



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:21 PM GMT

PDB ID : 3QS9
Title : Crystal structure of a human Flt3 ligand-receptor ternary complex
Authors : Verstraete, K.; Savvides, S.N.
Deposited on : 2011-02-20
Resolution : 7.80 Å(reported)

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

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

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

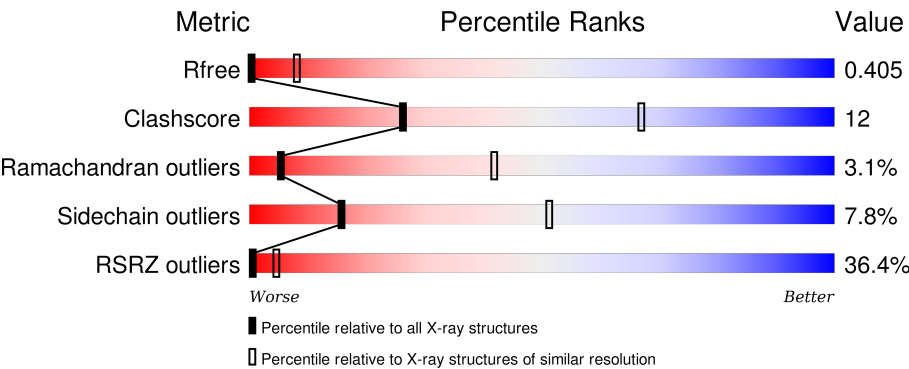
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.80 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	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	138	<div><div>13%</div><div><div></div><div>72%</div><div>20%</div><div>• 6%</div></div></div>
1	B	138	<div><div>5%</div><div><div></div><div>72%</div><div>19%</div><div>• 6%</div></div></div>
1	C	138	<div><div>10%</div><div><div></div><div>72%</div><div>19%</div><div>• 6%</div></div></div>
1	D	138	<div><div>11%</div><div><div></div><div>72%</div><div>19%</div><div>• 6%</div></div></div>
2	E	527	<div><div>36%</div><div><div></div><div>59%</div><div>16%</div><div>• 23%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	527	<div><div></div><div>19%</div><div>47%</div><div>14%</div><div>•</div><div>38%</div></div>
2	G	527	<div><div></div><div>35%</div><div>59%</div><div>17%</div><div>•</div><div>23%</div></div>
2	H	527	<div><div></div><div>41%</div><div>59%</div><div>16%</div><div>•</div><div>23%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13542 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 SL cytokine.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1033	657	181	187	8			
1	B	130	Total	C	N	O	S	0	0	0
			1033	657	181	187	8			
1	C	130	Total	C	N	O	S	0	0	0
			1033	657	181	187	8			
1	D	130	Total	C	N	O	S	0	0	0
			1033	657	181	187	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P49771
A	-2	SER	-	EXPRESSION TAG	UNP P49771
A	-1	HIS	-	EXPRESSION TAG	UNP P49771
A	0	MET	-	EXPRESSION TAG	UNP P49771
B	-3	GLY	-	EXPRESSION TAG	UNP P49771
B	-2	SER	-	EXPRESSION TAG	UNP P49771
B	-1	HIS	-	EXPRESSION TAG	UNP P49771
B	0	MET	-	EXPRESSION TAG	UNP P49771
C	-3	GLY	-	EXPRESSION TAG	UNP P49771
C	-2	SER	-	EXPRESSION TAG	UNP P49771
C	-1	HIS	-	EXPRESSION TAG	UNP P49771
C	0	MET	-	EXPRESSION TAG	UNP P49771
D	-3	GLY	-	EXPRESSION TAG	UNP P49771
D	-2	SER	-	EXPRESSION TAG	UNP P49771
D	-1	HIS	-	EXPRESSION TAG	UNP P49771
D	0	MET	-	EXPRESSION TAG	UNP P49771

- Molecule 2 is a protein called FL cytokine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	405	Total 2463	C 1586	N 427	O 433	S 17	0	0	0
2	F	329	Total 2021	C 1301	N 350	O 355	S 15	0	0	0
2	G	405	Total 2463	C 1586	N 427	O 433	S 17	0	0	0
2	H	405	Total 2463	C 1586	N 427	O 433	S 17	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	24	GLU	-	EXPRESSION TAG	UNP P36888
E	25	THR	-	EXPRESSION TAG	UNP P36888
E	26	GLY	-	EXPRESSION TAG	UNP P36888
E	541	GLY	-	EXPRESSION TAG	UNP P36888
E	542	GLY	-	EXPRESSION TAG	UNP P36888
E	543	THR	-	EXPRESSION TAG	UNP P36888
E	544	LYS	-	EXPRESSION TAG	UNP P36888
E	545	HIS	-	EXPRESSION TAG	UNP P36888
E	546	HIS	-	EXPRESSION TAG	UNP P36888
E	547	HIS	-	EXPRESSION TAG	UNP P36888
E	548	HIS	-	EXPRESSION TAG	UNP P36888
E	549	HIS	-	EXPRESSION TAG	UNP P36888
E	550	HIS	-	EXPRESSION TAG	UNP P36888
F	24	GLU	-	EXPRESSION TAG	UNP P36888
F	25	THR	-	EXPRESSION TAG	UNP P36888
F	26	GLY	-	EXPRESSION TAG	UNP P36888
F	541	GLY	-	EXPRESSION TAG	UNP P36888
F	542	GLY	-	EXPRESSION TAG	UNP P36888
F	543	THR	-	EXPRESSION TAG	UNP P36888
F	544	LYS	-	EXPRESSION TAG	UNP P36888
F	545	HIS	-	EXPRESSION TAG	UNP P36888
F	546	HIS	-	EXPRESSION TAG	UNP P36888
F	547	HIS	-	EXPRESSION TAG	UNP P36888
F	548	HIS	-	EXPRESSION TAG	UNP P36888
F	549	HIS	-	EXPRESSION TAG	UNP P36888
F	550	HIS	-	EXPRESSION TAG	UNP P36888
G	24	GLU	-	EXPRESSION TAG	UNP P36888
G	25	THR	-	EXPRESSION TAG	UNP P36888
G	26	GLY	-	EXPRESSION TAG	UNP P36888
G	541	GLY	-	EXPRESSION TAG	UNP P36888
G	542	GLY	-	EXPRESSION TAG	UNP P36888

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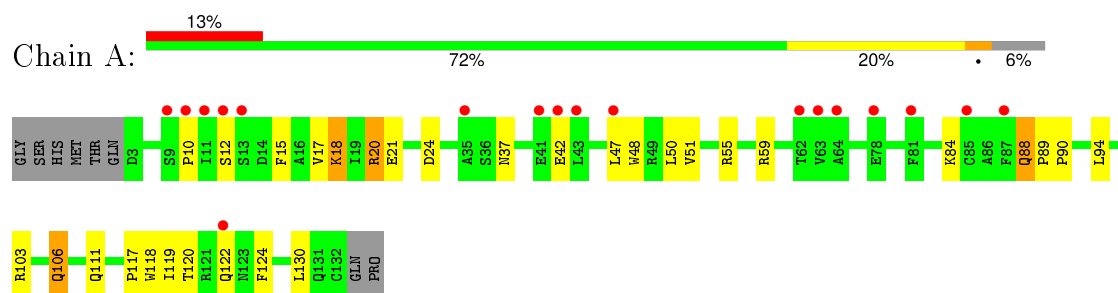
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Chain	Residue	Modelled	Actual	Comment	Reference
G	543	THR	-	EXPRESSION TAG	UNP P36888
G	544	LYS	-	EXPRESSION TAG	UNP P36888
G	545	HIS	-	EXPRESSION TAG	UNP P36888
G	546	HIS	-	EXPRESSION TAG	UNP P36888
G	547	HIS	-	EXPRESSION TAG	UNP P36888
G	548	HIS	-	EXPRESSION TAG	UNP P36888
G	549	HIS	-	EXPRESSION TAG	UNP P36888
G	550	HIS	-	EXPRESSION TAG	UNP P36888
H	24	GLU	-	EXPRESSION TAG	UNP P36888
H	25	THR	-	EXPRESSION TAG	UNP P36888
H	26	GLY	-	EXPRESSION TAG	UNP P36888
H	541	GLY	-	EXPRESSION TAG	UNP P36888
H	542	GLY	-	EXPRESSION TAG	UNP P36888
H	543	THR	-	EXPRESSION TAG	UNP P36888
H	544	LYS	-	EXPRESSION TAG	UNP P36888
H	545	HIS	-	EXPRESSION TAG	UNP P36888
H	546	HIS	-	EXPRESSION TAG	UNP P36888
H	547	HIS	-	EXPRESSION TAG	UNP P36888
H	548	HIS	-	EXPRESSION TAG	UNP P36888
H	549	HIS	-	EXPRESSION TAG	UNP P36888
H	550	HIS	-	EXPRESSION TAG	UNP P36888

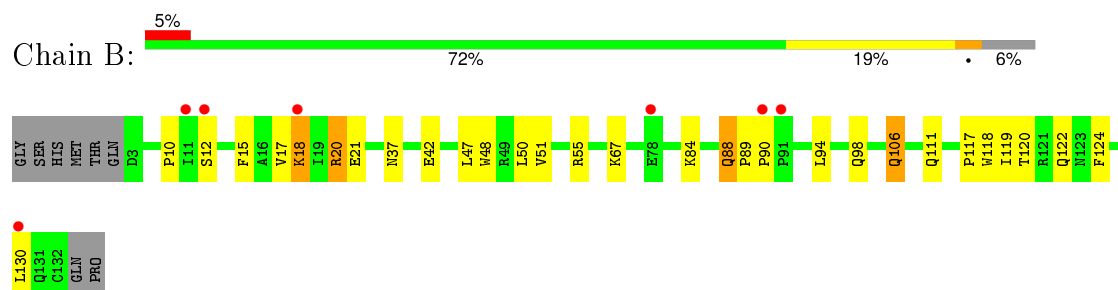
3 Residue-property plots [i](#)

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.

