Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2024 – 12:06 PM EDT

PDB ID	:	8V5S
Title	:	VZV glycoprotein E C-terminal domain (cleaved) in complex with human Fab 5A2
Authors	:	Harshbarger, W.; Malito, E.
Deposited on	:	2023-11-30
Resolution	:	3.53 Å(reported)

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

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

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

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

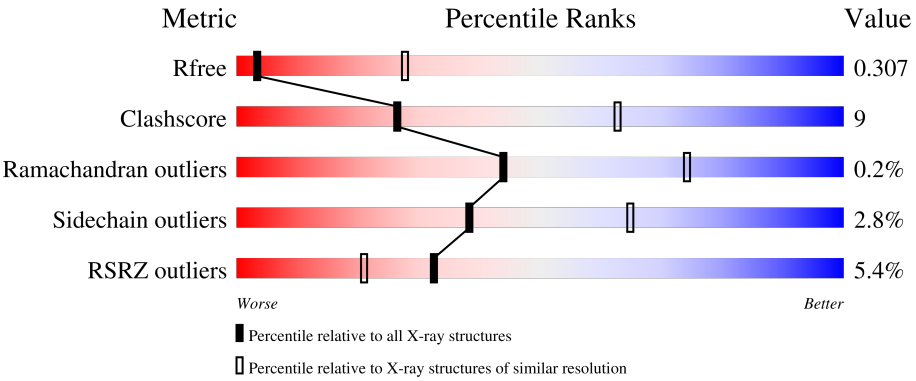
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.53 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}	164625	1272 (3.60-3.48)
Clashscore	180529	1360 (3.60-3.48)
Ramachandran outliers	177936	1347 (3.60-3.48)
Sidechain outliers	177891	1348 (3.60-3.48)
RSRZ outliers	164620	1271 (3.60-3.48)

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

Mol	Chain	Length	Quality of chain
1	A	242	3% 71% 16% • 12%
1	H	242	% 70% 18% 12%
2	B	210	9% 73% 26% •
2	L	210	8% 78% 21% •
3	C	254	2% 36% 14% 50%

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Mol	Chain	Length	Quality of chain
3	D	254	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8421 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 5A2 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	214	Total	C	N	O	S	0	0	0
			1616	1026	271	315	4			
1	A	214	Total	C	N	O	S	0	0	0
			1616	1026	271	315	4			

- Molecule 2 is a protein called 5A2 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	0	0
			1580	995	260	320	5			
2	B	210	Total	C	N	O	S	0	0	0
			1580	995	260	320	5			

- Molecule 3 is a protein called Envelope glycoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	128	Total	C	N	O	S	0	0	0
			1027	670	166	186	5			
3	D	125	Total	C	N	O	S	0	0	0
			1002	653	161	183	5			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	271	MET	-	initiating methionine	UNP A0A1B1JEP3
C	272	GLY	-	expression tag	UNP A0A1B1JEP3
C	273	THR	-	expression tag	UNP A0A1B1JEP3
C	274	VAL	-	expression tag	UNP A0A1B1JEP3
C	275	ASN	-	expression tag	UNP A0A1B1JEP3
C	276	LYS	-	expression tag	UNP A0A1B1JEP3
C	277	PRO	-	expression tag	UNP A0A1B1JEP3
C	278	VAL	-	expression tag	UNP A0A1B1JEP3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	279	VAL	-	expression tag	UNP A0A1B1JEP3
C	280	GLY	-	expression tag	UNP A0A1B1JEP3
C	281	VAL	-	expression tag	UNP A0A1B1JEP3
C	282	LEU	-	expression tag	UNP A0A1B1JEP3
C	283	MET	-	expression tag	UNP A0A1B1JEP3
C	284	GLY	-	expression tag	UNP A0A1B1JEP3
C	285	PHE	-	expression tag	UNP A0A1B1JEP3
C	286	GLY	-	expression tag	UNP A0A1B1JEP3
C	287	ILE	-	expression tag	UNP A0A1B1JEP3
C	288	ILE	-	expression tag	UNP A0A1B1JEP3
C	289	THR	-	expression tag	UNP A0A1B1JEP3
C	290	GLY	-	expression tag	UNP A0A1B1JEP3
C	291	THR	-	expression tag	UNP A0A1B1JEP3
C	292	LEU	-	expression tag	UNP A0A1B1JEP3
C	293	ARG	-	expression tag	UNP A0A1B1JEP3
C	294	ILE	-	expression tag	UNP A0A1B1JEP3
C	295	THR	-	expression tag	UNP A0A1B1JEP3
C	296	ASN	-	expression tag	UNP A0A1B1JEP3
C	297	PRO	-	expression tag	UNP A0A1B1JEP3
C	298	VAL	-	expression tag	UNP A0A1B1JEP3
C	299	ARG	-	expression tag	UNP A0A1B1JEP3
C	300	ALA	-	expression tag	UNP A0A1B1JEP3
C	517	GLY	-	expression tag	UNP A0A1B1JEP3
C	518	SER	-	expression tag	UNP A0A1B1JEP3
C	519	HIS	-	expression tag	UNP A0A1B1JEP3
C	520	HIS	-	expression tag	UNP A0A1B1JEP3
C	521	HIS	-	expression tag	UNP A0A1B1JEP3
C	522	HIS	-	expression tag	UNP A0A1B1JEP3
C	523	HIS	-	expression tag	UNP A0A1B1JEP3
C	524	HIS	-	expression tag	UNP A0A1B1JEP3
D	271	MET	-	initiating methionine	UNP A0A1B1JEP3
D	272	GLY	-	expression tag	UNP A0A1B1JEP3
D	273	THR	-	expression tag	UNP A0A1B1JEP3
D	274	VAL	-	expression tag	UNP A0A1B1JEP3
D	275	ASN	-	expression tag	UNP A0A1B1JEP3
D	276	LYS	-	expression tag	UNP A0A1B1JEP3
D	277	PRO	-	expression tag	UNP A0A1B1JEP3
D	278	VAL	-	expression tag	UNP A0A1B1JEP3
D	279	VAL	-	expression tag	UNP A0A1B1JEP3
D	280	GLY	-	expression tag	UNP A0A1B1JEP3
D	281	VAL	-	expression tag	UNP A0A1B1JEP3
D	282	LEU	-	expression tag	UNP A0A1B1JEP3

