Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2025 – 10:21 AM EST

PDB ID	:	9B9F
Title	:	Zebrafish Betaglycan Orphan Domain (zfBGo) in complex with TGF-B3 and extracellular domains of TGFBRI and TGFBRII
Authors	:	Wieteska, L.; Taylor, A.B.; Hinck, A.P.
Deposited on	:	2024-04-02
Resolution	:	3.00 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:

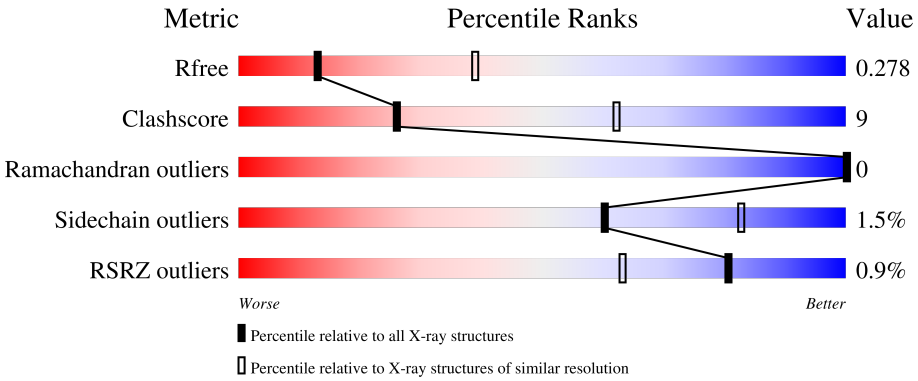
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 3.00 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	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	112	89% 11%
1	F	112	84% 16%
2	B	112	78% 22%
2	G	112	73% 27%
3	C	87	75% 14% 11%

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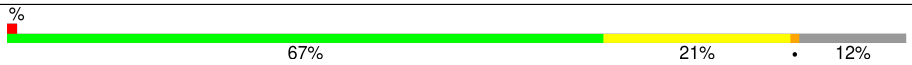
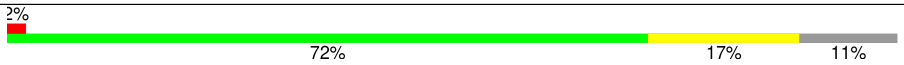
Mol	Chain	Length	Quality of chain
3	H	87	
4	D	113	
4	I	113	
5	E	338	
5	J	338	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11078 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 Transforming growth factor beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	0	0
			890	564	148	168	10			
1	F	112	Total	C	N	O	S	0	0	0
			890	564	148	168	10			

- Molecule 2 is a protein called Transforming growth factor beta-3 triple mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	112	Total	C	N	O	S	0	0	0
			879	556	142	171	10			
2	G	112	Total	C	N	O	S	0	0	0
			879	556	142	171	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	325	GLU	ARG	engineered mutation	UNP P10600
B	390	ALA	TYR	engineered mutation	UNP P10600
B	394	GLU	ARG	engineered mutation	UNP P10600
G	325	GLU	ARG	engineered mutation	UNP P10600
G	390	ALA	TYR	engineered mutation	UNP P10600
G	394	GLU	ARG	engineered mutation	UNP P10600

- Molecule 3 is a protein called Transforming growth factor beta receptor type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	77	Total	C	N	O	S	0	0	0
			586	361	99	115	11			
3	H	75	Total	C	N	O	S	0	0	0
			575	355	97	112	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	27	GLY	-	expression tag	UNP P36897
C	28	SER	-	expression tag	UNP P36897
H	27	GLY	-	expression tag	UNP P36897
H	28	SER	-	expression tag	UNP P36897

- Molecule 4 is a protein called Transforming growth factor beta receptor type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	105	Total	C	N	O	S	0	0	0
			831	519	136	161	15			
4	I	105	Total	C	N	O	S	0	0	0
			831	519	136	161	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	41	MET	-	initiating methionine	UNP P37173
I	41	MET	-	initiating methionine	UNP P37173