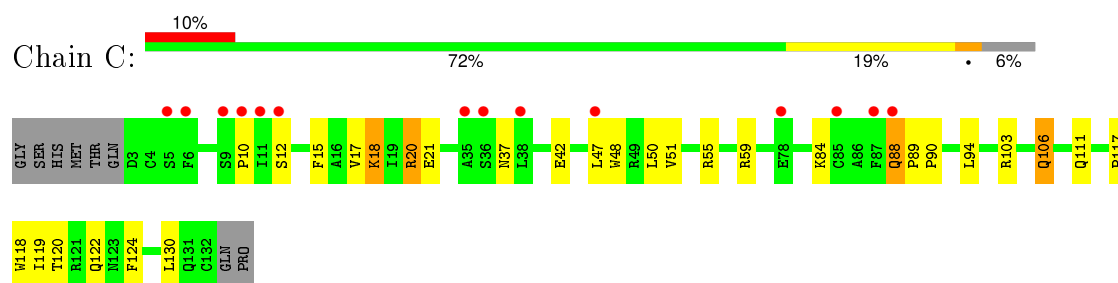
- Molecule 1: SL cytokine



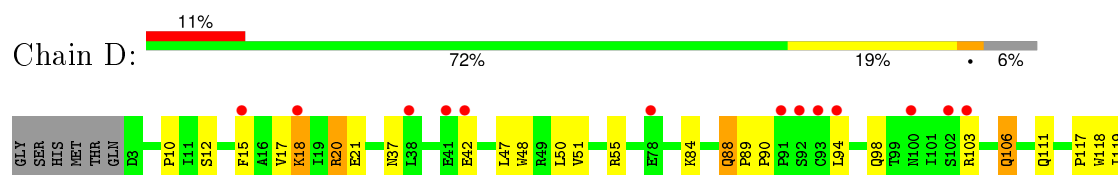
- Molecule 1: SL cytokine

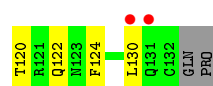


- Molecule 1: SL cytokine

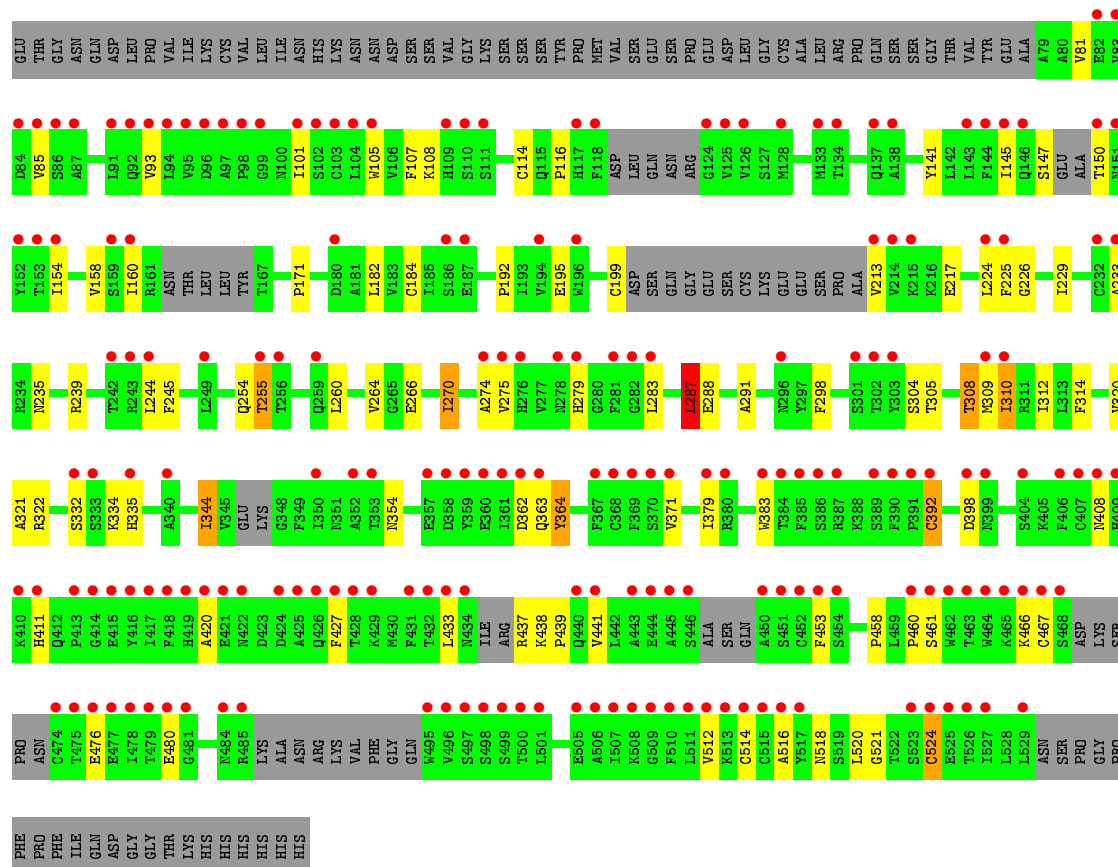


- Molecule 1: SL cytokine

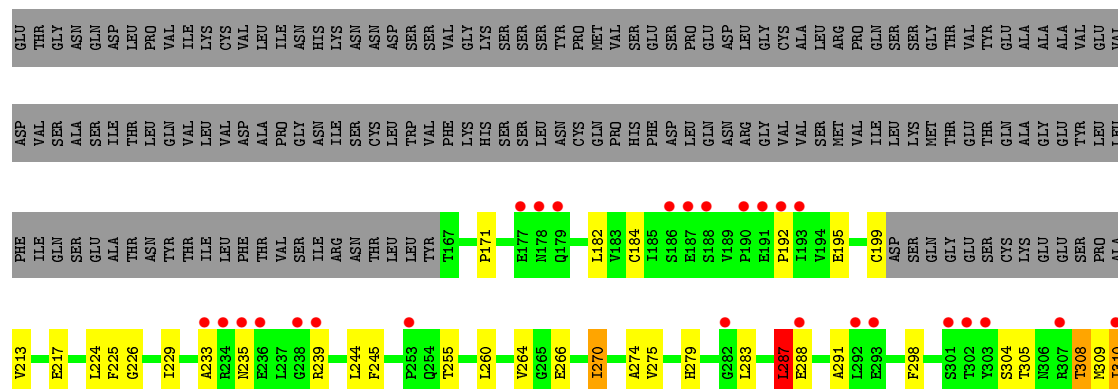


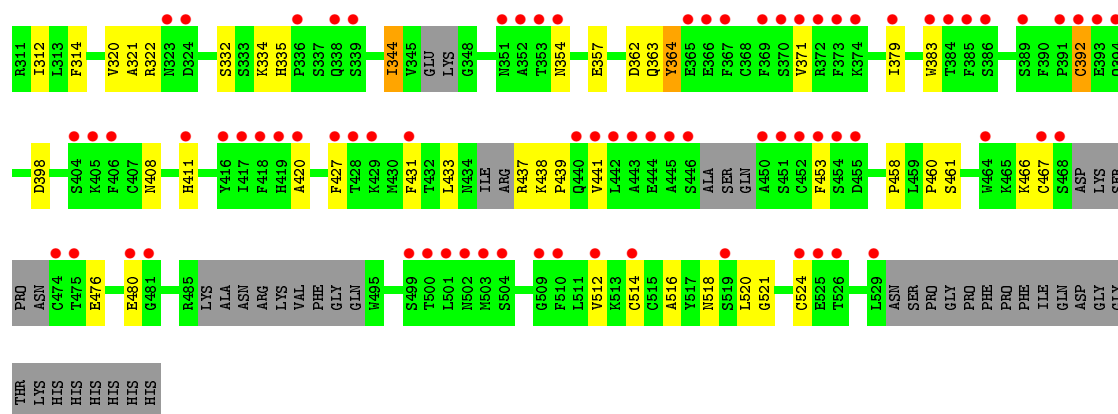


• Molecule 2: FL cytokine receptor

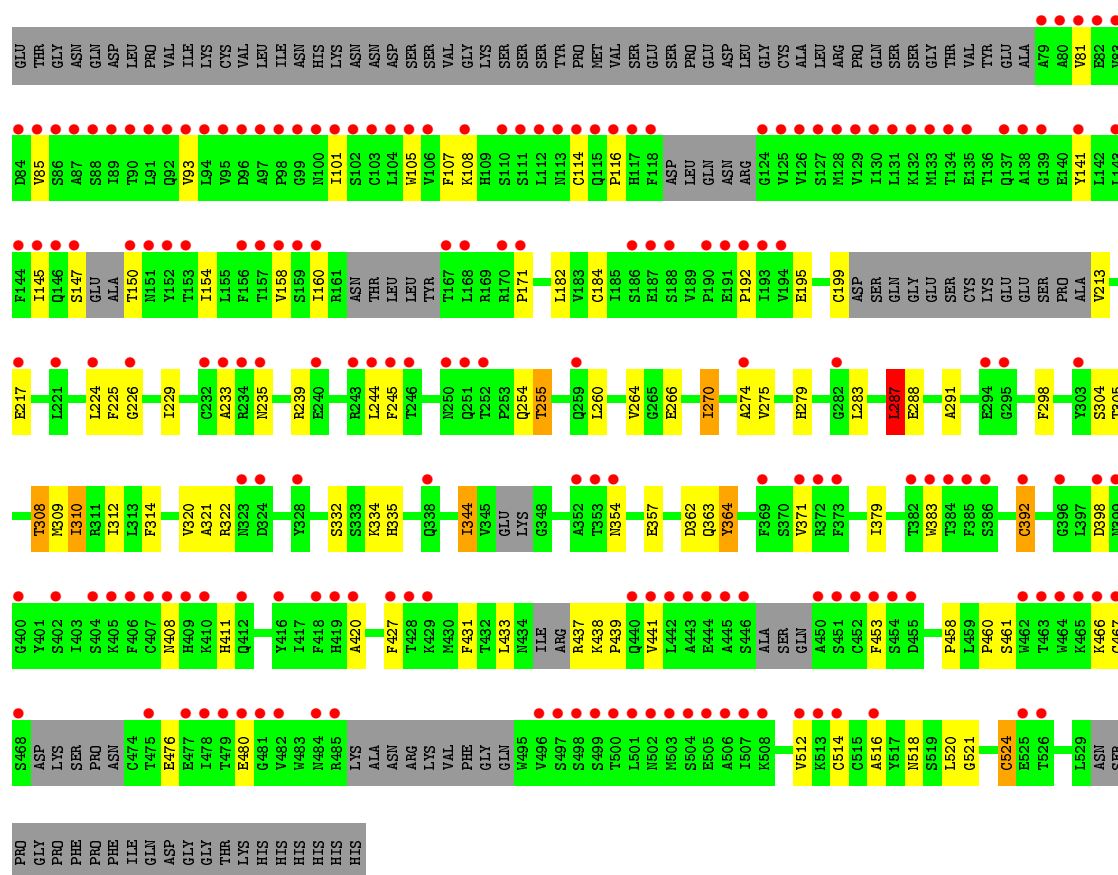


• Molecule 2: FL cytokine receptor

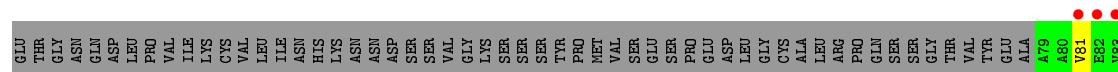
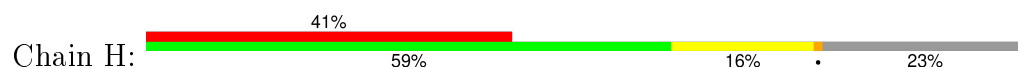


