



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:00 am GMT

PDB ID : 1RY7
Title : Crystal Structure of the 3 Ig form of FGFR3c in complex with FGF1
Authors : Olsen, S.K.; Ibrahimi, O.A.; Raucci, A.; Zhang, F.; Eliseenkova, A.V.; Yayon, A.; Basilico, C.; Linhardt, R.J.; Schlessinger, J.; Mohammadi, M.
Deposited on : 2003-12-19
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

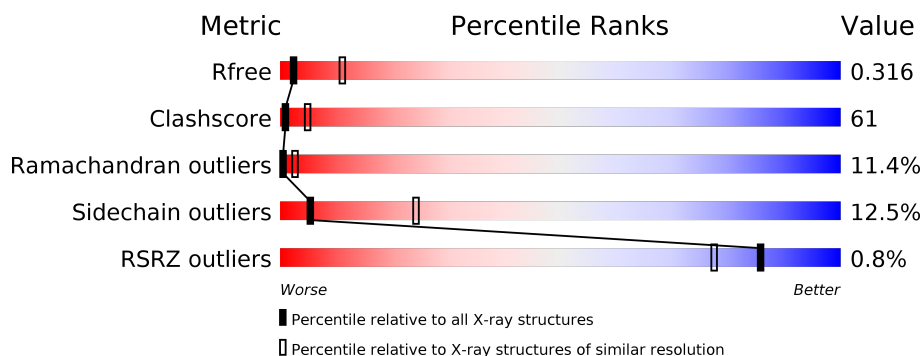
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	155	
2	B	334	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2766 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 Heparin-binding growth factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1181	750	201	226	4			

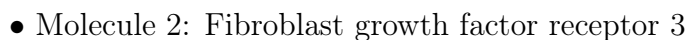
- Molecule 2 is a protein called Fibroblast growth factor receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1585	1010	277	292	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	32	MET	-	CLONING ARTIFACT	UNP P22607

- Molecule 1: Heparin-binding growth factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.22Å 64.75Å 99.93Å 90.00° 94.67° 90.00°	Depositor
Resolution (Å)	25.00 – 3.20 29.07 – 3.12	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-3.20) 90.5 (29.07-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.11Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.277 , 0.341 0.258 , 0.316	Depositor DCC
R_{free} test set	1085 reflections (10.33%)	DCC
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	2766	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% 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, 0.333 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	0.40	0/1209	0.69	0/1638
2	B	0.55	2/1629 (0.1%)	0.75	2/2233 (0.1%)
All	All	0.49	2/2838 (0.1%)	0.73	2/3871 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	170	ASN	CG-OD1	13.30	1.53	1.24
2	B	275	CYS	CB-SG	-5.32	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	170	ASN	CB-CG-OD1	-5.60	110.41	121.60
2	B	278	TYR	N-CA-C	-5.49	96.18	111.00

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	1181	0	1145	143	0
2	B	1585	0	1492	206	1
All	All	2766	0	2637	329	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 61.