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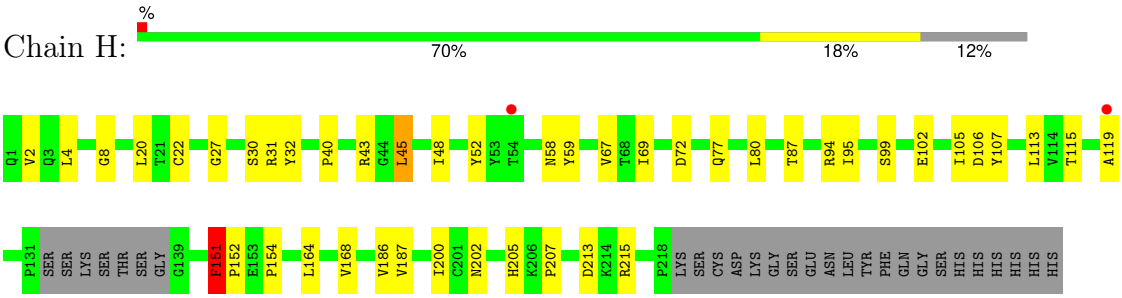
Chain	Residue	Modelled	Actual	Comment	Reference
D	283	MET	-	expression tag	UNP A0A1B1JEP3
D	284	GLY	-	expression tag	UNP A0A1B1JEP3
D	285	PHE	-	expression tag	UNP A0A1B1JEP3
D	286	GLY	-	expression tag	UNP A0A1B1JEP3
D	287	ILE	-	expression tag	UNP A0A1B1JEP3
D	288	ILE	-	expression tag	UNP A0A1B1JEP3
D	289	THR	-	expression tag	UNP A0A1B1JEP3
D	290	GLY	-	expression tag	UNP A0A1B1JEP3
D	291	THR	-	expression tag	UNP A0A1B1JEP3
D	292	LEU	-	expression tag	UNP A0A1B1JEP3
D	293	ARG	-	expression tag	UNP A0A1B1JEP3
D	294	ILE	-	expression tag	UNP A0A1B1JEP3
D	295	THR	-	expression tag	UNP A0A1B1JEP3
D	296	ASN	-	expression tag	UNP A0A1B1JEP3
D	297	PRO	-	expression tag	UNP A0A1B1JEP3
D	298	VAL	-	expression tag	UNP A0A1B1JEP3
D	299	ARG	-	expression tag	UNP A0A1B1JEP3
D	300	ALA	-	expression tag	UNP A0A1B1JEP3
D	517	GLY	-	expression tag	UNP A0A1B1JEP3
D	518	SER	-	expression tag	UNP A0A1B1JEP3
D	519	HIS	-	expression tag	UNP A0A1B1JEP3
D	520	HIS	-	expression tag	UNP A0A1B1JEP3
D	521	HIS	-	expression tag	UNP A0A1B1JEP3
D	522	HIS	-	expression tag	UNP A0A1B1JEP3
D	523	HIS	-	expression tag	UNP A0A1B1JEP3
D	524	HIS	-	expression tag	UNP A0A1B1JEP3