- Molecule 5 is a protein called Transforming growth factor beta receptor type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	298	Total	C	N	O	S	0	0	0
			2349	1498	411	431	9			
5	J	300	Total	C	N	O	S	0	0	0
			2368	1509	415	435	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	28	GLY	-	expression tag	UNP A0A0H3UK16
E	150	GLY	CYS	engineered mutation	UNP A0A0H3UK16
E	277	GLY	CYS	engineered mutation	UNP A0A0H3UK16
E	360	HIS	-	expression tag	UNP A0A0H3UK16
E	361	HIS	-	expression tag	UNP A0A0H3UK16
E	362	HIS	-	expression tag	UNP A0A0H3UK16
E	363	HIS	-	expression tag	UNP A0A0H3UK16
E	364	HIS	-	expression tag	UNP A0A0H3UK16
E	365	HIS	-	expression tag	UNP A0A0H3UK16
J	28	GLY	-	expression tag	UNP A0A0H3UK16
J	150	GLY	CYS	engineered mutation	UNP A0A0H3UK16
J	277	GLY	CYS	engineered mutation	UNP A0A0H3UK16
J	360	HIS	-	expression tag	UNP A0A0H3UK16

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Chain	Residue	Modelled	Actual	Comment	Reference
J	361	HIS	-	expression tag	UNP A0A0H3UK16
J	362	HIS	-	expression tag	UNP A0A0H3UK16
J	363	HIS	-	expression tag	UNP A0A0H3UK16
J	364	HIS	-	expression tag	UNP A0A0H3UK16
J	365	HIS	-	expression tag	UNP A0A0H3UK16

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: Transforming growth factor beta-3

Chain A:

• Molecule 1: Transforming growth factor beta-3

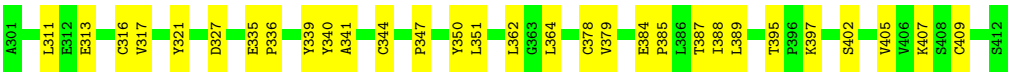
Chain F:

• Molecule 2: Transforming growth factor beta-3 triple mutant

Chain B:

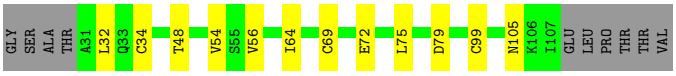
• Molecule 2: Transforming growth factor beta-3 triple mutant

Chain G:



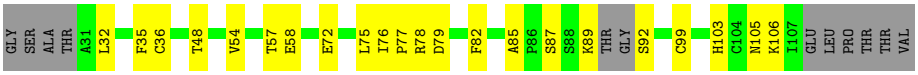
• Molecule 3: Transforming growth factor beta receptor type-1

Chain C:



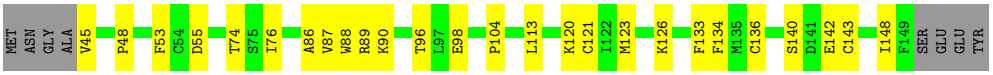
• Molecule 3: Transforming growth factor beta receptor type-1

Chain H:



• Molecule 4: Transforming growth factor beta receptor type-2

Chain D:

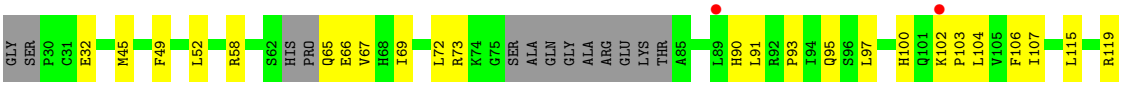


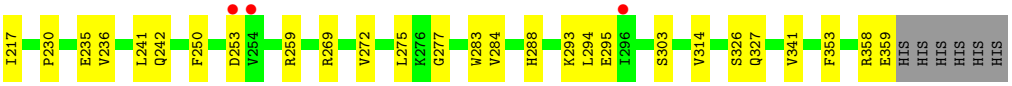
• Molecule 4: Transforming growth factor beta receptor type-2