All (329) 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:255:LEU:HD22	2:B:277:VAL:HG22	1.36	1.04
1:A:36:HIS:HB3	1:A:49:THR:H	1.20	1.03
2:B:190:LYS:HB2	2:B:195:PHE:HD2	1.25	1.01
2:B:189:LEU:HD11	2:B:227:THR:HB	1.46	0.96
2:B:288:LEU:HD13	2:B:306:VAL:HG21	1.48	0.96
1:A:58:GLN:H	1:A:58:GLN:HE21	1.10	0.95
2:B:312:ALA:HB1	2:B:325:SER:O	1.71	0.92
2:B:297:LYS:HE2	2:B:304:PRO:HB3	1.52	0.90
2:B:173:ARG:HB3	2:B:173:ARG:HH11	1.39	0.88
2:B:310:LYS:O	2:B:311:THR:HG23	1.72	0.88
2:B:256:GLN:OE1	2:B:276:LYS:HD2	1.74	0.87
1:A:27:LYS:HD2	1:A:149:PRO:HB3	1.55	0.87
1:A:72:LYS:HD2	1:A:79:TYR:HE2	1.40	0.84
1:A:6:ILE:HG22	1:A:7:THR:H	1.40	0.83
2:B:225:ASN:HA	2:B:242:THR:HA	1.62	0.81
1:A:58:GLN:N	1:A:58:GLN:HE21	1.77	0.80
1:A:79:TYR:CE1	1:A:94:PRO:HB3	2.17	0.79
2:B:270:ASP:HB2	2:B:327:HIS:ND1	1.98	0.78
2:B:171:THR:HG23	2:B:216:GLU:HG2	1.65	0.77
1:A:39:ARG:HD3	1:A:54:ASP:OD2	1.85	0.76
1:A:85:ASP:HB2	1:A:87:LEU:HG	1.67	0.75
1:A:58:GLN:H	1:A:58:GLN:NE2	1.85	0.75
2:B:190:LYS:HB2	2:B:195:PHE:CD2	2.16	0.74
1:A:89:TYR:HD1	1:A:90:GLY:H	1.36	0.73
2:B:252:ARG:HH11	2:B:252:ARG:HG2	1.54	0.73
2:B:297:LYS:HD3	2:B:297:LYS:O	1.87	0.73
1:A:59:LEU:HA	1:A:72:LYS:O	1.89	0.73
2:B:256:GLN:NE2	2:B:259:LEU:HD22	2.03	0.72
1:A:34:GLY:HA3	1:A:36:HIS:CE1	2.25	0.72
1:A:81:ALA:HB2	1:A:98:CYS:HB3	1.71	0.72
1:A:36:HIS:HB3	1:A:49:THR:N	2.01	0.71
2:B:253:PRO:HD3	2:B:343:ASN:CB	2.20	0.71
2:B:253:PRO:HD3	2:B:343:ASN:HB3	1.73	0.71
2:B:176:CYS:HG	2:B:228:CYS:CB	2.04	0.71
1:A:41:LEU:HD12	1:A:45:THR:OG1	1.90	0.71
1:A:58:GLN:N	1:A:58:GLN:NE2	2.38	0.70
2:B:226:TYR:N	2:B:241:TYR:O	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:LEU:HD11	2:B:337:TYR:CE2	2.26	0.70
1:A:95:ASN:HD21	1:A:97:GLU:HB2	1.54	0.69
2:B:190:LYS:C	2:B:192:GLY:H	1.96	0.69
2:B:266:VAL:HG12	2:B:267:LEU:HD12	1.73	0.69
1:A:148:LEU:HD11	2:B:246:LEU:HD22	1.75	0.69
2:B:357:LEU:H	2:B:357:LEU:HD12	1.57	0.68
2:B:281:ALA:HB3	2:B:343:ASN:HD21	1.59	0.68
2:B:267:LEU:HD23	2:B:331:PHE:HE1	1.59	0.68
2:B:190:LYS:HD2	2:B:195:PHE:CE2	2.29	0.68
1:A:65:SER:HA	2:B:284:HIS:ND1	2.08	0.68
2:B:258:GLY:O	2:B:261:ALA:HB2	1.94	0.68
1:A:80:LEU:HD22	1:A:100:PHE:CE2	2.29	0.67
1:A:6:ILE:HG22	1:A:7:THR:N	2.10	0.67
1:A:108:HIS:HD2	2:B:248:ARG:HB2	1.59	0.67
2:B:275:CYS:HG	2:B:339:CYS:HG	1.25	0.66
1:A:79:TYR:HE1	1:A:94:PRO:HB3	1.61	0.66