3 Residue-property plots (i)

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

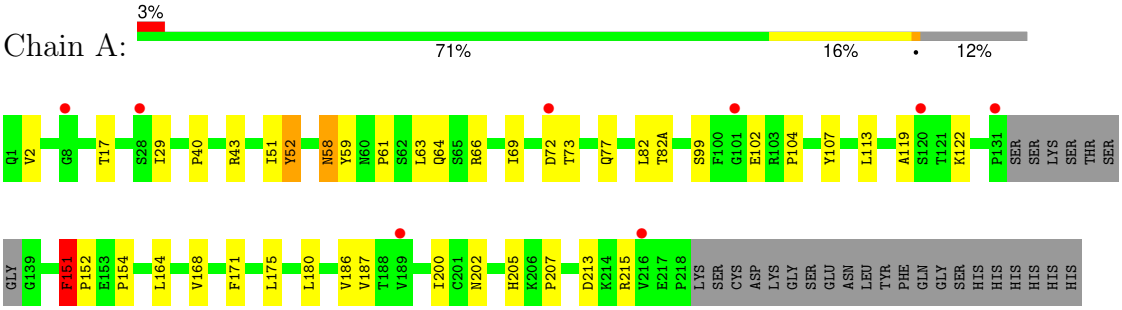
• Molecule 1: 5A2 Fab Heavy Chain

Chain H:



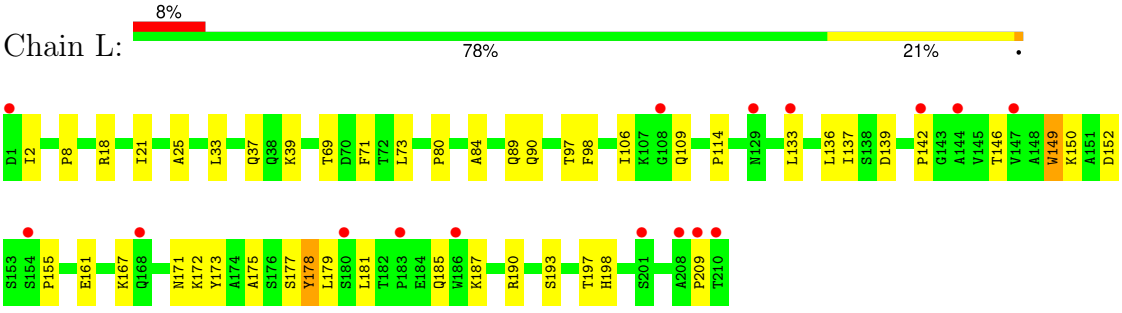
• Molecule 1: 5A2 Fab Heavy Chain

Chain A:



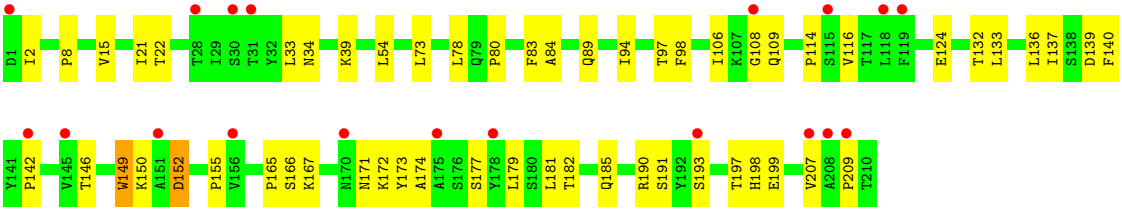
• Molecule 2: 5A2 Fab Light Chain

Chain L:

