	0.43
1:A:973:ILE:HD11	1:A:1001:LEU:HD11	2.00	0.43
1:D:848:HIS:CG	1:D:870:PRO:HA	2.53	0.43
1:B:1009:LYS:HB3	1:B:1030:LYS:HG2	2.00	0.43
1:D:1080:GLU:OE2	3:F:31:TYR:OH	2.35	0.43
3:E:78:HIS:CD2	3:E:96:GLN:HG2	2.53	0.43
3:G:150:LYS:HB3	3:G:150:LYS:HE2	1.77	0.43
1:D:1091:PRO:HB2	1:D:1094:CYS:HB2	2.01	0.43
1:C:911:VAL:HA	1:C:991:LYS:HD3	2.00	0.43
1:A:1090:ARG:HD2	1:A:1094:CYS:HB3	2.01	0.43
1:C:972:TYR:HE1	1:C:1000:VAL:HG22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:894:ASP:OD1	1:C:894:ASP:N	2.52	0.42
3:E:144:ILE:HG13	3:E:151:ILE:HG13	1.99	0.42
3:G:103:SER:HB3	3:G:116:ARG:HD3	2.01	0.42
3:E:40:LYS:O	3:E:121:LEU:HD11	2.19	0.42
3:F:60:LEU:HB3	3:F:85:LYS:HB2	2.00	0.42
1:C:1028:GLU:HG2	3:G:28:LYS:HB2	2.01	0.42
3:H:119:CYS:HB3	3:H:122:LYS:HG3	2.00	0.42
1:C:1071:GLY:HA3	3:G:73:SER:O	2.19	0.42
1:D:843:GLN:HB3	1:D:844:PHE:H	1.54	0.42
1:C:1076:PHE:O	1:C:1080:GLU:HG2	2.20	0.42
1:A:892:LEU:HG	1:A:925:LEU:HG	2.02	0.42
1:C:1082:LEU:HA	1:C:1087:ARG:HH12	1.85	0.42
1:A:1019:PHE:HD1	1:A:1061:PHE:CD2	2.38	0.42
1:D:1082:LEU:HA	1:D:1087:ARG:HH12	1.85	0.41
1:A:1090:ARG:NH1	1:A:1094:CYS:O	2.54	0.41
1:C:973:ILE:HD11	1:C:1001:LEU:HD11	2.02	0.41
1:C:945:LYS:NZ	1:C:1052:GLU:HB3	2.35	0.41
1:B:973:ILE:HD11	1:B:1001:LEU:HD11	2.01	0.41
3:E:65:ALA:HA	3:E:85:LYS:HG3	2.02	0.41
1:A:855:LEU:HD21	1:A:865:MET:HB2	2.03	0.41
1:D:1070:GLN:HE21	1:D:1070:GLN:H	1.68	0.41
3:H:69:LEU:O	3:H:82:LEU:HD12	2.20	0.41
1:D:853:GLN:HG2	1:D:865:MET:HB3	2.02	0.41
1:A:1023:PRO:HD2	1:A:1113:ARG:NH2	2.36	0.41
3:G:82:LEU:O	3:G:93:LEU:N	2.48	0.41
1:A:1060:GLU:O	1:A:1064:MET:HG3	2.21	0.41
1:A:1007:PTR:CD2	1:A:1030:LYS:HE3	2.50	0.41
1:C:1007:PTR:CD2	1:C:1030:LYS:HE3	2.50	0.41
1:C:1097:GLU:O	1:C:1101:ILE:HG13	2.21	0.41
1:C:888:THR:OG1	1:C:891:HIS:ND1	2.54	0.41
1:D:903:LYS:HG3	1:D:913:TYR:CE2	2.56	0.41
1:B:978:ALA:HA	1:B:1043:VAL:HG22	2.03	0.41
3:F:78:HIS:ND1	3:F:94:ARG:HD2	2.36	0.41
1:D:848:HIS:HA	1:D:872:GLN:NE2	2.36	0.41
1:B:908:ASP:O	1:B:991:LYS:NZ	2.40	0.41
3:F:96:GLN:NE2	3:F:105:GLN:HG3	2.35	0.41
1:A:958:SER:O	1:A:962:LYS:HG2	2.21	0.41
1:A:1039:SER:O	1:A:1043:VAL:HG23	2.21	0.41
1:A:1068:ASP:O	1:A:1070:GLN:HG3	2.21	0.41
3:G:40:LYS:HB3	3:G:121:LEU:HD11	2.03	0.41
1:C:1097:GLU:HG3	1:C:1126:ILE:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:ARG:NH2	1:D:908:ASP:OD1	2.54	0.40