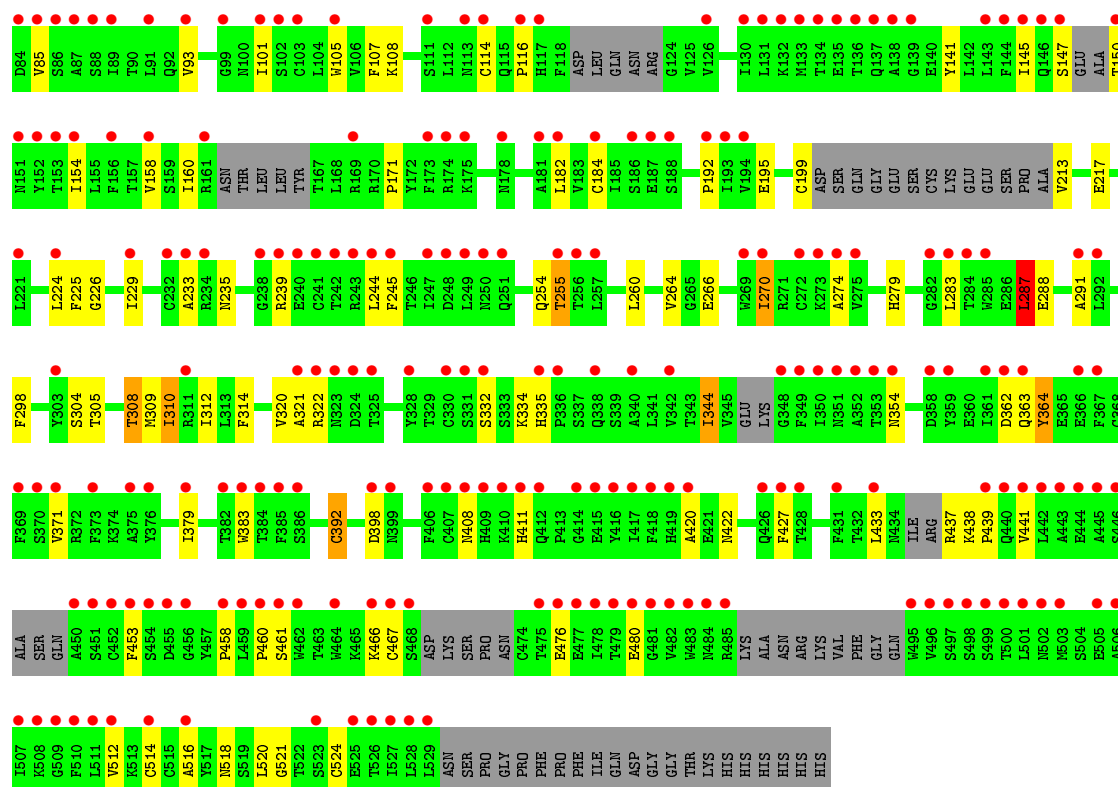


• Molecule 2: FL cytokine receptor



• Molecule 2: FL cytokine receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.75Å 153.55Å 133.87Å 90.00° 94.57° 90.00°	Depositor
Resolution (Å)	35.00 – 7.80 39.52 – 7.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (35.00-7.80) 97.9 (39.52-7.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 8.26Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.337 , 0.346 0.349 , 0.405	Depositor DCC
R_{free} test set	566 reflections (9.98%)	DCC
Wilson B-factor (Å ²)	422.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 563.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 5679 reflections	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	13542	wwPDB-VP
Average B, all atoms (Å ²)	363.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.33	0/1053	0.53	0/1428
1	B	0.34	0/1053	0.53	0/1428
1	C	0.33	0/1053	0.53	0/1428
1	D	0.34	0/1053	0.53	0/1428
2	E	0.62	0/2506	0.80	0/3464
2	F	0.64	0/2061	0.83	0/2848
2	G	0.62	0/2506	0.80	0/3464
2	H	0.62	0/2506	0.80	0/3464
All	All	0.55	0/13791	0.74	0/18952