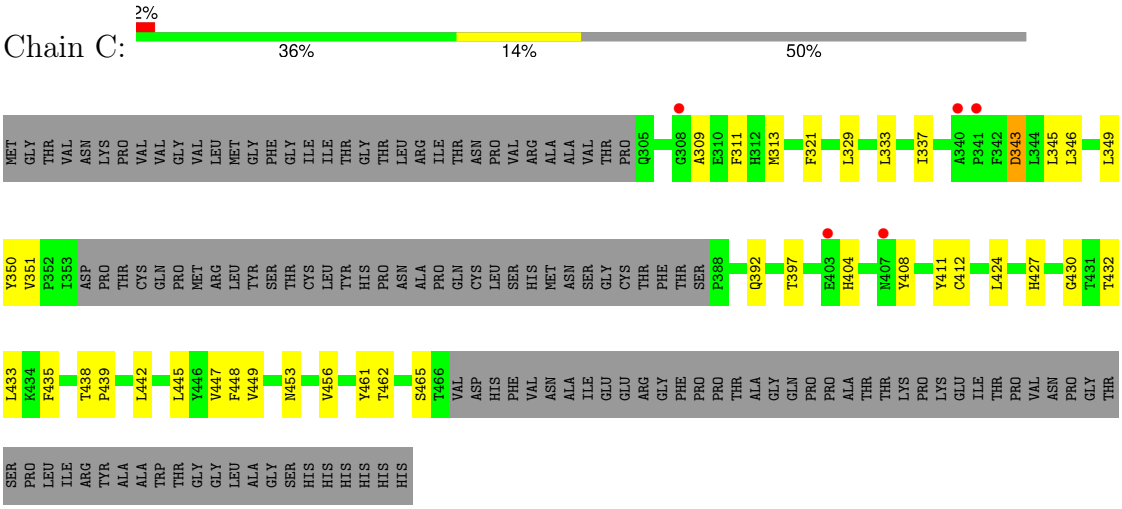


• Molecule 2: 5A2 Fab Light Chain

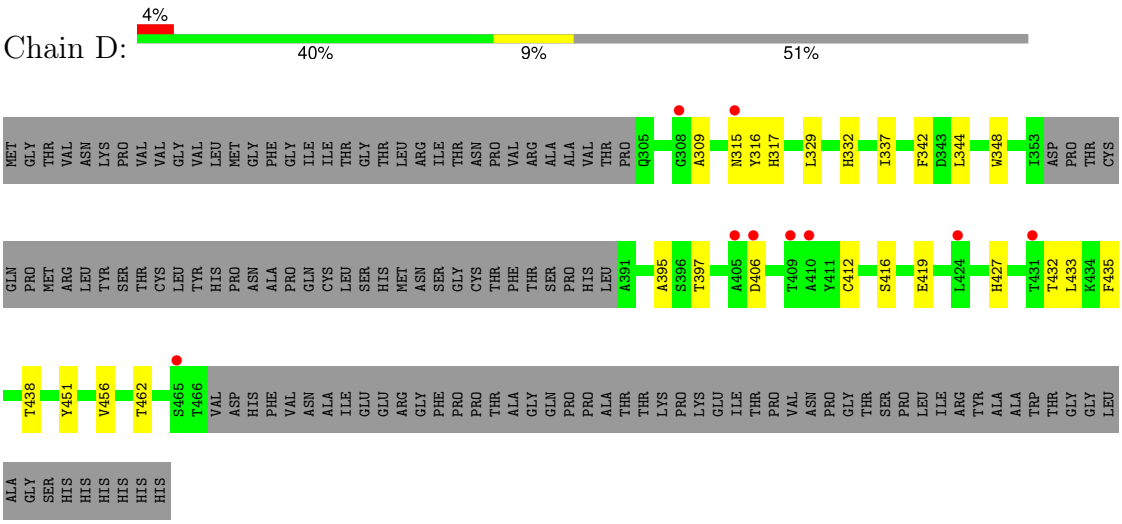
Chain B:



• Molecule 3: Envelope glycoprotein E



• Molecule 3: Envelope glycoprotein E



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.08Å 60.41Å 114.67Å 90.00° 93.89° 90.00°	Depositor
Resolution (Å)	40.02 – 3.53 40.02 – 3.53	Depositor EDS
% Data completeness (in resolution range)	90.7 (40.02-3.53) 88.8 (40.02-3.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.261 , 0.307 0.261 , 0.307	Depositor DCC
R_{free} test set	17240 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 20.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	8421	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.25	0/1657	0.54	0/2268
1	H	0.26	0/1657	0.55	0/2268
2	B	0.26	0/1618	0.51	1/2208 (0.0%)
2	L	0.26	0/1618	0.51	0/2208
3	C	0.27	0/1062	0.52	0/1450
3	D	0.25	0/1035	0.51	0/1413
All	All	0.26	0/8647	0.52	1/11815 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	33	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	PHE	Peptide
1	H	151	PHE	Peptide

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	1616	0	1594	25	0
1	H	1616	0	1594	26	0
2	B	1580	0	1553	40	0
2	L	1580	0	1553	30	0
3	C	1027	0	963	23	0
3	D	1002	0	937	14	0
All	All	8421	0	8194	152	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 9.