Chain I:

• Molecule 5: Transforming growth factor beta receptor type-3

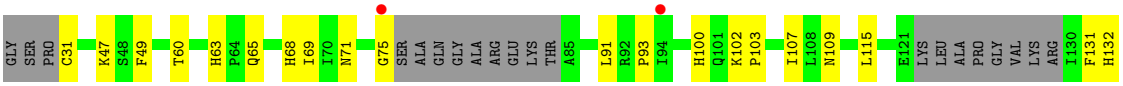
Chain E:

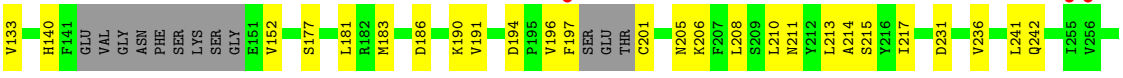




• Molecule 5: Transforming growth factor beta receptor type-3

Chain J:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	195.14Å 200.92Å 47.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.35 – 3.00 63.35 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.35-3.00) 99.9 (63.35-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.235 , 0.278 0.235 , 0.278	Depositor DCC
R_{free} test set	2024 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	105.3	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 85.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.001 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11078	wwPDB-VP
Average B, all atoms (Å^2)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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	0.28	0/915	0.51	0/1248
1	F	0.25	0/915	0.51	0/1248
2	B	0.27	0/903	0.50	0/1233
2	G	0.25	0/903	0.50	0/1233
3	C	0.30	0/596	0.51	0/810
3	H	0.33	0/584	0.52	0/792
4	D	0.29	0/848	0.53	0/1142
4	I	0.29	0/848	0.55	0/1142
5	E	0.30	0/2400	0.54	0/3256
5	J	0.29	0/2422	0.51	0/3290
All	All	0.29	0/11334	0.52	0/15394