2:B:190:LYS:HD2	2:B:195:PHE:HE2	1.61	0.66
1:A:108:HIS:CD2	2:B:248:ARG:HB2	2.31	0.66
1:A:103:ARG:HH11	1:A:103:ARG:HG2	1.60	0.66
1:A:138:THR:HA	1:A:142:GLN:OE1	1.95	0.66
1:A:95:ASN:ND2	1:A:97:GLU:HB2	2.11	0.65
1:A:27:LYS:CD	1:A:149:PRO:HB3	2.24	0.65
1:A:42:PRO:HG3	1:A:56:HIS:NE2	2.12	0.65
1:A:63:ALA:HB2	1:A:69:VAL:HG12	1.78	0.65
1:A:16:PHE:CD1	2:B:256:GLN:HB2	2.32	0.65
1:A:80:LEU:HD23	1:A:81:ALA:N	2.11	0.65
2:B:197:GLY:HA2	2:B:204:ILE:CD1	2.26	0.65
1:A:33:ASN:HB2	1:A:144:ALA:HA	1.79	0.65
2:B:156:PRO:HG2	2:B:157:GLU:H	1.62	0.65
2:B:229:VAL:HG11	2:B:238:ARG:HH21	1.62	0.65
1:A:72:LYS:HD2	1:A:79:TYR:CE2	2.27	0.64
1:A:76:THR:OG1	1:A:78:GLN:HG3	1.97	0.64
2:B:243:LEU:HD13	2:B:244:ASP:N	2.12	0.64
2:B:331:PHE:HA	2:B:356:VAL:CG2	2.27	0.64
1:A:51:ASP:C	1:A:53:SER:H	2.01	0.63
2:B:317:THR:HG22	2:B:318:ASP:N	2.13	0.63
1:A:105:GLU:O	1:A:108:HIS:N	2.31	0.63
1:A:36:HIS:HA	1:A:49:THR:O	1.99	0.63
2:B:171:THR:HA	2:B:216:GLU:HA	1.81	0.62
2:B:289:LYS:HE2	2:B:290:HIS:N	2.14	0.62
1:A:80:LEU:C	1:A:80:LEU:HD23	2.20	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD13	1:A:147:PHE:HE1	1.65	0.61
2:B:166:VAL:HG22	2:B:167:PRO:HD2	1.81	0.61
2:B:196:ARG:N	2:B:199:HIS:HB2	2.14	0.61
2:B:267:LEU:HD23	2:B:331:PHE:CE1	2.35	0.61
1:A:106:GLU:C	1:A:108:HIS:H	2.04	0.61
2:B:195:PHE:HE1	2:B:204:ILE:HG21	1.64	0.61
2:B:271:VAL:HG22	2:B:326:LEU:HB2	1.82	0.61
2:B:357:LEU:HD12	2:B:357:LEU:N	2.15	0.61
2:B:319:LYS:O	2:B:319:LYS:HD3	2.01	0.61
2:B:169:ALA:HA	2:B:217:SER:HA	1.83	0.61
1:A:23:TYR:CD2	2:B:283:PRO:HG3	2.36	0.61
1:A:95:ASN:O	1:A:97:GLU:N	2.33	0.60
2:B:173:ARG:NH1	2:B:173:ARG:HB3	2.13	0.60
2:B:273:PHE:O	2:B:323:VAL:HA	2.01	0.60
2:B:201:ILE:C	2:B:203:GLY:H	2.05	0.60
2:B:323:VAL:CG2	2:B:324:LEU:N	2.64	0.60
2:B:252:ARG:HG3	2:B:348:SER:HB2	1.83	0.60
2:B:312:ALA:CB	2:B:325:SER:O	2.47	0.60
2:B:197:GLY:HA2	2:B:204:ILE:HD11	1.84	0.60
1:A:28:LEU:HD22	1:A:57:ILE:HG13	1.82	0.59
1:A:129:ASN:HD21	1:A:131:SER:HB3	1.66	0.59
1:A:39:ARG:NE	1:A:41:LEU:HD21	2.18	0.59
1:A:89:TYR:CD1	1:A:90:GLY:N	2.71	0.59
1:A:103:ARG:NH1	1:A:103:ARG:HG2	2.16	0.59
1:A:133:LYS:HD3	1:A:138:THR:HG22	1.84	0.59
1:A:59:LEU:HD22	1:A:71:ILE:HG22	1.83	0.58
2:B:357:LEU:HB3	2:B:358:PRO:HD2	1.85	0.58
2:B:279:SER:O	2:B:280:ASP:C	2.42	0.58
2:B:157:GLU:HG2	2:B:158:ARG:N	2.18	0.58