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 [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	1033	0	1027	23	0
1	B	1033	0	1027	22	0
1	C	1033	0	1027	22	0
1	D	1033	0	1027	21	0
2	E	2463	0	1750	57	0
2	F	2021	0	1430	52	0
2	G	2463	0	1750	58	0
2	H	2463	0	1750	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13542	0	10788	300	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (300) 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)
2:H:287:LEU:HD23	2:H:288:GLU:H	1.38	0.88
2:G:287:LEU:HD23	2:G:288:GLU:H	1.38	0.88
2:E:287:LEU:HD23	2:E:288:GLU:H	1.38	0.86
2:F:287:LEU:HD23	2:F:288:GLU:H	1.38	0.86
2:F:520:LEU:HD12	2:F:521:GLY:N	1.96	0.81
2:H:438:LYS:HA	2:H:520:LEU:CD1	2.11	0.81
2:G:438:LYS:HA	2:G:520:LEU:CD1	2.11	0.81
2:E:438:LYS:HA	2:E:520:LEU:CD1	2.11	0.81
2:E:520:LEU:HD12	2:E:521:GLY:N	1.96	0.81
2:F:438:LYS:HA	2:F:520:LEU:CD1	2.11	0.80
2:G:520:LEU:HD12	2:G:521:GLY:N	1.96	0.80
1:B:106:GLN:HA	1:B:106:GLN:HE21	1.46	0.80
2:H:520:LEU:HD12	2:H:521:GLY:N	1.96	0.80
1:C:106:GLN:HE21	1:C:106:GLN:HA	1.47	0.79
2:E:514:CYS:O	2:E:524:CYS:SG	2.41	0.79
2:G:514:CYS:O	2:G:524:CYS:SG	2.41	0.79
1:D:106:GLN:HA	1:D:106:GLN:HE21	1.46	0.78
2:F:514:CYS:O	2:F:524:CYS:SG	2.41	0.78
2:H:514:CYS:O	2:H:524:CYS:SG	2.41	0.78
1:A:106:GLN:HE21	1:A:106:GLN:HA	1.47	0.77
1:A:88:GLN:HA	1:A:88:GLN:HE21	1.50	0.76
1:B:88:GLN:HE21	1:B:88:GLN:HA	1.50	0.75
1:C:88:GLN:HE21	1:C:88:GLN:HA	1.50	0.74
1:D:88:GLN:HE21	1:D:88:GLN:HA	1.50	0.74
2:E:520:LEU:HD12	2:E:521:GLY:H	1.53	0.73
2:F:520:LEU:HD12	2:F:521:GLY:H	1.53	0.73
2:E:304:SER:HB2	2:E:310:ILE:HD11	1.71	0.73
2:F:304:SER:HB2	2:F:310:ILE:HD11	1.71	0.72
2:G:322:ARG:HA	2:G:344:ILE:HG21	1.71	0.72
2:F:322:ARG:HA	2:F:344:ILE:HG21	1.71	0.71
2:G:304:SER:HB2	2:G:310:ILE:HD11	1.71	0.71
2:E:322:ARG:HA	2:E:344:ILE:HG21	1.71	0.71
2:H:304:SER:HB2	2:H:310:ILE:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:520:LEU:HD12	2:H:521:GLY:H	1.53	0.70
2:G:520:LEU:HD12	2:G:521:GLY:H	1.53	0.70
2:H:322:ARG:HA	2:H:344:ILE:HG21	1.71	0.70
2:E:147:SER:HG	2:E:150:THR:N	1.89	0.70
2:F:466:LYS:CB	2:F:512:VAL:HG12	2.23	0.69
2:H:466:LYS:CB	2:H:512:VAL:HG12	2.24	0.68
2:E:466:LYS:CB	2:E:512:VAL:HG12	2.24	0.68
2:G:466:LYS:CB	2:G:512:VAL:HG12	2.23	0.68
2:G:147:SER:HG	2:G:150:THR:N	1.91	0.68
2:H:147:SER:HG	2:H:150:THR:N	1.93	0.67
2:E:437:ARG:O	2:E:520:LEU:HD11	1.96	0.66
2:H:379:ILE:HD13	2:H:420:ALA:HB1	1.78	0.65
2:F:437:ARG:O	2:F:520:LEU:HD11	1.97	0.65
2:G:379:ILE:HD13	2:G:420:ALA:HB1	1.78	0.65
2:H:437:ARG:O	2:H:520:LEU:HD11	1.96	0.64
2:E:379:ILE:HD13	2:E:420:ALA:HB1	1.78	0.64
2:G:437:ARG:O	2:G:520:LEU:HD11	1.96	0.64
2:F:379:ILE:HD13	2:F:420:ALA:HB1	1.78	0.64
1:C:20:ARG:HD2	1:C:21:GLU:HG3	1.80	0.64
1:A:20:ARG:HD2	1:A:21:GLU:HG3	1.80	0.64
2:G:438:LYS:HA	2:G:520:LEU:HD11	1.80	0.63
1:D:20:ARG:HD2	1:D:21:GLU:HG3	1.79	0.63
2:F:438:LYS:HA	2:F:520:LEU:HD13	1.81	0.62
1:B:20:ARG:HD2	1:B:21:GLU:HG3	1.79	0.62
2:G:439:PRO:CG	2:G:518:ASN:HB2	2.29	0.62
2:F:438:LYS:HA	2:F:520:LEU:HD11	1.81	0.62
2:F:439:PRO:CG	2:F:518:ASN:HB2	2.30	0.62
2:H:438:LYS:HA	2:H:520:LEU:HD13	1.81	0.62
2:E:438:LYS:HA	2:E:520:LEU:HD11	1.81	0.62
2:E:439:PRO:CG	2:E:518:ASN:HB2	2.30	0.62
2:H:439:PRO:CG	2:H:518:ASN:HB2	2.30	0.61
1:C:122:GLN:HB2	1:C:124:PHE:CZ	2.36	0.61
2:E:438:LYS:HA	2:E:520:LEU:HD13	1.81	0.61
2:H:438:LYS:HA	2:H:520:LEU:HD11	1.80	0.61
1:A:122:GLN:HB2	1:A:124:PHE:CZ	2.36	0.61
2:G:182:LEU:HB2	2:G:224:LEU:HD21	1.84	0.60
2:G:438:LYS:HA	2:G:520:LEU:HD13	1.81	0.60
1:B:122:GLN:HB2	1:B:124:PHE:CZ	2.37	0.60
1:D:122:GLN:HB2	1:D:124:PHE:CZ	2.37	0.60
2:F:182:LEU:HB2	2:F:224:LEU:HD21	1.84	0.60
2:H:182:LEU:HB2	2:H:224:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:LEU:HB2	2:E:224:LEU:HD21	1.84	0.59
2:H:518:ASN:OD1	2:H:520:LEU:HG	2.02	0.59
2:E:518:ASN:OD1	2:E:520:LEU:HG	2.02	0.59
2:F:441:VAL:HG23	2:F:453:PHE:O	2.03	0.59
2:F:518:ASN:OD1	2:F:520:LEU:HG	2.02	0.59
2:G:441:VAL:HG23	2:G:453:PHE:O	2.03	0.59
2:H:171:PRO:HB3	2:H:184:CYS:SG	2.43	0.59
2:F:171:PRO:HB3	2:F:184:CYS:SG	2.43	0.59
2:G:171:PRO:HB3	2:G:184:CYS:SG	2.43	0.59
2:E:441:VAL:HG23	2:E:453:PHE:O	2.03	0.59
2:G:518:ASN:OD1	2:G:520:LEU:HG	2.02	0.58
1:D:17:VAL:O	1:D:20:ARG:HG3	2.03	0.58
2:E:171:PRO:HB3	2:E:184:CYS:SG	2.43	0.58
1:C:119:ILE:HG23	1:C:120:THR:HG23	1.85	0.58
1:A:119:ILE:HG23	1:A:120:THR:HG23	1.85	0.58
2:E:332:SER:CB	2:E:335:HIS:HB2	2.34	0.58
2:H:441:VAL:HG23	2:H:453:PHE:O	2.03	0.58
2:H:332:SER:CB	2:H:335:HIS:HB2	2.34	0.58
2:E:441:VAL:HG13	2:E:441:VAL:O	2.04	0.58
2:G:320:VAL:HB	2:G:344:ILE:HD11	1.85	0.57
2:H:441:VAL:O	2:H:441:VAL:HG13	2.04	0.57
1:C:17:VAL:O	1:C:20:ARG:HG3	2.05	0.57
2:F:320:VAL:HB	2:F:344:ILE:HD11	1.85	0.57
2:E:320:VAL:HB	2:E:344:ILE:HD11	1.85	0.57
1:B:17:VAL:O	1:B:20:ARG:HG3	2.03	0.57
2:F:332:SER:CB	2:F:335:HIS:HB2	2.34	0.57
2:H:320:VAL:HB	2:H:344:ILE:HD11	1.85	0.57
2:F:441:VAL:O	2:F:441:VAL:HG13	2.04	0.57
2:G:332:SER:CB	2:G:335:HIS:HB2	2.34	0.57
1:D:119:ILE:HG23	1:D:120:THR:HG23	1.87	0.57
1:B:88:GLN:HA	1:B:88:GLN:NE2	2.19	0.57
2:E:466:LYS:CA	2:E:512:VAL:HG12	2.35	0.57
1:A:17:VAL:O	1:A:20:ARG:HG3	2.05	0.56
2:G:441:VAL:HG13	2:G:441:VAL:O	2.04	0.56
1:D:55:ARG:HH12	1:D:90:PRO:HD3	1.71	0.56
2:H:466:LYS:CA	2:H:512:VAL:HG12	2.35	0.56
2:G:466:LYS:CA	2:G:512:VAL:HG12	2.35	0.56
1:A:59:ARG:HH11	1:D:98:GLN:HE22	1.54	0.56
1:A:88:GLN:NE2	1:A:88:GLN:HA	2.20	0.56
2:F:466:LYS:CA	2:F:512:VAL:HG12	2.35	0.56
2:E:245:PHE:HD2	2:E:270:ILE:HG23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ARG:HH12	1:B:90:PRO:HD3	1.70	0.55
2:G:245:PHE:HD2	2:G:270:ILE:HG23	1.72	0.55
1:B:119:ILE:HG23	1:B:120:THR:HG23	1.87	0.55
1:B:98:GLN:HE22	1:C:59:ARG:HH11	1.54	0.55
1:D:88:GLN:NE2	1:D:88:GLN:HA	2.19	0.55
1:A:55:ARG:HH12	1:A:90:PRO:HD3	1.72	0.55
2:H:287:LEU:CD2	2:H:288:GLU:H	2.16	0.54
2:G:287:LEU:CD2	2:G:288:GLU:H	2.16	0.54
2:F:458:PRO:O	2:F:460:PRO:HD3	2.07	0.54
2:H:199:CYS:HA	2:H:213:VAL:HA	1.90	0.54
2:E:458:PRO:O	2:E:460:PRO:HD3	2.07	0.54
2:H:245:PHE:HD2	2:H:270:ILE:HG23	1.71	0.54
2:F:245:PHE:HD2	2:F:270:ILE:HG23	1.71	0.54
1:C:55:ARG:HH12	1:C:90:PRO:HD3	1.72	0.54
2:E:437:ARG:O	2:E:520:LEU:HD21	2.08	0.54
2:G:437:ARG:O	2:G:520:LEU:HD21	2.08	0.53
2:F:287:LEU:CD2	2:F:288:GLU:H	2.16	0.53
2:F:437:ARG:O	2:F:520:LEU:HD21	2.08	0.53
2:E:199:CYS:HA	2:E:213:VAL:HA	1.90	0.53
2:E:101:ILE:HG12	2:E:147:SER:HA	1.91	0.53
2:H:458:PRO:O	2:H:460:PRO:HD3	2.08	0.53
2:G:458:PRO:O	2:G:460:PRO:HD3	2.08	0.53
1:D:117:PRO:HG2	1:D:118:TRP:CD1	2.44	0.53
2:F:199:CYS:HA	2:F:213:VAL:HA	1.90	0.53
2:G:199:CYS:HA	2:G:213:VAL:HA	1.90	0.53
1:C:117:PRO:HG2	1:C:118:TRP:CD1	2.44	0.53
1:C:88:GLN:NE2	1:C:88:GLN:HA	2.20	0.53
1:A:117:PRO:HG2	1:A:118:TRP:CD1	2.44	0.53
2:H:437:ARG:O	2:H:520:LEU:HD21	2.08	0.52
2:G:466:LYS:HA	2:G:512:VAL:HG12	1.91	0.52
2:F:466:LYS:HA	2:F:512:VAL:HG12	1.91	0.52
2:H:466:LYS:HA	2:H:512:VAL:HG12	1.91	0.52
2:H:101:ILE:HG12	2:H:147:SER:HA	1.91	0.52
2:H:439:PRO:HD3	2:H:520:LEU:HD11	1.92	0.52
1:A:106:GLN:NE2	1:A:106:GLN:HA	2.22	0.52
2:E:439:PRO:HD3	2:E:520:LEU:HD11	1.92	0.52