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	890	0	847	7	0
1	F	890	0	847	10	0
2	B	879	0	829	20	0
2	G	879	0	829	25	0
3	C	586	0	558	7	0
3	H	575	0	547	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	831	0	794	16	0
4	I	831	0	794	13	0
5	E	2349	0	2352	56	0
5	J	2368	0	2366	40	0
All	All	11078	0	10763	202	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 (202) 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)
3:H:57:THR:HG23	3:H:92:SER:CB	1.97	0.94
3:H:57:THR:HG23	3:H:92:SER:HB2	1.59	0.85
1:A:379:VAL:HG21	2:B:379:VAL:HG21	1.58	0.85
2:B:350:TYR:CE2	2:B:351:LEU:HG	2.14	0.83
5:E:190:LYS:HB2	5:E:211:ASN:HB3	1.60	0.83
1:F:379:VAL:HG21	2:G:379:VAL:HG21	1.62	0.81
5:J:68:HIS:HD1	5:J:177:SER:HG	1.26	0.80
5:E:58:ARG:HD3	5:E:195:PRO:HA	1.69	0.74
4:I:140:SER:HB2	4:I:143:CYS:HB3	1.70	0.73
5:J:208:LEU:HD21	5:J:213:LEU:HD21	1.72	0.72
5:E:65:GLN:HB2	5:E:103:PRO:O	1.90	0.71
2:G:395:THR:CG2	2:G:397:LYS:HE2	2.21	0.71
2:G:395:THR:HG21	2:G:397:LYS:HE2	1.74	0.69
5:J:196:VAL:HG13	5:J:197:PHE:CD2	2.27	0.69
5:E:115:LEU:HB3	5:E:140:HIS:HE1	1.57	0.69
5:J:47:LYS:HE2	5:J:49:PHE:CZ	2.28	0.69
4:D:140:SER:HB2	4:D:143:CYS:HB3	1.75	0.69
2:G:350:TYR:CE2	2:G:351:LEU:HG	2.29	0.68
3:H:35:PHE:CZ	3:H:103:HIS:HB3	2.29	0.67
5:E:73:ARG:NH1	5:E:180:GLU:OE2	2.28	0.66
3:H:57:THR:CG2	3:H:92:SER:CB	2.71	0.66
5:E:181:LEU:HD13	5:E:214:ALA:HB2	1.77	0.65
3:H:54:VAL:HB	3:H:105:ASN:HB2	1.78	0.65
5:E:130:ILE:HA	5:E:151:GLU:HB3	1.77	0.65
4:D:87:VAL:HG12	4:D:98:GLU:HB3	1.79	0.64
3:C:54:VAL:HB	3:C:105:ASN:HB2	1.79	0.64
3:H:72:GLU:HA	3:H:75:LEU:HD12	1.80	0.64
3:H:58:GLU:O	3:H:58:GLU:OE1	2.16	0.64
4:D:87:VAL:CG1	4:D:98:GLU:HB3	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:49:PHE:HB3	5:E:213:LEU:HD22	1.82	0.62
4:D:88:TRP:HB3	4:D:134:PHE:HB2	1.80	0.61
5:J:91:LEU:HD22	5:J:191:VAL:HB	1.83	0.60
3:C:99:CYS:HA	4:D:45:VAL:HG23	1.84	0.59
5:E:58:ARG:HH11	5:E:195:PRO:CB	2.16	0.59
4:I:104:PRO:HA	4:I:113:LEU:HD12	1.85	0.58
3:H:35:PHE:CE2	3:H:106:LYS:HB2	2.39	0.58
5:E:91:LEU:HD21	5:E:106:PHE:HZ	1.70	0.56
5:E:236:VAL:HG13	5:E:341:VAL:HA	1.86	0.56
5:J:181:LEU:HD13	5:J:214:ALA:HB2	1.87	0.56
5:E:236:VAL:HG23	5:E:272:VAL:HB	1.87	0.56
5:E:32:GLU:HB3	5:E:326:SER:HB3	1.88	0.56
2:B:350:TYR:CD2	2:B:351:LEU:HG	2.39	0.56
2:B:350:TYR:CE1	2:B:364:LEU:HB2	2.41	0.56
5:J:47:LYS:HA	5:J:217:ILE:HG22	1.88	0.56
5:E:272:VAL:HG22	5:E:295:GLU:HB2	1.88	0.55
5:E:52:LEU:HD21	5:E:182:ARG:HD3	1.87	0.55
5:E:58:ARG:O	5:E:58:ARG:HG2	2.05	0.55
3:C:72:GLU:HA	3:C:75:LEU:HD12	1.88	0.55
3:H:35:PHE:HE2	3:H:106:LYS:HB2	1.71	0.55
3:H:57:THR:CG2	3:H:92:SER:HB2	2.32	0.55
2:B:396:PRO:HB2	5:E:208:LEU:HD12	1.88	0.54