2:B:186:ILE:O	2:B:186:ILE:HG23	2.04	0.57
2:B:333:ASP:N	2:B:333:ASP:OD1	2.36	0.57
1:A:11:ALA:O	1:A:12:LEU:HB2	2.03	0.57
2:B:223:ARG:CB	2:B:244:ASP:HA	2.34	0.57
2:B:343:ASN:OD1	2:B:344:SER:N	2.38	0.57
1:A:33:ASN:HD21	1:A:128:LYS:N	2.03	0.57
1:A:83:ASP:OD1	1:A:87:LEU:HD12	2.05	0.57
2:B:290:HIS:HA	2:B:306:VAL:HG12	1.85	0.56
1:A:59:LEU:HD23	1:A:72:LYS:O	2.05	0.56
2:B:348:SER:O	2:B:349:HIS:HB3	2.05	0.56
2:B:289:LYS:O	2:B:306:VAL:HA	2.06	0.56
2:B:254:ILE:C	2:B:255:LEU:HD23	2.26	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:HIS:CB	1:A:49:THR:H	2.06	0.55
2:B:176:CYS:SG	2:B:228:CYS:SG	3.03	0.55
2:B:265:ALA:O	2:B:356:VAL:HA	2.06	0.55
1:A:145:ILE:HG13	1:A:146:LEU:HD23	1.87	0.55
2:B:154:THR:OG1	2:B:177:PRO:HB2	2.07	0.55
2:B:195:PHE:HA	2:B:199:HIS:ND1	2.21	0.55
2:B:173:ARG:HH11	2:B:173:ARG:CB	2.17	0.54
1:A:18:LEU:HB3	2:B:278:TYR:HB2	1.88	0.54
2:B:190:LYS:O	2:B:192:GLY:N	2.38	0.54
1:A:85:ASP:OD2	1:A:85:ASP:N	2.39	0.54
1:A:51:ASP:O	1:A:53:SER:N	2.39	0.54
2:B:230:VAL:O	2:B:236:SER:HA	2.08	0.54
2:B:196:ARG:C	2:B:198:GLU:H	2.11	0.54
1:A:38:LEU:HD13	1:A:147:PHE:CE1	2.42	0.53
1:A:9:PHE:O	1:A:11:ALA:N	2.41	0.53
2:B:229:VAL:CG1	2:B:238:ARG:HH21	2.21	0.53
1:A:88:LEU:HD13	1:A:124:VAL:HG13	1.89	0.53
2:B:276:LYS:HG2	2:B:321:LEU:CD2	2.38	0.53
2:B:266:VAL:HG13	2:B:358:PRO:O	2.08	0.53
2:B:310:LYS:O	2:B:311:THR:CG2	2.53	0.53
2:B:288:LEU:HD11	2:B:340:LEU:HD12	1.90	0.53
2:B:187:SER:CB	2:B:229:VAL:HB	2.39	0.53
2:B:223:ARG:HB2	2:B:244:ASP:HA	1.91	0.53
1:A:37:PHE:O	1:A:38:LEU:C	2.45	0.52
1:A:34:GLY:HA3	1:A:36:HIS:HE1	1.71	0.52
2:B:189:LEU:HA	2:B:195:PHE:N	2.24	0.52
1:A:109:TYR:HD2	1:A:146:LEU:HD13	1.74	0.52
2:B:357:LEU:CB	2:B:358:PRO:HD2	2.38	0.52
2:B:264:THR:HG22	2:B:265:ALA:N	2.25	0.52
1:A:110:ASN:OD1	2:B:248:ARG:NH1	2.40	0.52
1:A:39:ARG:NH2	1:A:47:ASP:OD2	2.33	0.52
2:B:281:ALA:HB3	2:B:343:ASN:ND2	2.24	0.52
2:B:218:VAL:HB	2:B:245:VAL:HG21	1.92	0.51
1:A:79:TYR:CD1	1:A:94:PRO:HB3	2.45	0.51
2:B:151:PRO:HA	2:B:179:ALA:O	2.11	0.51
1:A:108:HIS:HB3	2:B:248:ARG:HG3	1.92	0.51
2:B:207:ARG:C	2:B:209:GLN:H	2.14	0.51
2:B:204:ILE:HG13	2:B:205:LYS:N	2.26	0.51
2:B:190:LYS:C	2:B:192:GLY:N	2.64	0.51
2:B:318:ASP:HB3	2:B:321:LEU:HB2	1.93	0.51
1:A:42:PRO:HG3	1:A:56:HIS:CD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLU:HG2	1:A:115:LYS:HD2	1.92	0.51