1:D:867:ARG:NH2	1:D:874:ASN:OD1	2.54	0.40
1:D:1056:SER:HB2	1:D:1059:VAL:HG23	2.02	0.40
1:A:957:THR:HG23	1:A:1040:PHE:HZ	1.86	0.40
3:H:78:HIS:CD2	3:H:96:GLN:HG2	2.57	0.40
1:C:1007:PTR:HE2	1:C:1009:LYS:HD3	2.03	0.40
1:A:848:HIS:HB2	1:A:868:TYR:CE1	2.57	0.40
1:A:946:GLU:CD	1:A:946:GLU:H	2.24	0.40
1:D:894:ASP:N	1:D:894:ASP:OD1	2.54	0.40
1:A:1124:ASP:HA	1:A:1127:ARG:HB2	2.03	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)
1:C:1056:SER:OG	3:H:63:GLU:OE1[5_455]	2.19	0.01

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	278/297 (94%)	262 (94%)	16 (6%)	0	100	100
1	B	274/297 (92%)	262 (96%)	12 (4%)	0	100	100
1	C	278/297 (94%)	263 (95%)	14 (5%)	1 (0%)	39	79
1	D	278/297 (94%)	263 (95%)	15 (5%)	0	100	100
2	I	5/15 (33%)	5 (100%)	0	0	100	100
2	J	6/15 (40%)	5 (83%)	1 (17%)	0	100	100
2	K	5/15 (33%)	5 (100%)	0	0	100	100
2	L	5/15 (33%)	5 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	118/143 (82%)	117 (99%)	1 (1%)	0	100	100
3	F	120/143 (84%)	117 (98%)	3 (2%)	0	100	100
3	G	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
3	H	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
All	All	1605/1820 (88%)	1540 (96%)	64 (4%)	1 (0%)	56	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1053	LYS

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	260/271 (96%)	253 (97%)	7 (3%)	52	80
1	B	255/271 (94%)	249 (98%)	6 (2%)	57	82
1	C	258/271 (95%)	251 (97%)	7 (3%)	52	80
1	D	259/271 (96%)	250 (96%)	9 (4%)	43	76
2	I	7/12 (58%)	7 (100%)	0	100	100
2	J	8/12 (67%)	8 (100%)	0	100	100
2	K	7/12 (58%)	7 (100%)	0	100	100
2	L	7/12 (58%)	7 (100%)	0	100	100
3	E	110/122 (90%)	110 (100%)	0	100	100
3	F	110/122 (90%)	110 (100%)	0	100	100
3	G	110/122 (90%)	109 (99%)	1 (1%)	84	92
3	H	110/122 (90%)	110 (100%)	0	100	100
All	All	1501/1620 (93%)	1471 (98%)	30 (2%)	63	86

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	886	HIS
1	A	1049	THR
1	A	1056	SER
1	A	1061	PHE
1	A	1069	LYS
1	A	1070	GLN
1	A	1121	LEU
1	B	886	HIS
1	B	969	THR
1	B	1050	TYR
1	B	1056	SER
1	B	1061	PHE
1	B	1070	GLN
1	C	938	ARG
1	C	977	LEU
1	C	989	ARG
1	C	1054	SER
1	C	1061	PHE
1	C	1070	GLN
1	C	1121	LEU
1	D	938	ARG
1	D	969	THR
1	D	977	LEU
1	D	1054	SER
1	D	1056	SER
1	D	1061	PHE
1	D	1070	GLN
1	D	1097	GLU
1	D	1121	LEU
3	G	150	LYS