All (152) 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:B:133:LEU:HD11	2:B:149:TRP:HE1	1.43	0.82
2:L:133:LEU:HD11	2:L:149:TRP:HE1	1.43	0.82
1:H:2:VAL:HG22	1:H:107:TYR:HD2	1.46	0.77
2:B:39:LYS:HG3	2:B:84:ALA:HB2	1.68	0.76
3:C:309:ALA:HB1	3:C:337:ILE:HG22	1.66	0.76
3:C:427:HIS:HB3	3:C:432:THR:HG23	1.69	0.74
2:B:150:LYS:HB2	2:B:193:SER:HB3	1.70	0.73
2:L:167:LYS:HG2	2:L:173:TYR:HE1	1.55	0.72
1:A:164:LEU:HD21	1:A:187:VAL:HG11	1.73	0.71
1:H:113:LEU:HD23	1:H:154:PRO:HD3	1.74	0.69
1:A:200:ILE:HG12	1:A:215:ARG:HG3	1.74	0.69
1:A:72:ASP:HB3	1:A:77:GLN:HG3	1.75	0.69
1:H:164:LEU:HD21	1:H:187:VAL:HG11	1.74	0.68
2:B:146:THR:HG1	2:B:197:THR:HG1	1.42	0.68
2:L:21:ILE:HD11	2:L:73:LEU:HD23	1.75	0.66
2:L:150:LYS:HB2	2:L:193:SER:HB3	1.76	0.66
2:L:114:PRO:HD3	2:L:198:HIS:HD1	1.61	0.66
1:A:113:LEU:HD23	1:A:154:PRO:HD3	1.78	0.65
1:H:72:ASP:HB3	1:H:77:GLN:HG3	1.79	0.64
2:B:8:PRO:HD2	2:B:21:ILE:HG22	1.78	0.63
1:A:2:VAL:HG22	1:A:107:TYR:HD2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:VAL:HG22	1:H:107:TYR:CD2	2.30	0.63
2:B:80:PRO:HA	2:B:106:ILE:HD13	1.81	0.62
1:H:40:PRO:HB2	1:H:43:ARG:HB2	1.81	0.62
1:H:200:ILE:HG12	1:H:215:ARG:HG3	1.82	0.61
1:A:99:SER:HB3	1:A:102:GLU:HG3	1.84	0.60
2:L:18:ARG:HD3	2:B:22:THR:HG21	1.82	0.59
2:L:139:ASP:HA	2:L:172:LYS:HB3	1.84	0.58
2:L:80:PRO:HA	2:L:106:ILE:HD13	1.85	0.58
1:A:63:LEU:HB2	1:A:66:ARG:HD3	1.85	0.58
3:D:397:THR:HG23	3:D:416:SER:HB3	1.85	0.57
2:B:149:TRP:CD1	2:B:179:LEU:HD22	2.39	0.57
2:B:152:ASP:OD2	2:B:191:SER:N	2.28	0.57
3:D:427:HIS:HB3	3:D:432:THR:HG23	1.86	0.57
2:L:146:THR:HG1	2:L:197:THR:HG1	1.49	0.57
2:L:142:PRO:HG2	2:L:198:HIS:NE2	2.20	0.57
1:H:95:ILE:HG12	1:H:105:ILE:HG12	1.86	0.57
3:C:346:LEU:HB3	3:C:448:PHE:CE1	2.40	0.57
1:A:40:PRO:HB2	1:A:43:ARG:HB2	1.87	0.56
1:H:99:SER:HB3	1:H:102:GLU:HG3	1.85	0.56
2:B:21:ILE:HD11	2:B:73:LEU:HD23	1.86	0.56
3:D:309:ALA:HB1	3:D:337:ILE:HG22	1.88	0.56
1:H:2:VAL:CG1	1:H:27:GLY:HA3	2.35	0.56
2:B:182:THR:OG1	2:B:185:GLN:OE1	2.23	0.56
2:B:94:ILE:HB	3:D:316:TYR:HB2	1.87	0.56
2:B:124:GLU:OE1	2:B:124:GLU:N	2.35	0.56
1:A:29:ILE:HG21	1:A:73:THR:HA	1.88	0.55
2:B:15:VAL:HG23	2:B:108:GLY:HA3	1.89	0.55
1:H:205:HIS:CD2	1:H:207:PRO:HD2	2.42	0.55
1:H:2:VAL:HG12	1:H:27:GLY:HA3	1.89	0.55
2:L:149:TRP:CD1	2:L:179:LEU:HD22	2.41	0.55
1:A:205:HIS:CD2	1:A:207:PRO:HD2	2.43	0.54
2:B:89:GLN:HB2	2:B:98:PHE:CD2	2.43	0.54
2:B:83:PHE:CE2	2:B:166:SER:HB3	2.43	0.53
2:L:39:LYS:HG3	2:L:84:ALA:HB2	1.90	0.53
1:A:2:VAL:HG22	1:A:107:TYR:CD2	2.43	0.53