2:B:220:PRO:HA	2:B:245:VAL:HB	1.92	0.51
2:B:166:VAL:HG22	2:B:167:PRO:CD	2.41	0.51
2:B:309:LEU:HD13	2:B:324:LEU:HD11	1.92	0.51
2:B:255:LEU:HD23	2:B:255:LEU:N	2.26	0.50
2:B:162:LYS:CB	2:B:241:TYR:HA	2.41	0.50
2:B:276:LYS:HG2	2:B:321:LEU:HD21	1.93	0.50
2:B:337:TYR:N	2:B:337:TYR:CD1	2.76	0.50
1:A:30:TYR:HB3	1:A:148:LEU:O	2.11	0.50
2:B:195:PHE:CE1	2:B:204:ILE:HG21	2.46	0.50
1:A:39:ARG:O	1:A:46:VAL:HA	2.11	0.50
2:B:198:GLU:C	2:B:200:ARG:H	2.15	0.50
2:B:223:ARG:NH1	2:B:223:ARG:HB2	2.27	0.50
2:B:230:VAL:HB	2:B:237:ILE:HG13	1.93	0.50
2:B:270:ASP:C	2:B:270:ASP:OD2	2.50	0.49
2:B:253:PRO:HD3	2:B:343:ASN:HB2	1.92	0.49
1:A:51:ASP:C	1:A:53:SER:N	2.66	0.49
2:B:266:VAL:O	2:B:269:SER:OG	2.31	0.49
2:B:309:LEU:HD22	2:B:310:LYS:HE3	1.95	0.49
2:B:252:ARG:HH11	2:B:252:ARG:CG	2.24	0.49
2:B:186:ILE:HD12	2:B:211:TRP:HA	1.93	0.49
1:A:81:ALA:O	1:A:88:LEU:HA	2.12	0.48
1:A:6:ILE:CG2	1:A:7:THR:H	2.20	0.48
2:B:243:LEU:HD11	2:B:245:VAL:HG23	1.95	0.48
2:B:278:TYR:CD2	2:B:279:SER:N	2.82	0.48
2:B:309:LEU:CD1	2:B:324:LEU:HD11	2.43	0.48
1:A:65:SER:HA	2:B:284:HIS:CE1	2.48	0.48
2:B:340:LEU:HD22	2:B:347:PHE:HD2	1.79	0.48
1:A:33:ASN:ND2	1:A:128:LYS:N	2.60	0.48
2:B:153:TRP:O	2:B:156:PRO:HD3	2.13	0.48
2:B:360:GLU:O	2:B:361:GLU:CB	2.61	0.48
2:B:271:VAL:HG21	2:B:354:LEU:CD1	2.44	0.48
2:B:278:TYR:O	2:B:279:SER:HB2	2.14	0.48
1:A:36:HIS:N	1:A:36:HIS:ND1	2.61	0.48
2:B:337:TYR:N	2:B:337:TYR:HD1	2.11	0.48
1:A:89:TYR:HD1	1:A:90:GLY:N	2.03	0.47
2:B:152:TYR:N	2:B:152:TYR:CD1	2.81	0.47
2:B:176:CYS:SG	2:B:228:CYS:CB	3.01	0.47
1:A:79:TYR:HD1	1:A:94:PRO:CA	2.27	0.47
1:A:81:ALA:HB1	1:A:97:GLU:O	2.15	0.47
2:B:189:LEU:O	2:B:189:LEU:HD12	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASN:HD21	2:B:248:ARG:HH22	1.61	0.47
1:A:39:ARG:HD3	1:A:54:ASP:CG	2.35	0.47
2:B:252:ARG:HD2	2:B:347:PHE:O	2.14	0.47
2:B:349:HIS:C	2:B:350:HIS:HD1	2.17	0.47
2:B:198:GLU:O	2:B:200:ARG:N	2.48	0.47
2:B:171:THR:CG2	2:B:216:GLU:HG2	2.40	0.47
2:B:330:THR:C	2:B:332:GLU:H	2.17	0.47
2:B:336:GLU:HG3	2:B:353:TRP:CE2	2.50	0.47
2:B:310:LYS:HD2	2:B:310:LYS:N	2.30	0.47
1:A:114:SER:O	1:A:115:LYS:C	2.53	0.46
1:A:81:ALA:HB3	1:A:89:TYR:CE1	2.50	0.46
2:B:220:PRO:O	2:B:223:ARG:HG2	2.15	0.46
1:A:18:LEU:CB	2:B:278:TYR:HB2	2.45	0.46
1:A:134:ARG:O	1:A:135:GLY:C	2.54	0.46
2:B:255:LEU:O	2:B:256:GLN:C	2.53	0.46