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

Mol	Chain	Res	Type
1	A	874	ASN
1	B	1109	ASN
1	C	1125	GLN
1	D	986	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PTR	A	1007	1	14,16,17	1.16	1 (7%)	18,22,24	0.66	0
1	PTR	A	1008	1	14,16,17	1.16	1 (7%)	18,22,24	0.65	0
1	PTR	B	1007	1	14,16,17	1.14	1 (7%)	18,22,24	0.67	0
1	PTR	B	1008	1	14,16,17	1.18	1 (7%)	18,22,24	0.68	0
1	PTR	C	1007	1	14,16,17	1.16	1 (7%)	18,22,24	0.69	0
1	PTR	C	1008	1	14,16,17	1.16	1 (7%)	18,22,24	0.63	0
1	PTR	D	1007	1	14,16,17	1.14	1 (7%)	18,22,24	0.63	0
1	PTR	D	1008	1	14,16,17	1.14	1 (7%)	18,22,24	0.63	0
2	PTR	I	757	2	14,16,17	1.19	1 (7%)	18,22,24	0.66	0
2	PTR	J	757	2	14,16,17	1.15	1 (7%)	18,22,24	0.66	0
2	PTR	K	757	2	14,16,17	1.23	1 (7%)	18,22,24	0.67	0
2	PTR	L	757	2	14,16,17	1.18	1 (7%)	18,22,24	0.67	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
1	PTR	A	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1008	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1008	1	-	0/9/11/13	0/1/1/1
1	PTR	C	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	C	1008	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1008	1	-	0/9/11/13	0/1/1/1
2	PTR	I	757	2	-	0/9/11/13	0/1/1/1
2	PTR	J	757	2	-	0/9/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	K	757	2	-	0/9/11/13	0/1/1/1
2	PTR	L	757	2	-	0/9/11/13	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	757	PTR	OH-CZ	-4.39	1.30	1.40
2	I	757	PTR	OH-CZ	-4.23	1.30	1.40
1	B	1008	PTR	OH-CZ	-4.20	1.30	1.40
2	L	757	PTR	OH-CZ	-4.19	1.30	1.40
1	C	1008	PTR	OH-CZ	-4.12	1.30	1.40
1	A	1007	PTR	OH-CZ	-4.12	1.30	1.40
2	J	757	PTR	OH-CZ	-4.12	1.30	1.40
1	C	1007	PTR	OH-CZ	-4.11	1.30	1.40
1	A	1008	PTR	OH-CZ	-4.10	1.30	1.40
1	D	1007	PTR	OH-CZ	-4.05	1.30	1.40
1	B	1007	PTR	OH-CZ	-4.04	1.30	1.40
1	D	1008	PTR	OH-CZ	-4.02	1.30	1.40

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1007	PTR	1	0
1	B	1007	PTR	1	0
1	C	1007	PTR	2	0
1	D	1007	PTR	1	0
1	D	1008	PTR	1	0
2	I	757	PTR	2	0
2	J	757	PTR	1	0
2	K	757	PTR	3	0
2	L	757	PTR	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
4	IZA	A	2001	-	22,26,26	3.38	9 (40%)	25,41,41	1.80	5 (20%)
4	IZA	B	1201	-	22,26,26	3.40	9 (40%)	25,41,41	1.83	6 (24%)
5	PO4	B	1202	-	4,4,4	0.47	0	6,6,6	0.27	0
4	IZA	C	1201	-	22,26,26	3.39	9 (40%)	25,41,41	1.84	6 (24%)
4	IZA	D	1201	-	22,26,26	3.41	9 (40%)	25,41,41	1.85	6 (24%)