5:J:75:GLY:HA3	5:J:183:MET:HE2	1.88	0.54
2:B:350:TYR:CE2	2:B:351:LEU:CG	2.89	0.54
4:D:126:LYS:HB2	4:D:133:PHE:HD2	1.73	0.54
2:G:389:LEU:HB2	5:J:210:LEU:HD21	1.91	0.53
5:E:294:LEU:HD23	5:E:314:VAL:HG22	1.91	0.53
5:E:91:LEU:HD21	5:E:106:PHE:CZ	2.44	0.53
4:I:48:PRO:HB2	4:I:76:ILE:HG22	1.89	0.53
1:A:379:VAL:HG13	1:A:380:PRO:HD2	1.89	0.52
2:G:350:TYR:CE2	2:G:351:LEU:CD1	2.93	0.52
5:E:104:LEU:HB2	5:E:106:PHE:CE2	2.45	0.52
5:J:231:ASP:O	5:J:231:ASP:OD1	2.28	0.52
3:H:99:CYS:HA	4:I:45:VAL:HG23	1.92	0.52
2:G:350:TYR:CE1	2:G:364:LEU:HB2	2.45	0.52
5:J:47:LYS:HE2	5:J:49:PHE:HZ	1.69	0.52
5:J:242:GLN:HB2	5:J:348:PRO:O	2.11	0.51
5:E:97:LEU:H	5:E:97:LEU:HD23	1.76	0.51
5:J:194:ASP:HB3	5:J:196:VAL:HG12	1.93	0.51
2:G:313:GLU:O	2:G:347:PRO:HD2	2.10	0.51
5:E:241:LEU:O	5:E:277:GLY:HA2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:TYR:CE2	2:B:351:LEU:CD1	2.94	0.50
3:H:58:GLU:H	3:H:92:SER:HB2	1.76	0.50
5:E:241:LEU:HD23	5:E:242:GLN:N	2.27	0.50
2:G:384:GLU:OE1	2:G:407:LYS:NZ	2.45	0.50
5:E:230:PRO:HG3	5:E:358:ARG:HH21	1.76	0.49
5:E:58:ARG:HB2	5:E:197:PHE:O	2.12	0.49
5:J:49:PHE:HB3	5:J:213:LEU:HD13	1.94	0.49
5:J:49:PHE:CE1	5:J:215:SER:HB3	2.48	0.49
5:J:236:VAL:HG13	5:J:341:VAL:HA	1.94	0.49
5:J:190:LYS:HD3	5:J:211:ASN:CG	2.33	0.49
2:G:389:LEU:HB2	5:J:210:LEU:CD2	2.42	0.49
1:F:389:LEU:HD11	1:F:396:PRO:HB2	1.94	0.49
5:J:241:LEU:HD23	5:J:242:GLN:N	2.28	0.48
5:J:100:HIS:CE1	5:J:102:LYS:HB2	2.48	0.48
5:E:100:HIS:NE2	5:E:104:LEU:HD21	2.28	0.48
3:C:105:ASN:OD1	3:C:105:ASN:N	2.46	0.48
2:G:387:THR:HG22	5:J:210:LEU:HD11	1.96	0.48
5:E:327:GLN:N	5:E:327:GLN:OE1	2.47	0.48
5:J:100:HIS:CG	5:J:191:VAL:HG22	2.49	0.48
1:F:384:GLU:OE1	1:F:407:LYS:NZ	2.47	0.47
1:A:385:PRO:HB3	1:A:402:SER:HA	1.95	0.47
5:E:170:HIS:HB3	5:E:171:ARG:HH11	1.79	0.47
2:B:318:ARG:HG3	2:B:345:SER:HB3	1.96	0.47
5:J:65:GLN:HG2	5:J:103:PRO:HG2	1.96	0.47
5:J:107:ILE:HA	5:J:132:HIS:HB2	1.97	0.47
5:E:275:LEU:HB3	5:E:283:TRP:CE2	2.49	0.47
2:G:317:VAL:HG22	2:G:409:CYS:SG	2.54	0.47
3:H:32:LEU:HB3	3:H:48:THR:HG22	1.97	0.46
5:J:196:VAL:HG13	5:J:197:PHE:N	2.30	0.46
5:E:69:ILE:HG12	5:E:107:ILE:HD12	1.98	0.46
5:J:93:PRO:HA	5:J:190:LYS:HG3	1.98	0.46
3:H:57:THR:HG23	3:H:92:SER:OG	2.15	0.46
5:J:242:GLN:HG3	5:J:348:PRO:HA	1.98	0.46
4:D:104:PRO:HA	4:D:113:LEU:HD12	1.97	0.46
5:E:100:HIS:NE2	5:E:102:LYS:O	2.49	0.46
5:E:45:MET:HB3	5:E:217:ILE:HG22	1.98	0.45
1:A:357:THR:HG23	5:E:250:PHE:HE2	1.81	0.45
2:B:380:PRO:HB3	2:B:406:VAL:HG22	1.98	0.45
2:G:336:PRO:HD2	2:G:388:ILE:HG22	1.98	0.45
3:H:106:LYS:O	3:H:106:LYS:HG2	2.17	0.45
5:J:93:PRO:HB3	5:J:191:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LEU:HD11	1:A:396:PRO:HB2	1.99	0.45