1:A:113:ILE:O	1:A:115:LYS:N	2.49	0.46
2:B:343:ASN:C	2:B:343:ASN:OD1	2.54	0.46
2:B:338:THR:HG23	2:B:350:HIS:O	2.15	0.46
2:B:285:ILE:HG13	2:B:322:GLU:OE2	2.15	0.46
1:A:124:VAL:HG12	1:A:124:VAL:O	2.16	0.46
1:A:88:LEU:CD1	1:A:124:VAL:HG13	2.45	0.46
1:A:24:LYS:HD2	2:B:319:LYS:O	2.16	0.46
1:A:6:ILE:O	1:A:7:THR:HB	2.16	0.46
2:B:207:ARG:C	2:B:209:GLN:N	2.70	0.46
2:B:174:PHE:O	2:B:213:LEU:N	2.49	0.46
2:B:243:LEU:C	2:B:243:LEU:HD13	2.36	0.46
2:B:274:HIS:O	2:B:275:CYS:SG	2.74	0.46
1:A:15:LYS:O	2:B:256:GLN:HG3	2.16	0.46
1:A:41:LEU:HD11	1:A:47:ASP:OD1	2.16	0.45
2:B:293:VAL:O	2:B:294:ASN:C	2.54	0.45
1:A:83:ASP:HB3	1:A:89:TYR:HE2	1.81	0.45
2:B:219:VAL:HG13	2:B:220:PRO:HD2	1.98	0.45
2:B:153:TRP:CE2	2:B:237:ILE:HD12	2.51	0.45
2:B:277:VAL:O	2:B:277:VAL:HG12	2.15	0.45
1:A:103:ARG:CG	1:A:103:ARG:HH11	2.28	0.45
1:A:79:TYR:O	1:A:80:LEU:C	2.55	0.45
1:A:83:ASP:HB3	1:A:89:TYR:CE2	2.51	0.45
2:B:266:VAL:HB	2:B:269:SER:OG	2.17	0.45
2:B:152:TYR:CE1	2:B:179:ALA:HB3	2.52	0.45
1:A:109:TYR:CD2	1:A:146:LEU:HD13	2.50	0.45
2:B:206:LEU:HD12	2:B:206:LEU:C	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LEU:N	2:B:246:LEU:HD12	2.31	0.45
2:B:259:LEU:HA	2:B:260:PRO:C	2.37	0.45
2:B:266:VAL:HG12	2:B:267:LEU:N	2.31	0.45
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.80	0.45
2:B:253:PRO:CG	2:B:343:ASN:HB2	2.47	0.45
2:B:316:THR:HB	2:B:317:THR:H	1.56	0.44
2:B:230:VAL:HB	2:B:237:ILE:CG1	2.47	0.44
1:A:32:SER:HB2	1:A:146:LEU:HB2	1.99	0.44
2:B:223:ARG:HB2	2:B:223:ARG:CZ	2.47	0.44
2:B:174:PHE:CD1	2:B:241:TYR:CD1	3.06	0.44
2:B:330:THR:C	2:B:332:GLU:N	2.71	0.44
1:A:148:LEU:C	1:A:148:LEU:HD12	2.38	0.44
1:A:39:ARG:O	1:A:46:VAL:HG13	2.17	0.44
2:B:331:PHE:HA	2:B:356:VAL:HG21	1.99	0.44
1:A:6:ILE:CG2	1:A:7:THR:N	2.81	0.44
2:B:189:LEU:HA	2:B:195:PHE:H	1.82	0.44
2:B:196:ARG:CA	2:B:199:HIS:HB2	2.47	0.44
2:B:169:ALA:HA	2:B:217:SER:CA	2.46	0.43
2:B:326:LEU:HD11	2:B:337:TYR:CZ	2.52	0.43
2:B:345:ILE:O	2:B:346:GLY:O	2.35	0.43
1:A:117:HIS:O	1:A:118:ALA:C	2.56	0.43
1:A:80:LEU:HD22	1:A:100:PHE:HE2	1.80	0.43
1:A:95:ASN:H	1:A:98:CYS:HG	1.64	0.43
1:A:41:LEU:O	1:A:44:GLY:N	2.51	0.43
2:B:188:TRP:CD1	2:B:206:LEU:HD22	2.53	0.43
2:B:198:GLU:C	2:B:200:ARG:N	2.71	0.43
1:A:86:GLY:O	1:A:135:GLY:N	2.47	0.43
2:B:176:CYS:HG	2:B:228:CYS:HB2	1.78	0.43
1:A:24:LYS:HB3	2:B:319:LYS:NZ	2.33	0.43