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
4	IZA	A	2001	-	-	0/6/6/6	0/4/4/4
4	IZA	B	1201	-	-	0/6/6/6	0/4/4/4
5	PO4	B	1202	-	-	0/0/0/0	0/0/0/0
4	IZA	C	1201	-	-	0/6/6/6	0/4/4/4
4	IZA	D	1201	-	-	0/6/6/6	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1201	IZA	C14-C2	-2.35	1.49	1.53
4	C	1201	IZA	C14-C2	-2.30	1.49	1.53
4	B	1201	IZA	C14-C2	-2.21	1.49	1.53
4	A	2001	IZA	C14-C2	-2.21	1.49	1.53
4	D	1201	IZA	C3-C8	-2.15	1.38	1.44
4	B	1201	IZA	C3-C8	-2.14	1.38	1.44
4	C	1201	IZA	C3-C8	-2.13	1.38	1.44
4	A	2001	IZA	C3-C8	-2.13	1.38	1.44
4	A	2001	IZA	C7-C6	2.13	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1201	IZA	C7-C6	2.19	1.39	1.35
4	D	1201	IZA	C7-C6	2.24	1.39	1.35
4	C	1201	IZA	C7-C6	2.26	1.39	1.35
4	A	2001	IZA	C12-N2	3.80	1.42	1.34
4	C	1201	IZA	C12-N2	3.82	1.42	1.34
4	D	1201	IZA	C12-N2	3.82	1.42	1.34
4	B	1201	IZA	C12-N2	3.82	1.42	1.34
4	D	1201	IZA	C13-C9	3.84	1.48	1.41
4	C	1201	IZA	C13-C9	3.84	1.48	1.41
4	B	1201	IZA	C13-C9	3.91	1.49	1.41
4	A	2001	IZA	C13-C9	3.91	1.49	1.41
4	A	2001	IZA	C8-C10	4.91	1.48	1.41
4	C	1201	IZA	C8-C10	4.93	1.48	1.41
4	B	1201	IZA	C8-C10	5.00	1.48	1.41
4	D	1201	IZA	C8-C10	5.05	1.48	1.41
4	C	1201	IZA	C11-N2	6.10	1.44	1.33
4	B	1201	IZA	C11-N2	6.12	1.44	1.33
4	A	2001	IZA	C11-N2	6.15	1.44	1.33
4	D	1201	IZA	C11-N2	6.17	1.44	1.33
4	C	1201	IZA	C11-C10	6.73	1.52	1.41
4	A	2001	IZA	C11-C10	6.74	1.52	1.41
4	D	1201	IZA	C11-C10	6.76	1.52	1.41
4	B	1201	IZA	C11-C10	6.79	1.52	1.41
4	A	2001	IZA	C13-C12	9.16	1.48	1.36
4	B	1201	IZA	C13-C12	9.21	1.48	1.36
4	D	1201	IZA	C13-C12	9.22	1.48	1.36
4	C	1201	IZA	C13-C12	9.23	1.48	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1201	IZA	C13-C12-N2	-5.48	119.06	123.91
4	D	1201	IZA	C13-C12-N2	-5.38	119.16	123.91
4	A	2001	IZA	C13-C12-N2	-5.35	119.18	123.91
4	B	1201	IZA	C13-C12-N2	-5.30	119.22	123.91
4	D	1201	IZA	C13-C9-C1	-3.19	118.03	122.61
4	C	1201	IZA	C13-C9-C1	-3.14	118.10	122.61
4	B	1201	IZA	C5-C6-C7	-3.09	119.92	123.51
4	B	1201	IZA	C13-C9-C1	-3.06	118.22	122.61
4	A	2001	IZA	C13-C9-C1	-3.04	118.25	122.61
4	C	1201	IZA	C5-C6-C7	-3.02	120.00	123.51
4	D	1201	IZA	C5-C6-C7	-3.02	120.01	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	IZA	C5-C6-C7	-3.00	120.03	123.51
4	C	1201	IZA	C4-C3-C0	-2.72	118.71	122.61