5:E:66:GLU:HB2	5:E:104:LEU:HD22	1.99	0.45
3:C:32:LEU:HB3	3:C:48:THR:HG22	1.99	0.45
5:J:327:GLN:OE1	5:J:327:GLN:N	2.50	0.45
5:E:235:GLU:HG3	5:E:269:ARG:CZ	2.47	0.45
5:E:269:ARG:NH2	5:E:359:GLU:OE2	2.50	0.45
4:D:126:LYS:HB2	4:D:133:PHE:CD2	2.51	0.44
5:E:72:LEU:HD12	5:E:181:LEU:HB2	1.99	0.44
5:E:241:LEU:HD12	5:E:353:PHE:HE1	1.83	0.44
5:E:139:VAL:HG22	5:E:152:VAL:HG22	1.98	0.44
5:J:272:VAL:HG22	5:J:295:GLU:HB2	1.99	0.44
2:B:312:GLU:HG2	2:B:352:ARG:HH22	1.81	0.44
5:E:190:LYS:HG2	5:E:191:VAL:N	2.33	0.44
2:G:344:CYS:HB3	2:G:378:CYS:SG	2.58	0.44
4:I:87:VAL:CG1	4:I:98:GLU:HB3	2.48	0.44
1:A:317:VAL:HG22	1:A:409:CYS:SG	2.57	0.44
4:D:48:PRO:HB2	4:D:76:ILE:HG22	2.00	0.44
5:E:190:LYS:HE3	5:E:211:ASN:HD22	1.83	0.44
2:G:395:THR:HG22	2:G:397:LYS:HE2	1.99	0.44
5:E:65:GLN:N	5:E:65:GLN:OE1	2.51	0.44
2:B:384:GLU:OE1	2:B:407:LYS:NZ	2.51	0.43
2:B:344:CYS:HB3	2:B:378:CYS:SG	2.58	0.43
4:D:89:ARG:HB2	4:D:96:THR:HG22	1.99	0.43
4:D:120:LYS:HD3	4:D:148:ILE:HD13	1.99	0.43
5:E:73:ARG:CZ	5:E:180:GLU:OE2	2.66	0.43
5:E:90:HIS:CE1	5:E:119:ARG:HD2	2.53	0.43
5:E:190:LYS:HE3	5:E:211:ASN:ND2	2.33	0.43
2:G:384:GLU:HB2	2:G:405:VAL:HG13	1.99	0.43
5:J:241:LEU:HD12	5:J:353:PHE:HE1	1.82	0.43
5:J:264:ASP:O	5:J:289:LYS:NZ	2.43	0.43
3:H:57:THR:CG2	3:H:92:SER:HB3	2.48	0.43
5:J:205:ASN:OD1	5:J:206:LYS:NZ	2.49	0.43
2:B:312:GLU:HG2	2:B:352:ARG:NH2	2.34	0.43
2:G:335:GLU:HB2	2:G:389:LEU:HB3	2.01	0.43
5:J:60:THR:HA	5:J:63:HIS:O	2.19	0.43
5:J:275:LEU:HB3	5:J:283:TRP:CE2	2.53	0.43
1:F:385:PRO:HB3	1:F:402:SER:HA	2.00	0.43
2:G:311:LEU:HD23	2:G:311:LEU:HA	1.87	0.43
3:C:34:CYS:HB2	3:C:69:CYS:SG	2.59	0.42
4:D:74:THR:OG1	4:D:142:GLU:OE2	2.26	0.42
5:E:208:LEU:HD23	5:E:208:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:86:ALA:HB3	4:I:136:CYS:SG	2.59	0.42
2:B:355:ASP:HB2	2:B:410:LYS:HD2	2.01	0.42
4:I:89:ARG:HA	4:I:132:THR:O	2.19	0.42
4:I:116:ALA:O	4:I:139:SER:OG	2.34	0.42
4:D:55:ASP:O	4:D:98:GLU:HA	2.19	0.42
5:E:67:VAL:HB	5:E:175:VAL:HA	2.01	0.42
5:E:190:LYS:HB3	5:E:212:TYR:HE1	1.84	0.42
3:H:89:LYS:HE3	3:H:89:LYS:HB2	1.84	0.42
5:E:284:VAL:HG22	5:E:303:SER:HB2	2.02	0.42
3:H:76:ILE:O	3:H:82:PHE:HD2	2.02	0.42
4:I:127:LYS:HE2	4:I:127:LYS:HB2	1.92	0.42
2:G:350:TYR:CE2	2:G:351:LEU:CG	3.00	0.42
3:H:85:ALA:O	3:H:87:SER:OG	2.23	0.42
1:F:339:TYR:CZ	1:F:341:ALA:HB2	2.55	0.42
4:D:86:ALA:HB3	4:D:136:CYS:SG	2.60	0.42
2:B:336:PRO:HD2	2:B:388:ILE:HG22	2.01	0.41
5:E:93:PRO:HG2	5:E:95:GLN:HG2	2.02	0.41
2:B:305:ASN:O	2:B:309:ARG:HG2	2.20	0.41
5:E:259:ARG:HG3	5:E:288:HIS:HB2	2.02	0.41
3:H:76:ILE:HA	3:H:77:PRO:HA	1.88	0.41
4:I:128:LYS:HE3	4:I:128:LYS:HB3	1.88	0.41