2:E:466:LYS:HA	2:E:512:VAL:HG12	1.91	0.52
2:F:439:PRO:HG3	2:F:518:ASN:HB2	1.92	0.52
1:B:117:PRO:HG2	1:B:118:TRP:CD1	2.44	0.52
2:G:101:ILE:HG12	2:G:147:SER:HA	1.91	0.52
1:B:98:GLN:HE22	1:C:59:ARG:HD3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:437:ARG:N	2:G:520:LEU:HD21	2.25	0.52
2:H:437:ARG:N	2:H:520:LEU:HD21	2.25	0.52
2:F:439:PRO:HD3	2:F:520:LEU:HD11	1.92	0.51
1:D:84:LYS:HE3	2:G:279:HIS:CE1	2.46	0.51
2:E:81:VAL:HB	2:E:158:VAL:HA	1.93	0.51
2:G:225:PHE:HA	2:G:312:ILE:HD11	1.92	0.51
1:D:12:SER:O	1:D:15:PHE:HD2	1.94	0.51
2:E:298:PHE:HB3	2:E:314:PHE:CE1	2.46	0.51
2:G:439:PRO:HD3	2:G:520:LEU:HD11	1.92	0.51
2:E:437:ARG:N	2:E:520:LEU:HD21	2.25	0.51
1:B:84:LYS:HE3	2:F:279:HIS:CE1	2.46	0.51
2:E:439:PRO:HG3	2:E:518:ASN:HB2	1.92	0.51
1:B:12:SER:O	1:B:15:PHE:HD2	1.93	0.51
2:F:437:ARG:N	2:F:520:LEU:HD21	2.25	0.51
2:F:298:PHE:HB3	2:F:314:PHE:CE1	2.46	0.51
2:H:439:PRO:HG3	2:H:518:ASN:HB2	1.92	0.51
2:G:439:PRO:HG3	2:G:518:ASN:HB2	1.92	0.51
2:H:245:PHE:CD2	2:H:270:ILE:HG23	2.46	0.51
2:E:225:PHE:HA	2:E:312:ILE:HD11	1.92	0.51
2:E:287:LEU:CD2	2:E:288:GLU:H	2.16	0.50
2:G:298:PHE:HB3	2:G:314:PHE:CE1	2.46	0.50
2:H:458:PRO:N	2:H:518:ASN:HD21	2.09	0.50
1:B:47:LEU:O	1:B:51:VAL:HG23	2.12	0.50
2:G:81:VAL:HB	2:G:158:VAL:HA	1.92	0.50
2:E:458:PRO:N	2:E:518:ASN:HD21	2.09	0.50
2:G:245:PHE:CD2	2:G:270:ILE:HG23	2.46	0.50
2:F:458:PRO:N	2:F:518:ASN:HD21	2.10	0.50
2:H:298:PHE:HB3	2:H:314:PHE:CE1	2.46	0.50
2:H:81:VAL:HB	2:H:158:VAL:HA	1.93	0.50
2:E:245:PHE:CD2	2:E:270:ILE:HG23	2.46	0.50
2:H:225:PHE:HA	2:H:312:ILE:HD11	1.92	0.50
2:F:245:PHE:CD2	2:F:270:ILE:HG23	2.46	0.50
1:C:47:LEU:O	1:C:51:VAL:HG23	2.12	0.50
1:C:84:LYS:HE3	2:H:279:HIS:CE1	2.47	0.50
1:D:47:LEU:O	1:D:51:VAL:HG23	2.11	0.50
2:G:458:PRO:N	2:G:518:ASN:HD21	2.10	0.49
1:A:84:LYS:HE3	2:E:279:HIS:CE1	2.47	0.49
2:F:225:PHE:HA	2:F:312:ILE:HD11	1.92	0.49
1:A:47:LEU:O	1:A:51:VAL:HG23	2.12	0.49
1:B:106:GLN:NE2	1:B:106:GLN:HA	2.21	0.49
2:F:264:VAL:HG13	2:F:321:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:264:VAL:HG13	2:E:321:ALA:HA	1.95	0.48
2:E:105:TRP:HD1	2:E:114:CYS:HB3	1.79	0.48
2:H:264:VAL:HG13	2:H:321:ALA:HA	1.95	0.48
1:D:106:GLN:HA	1:D:106:GLN:NE2	2.21	0.48
1:C:106:GLN:NE2	1:C:106:GLN:HA	2.23	0.48
2:H:105:TRP:HD1	2:H:114:CYS:HB3	1.79	0.48
1:D:50:LEU:HG	1:D:111:GLN:HE21	1.79	0.47
2:G:264:VAL:HG13	2:G:321:ALA:HA	1.95	0.47
2:G:105:TRP:HD1	2:G:114:CYS:HB3	1.79	0.47
1:B:50:LEU:HG	1:B:111:GLN:HE21	1.79	0.47
2:F:437:ARG:C	2:F:520:LEU:HD21	2.35	0.47
2:E:437:ARG:C	2:E:520:LEU:HD21	2.35	0.47
1:C:50:LEU:HG	1:C:111:GLN:HE21	1.80	0.47
2:F:266:GLU:O	2:F:320:VAL:HG22	2.15	0.46
2:H:266:GLU:O	2:H:320:VAL:HG22	2.15	0.46
1:A:12:SER:O	1:A:15:PHE:HD2	1.98	0.46
2:G:437:ARG:C	2:G:520:LEU:HD21	2.35	0.46
2:H:467:CYS:CB	2:H:476:GLU:CB	2.94	0.46
2:E:467:CYS:CB	2:E:476:GLU:CB	2.94	0.46
2:H:437:ARG:C	2:H:520:LEU:HD21	2.35	0.46
1:C:12:SER:O	1:C:15:PHE:HD2	1.99	0.46
2:F:467:CYS:CB	2:F:476:GLU:CB	2.94	0.46
1:A:50:LEU:HG	1:A:111:GLN:HE21	1.80	0.46
2:E:192:PRO:HB3	2:E:235:ASN:HB3	1.98	0.46
1:A:103:ARG:HA	1:A:103:ARG:HD2	1.73	0.45
1:A:18:LYS:HD2	1:A:18:LYS:N	2.31	0.45
2:G:192:PRO:HB3	2:G:235:ASN:HB3	1.98	0.45
1:C:18:LYS:N	1:C:18:LYS:HD2	2.31	0.45
2:H:192:PRO:HB3	2:H:235:ASN:HB3	1.98	0.45
2:G:467:CYS:CB	2:G:476:GLU:CB	2.94	0.45
2:F:461:SER:O	2:F:516:ALA:HA	2.17	0.45
2:H:107:PHE:HA	2:H:141:TYR:HD2	1.81	0.45
1:A:37:ASN:OD1	1:A:94:LEU:HD12	2.17	0.45
2:E:266:GLU:O	2:E:320:VAL:HG22	2.15	0.45
2:E:233:ALA:O	2:E:239:ARG:HA	2.17	0.45
1:C:10:PRO:HB3	2:H:279:HIS:CE1	2.53	0.44
2:G:107:PHE:HA	2:G:141:TYR:HD2	1.81	0.44
2:G:461:SER:O	2:G:516:ALA:HA	2.17	0.44
1:A:10:PRO:HB3	2:E:279:HIS:CE1	2.53	0.44
2:G:233:ALA:O	2:G:239:ARG:HA	2.17	0.44
2:G:266:GLU:O	2:G:320:VAL:HG22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:192:PRO:HB3	2:F:235:ASN:HB3	1.98	0.44
2:E:107:PHE:HA	2:E:141:TYR:HD2	1.82	0.44
2:F:274:ALA:HB3	2:F:283:LEU:HD11	1.99	0.44
1:D:37:ASN:OD1	1:D:94:LEU:HD12	2.18	0.44
2:E:461:SER:O	2:E:516:ALA:HA	2.17	0.44
2:H:233:ALA:O	2:H:239:ARG:HA	2.17	0.44
2:G:274:ALA:HB3	2:G:283:LEU:HD11	1.99	0.44
1:B:37:ASN:OD1	1:B:94:LEU:HD12	2.18	0.44
2:H:461:SER:O	2:H:516:ALA:HA	2.17	0.44
2:F:233:ALA:O	2:F:239:ARG:HA	2.17	0.43
1:B:18:LYS:HD2	1:B:18:LYS:N	2.33	0.43
1:D:18:LYS:N	1:D:18:LYS:HD2	2.33	0.43
2:F:195:GLU:HA	2:F:217:GLU:HA	2.01	0.43
1:C:37:ASN:OD1	1:C:94:LEU:HD12	2.17	0.43
2:G:195:GLU:HA	2:G:217:GLU:HA	2.01	0.43
2:H:274:ALA:HB3	2:H:283:LEU:HD11	1.99	0.43
2:E:274:ALA:HB3	2:E:283:LEU:HD11	1.99	0.43
1:B:10:PRO:HB3	2:F:279:HIS:CE1	2.54	0.43
2:E:354:ASN:HB3	2:E:427:PHE:CE1	2.54	0.43
1:C:103:ARG:HD2	1:C:103:ARG:HA	1.73	0.43
1:D:10:PRO:HB3	2:G:279:HIS:CE1	2.54	0.43
1:A:24:ASP:O	1:B:67:LYS:HB2	2.19	0.43
2:E:195:GLU:HA	2:E:217:GLU:HA	2.01	0.42
2:H:362:ASP:O	2:H:364:TYR:N	2.53	0.42
2:H:195:GLU:HA	2:H:217:GLU:HA	2.01	0.42
2:F:354:ASN:HB3	2:F:427:PHE:CE1	2.54	0.42
2:G:354:ASN:HB3	2:G:427:PHE:CE1	2.54	0.42
2:G:362:ASP:O	2:G:364:TYR:N	2.53	0.42
2:H:354:ASN:HB3	2:H:427:PHE:CE1	2.54	0.42
1:D:103:ARG:HA	1:D:103:ARG:HD2	1.72	0.42
2:G:304:SER:HB3	2:G:308:THR:HB	2.02	0.42
2:H:304:SER:HB3	2:H:308:THR:HB	2.02	0.42
2:H:467:CYS:CB	2:H:476:GLU:H	2.33	0.42
1:B:48:TRP:CD1	1:B:130:LEU:HG	2.55	0.42
2:E:304:SER:HB3	2:E:308:THR:HB	2.02	0.42
1:A:88:GLN:HE21	1:A:89:PRO:HD2	1.85	0.41
2:E:467:CYS:CB	2:E:476:GLU:H	2.33	0.41
1:C:48:TRP:CD1	1:C:130:LEU:HG	2.55	0.41
1:B:88:GLN:HE21	1:B:89:PRO:HD2	1.85	0.41
1:C:88:GLN:HE21	1:C:89:PRO:HD2	1.85	0.41
2:E:362:ASP:O	2:E:364:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:275:VAL:HG22	2:E:310:ILE:HG23	2.02	0.41
2:G:467:CYS:CB	2:G:476:GLU:H	2.33	0.41
1:D:48:TRP:CD1	1:D:130:LEU:HG	2.55	0.41
1:A:106:GLN:CA	1:A:106:GLN:HE21	2.23	0.41
1:D:88:GLN:HE21	1:D:89:PRO:HD2	1.86	0.41
2:F:304:SER:HB3	2:F:308:THR:HB	2.02	0.41
2:F:467:CYS:CB	2:F:476:GLU:H	2.33	0.41
2:H:383:TRP:CD1	2:H:392:CYS:HB3	2.56	0.41
2:F:362:ASP:O	2:F:364:TYR:N	2.53	0.41
2:F:275:VAL:HG22	2:F:310:ILE:HG23	2.02	0.40
2:H:254:GLN:O	2:H:255:THR:C	2.60	0.40
2:F:383:TRP:CD1	2:F:392:CYS:HB3	2.56	0.40
2:E:254:GLN:O	2:E:255:THR:C	2.59	0.40
1:A:48:TRP:CD1	1:A:130:LEU:HG	2.55	0.40
2:G:383:TRP:CD1	2:G:392:CYS:HB3	2.56	0.40
2:H:379:ILE:HG22	2:H:422:ASN:HB3	2.04	0.40
2:G:275:VAL:HG22	2:G:310:ILE:HG23	2.02	0.40
2:G:254:GLN:O	2:G:255:THR:C	2.60	0.40
2:E:383:TRP:CD1	2:E:392:CYS:HB3	2.56	0.40
2:F:357:GLU:O	2:F:431:PHE:HA	2.22	0.40
2:G:357:GLU:O	2:G:431:PHE:HA	2.22	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	128/138 (93%)	120 (94%)	7 (6%)	1 (1%)	24	69
1	B	128/138 (93%)	120 (94%)	7 (6%)	1 (1%)	24	69
1	C	128/138 (93%)	120 (94%)	7 (6%)	1 (1%)	24	69
1	D	128/138 (93%)	120 (94%)	7 (6%)	1 (1%)	24	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	385/527 (73%)	333 (86%)	37 (10%)	15 (4%)	4	36
2	F	315/527 (60%)	273 (87%)	30 (10%)	12 (4%)	4	37
2	G	385/527 (73%)	333 (86%)	37 (10%)	15 (4%)	4	36
2	H	385/527 (73%)	333 (86%)	37 (10%)	15 (4%)	4	36
All	All	1982/2660 (74%)	1752 (88%)	169 (8%)	61 (3%)	5	42