4	D	1201	IZA	C4-C3-C0	-2.70	118.74	122.61
4	B	1201	IZA	C4-C3-C0	-2.66	118.79	122.61
4	A	2001	IZA	C4-C3-C0	-2.55	118.96	122.61
4	B	1201	IZA	C13-C9-C10	2.05	121.00	117.39
4	C	1201	IZA	C13-C9-C10	2.06	121.02	117.39
4	D	1201	IZA	C13-C9-C10	2.16	121.20	117.39
4	A	2001	IZA	C6-C7-C8	3.31	121.24	118.74
4	C	1201	IZA	C6-C7-C8	3.35	121.27	118.74
4	D	1201	IZA	C6-C7-C8	3.47	121.36	118.74
4	B	1201	IZA	C6-C7-C8	3.54	121.42	118.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	IZA	1	0
4	B	1201	IZA	1	0
4	C	1201	IZA	2	0
4	D	1201	IZA	2	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	282/297 (94%)	0.97	37 (13%)	5	4	125, 186, 246, 261	0
1	B	280/297 (94%)	0.92	42 (15%)	3	3	144, 189, 249, 262	0
1	C	282/297 (94%)	0.96	36 (12%)	5	5	122, 183, 254, 269	0
1	D	282/297 (94%)	0.98	47 (16%)	2	2	139, 190, 254, 278	0
2	I	7/15 (46%)	1.13	2 (28%)	1	1	176, 215, 231, 232	0
2	J	8/15 (53%)	1.63	3 (37%)	0	1	189, 216, 244, 247	0
2	K	7/15 (46%)	4.02	5 (71%)	0	0	178, 214, 241, 241	0
2	L	7/15 (46%)	3.55	6 (85%)	0	0	206, 215, 237, 239	0
3	E	124/143 (86%)	0.98	16 (12%)	5	4	124, 157, 238, 250	0
3	F	126/143 (88%)	0.77	13 (10%)	9	6	135, 187, 247, 263	0
3	G	125/143 (87%)	0.93	13 (10%)	8	6	135, 165, 229, 259	0
3	H	125/143 (87%)	0.98	23 (18%)	2	2	144, 191, 246, 266	0
All	All	1655/1820 (90%)	0.97	243 (14%)	3	3	122, 185, 249, 278	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	762	HIS	8.4
3	H	150	LYS	7.6
2	K	760	VAL	6.3
2	K	759	THR	5.9
1	A	1130	ILE	5.7
2	L	762	HIS	5.3
1	B	892	LEU	5.3
3	E	22	LEU	5.0
1	D	871	LEU	5.0
3	H	143	TYR	4.9
1	C	860	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	927	LEU	4.5
1	C	917	CYS	4.4
2	L	755	VAL	4.3
1	D	925	LEU	4.2
2	I	762	HIS	4.1
1	D	993	GLY	4.1
3	H	144	ILE	4.1
2	L	760	VAL	4.0
2	J	760	VAL	3.9
1	A	975	ARG	3.9
1	A	925	LEU	3.9
1	B	855	LEU	3.8
3	E	23	LYS	3.8
1	B	884	LEU	3.8
3	H	145	TYR	3.8
1	C	882	LYS	3.7
2	J	761	VAL	3.6
1	C	884	LEU	3.6
1	A	985	GLU	3.6
1	B	1013	PRO	3.6
1	B	997	LEU	3.5
3	E	141	ALA	3.5
2	L	761	VAL	3.5
1	D	888	THR	3.5
1	D	962	LYS	3.4
1	B	925	LEU	3.4
1	C	867	ARG	3.4
1	C	916	VAL	3.4
1	C	918	TYR	3.4
1	B	966	TYR	3.4
1	A	984	VAL	3.4
3	H	25	PHE	3.4
1	D	852	LEU	3.3
3	E	60	LEU	3.3
1	B	977	LEU	3.3
1	C	981	ASN	3.2
3	G	102	PHE	3.2
1	C	925	LEU	3.2
1	A	882	LYS	3.2
2	L	758	SER	3.2
3	H	60	LEU	3.1