4:I:128:LYS:HD3	4:I:133:PHE:CD2	2.55	0.41
5:J:69:ILE:HG12	5:J:107:ILE:HD12	2.01	0.41
3:C:56:VAL:HA	3:C:64:ILE:O	2.21	0.41
5:E:275:LEU:HB3	5:E:283:TRP:CZ2	2.55	0.41
5:J:115:LEU:HB3	5:J:140:HIS:HE1	1.86	0.41
1:A:321:TYR:HB2	1:A:340:TYR:CE1	2.56	0.41
4:D:123:MET:HA	4:D:136:CYS:HB3	2.03	0.41
5:E:52:LEU:HD11	5:E:182:ARG:HG2	2.02	0.41
2:G:350:TYR:CZ	2:G:351:LEU:HG	2.56	0.41
2:G:385:PRO:HB3	2:G:402:SER:HA	2.03	0.41
4:I:120:LYS:HD3	4:I:148:ILE:HD13	2.03	0.41
5:J:71:ASN:OD1	5:J:109:ASN:ND2	2.50	0.41
2:B:384:GLU:HB2	2:B:405:VAL:HG13	2.01	0.41
2:B:385:PRO:HB3	2:B:402:SER:HA	2.01	0.41
1:F:317:VAL:HG22	1:F:409:CYS:SG	2.61	0.41
5:J:190:LYS:HB3	5:J:190:LYS:HE2	1.86	0.41
2:B:402:SER:HB3	5:E:253:ASP:CG	2.42	0.41
2:G:321:TYR:HB2	2:G:340:TYR:CE1	2.57	0.41
4:D:90:LYS:O	4:D:90:LYS:HG2	2.20	0.40
1:F:343:PHE:HB3	2:G:362:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:131:PHE:HB2	5:J:152:VAL:HG22	2.03	0.40
1:F:318:ARG:HG3	1:F:345:SER:HB3	2.03	0.40
2:G:339:TYR:CZ	2:G:341:ALA:HB2	2.56	0.40
5:E:293:LYS:HB2	5:E:293:LYS:HE2	1.83	0.40
1:F:380:PRO:HB3	1:F:406:VAL:CG2	2.52	0.40
5:E:58:ARG:CB	5:E:197:PHE:O	2.69	0.40
1:F:368:LEU:HD12	2:G:327:ASP:O	2.22	0.40
4:I:55:ASP:O	4:I:98:GLU:HA	2.22	0.40
2:B:350:TYR:CZ	2:B:351:LEU:HG	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	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
1	F	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
2	B	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
2	G	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
3	C	75/87 (86%)	69 (92%)	6 (8%)	0	100	100
3	H	71/87 (82%)	62 (87%)	9 (13%)	0	100	100
4	D	103/113 (91%)	94 (91%)	9 (9%)	0	100	100
4	I	103/113 (91%)	94 (91%)	9 (9%)	0	100	100
5	E	284/338 (84%)	264 (93%)	20 (7%)	0	100	100
5	J	290/338 (86%)	269 (93%)	21 (7%)	0	100	100
All	All	1366/1524 (90%)	1275 (93%)	91 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	102/102 (100%)	101 (99%)	1 (1%)	73	88
1	F	102/102 (100%)	101 (99%)	1 (1%)	73	88
2	B	101/101 (100%)	100 (99%)	1 (1%)	73	88
2	G	101/101 (100%)	100 (99%)	1 (1%)	73	88
3	C	72/80 (90%)	71 (99%)	1 (1%)	62	83
3	H	71/80 (89%)	68 (96%)	3 (4%)	25	59
4	D	101/107 (94%)	99 (98%)	2 (2%)	50	78
4	I	101/107 (94%)	99 (98%)	2 (2%)	50	78
5	E	267/299 (89%)	264 (99%)	3 (1%)	70	87
5	J	269/299 (90%)	265 (98%)	4 (2%)	60	83
All	All	1287/1378 (93%)	1268 (98%)	19 (2%)	60	83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	CYS
2	B	316	CYS
3	C	79	ASP
4	D	53	PHE
4	D	121	CYS
5	E	130	ILE
5	E	133	VAL
5	E	212	TYR
1	F	316	CYS
2	G	316	CYS
3	H	36	CYS
3	H	78	ARG
3	H	79	ASP
4	I	53	PHE
4	I	121	CYS
5	J	31	CYS