2:B:201:ILE:C	2:B:203:GLY:N	2.71	0.43
1:A:106:GLU:C	1:A:108:HIS:N	2.71	0.43
1:A:29:LEU:O	1:A:30:TYR:O	2.37	0.43
1:A:54:ASP:O	1:A:57:ILE:HG12	2.18	0.43
2:B:289:LYS:HZ3	2:B:291:VAL:N	2.17	0.43
1:A:76:THR:OG1	1:A:77:GLY:N	2.51	0.43
2:B:293:VAL:HB	2:B:305:TYR:CE1	2.54	0.43
2:B:207:ARG:O	2:B:209:GLN:N	2.52	0.42
1:A:61:LEU:N	1:A:61:LEU:HD12	2.34	0.42
1:A:90:GLY:O	1:A:91:SER:O	2.37	0.42
2:B:151:PRO:HB3	2:B:184:PRO:HG3	2.01	0.42
1:A:135:GLY:O	1:A:137:ARG:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:CD	1:A:54:ASP:OD2	2.62	0.42
1:A:17:ASN:C	1:A:18:LEU:HD22	2.40	0.42
1:A:8:THR:O	1:A:12:LEU:HB2	2.19	0.42
1:A:90:GLY:O	1:A:91:SER:C	2.58	0.42
2:B:252:ARG:NH1	2:B:252:ARG:HG2	2.29	0.42
1:A:39:ARG:HG3	1:A:56:HIS:HB2	2.02	0.42
2:B:185:SER:O	2:B:230:VAL:HA	2.20	0.42
2:B:290:HIS:HB3	2:B:297:LYS:HE3	2.01	0.42
2:B:323:VAL:HG23	2:B:324:LEU:N	2.34	0.42
1:A:105:GLU:HG3	1:A:111:THR:HG23	2.01	0.42
1:A:72:LYS:HG2	1:A:73:SER:N	2.35	0.42
1:A:110:ASN:ND2	2:B:248:ARG:HH22	2.18	0.42
1:A:150:LEU:HD11	2:B:165:ALA:HB2	2.01	0.42
2:B:181:ASN:HA	2:B:182:PRO:HA	1.83	0.42
2:B:156:PRO:HG2	2:B:157:GLU:N	2.32	0.41
2:B:276:LYS:CG	2:B:321:LEU:HD21	2.50	0.41
2:B:349:HIS:C	2:B:349:HIS:CD2	2.94	0.41
1:A:95:ASN:C	1:A:97:GLU:N	2.72	0.41
1:A:9:PHE:O	1:A:10:THR:C	2.58	0.41
2:B:169:ALA:CA	2:B:217:SER:HA	2.51	0.41
2:B:252:ARG:NH1	2:B:252:ARG:CG	2.84	0.41
1:A:30:TYR:CE2	2:B:163:LEU:HD12	2.55	0.41
1:A:80:LEU:C	1:A:80:LEU:CD2	2.88	0.41
2:B:274:HIS:CG	2:B:321:LEU:HD13	2.54	0.41
2:B:291:VAL:HG22	2:B:292:GLU:N	2.35	0.41
2:B:270:ASP:N	2:B:327:HIS:O	2.54	0.41
2:B:223:ARG:HA	2:B:243:LEU:CD1	2.51	0.41
1:A:43:ASP:CG	1:A:44:GLY:N	2.74	0.41
1:A:28:LEU:HD13	1:A:37:PHE:CD1	2.56	0.41
1:A:155:ASP:OD1	2:B:223:ARG:CD	2.68	0.41
1:A:79:TYR:HD1	1:A:94:PRO:HA	1.86	0.41
2:B:289:LYS:HE2	2:B:290:HIS:H	1.85	0.41
1:A:54:ASP:C	1:A:56:HIS:H	2.24	0.41
2:B:227:THR:OG1	2:B:240:THR:HG23	2.21	0.41
2:B:301:ASP:C	2:B:303:THR:H	2.24	0.41
2:B:169:ALA:C	2:B:217:SER:HA	2.40	0.41
1:A:31:CYS:SG	1:A:126:LEU:HB2	2.61	0.40
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.80	0.40
2:B:267:LEU:HG	2:B:331:PHE:CZ	2.56	0.40
1:A:127:LYS:O	1:A:130:GLY:N	2.35	0.40
1:A:16:PHE:HB2	2:B:256:GLN:OE1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:MET:HE3	1:A:88:LEU:HD21	2.02	0.40