3	H	24	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	1119	LEU	3.1
1	D	873	ASP	3.1
1	D	1054	SER	3.1
1	A	884	LEU	3.1
1	A	941	LEU	3.1
3	G	150	LYS	3.1
1	D	865	MET	3.1
3	H	31	TYR	3.1
2	K	758	SER	3.1
1	A	860	PHE	3.1
1	A	1048	PHE	3.0
1	B	1031	PHE	3.0
1	D	1061	PHE	3.0
1	C	948	ILE	3.0
1	C	1011	LYS	3.0
1	C	1048	PHE	2.9
3	F	143	TYR	2.9
1	B	857	LYS	2.9
2	L	759	THR	2.8
1	C	941	LEU	2.8
3	G	60	LEU	2.8
1	D	948	ILE	2.8
1	C	911	VAL	2.8
3	G	90	THR	2.8
1	B	895	PHE	2.8
1	C	1018	ILE	2.8
1	B	1033	VAL	2.8
3	E	90	THR	2.8
3	F	127	TYR	2.8
3	H	22	LEU	2.8
1	A	917	CYS	2.8
2	J	762	HIS	2.7
1	B	1048	PHE	2.7
3	H	23	LYS	2.7
1	B	844	PHE	2.7
1	B	1026	LEU	2.7
1	B	990	VAL	2.7
1	C	990	VAL	2.7
1	D	870	PRO	2.7
1	D	1051	ILE	2.7
1	D	1057	PRO	2.7
1	C	956	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
3	F	60	LEU	2.7
1	D	1018	ILE	2.7
1	D	855	LEU	2.7
3	F	104	LEU	2.7
1	A	1013	PRO	2.7
1	C	849	LEU	2.6
1	A	878	VAL	2.6
1	A	926	ARG	2.6
1	B	860	PHE	2.6
1	D	895	PHE	2.6
1	B	1108	ASN	2.6
3	E	159	LEU	2.6
1	B	882	LYS	2.6
2	K	761	VAL	2.6
1	B	1114	PRO	2.6
1	D	1116	PHE	2.6
3	F	82	LEU	2.6
1	A	1003	GLN	2.6
1	B	985	GLU	2.6
1	B	967	LEU	2.6
1	C	957	THR	2.6
1	D	965	GLU	2.6
1	D	1013	PRO	2.6
1	B	975	ARG	2.6
3	H	104	LEU	2.6
3	F	120	VAL	2.6
3	H	92	ASN	2.6
3	H	151	ILE	2.5
1	A	849	LEU	2.5
3	H	127	TYR	2.5
2	I	760	VAL	2.5
3	E	69	LEU	2.5
1	B	1076	PHE	2.5
1	B	852	LEU	2.5
1	C	954	LEU	2.5
3	H	153	LEU	2.5
1	D	1048	PHE	2.5
1	C	985	GLU	2.5
1	D	984	VAL	2.5
1	B	957	THR	2.5
3	E	80	PHE	2.5
3	E	114	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1065	ILE	2.5
1	C	1047	LEU	2.4
3	E	56	ALA	2.4
3	H	26	SER	2.4
1	C	977	LEU	2.4
3	F	24	THR	2.4
3	E	102	PHE	2.4
3	F	144	ILE	2.4
1	B	960	ILE	2.4
1	B	858	GLY	2.4
3	H	59	LEU	2.4
3	G	24	THR	2.4
1	D	941	LEU	2.4
1	A	879	VAL	2.4
1	A	1047	LEU	2.3
1	C	929	MET	2.3
1	B	875	THR	2.3
1	B	995	PHE	2.3
1	D	1005	LYS	2.3
1	C	844	PHE	2.3
1	A	916	VAL	2.3
1	C	940	TYR	2.3
3	F	31	TYR	2.3
1	D	1067	ASN	2.3
1	A	1078	LEU	2.3
1	C	983	LEU	2.3
1	A	1018	ILE	2.3
1	A	868	TYR	2.3
1	D	868	TYR	2.3
3	E	87	GLN	2.3
1	D	995	PHE	2.3
3	H	80	PHE	2.3
3	E	118	ASP	2.3
3	H	91	LYS	2.3
1	C	975	ARG	2.3
1	A	895	PHE	2.3
1	A	1027	THR	2.3
1	D	957	THR	2.3
3	G	69	LEU	2.3
1	C	1067	ASN	2.3
1	D	937	LEU	2.2
1	A	1067	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1047	LEU	2.2
1	D	891	HIS	2.2
1	A	1075	VAL	2.2