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Mol	Chain	Res	Type
5	J	133	VAL
5	J	186	ASP
5	J	201	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	140	HIS
5	J	140	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 oligosaccharides 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, 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	112/112 (100%)	-0.61	0 100 100	85, 110, 159, 225	0
1	F	112/112 (100%)	-0.57	0 100 100	101, 125, 190, 244	0
2	B	112/112 (100%)	-0.39	0 100 100	92, 129, 173, 206	0
2	G	112/112 (100%)	-0.52	0 100 100	100, 149, 212, 249	0
3	C	77/87 (88%)	-0.35	0 100 100	116, 154, 221, 253	0
3	H	75/87 (86%)	-0.43	0 100 100	123, 152, 235, 254	0
4	D	105/113 (92%)	-0.52	0 100 100	98, 139, 190, 211	0
4	I	105/113 (92%)	-0.65	0 100 100	89, 116, 150, 185	0
5	E	298/338 (88%)	-0.12	5 (1%) 69 47	108, 163, 244, 326	0
5	J	300/338 (88%)	-0.32	7 (2%) 61 39	133, 187, 247, 328	0
All	All	1408/1524 (92%)	-0.39	12 (0%) 81 63	85, 149, 230, 328	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	256	VAL	3.3
5	J	353	PHE	2.7
5	E	296	ILE	2.6
5	E	254	VAL	2.6
5	E	253	ASP	2.4
5	E	89	LEU	2.3
5	J	75	GLY	2.2
5	J	275	LEU	2.1
5	J	255	ILE	2.1
5	J	94	ILE	2.1
5	J	197	PHE	2.0
5	E	102	LYS	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.