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	85	VAL
2	E	255	THR
2	E	305	THR
2	E	334	LYS
2	E	363	GLN
2	F	255	THR
2	F	305	THR
2	F	334	LYS
2	F	363	GLN
2	G	85	VAL
2	G	255	THR
2	G	305	THR
2	G	334	LYS
2	G	363	GLN
2	H	85	VAL
2	H	255	THR
2	H	305	THR
2	H	334	LYS
2	H	363	GLN
2	E	291	ALA
2	F	291	ALA
2	G	291	ALA
2	H	291	ALA
2	E	108	LYS
2	E	226	GLY
2	E	364	TYR
2	F	226	GLY
2	F	364	TYR
2	G	108	LYS
2	G	226	GLY
2	G	364	TYR
2	H	108	LYS

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Mol	Chain	Res	Type
2	H	364	TYR
1	A	42	GLU
1	C	42	GLU
2	E	398	ASP
2	E	408	ASN
2	E	480	GLU
2	F	398	ASP
2	F	408	ASN
2	F	480	GLU
2	G	398	ASP
2	G	408	ASN
2	G	480	GLU
2	H	226	GLY
2	H	398	ASP
2	H	408	ASN
2	H	480	GLU
1	B	42	GLU
1	D	42	GLU
2	E	411	HIS
2	F	411	HIS
2	G	411	HIS
2	H	411	HIS
2	E	116	PRO
2	E	287	LEU
2	F	287	LEU
2	G	116	PRO
2	G	287	LEU
2	H	116	PRO
2	H	287	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	115/127 (91%)	111 (96%)	4 (4%)	43 74
1	B	115/127 (91%)	111 (96%)	4 (4%)	43 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	115/127 (91%)	111 (96%)	4 (4%)	43	74
1	D	115/127 (91%)	111 (96%)	4 (4%)	43	74
2	E	139/473 (29%)	122 (88%)	17 (12%)	6	31
2	F	117/473 (25%)	105 (90%)	12 (10%)	9	37
2	G	139/473 (29%)	122 (88%)	17 (12%)	6	31
2	H	139/473 (29%)	123 (88%)	16 (12%)	7	32
All	All	994/2400 (41%)	916 (92%)	78 (8%)	16	51

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	20	ARG
1	A	88	GLN
1	A	106	GLN
1	B	18	LYS
1	B	20	ARG
1	B	88	GLN
1	B	106	GLN
1	C	18	LYS
1	C	20	ARG
1	C	88	GLN
1	C	106	GLN
1	D	18	LYS
1	D	20	ARG
1	D	88	GLN
1	D	106	GLN
2	E	93	VAL
2	E	145	ILE
2	E	154	ILE
2	E	160	ILE
2	E	229	ILE
2	E	244	LEU
2	E	260	LEU
2	E	270	ILE
2	E	287	LEU
2	E	308	THR
2	E	309	MET
2	E	310	ILE
2	E	344	ILE

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Mol	Chain	Res	Type
2	E	371	VAL
2	E	392	CYS
2	E	433	LEU
2	E	524	CYS
2	F	229	ILE
2	F	244	LEU
2	F	260	LEU
2	F	270	ILE
2	F	287	LEU
2	F	308	THR
2	F	309	MET
2	F	310	ILE
2	F	344	ILE
2	F	371	VAL
2	F	392	CYS
2	F	433	LEU
2	G	93	VAL
2	G	145	ILE
2	G	154	ILE
2	G	160	ILE
2	G	229	ILE
2	G	244	LEU
2	G	260	LEU
2	G	270	ILE
2	G	287	LEU
2	G	308	THR
2	G	309	MET
2	G	310	ILE
2	G	344	ILE
2	G	371	VAL
2	G	392	CYS
2	G	433	LEU
2	G	524	CYS
2	H	93	VAL
2	H	145	ILE
2	H	154	ILE
2	H	160	ILE
2	H	229	ILE
2	H	244	LEU
2	H	260	LEU
2	H	270	ILE
2	H	287	LEU

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Mol	Chain	Res	Type
2	H	308	THR
2	H	309	MET
2	H	310	ILE
2	H	344	ILE
2	H	371	VAL
2	H	392	CYS
2	H	433	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	80	HIS
1	A	88	GLN
1	A	106	GLN
1	A	111	GLN
1	A	122	GLN
1	B	28	GLN
1	B	80	HIS
1	B	88	GLN
1	B	98	GLN
1	B	106	GLN
1	B	111	GLN
1	B	122	GLN
1	C	28	GLN
1	C	80	HIS
1	C	88	GLN
1	C	106	GLN
1	C	111	GLN
1	C	122	GLN
1	D	28	GLN
1	D	80	HIS
1	D	88	GLN
1	D	98	GLN
1	D	106	GLN
1	D	111	GLN
1	D	122	GLN
2	E	279	HIS
2	F	279	HIS
2	G	279	HIS
2	H	279	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	130/138 (94%)	1.05	18 (13%)	4 10	306, 306, 306, 306	0
1	B	130/138 (94%)	0.86	7 (5%)	29 30	289, 289, 289, 289	0
1	C	130/138 (94%)	0.84	14 (10%)	8 13	344, 344, 344, 344	0
1	D	130/138 (94%)	0.78	15 (11%)	6 12	293, 293, 293, 293	0
2	E	405/527 (76%)	2.17	192 (47%)	0 4	326, 383, 441, 441	0
2	F	329/527 (62%)	1.58	102 (31%)	1 5	330, 330, 432, 432	0
2	G	405/527 (76%)	2.26	187 (46%)	0 4	374, 383, 455, 455	0
2	H	405/527 (76%)	2.46	216 (53%)	0 4	381, 388, 469, 469	0
All	All	2064/2660 (77%)	1.83	751 (36%)	0 4	289, 381, 455, 469	0

All (751) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	485	ARG	13.9
2	G	502	ASN	13.8
2	G	126	VAL	12.3
2	H	484	ASN	12.1
2	G	504	SER	11.4
2	G	503	MET	11.0
2	G	116	PRO	9.9
2	E	359	TYR	9.6
2	G	117	HIS	9.2
2	H	480	GLU	8.9
2	H	497	SER	8.7
2	H	498	SER	8.7
2	H	409	HIS	8.7
2	H	499	SER	8.1
2	H	483	TRP	8.0
2	G	86	SER	7.7

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Mol	Chain	Res	Type	RSRZ
2	G	93	VAL	7.7
2	E	361	ILE	7.7
2	G	103	CYS	7.7
2	H	444	GLU	7.5
2	F	366	GLU	7.4
2	E	360	GLU	7.4
2	H	352	ALA	7.4
2	E	145	ILE	7.3
2	H	496	VAL	7.3
2	H	86	SER	7.2
2	H	452	CYS	7.2
2	E	103	CYS	7.2
2	E	102	SER	7.1
2	E	144	PHE	7.0
2	H	481	GLY	6.9
2	H	416	TYR	6.9
2	F	371	VAL	6.9
2	H	408	ASN	6.8
2	E	434	ASN	6.8
2	G	102	SER	6.8
2	E	85	VAL	6.7
2	E	124	GLY	6.7
2	H	274	ALA	6.6
2	G	133	MET	6.5
2	G	124	GLY	6.5
2	G	371	VAL	6.5
2	G	125	VAL	6.4
2	G	464	TRP	6.2
2	G	83	VAL	6.2
2	G	85	VAL	6.2
2	G	444	GLU	6.1
2	F	442	LEU	6.1
2	G	462	TRP	6.0
2	H	84	ASP	6.0
2	H	273	LYS	5.9
2	E	409	HIS	5.9
2	H	87	ALA	5.9
2	G	87	ALA	5.9
2	H	137	GLN	5.9
2	G	479	THR	5.8
2	G	501	LEU	5.8
2	G	192	PRO	5.8

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Mol	Chain	Res	Type	RSRZ
2	G	450	ALA	5.8
2	G	92	GLN	5.8
2	H	479	THR	5.8
2	F	443	ALA	5.8
2	H	133	MET	5.7
2	G	130	ILE	5.7
2	H	353	THR	5.7
2	E	95	VAL	5.7
2	H	248	ASP	5.7
2	G	233	ALA	5.6
2	E	431	PHE	5.6
2	G	145	ILE	5.6
2	H	249	LEU	5.6
2	H	443	ALA	5.5
2	G	128	MET	5.5
2	E	96	ASP	5.5
2	G	127	SER	5.5
2	E	463	THR	5.4
2	G	115	GLN	5.4
2	E	97	ALA	5.4
2	G	88	SER	5.4
2	H	250	ASN	5.4
2	G	193	ILE	5.4
2	E	371	VAL	5.4
2	E	420	ALA	5.4
2	G	91	LEU	5.4
2	H	351	ASN	5.4
2	E	362	ASP	5.3
2	H	454	SER	5.3
2	E	152	TYR	5.3
2	E	427	PHE	5.3
2	H	282	GLY	5.2
2	E	433	LEU	5.2
2	E	369	PHE	5.2
2	E	415	GLU	5.2
2	H	145	ILE	5.2
2	G	186	SER	5.2
2	F	446	SER	5.1
2	E	87	ALA	5.1
2	E	98	PRO	5.1
2	H	526	THR	5.1
2	E	464	TRP	5.1

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Mol	Chain	Res	Type	RSRZ
2	G	352	ALA	5.1
2	H	500	THR	5.1
2	G	418	PHE	5.1
2	H	85	VAL	5.1
2	G	118	PHE	5.0
2	E	302	THR	5.0
2	F	418	PHE	5.0
2	G	383	TRP	5.0
2	G	89	ILE	5.0
2	G	105	TRP	5.0
2	H	446	SER	5.0
2	G	452	CYS	5.0
2	F	404	SER	4.9
2	H	509	GLY	4.9
1	A	62	THR	4.9
2	E	358	ASP	4.9
2	E	426	GLN	4.9
2	H	525	GLU	4.9
2	H	151	ASN	4.9
2	H	283	LEU	4.9
2	E	432	THR	4.9
2	H	417	ILE	4.8
2	G	98	PRO	4.8
2	G	111	SER	4.8
2	G	129	VAL	4.8
2	G	194	VAL	4.8
2	G	81	VAL	4.8
2	E	379	ILE	4.8
2	E	462	TRP	4.8
2	E	475	THR	4.8
2	G	505	GLU	4.8
2	E	274	ALA	4.7
2	H	186	SER	4.7
2	E	84	ASP	4.7
2	E	186	SER	4.7
2	F	444	GLU	4.7
2	H	527	ILE	4.7
2	E	452	CYS	4.7
2	E	485	ARG	4.7
2	H	134	THR	4.7
2	H	324	ASP	4.7
1	A	12	SER	4.7