1	A	973	ILE	2.2
1	D	983	LEU	2.2
3	G	97	CYS	2.2
3	E	104	LEU	2.2
3	G	127	TYR	2.2
1	A	1051	ILE	2.2
1	B	1061	PHE	2.2
1	A	918	TYR	2.2
1	D	975	ARG	2.2
1	D	1053	LYS	2.2
1	C	953	LEU	2.2
1	C	995	PHE	2.2
1	D	987	GLU	2.2
1	D	1114	PRO	2.2
1	B	850	LYS	2.1
3	G	56	ALA	2.1
1	B	940	TYR	2.1
1	B	980	ARG	2.1
3	G	70	ILE	2.1
1	B	984	VAL	2.1
3	H	142	TYR	2.1
3	H	90	THR	2.1
3	F	150	LYS	2.1
1	A	950	HIS	2.1
3	F	70	ILE	2.1
3	G	104	LEU	2.1
1	A	1031	PHE	2.1
3	E	97	CYS	2.1
1	D	997	LEU	2.1
1	D	844	PHE	2.1
3	H	109	ARG	2.1
1	B	865	MET	2.1
1	D	877	GLU	2.1
1	C	868	TYR	2.1
1	A	1050	TYR	2.1
1	B	1021	TYR	2.1
3	G	52	THR	2.1
1	D	857	LYS	2.1
3	G	57	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	940	TYR	2.1
1	A	1074	ILE	2.1
1	D	884	LEU	2.1
1	D	932	LEU	2.1
1	B	962	LYS	2.1
1	C	1097	GLU	2.1
1	A	1054	SER	2.1
1	A	1088	LEU	2.1
1	D	849	LEU	2.1
1	A	967	LEU	2.1
1	D	999	LYS	2.0
3	F	114	VAL	2.0
1	C	1070	GLN	2.0
1	B	956	TYR	2.0
1	D	1021	TYR	2.0
1	D	1011	LYS	2.0
1	B	1074	ILE	2.0
1	D	1019	PHE	2.0
1	B	1018	ILE	2.0
3	F	30	GLU	2.0
3	H	154	VAL	2.0
3	E	117	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{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	LLDF	B-factors(Å^2)	Q<0.9
1	PTR	C	1008	16/17	0.69	0.54	-	175,205,218,223	4
1	PTR	D	1007	16/17	0.68	0.38	-	210,227,238,241	0
1	PTR	B	1007	16/17	0.48	0.47	-	205,228,253,260	0
2	PTR	L	757	16/17	0.92	0.23	-	176,182,211,215	0
1	PTR	C	1007	16/17	0.75	0.30	-	175,199,216,220	0
2	PTR	I	757	16/17	0.84	0.21	-	145,165,210,218	0
2	PTR	K	757	16/17	0.86	0.24	-	146,164,202,217	0
1	PTR	A	1008	16/17	0.48	0.81	-	197,214,223,225	4
1	PTR	B	1008	16/17	0.58	0.46	-	201,219,238,238	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	PTR	A	1007	16/17	0.56	0.38	-	194,217,232,239	0
2	PTR	J	757	16/17	0.84	0.21	-	176,184,214,215	0
1	PTR	D	1008	16/17	0.56	0.41	-	205,213,222,225	4

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^{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	LLDF	B-factors(Å^2)	Q<0.9
4	IZA	B	1201	23/23	0.92	1.01	2.91	183,196,206,209	0
4	IZA	D	1201	23/23	0.90	0.70	1.76	182,189,196,201	0
4	IZA	C	1201	23/23	0.91	0.66	0.95	183,192,202,204	0
4	IZA	A	2001	23/23	0.94	0.51	0.52	158,177,185,188	0
5	PO4	B	1202	5/5	0.69	0.26	-1.48	197,203,214,216	0

6.5 Other polymers (i)

There are no such residues in this entry.