2:B:223:ARG:HA	2:B:243:LEU:HD12	2.02	0.40
2:B:288:LEU:HB2	2:B:338:THR:HB	2.04	0.40
2:B:175:ARG:HA	2:B:211:TRP:O	2.21	0.40
1:A:139:HIS:O	1:A:142:GLN:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:HIS:CE1	2:B:327:HIS:CE1[2_656]	2.06	0.14

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	149/155 (96%)	105 (70%)	23 (15%)	21 (14%)	0	1
2	B	211/334 (63%)	147 (70%)	44 (21%)	20 (10%)	1	4
All	All	360/489 (74%)	252 (70%)	67 (19%)	41 (11%)	0	3

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	30	TYR
1	A	51	ASP
1	A	52	ARG
1	A	80	LEU
1	A	96	GLU
1	A	114	SER
2	B	169	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	198	GLU
2	B	205	LYS
2	B	311	THR
2	B	317	THR
2	B	358	PRO
2	B	361	GLU
1	A	7	THR
1	A	55	GLN
1	A	91	SER
1	A	108	HIS
2	B	194	GLU
2	B	199	HIS
2	B	279	SER
2	B	294	ASN
2	B	346	GLY
1	A	32	SER
1	A	77	GLY
1	A	84	THR
1	A	128	LYS
2	B	208	HIS
2	B	270	ASP
2	B	310	LYS
1	A	9	PHE
1	A	135	GLY
2	B	168	ALA
2	B	201	ILE
2	B	225	ASN
2	B	300	PRO
1	A	14	GLU
2	B	329	VAL
1	A	49	THR
1	A	136	PRO
1	A	35	GLY

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	128/135 (95%)	118 (92%)	10 (8%)	15	50
2	B	161/278 (58%)	135 (84%)	26 (16%)	3	13
All	All	289/413 (70%)	253 (88%)	36 (12%)	5	24

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	43	ASP
1	A	49	THR
1	A	58	GLN
1	A	64	GLU
1	A	66	VAL
1	A	84	THR
1	A	85	ASP
1	A	104	LEU
1	A	132	CYS
2	B	152	TYR
2	B	157	GLU
2	B	163	LEU
2	B	166	VAL
2	B	189	LEU
2	B	200	ARG
2	B	223	ARG
2	B	232	ASN
2	B	247	GLU
2	B	251	HIS
2	B	255	LEU
2	B	259	LEU
2	B	267	LEU
2	B	289	LYS
2	B	310	LYS
2	B	323	VAL
2	B	324	LEU
2	B	327	HIS
2	B	330	THR
2	B	333	ASP
2	B	337	TYR
2	B	340	LEU
2	B	344	SER
2	B	349	HIS
2	B	350	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	357	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	58	GLN
1	A	95	ASN
1	A	129	ASN
2	B	232	ASN
2	B	286	GLN
2	B	294	ASN
2	B	349	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	151/155 (97%)	-0.42	0 100 100	7, 39, 65, 71	0
2	B	213/334 (63%)	-0.12	3 (1%) 75 63	2, 46, 82, 91	0
All	All	364/489 (74%)	-0.25	3 (0%) 86 77	2, 44, 74, 91	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	197	GLY	3.8
2	B	315	ASN	2.2
2	B	198	GLU	2.2

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 carbohydrates 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.