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Mol	Chain	Res	Type	RSRZ
2	H	464	TRP	4.6
2	H	482	VAL	4.6
2	F	502	ASN	4.6
2	G	138	ALA	4.6
2	E	153	THR	4.6
2	G	135	GLU	4.6
2	H	383	TRP	4.6
2	H	332	SER	4.6
2	G	97	ALA	4.6
2	F	501	LEU	4.6
2	E	467	CYS	4.6
2	H	418	PHE	4.6
2	G	160	ILE	4.6
2	E	357	GLU	4.6
2	E	418	PHE	4.6
2	F	373	PHE	4.6
2	F	451	SER	4.5
2	H	150	THR	4.5
2	H	451	SER	4.5
2	E	408	ASN	4.5
2	E	421	GLU	4.5
2	E	480	GLU	4.5
2	F	474	CYS	4.5
2	H	103	CYS	4.5
2	G	131	LEU	4.5
2	H	460	PRO	4.5
2	E	516	ALA	4.5
2	G	445	ALA	4.5
2	H	495	TRP	4.4
2	G	159	SER	4.4
2	H	354	ASN	4.4
2	G	406	PHE	4.4
2	H	406	PHE	4.4
2	G	101	ILE	4.4
2	E	497	SER	4.4
2	F	192	PRO	4.4
2	G	478	ILE	4.4
2	H	233	ALA	4.4
2	E	416	TYR	4.4
2	G	443	ALA	4.4
2	G	451	SER	4.4
2	H	348	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
2	H	371	VAL	4.3
2	H	431	PHE	4.3
2	F	445	ALA	4.3
2	E	143	LEU	4.3
1	C	11	ILE	4.3
2	E	514	CYS	4.3
2	E	466	LYS	4.3
2	G	84	ASP	4.3
2	F	383	TRP	4.3
2	H	412	GLN	4.3
2	G	90	THR	4.3
2	H	147	SER	4.3
2	E	417	ILE	4.3
2	F	352	ALA	4.3
2	H	384	THR	4.3
2	H	459	LEU	4.3
2	F	510	PHE	4.2
2	F	238	GLY	4.2
2	G	408	ASN	4.2
2	H	146	GLN	4.2
2	F	367	PHE	4.2
2	H	247	ILE	4.2
2	H	445	ALA	4.2
2	G	466	LYS	4.2
2	H	427	PHE	4.2
2	H	462	TRP	4.2
2	G	94	LEU	4.2
2	G	99	GLY	4.2
2	H	350	ILE	4.1
2	E	384	THR	4.1
2	E	406	PHE	4.1
2	H	501	LEU	4.1
2	H	399	ASN	4.1
2	E	86	SER	4.1
2	H	83	VAL	4.1
2	G	234	ARG	4.1
2	H	192	PRO	4.1
2	G	82	GLU	4.1
2	G	463	THR	4.1
2	E	233	ALA	4.1
2	E	508	LYS	4.1
2	H	311	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
2	E	301	SER	4.0
2	E	282	GLY	4.0
2	H	138	ALA	4.0
2	E	370	SER	4.0
2	H	363	GLN	4.0
2	F	441	VAL	4.0
2	F	452	CYS	4.0
2	G	404	SER	4.0
1	B	12	SER	4.0
2	E	512	VAL	4.0
2	G	499	SER	4.0
2	E	461	SER	4.0
2	F	370	SER	4.0
2	G	373	PHE	4.0
2	G	497	SER	4.0
2	H	102	SER	4.0
2	G	250	ASN	4.0
2	F	450	ALA	3.9
2	H	136	THR	3.9
2	E	83	VAL	3.9
1	C	10	PRO	3.9
2	G	465	LYS	3.9
1	A	11	ILE	3.9
2	E	243	ARG	3.9
2	E	479	THR	3.9
2	G	409	HIS	3.9
2	E	386	SER	3.9
2	G	191	GLU	3.9
2	H	441	VAL	3.9
2	H	512	VAL	3.9
2	H	135	GLU	3.9
2	H	510	PHE	3.9
2	E	118	PHE	3.8
2	H	323	ASN	3.8
2	H	477	GLU	3.8
2	F	233	ALA	3.8
2	H	234	ARG	3.8
2	F	351	ASN	3.8
2	G	152	TYR	3.8
2	G	514	CYS	3.8
2	H	328	TYR	3.8
2	E	93	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
2	E	509	GLY	3.7
2	E	99	GLY	3.7
2	E	104	LEU	3.7
1	A	42	GLU	3.7
2	H	506	ALA	3.7
2	E	146	GLN	3.7
2	H	505	GLU	3.7
2	H	255	THR	3.7
2	G	96	ASP	3.7
2	G	132	LYS	3.7
2	E	507	ILE	3.7
2	H	369	PHE	3.7
2	H	458	PRO	3.7
2	H	508	LYS	3.7
2	G	114	CYS	3.7
2	F	186	SER	3.7
2	G	500	THR	3.7
2	H	516	ALA	3.7
2	H	507	ILE	3.7
2	F	503	MET	3.6
2	F	384	THR	3.6
2	E	383	TRP	3.6
2	E	474	CYS	3.6
2	E	515	CYS	3.6
2	F	302	THR	3.6
2	G	480	GLU	3.6
2	E	332	SER	3.6
2	F	440	GLN	3.6
2	H	450	ALA	3.6
2	F	323	ASN	3.6
2	G	416	TYR	3.6
2	H	410	LYS	3.6
2	G	158	VAL	3.6
2	G	405	LYS	3.6
2	E	367	PHE	3.5
2	E	454	SER	3.5
2	G	243	ARG	3.5
2	G	323	ASN	3.5
2	H	256	THR	3.5
2	E	525	GLU	3.5
2	F	191	GLU	3.5
2	F	392	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	10	PRO	3.5
2	H	113	ASN	3.5
2	G	481	GLY	3.5
2	F	234	ARG	3.5
2	E	484	ASN	3.5
2	H	529	LEU	3.5
2	H	88	SER	3.5
2	G	384	THR	3.5
2	E	187	GLU	3.5
2	G	151	ASN	3.4
2	F	253	PRO	3.4
2	F	526	THR	3.4
2	E	444	GLU	3.4
2	E	481	GLY	3.4
2	G	80	ALA	3.4
2	G	240	GLU	3.4
2	G	95	VAL	3.4
2	F	500	THR	3.4
2	E	368	CYS	3.4
2	E	353	THR	3.4
2	E	451	SER	3.4
2	H	415	GLU	3.4
2	G	454	SER	3.4
2	E	94	LEU	3.4
2	F	187	GLU	3.4
2	F	338	GLN	3.4
2	F	475	THR	3.4
2	G	144	PHE	3.4
2	G	512	VAL	3.4
2	H	241	CYS	3.3
2	H	349	PHE	3.3
2	F	394	GLN	3.3
2	E	496	VAL	3.3
2	F	468	SER	3.3
2	H	284	THR	3.3
2	H	373	PHE	3.3
1	A	43	LEU	3.3
2	H	467	CYS	3.3
2	E	419	HIS	3.3
2	F	324	ASP	3.3
2	H	101	ILE	3.3
2	G	134	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	G	143	LEU	3.3
2	H	419	HIS	3.3
2	H	414	GLY	3.3
2	E	105	TRP	3.3
2	E	441	VAL	3.3
2	G	477	GLU	3.3
2	E	111	SER	3.2
2	H	453	PHE	3.2
2	G	188	SER	3.2
2	H	528	LEU	3.2
2	H	187	GLU	3.2
2	H	239	ARG	3.2
2	E	468	SER	3.2
2	H	468	SER	3.2
2	E	529	LEU	3.2
2	E	476	GLU	3.2
2	F	481	GLY	3.2
2	G	385	PHE	3.2
2	E	283	LEU	3.2
2	E	465	LYS	3.2
2	E	411	HIS	3.2
2	G	419	HIS	3.2
2	G	153	THR	3.2
2	E	279	HIS	3.2
2	H	243	ARG	3.2
2	E	422	ASN	3.2
2	E	524	CYS	3.2
2	H	132	LYS	3.2
2	H	193	ILE	3.2
2	G	372	ARG	3.2
2	H	375	ALA	3.2
2	E	523	SER	3.2
2	G	407	CYS	3.2
1	C	85	CYS	3.1
2	E	137	GLN	3.1
2	F	235	ASN	3.1
2	E	244	LEU	3.1
2	E	428	THR	3.1
2	H	442	LEU	3.1
2	G	506	ALA	3.1
2	F	303	TYR	3.1
2	G	110	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	309	MET	3.1
2	H	466	LYS	3.1
1	C	78	GLU	3.1
2	G	441	VAL	3.1
2	E	126	VAL	3.1
2	E	513	LYS	3.1
2	H	503	MET	3.1
1	D	78	GLU	3.1
2	F	429	LYS	3.1
2	F	455	ASP	3.1
2	G	106	VAL	3.1
2	H	461	SER	3.0
2	G	440	GLN	3.0
2	H	285	TRP	3.0
2	H	456	GLY	3.0
2	F	393	GLU	3.0
2	H	130	ILE	3.0
2	E	407	CYS	3.0
2	H	385	PHE	3.0
2	E	117	HIS	3.0
2	E	109	HIS	3.0
2	E	443	ALA	3.0
2	G	420	ALA	3.0
2	E	352	ALA	3.0
1	D	38	LEU	3.0
2	E	398	ASP	3.0
2	G	427	PHE	3.0
2	H	182	LEU	3.0
2	H	428	THR	3.0
2	F	480	GLU	3.0
2	H	105	TRP	3.0
2	F	427	PHE	3.0
2	G	245	PHE	3.0
2	H	523	SER	3.0
2	G	259	GLN	3.0
2	G	79	ALA	2.9
2	E	414	GLY	2.9
2	E	151	ASN	2.9
2	G	294	GLU	2.9
2	G	274	ALA	2.9
1	B	90	PRO	2.9
1	A	85	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	499	SER	2.9
2	F	411	HIS	2.9
2	G	100	ASN	2.9
2	F	420	ALA	2.9
2	H	175	LYS	2.9
2	H	158	VAL	2.9
2	E	110	SER	2.9
2	F	405	LYS	2.9
2	H	152	TYR	2.9