2:B:149:TRP:HH2	2:B:177:SER:HB3	1.74	0.52
3:C:350:TYR:O	3:C:392:GLN:N	2.41	0.52
1:A:59:TYR:HE1	1:A:69:ILE:HG13	1.75	0.51
2:L:181:LEU:HD12	2:L:185:GLN:HB3	1.91	0.51
2:B:181:LEU:HD12	2:B:185:GLN:HB3	1.93	0.50
2:B:190:ARG:O	2:B:209:PRO:HD3	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:351:VAL:HG13	3:C:445:LEU:HB3	1.91	0.50
1:H:202:ASN:ND2	1:H:213:ASP:OD1	2.44	0.50
2:L:89:GLN:NE2	2:L:90:GLN:O	2.45	0.50
1:A:168:VAL:HG22	1:A:187:VAL:HG22	1.93	0.50
2:L:2:ILE:O	2:L:97:THR:HG21	2.11	0.49
2:B:2:ILE:O	2:B:97:THR:HG21	2.13	0.49
2:B:109:GLN:HG3	2:B:171:ASN:HB2	1.93	0.49
3:C:349:LEU:HB2	3:C:447:VAL:HG22	1.95	0.49
2:L:89:GLN:HB2	2:L:98:PHE:CD2	2.48	0.48
3:D:317:HIS:HB2	3:D:462:THR:HB	1.94	0.48
3:D:342:PHE:HE2	3:D:344:LEU:HG	1.77	0.48
2:L:8:PRO:HD2	2:L:21:ILE:HG22	1.96	0.48
2:B:139:ASP:HA	2:B:172:LYS:HB3	1.96	0.48
2:B:149:TRP:O	2:B:155:PRO:HA	2.13	0.48
3:D:348:TRP:HB2	3:D:395:ALA:HB3	1.96	0.48
3:C:343:ASP:N	3:C:453:ASN:OD1	2.42	0.48
3:D:435:PHE:HB3	3:D:438:THR:CG2	2.44	0.48
2:L:167:LYS:HG2	2:L:173:TYR:CE1	2.43	0.48
3:D:451:TYR:CE1	3:D:456:VAL:HG22	2.49	0.47
3:D:435:PHE:HB3	3:D:438:THR:HG21	1.96	0.47
2:B:167:LYS:HG2	2:B:173:TYR:CE1	2.50	0.47
1:H:106:ASP:OD1	1:H:106:ASP:N	2.37	0.47
2:L:109:GLN:HG3	2:L:171:ASN:HB2	1.96	0.47
1:A:119:ALA:HB3	1:A:151:PHE:HE2	1.80	0.47
2:B:167:LYS:HG2	2:B:173:TYR:HE1	1.80	0.47
2:B:137:ILE:O	2:B:174:ALA:HA	2.15	0.47
2:L:139:ASP:HB3	2:L:172:LYS:HD3	1.97	0.47
2:B:142:PRO:HD2	2:B:198:HIS:CE1	2.50	0.47
1:H:20:LEU:HD12	1:H:80:LEU:HD23	1.97	0.46
1:H:119:ALA:HB3	1:H:151:PHE:HE2	1.78	0.46
1:H:87:THR:HG23	1:H:115:THR:HA	1.98	0.46
2:L:137:ILE:HD11	2:L:175:ALA:HB3	1.97	0.46
2:B:191:SER:HA	2:B:207:VAL:O	2.15	0.46
3:C:311:PHE:HD2	3:C:333:LEU:HD11	1.80	0.46
2:L:149:TRP:O	2:L:155:PRO:HA	2.16	0.46
1:H:59:TYR:HE1	1:H:69:ILE:HG13	1.81	0.46
1:A:186:VAL:HG11	2:B:136:LEU:HD11	1.98	0.46
2:B:199:GLU:N	2:B:199:GLU:OE1	2.49	0.46
1:A:171:PHE:HE2	2:B:174:ALA:O	2.00	0.45
1:H:48:ILE:HD11	1:H:67:VAL:HG11	1.98	0.45
2:L:149:TRP:HH2	2:L:177:SER:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:424:LEU:HD13	3:C:424:LEU:HA	1.86	0.45
2:B:114:PRO:HB3	2:B:140:PHE:HB3	1.99	0.44
2:L:161:GLU:O	2:L:177:SER:HA	2.16	0.44
1:A:63:LEU:HD12	1:A:82:LEU:HD11	1.99	0.44
1:H:32:TYR:CD2	1:H:94:ARG:HD2	2.53	0.44
2:B:142:PRO:HD2	2:B:198:HIS:HE1	1.82	0.44
1:H:119:ALA:HB3	1:H:151:PHE:CE2	2.53	0.43
1:H:4:LEU:HB3	1:H:22:CYS:SG	2.58	0.43
1:A:122:LYS:HA	1:A:122:LYS:HD2	1.87	0.43
3:C:397:THR:HG21	3:C:430:GLY:HA3	2.00	0.43
1:A:61:PRO:HA	1:A:64:GLN:HB2	2.00	0.43
3:C:346:LEU:HB3	3:C:448:PHE:CZ	2.53	0.43
3:C:445:LEU:HD21	3:C:461:TYR:HD2	1.83	0.43
3:D:342:PHE:CE2	3:D:344:LEU:HG	2.53	0.43
1:H:45:LEU:H	1:H:45:LEU:HD23	1.84	0.43
2:L:33:LEU:HD21	2:L:71:PHE:CG	2.54	0.43
2:B:132:THR:HA	2:B:179:LEU:O	2.18	0.43
1:A:202:ASN:ND2	1:A:213:ASP:OD1	2.52	0.43
3:C:424:LEU:HB3	3:C:433:LEU:HD12	2.01	0.42
1:H:168:VAL:HG22	1:H:187:VAL:HG22	2.01	0.42
3:D:451:TYR:HE1	3:D:456:VAL:HG22	1.83	0.42
2:L:25:ALA:O	2:L:69:THR:OG1	2.35	0.42
2:L:190:ARG:O	2:L:209:PRO:HD3	2.18	0.42
1:A:51:ILE:HG12	1:A:52:TYR:O	2.18	0.42
3:C:351:VAL:CG1	3:C:445:LEU:HB3	2.49	0.42
2:B:116:VAL:HG22	2:B:137:ILE:HG22	2.01	0.42
3:C:329:LEU:HD21	3:C:462:THR:HG21	2.01	0.42
2:B:139:ASP:HB3	2:B:172:LYS:HD3	2.02	0.42
3:C:345:LEU:HD12	3:C:397:THR:O	2.20	0.42
1:A:17:THR:HG22	1:A:82(A):THR:HA	2.02	0.41
1:A:58:ASN:OD1	1:A:58:ASN:N	2.53	0.41
1:A:104:PRO:HA	2:B:34:ASN:ND2	2.34	0.41
3:C:435:PHE:HB3	3:C:438:THR:HG22	2.01	0.41
1:A:175:LEU:HD12	1:A:180:LEU:O	2.20	0.41
2:B:83:PHE:HE2	2:B:166:SER:HB3	1.84	0.41
2:L:161:GLU:HB2	2:L:178:TYR:HD1	1.85	0.41
2:B:54:LEU:HD23	2:B:54:LEU:HA	1.91	0.41
3:C:449:VAL:HG23	3:C:456:VAL:HG13	2.03	0.41
1:H:186:VAL:HG11	2:L:136:LEU:HD11	2.03	0.41
2:B:165:PRO:HD3	2:B:174:ALA:O	2.21	0.41
3:C:439:PRO:HD2	3:C:442:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:404:HIS:CD2	3:C:411:TYR:HD2	2.38	0.41
3:D:329:LEU:HD21	3:D:462:THR:HG21	2.02	0.41
3:C:313:MET:SD	3:C:448:PHE:HD2	2.44	0.41
1:H:8:GLY:HA3	1:H:20:LEU:HD23	2.03	0.40
2:L:37:GLN:HG3	2:L:84:ALA:HB3	2.03	0.40
3:C:424:LEU:HD11	3:C:435:PHE:CE2	2.57	0.40
3:C:424:LEU:HD11	3:C:435:PHE:CD2	2.56	0.40
3:D:348:TRP:CE2	3:D:433:LEU:HD13	2.56	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	210/242 (87%)	195 (93%)	14 (7%)	1 (0%)	25	59
1	H	210/242 (87%)	194 (92%)	15 (7%)	1 (0%)	25	59
2	B	208/210 (99%)	191 (92%)	17 (8%)	0	100	100
2	L	208/210 (99%)	192 (92%)	16 (8%)	0	100	100
3	C	124/254 (49%)	109 (88%)	15 (12%)	0	100	100
3	D	121/254 (48%)	108 (89%)	13 (11%)	0	100	100
All	All	1081/1412 (77%)	989 (92%)	90 (8%)	2 (0%)	44	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	PRO
1	H	152	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/209 (88%)	181 (98%)	3 (2%)	58	76
1	H	184/209 (88%)	178 (97%)	6 (3%)	33	61
2	B	179/179 (100%)	176 (98%)	3 (2%)	56	76
2	L	179/179 (100%)	175 (98%)	4 (2%)	47	70
3	C	111/216 (51%)	106 (96%)	5 (4%)	23	53
3	D	108/216 (50%)	103 (95%)	5 (5%)	23	52
All	All	945/1208 (78%)	919 (97%)	26 (3%)	38	65