2	H	143	LEU	2.9
2	H	398	ASP	2.9
2	F	178	ASN	2.9
2	G	235	ASN	2.9
2	H	502	ASN	2.9
2	E	125	VAL	2.9
2	F	369	PHE	2.8
2	H	144	PHE	2.8
2	H	382	THR	2.8
2	H	292	LEU	2.8
1	A	78	GLU	2.8
2	E	296	ASN	2.8
2	E	310	ILE	2.8
2	G	399	ASN	2.8
2	H	232	CYS	2.8
2	H	433	LEU	2.8
2	H	455	ASP	2.8
2	E	255	THR	2.8
2	H	367	PHE	2.8
2	F	177	GLU	2.8
2	H	411	HIS	2.8
2	E	101	ILE	2.8
2	F	379	ILE	2.8
2	F	428	THR	2.8
2	F	504	SER	2.8
2	H	181	ALA	2.8
2	G	396	GLY	2.8
2	F	353	THR	2.8
2	G	246	THR	2.8
2	F	524	CYS	2.8
2	E	180	ASP	2.8
2	E	256	THR	2.7
1	B	130	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	128	MET	2.7
2	E	429	LYS	2.7
2	E	477	GLU	2.7
2	H	111	SER	2.7
2	F	416	TYR	2.7
1	B	11	ILE	2.7
1	C	9	SER	2.7
2	G	455	ASP	2.7
2	H	478	ILE	2.7
2	H	514	CYS	2.7
2	E	453	PHE	2.7
2	G	244	LEU	2.7
2	G	353	THR	2.7
2	G	402	SER	2.7
2	G	442	LEU	2.7
2	H	244	LEU	2.7
2	E	410	LYS	2.7
2	H	188	SER	2.7
2	E	213	VAL	2.7
1	D	91	PRO	2.7
2	E	335	HIS	2.7
2	E	303	TYR	2.7
2	G	113	ASN	2.7
2	E	425	ALA	2.7
2	G	400	GLY	2.7
2	G	453	PHE	2.7
2	H	407	CYS	2.7
1	A	35	ALA	2.7
2	H	321	ALA	2.6
2	H	335	HIS	2.6
1	B	78	GLU	2.6
2	H	359	TYR	2.6
2	F	454	SER	2.6
2	H	272	CYS	2.6
2	H	376	TYR	2.6
2	G	190	PRO	2.6
2	H	114	CYS	2.6
2	F	365	GLU	2.6
2	E	281	PHE	2.6
2	E	133	MET	2.6
2	E	82	GLU	2.6
2	E	154	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	141	TYR	2.6
1	D	18	LYS	2.6
1	D	42	GLU	2.6
2	E	495	TRP	2.6
2	H	331	SER	2.6
2	F	406	PHE	2.6
2	E	160	ILE	2.6
2	H	161	ARG	2.6
2	E	500	THR	2.6
2	F	499	SER	2.6
2	F	529	LEU	2.6
2	H	338	GLN	2.6
2	G	382	THR	2.6
2	H	116	PRO	2.6
1	B	91	PRO	2.6
2	H	194	VAL	2.6
2	H	224	LEU	2.6
1	D	131	GLN	2.6
2	G	446	SER	2.6
2	F	236	GLU	2.6
2	F	519	SER	2.6
2	G	525	GLU	2.6
2	E	385	PHE	2.5
2	G	156	PHE	2.5
2	H	476	GLU	2.5
2	F	509	GLY	2.5
2	H	153	THR	2.5
2	G	104	LEU	2.5
2	E	278	ASN	2.5
2	E	363	GLN	2.5
2	G	170	ARG	2.5
2	G	508	LYS	2.5
2	G	369	PHE	2.5
2	H	342	VAL	2.5
2	E	215	LYS	2.5
2	G	498	SER	2.5
2	G	168	LEU	2.5
2	H	386	SER	2.5
2	G	398	ASP	2.5
2	F	288	GLU	2.5
2	F	292	LEU	2.5
1	C	87	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	336	PRO	2.5
2	G	187	GLU	2.5
2	F	467	CYS	2.5
2	G	251	GLN	2.5
1	A	13	SER	2.4
2	F	188	SER	2.4
2	E	214	VAL	2.4
2	H	379	ILE	2.4
2	E	159	SER	2.4
2	H	238	GLY	2.4
2	E	478	ILE	2.4
2	H	269	TRP	2.4
1	D	41	GLU	2.4
2	F	464	TRP	2.4
2	E	526	THR	2.4
2	H	440	GLN	2.4
2	H	240	GLU	2.4
2	E	392	CYS	2.4
1	A	122	GLN	2.4
2	H	336	PRO	2.4
2	F	293	GLU	2.4
2	H	366	GLU	2.4
1	C	38	LEU	2.4
2	G	412	GLN	2.4
1	C	12	SER	2.4
2	F	301	SER	2.4
2	E	150	THR	2.4
2	G	482	VAL	2.4
2	G	147	SER	2.4
1	D	15	PHE	2.4
2	H	251	GLN	2.4
1	B	18	LYS	2.4
2	E	511	LEU	2.4
2	E	510	PHE	2.4
2	G	221	LEU	2.4
2	G	167	THR	2.4
2	H	330	CYS	2.3
2	E	138	ALA	2.3
2	G	171	PRO	2.3
2	E	225	PHE	2.3
2	E	134	THR	2.3
2	F	525	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	36	SER	2.3
2	E	404	SER	2.3
2	E	498	SER	2.3
2	G	507	ILE	2.3
2	E	194	VAL	2.3
2	E	259	GLN	2.3
2	E	460	PRO	2.3
2	H	361	ILE	2.3
2	H	221	LEU	2.3
2	F	514	CYS	2.3
2	G	392	CYS	2.3
2	G	150	THR	2.3
2	H	511	LEU	2.3
2	E	242	THR	2.3
2	G	386	SER	2.3
2	F	307	ARG	2.3
2	H	173	PHE	2.3
2	E	391	PRO	2.3
2	F	374	LYS	2.3
2	F	417	ILE	2.3
2	H	82	GLU	2.3
1	A	81	PHE	2.3
1	C	5	SER	2.3
2	F	389	SER	2.3
2	G	526	THR	2.3
2	H	275	VAL	2.3
2	F	372	ARG	2.3
1	D	130	LEU	2.3
2	E	249	LEU	2.3
2	G	410	LYS	2.3
2	G	429	LYS	2.3
2	G	137	GLN	2.3
2	G	354	ASN	2.3
2	G	516	ALA	2.3
2	F	512	VAL	2.3
2	E	399	ASN	2.2
2	E	517	TYR	2.2
2	H	322	ARG	2.2
2	H	420	ALA	2.2
2	F	193	ILE	2.2
2	H	174	ARG	2.2
2	E	506	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	242	THR	2.2
2	E	196	TRP	2.2
2	E	440	GLN	2.2
2	E	413	PRO	2.2
2	E	91	LEU	2.2
2	F	453	PHE	2.2
2	H	156	PHE	2.2
1	A	47	LEU	2.2
1	C	35	ALA	2.2
2	H	139	GLY	2.2
2	H	475	THR	2.2
2	F	190	PRO	2.2
1	C	88	GLN	2.2
2	E	450	ALA	2.2
2	H	131	LEU	2.2
1	D	92	SER	2.2
2	E	387	ARG	2.2
2	F	339	SER	2.2
2	G	139	GLY	2.2
2	G	146	GLN	2.2
2	E	276	HIS	2.2
2	H	117	HIS	2.2
1	A	9	SER	2.2
1	D	102	SER	2.2
2	G	428	THR	2.2
2	G	303	TYR	2.2
2	E	380	ARG	2.2
2	F	385	PHE	2.2
2	G	232	CYS	2.2
2	H	439	PRO	2.2
1	D	94	LEU	2.2
2	G	282	GLY	2.2
2	G	328	TYR	2.2
2	H	93	VAL	2.2
2	E	445	ALA	2.1
2	E	390	PHE	2.1
2	H	358	ASP	2.1
2	E	350	ILE	2.1
2	E	333	SER	2.1
1	D	93	CYS	2.1
2	E	275	VAL	2.1
2	E	389	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	446	SER	2.1
1	C	47	LEU	2.1
2	H	370	SER	2.1
2	E	92	GLN	2.1
2	F	239	ARG	2.1
2	E	505	GLU	2.1
2	E	340	ALA	2.1
2	G	108	LYS	2.1
2	G	468	SER	2.1
2	F	391	PRO	2.1
2	H	270	ILE	2.1
2	F	419	HIS	2.1
2	H	169	ARG	2.1
2	F	282	GLY	2.1
2	H	178	ASN	2.1
2	G	338	GLN	2.1
2	G	496	VAL	2.1
2	G	224	LEU	2.1
2	G	484	ASN	2.1
2	H	362	ASP	2.1
2	H	426	GLN	2.1
2	E	232	CYS	2.1
1	A	64	ALA	2.1
2	H	99	GLY	2.1
2	H	154	ILE	2.1
1	A	63	VAL	2.1
2	H	126	VAL	2.1
2	G	157	THR	2.1
2	G	324	ASP	2.1
2	E	424	ASP	2.1
2	G	295	GLY	2.1
2	F	354	ASN	2.1
2	H	81	VAL	2.1
1	D	100	ASN	2.0
2	F	179	GLN	2.0
2	H	245	PHE	2.0
2	G	112	LEU	2.0
2	H	303	TYR	2.0
2	G	467	CYS	2.0
2	G	485	ARG	2.0
2	H	291	ALA	2.0
2	G	226	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	6	PHE	2.0
2	F	386	SER	2.0
2	G	252	THR	2.0
1	A	41	GLU	2.0
2	H	184	CYS	2.0
2	F	431	PHE	2.0
2	H	340	ALA	2.0
2	E	224	LEU	2.0
2	E	527	ILE	2.0
2	G	475	THR	2.0
2	H	325	THR	2.0
1	D	103	ARG	2.0
2	H	89	ILE	2.0
2	H	257	LEU	2.0
2	G	217	GLU	2.0
2	H	229	ILE	2.0
1	A	87	PHE	2.0
2	F	310	ILE	2.0
2	G	513	LYS	2.0
2	E	501	LEU	2.0
2	H	91	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.