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	30	SER
1	H	31	ARG
1	H	45	LEU
1	H	52	TYR
1	H	58	ASN
1	H	151	PHE
2	L	149	TRP
2	L	152	ASP
2	L	178	TYR
2	L	187	LYS
1	A	52	TYR
1	A	58	ASN
1	A	151	PHE
2	B	78	LEU
2	B	149	TRP
2	B	152	ASP
3	C	321	PHE
3	C	343	ASP
3	C	408	TYR
3	C	412	CYS
3	C	465	SER
3	D	315	ASN

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Mol	Chain	Res	Type
3	D	332	HIS
3	D	406	ASP
3	D	412	CYS
3	D	419	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	214/242 (88%)	0.63	8 (3%)	45	29	18, 43, 68, 79	0
1	H	214/242 (88%)	0.49	2 (0%)	81	61	11, 29, 71, 87	0
2	B	210/210 (100%)	0.78	19 (9%)	17	11	17, 38, 92, 102	0
2	L	210/210 (100%)	0.68	16 (7%)	21	15	10, 38, 90, 101	0
3	C	128/254 (50%)	0.60	5 (3%)	44	28	19, 44, 73, 102	0
3	D	125/254 (49%)	0.83	9 (7%)	23	16	26, 47, 98, 130	0
All	All	1101/1412 (77%)	0.66	59 (5%)	32	21	10, 41, 86, 130	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	119	ALA	4.4
3	D	405	ALA	3.8
3	D	424	LEU	3.7
2	B	30	SER	3.5
2	L	209	PRO	3.5
2	L	180	SER	3.4
2	L	144	ALA	3.4
2	B	193	SER	3.3
1	A	216	VAL	3.3
2	L	210	THR	3.0
3	D	409	THR	3.0
2	L	108	GLY	2.8
2	L	208	ALA	2.8
2	B	208	ALA	2.8
2	B	142	PRO	2.8
3	C	341	PRO	2.7
3	D	308	GLY	2.7
2	B	1	ASP	2.7
2	B	156	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	207	VAL	2.6
2	B	108	GLY	2.5
3	D	431	THR	2.5
2	B	119	PHE	2.5
1	A	8	GLY	2.5
2	B	175	ALA	2.5
3	C	403	GLU	2.5
2	B	151	ALA	2.4
3	D	315	ASN	2.4
3	C	340	ALA	2.4
2	B	31	THR	2.4
1	A	101	GLY	2.4
1	A	189	VAL	2.4
2	B	209	PRO	2.4
2	L	129	ASN	2.4
1	A	131	PRO	2.4
2	B	115	SER	2.4
3	C	308	GLY	2.3
3	D	410	ALA	2.3
1	H	54	THR	2.3
2	B	178	TYR	2.3
1	A	120	SER	2.3
2	L	1	ASP	2.3
2	L	133	LEU	2.3
2	B	28	THR	2.3
2	L	183	PRO	2.2
2	L	186	TRP	2.2
3	D	465	SER	2.2
2	L	201	SER	2.2
2	B	170	ASN	2.2
2	L	147	VAL	2.1
2	B	118	LEU	2.1
2	L	142	PRO	2.1
1	A	28	SER	2.1
2	B	145	VAL	2.1
3	C	407	ASN	2.1
3	D	406	ASP	2.0
2	L	154	SER	2.0
1	A	72	ASP	2.0
2	L	168	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.