



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:23 PM UTC

PDB ID : 1SHY / pdb_00001shy
Title : The Crystal Structure of HGF beta-chain in Complex with the Sema Domain of the Met Receptor.
Authors : Stamos, J.; Wiesmann, C.
Deposited on : 2004-02-26
Resolution : 3.22 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

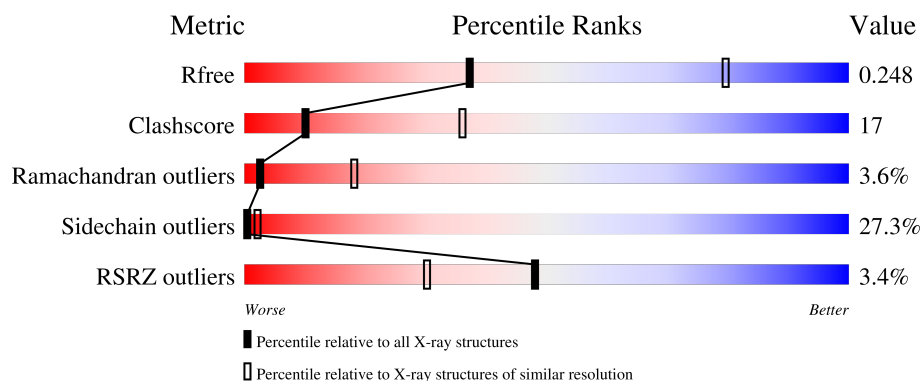
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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 $\leq 5\%$. 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	234	5% 50% 37% 9% ..
2	B	551	2% 44% 34% 11% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5735 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 Hepatocyte growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1773	1127	315	317	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	604	SER	CYS	engineered mutation	UNP P14210

- Molecule 2 is a protein called Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	499	Total	C	N	O	S	0	0	0
			3962	2517	674	742	29			

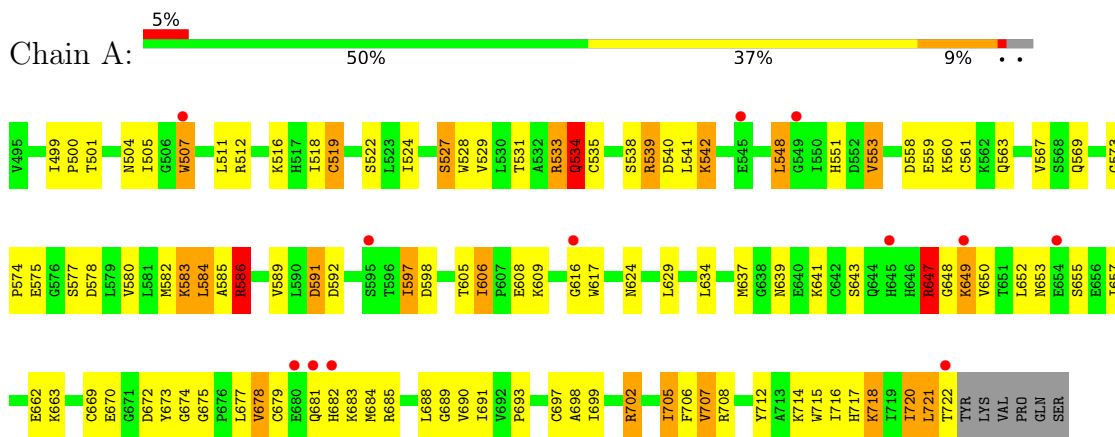
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	303	LEU	LYS	SEE REMARK 999	UNP P08581
B	304	VAL	ARG	SEE REMARK 999	UNP P08581
B	305	PRO	LYS	SEE REMARK 999	UNP P08581
B	306	ARG	LYS	SEE REMARK 999	UNP P08581
B	307	GLY	ARG	SEE REMARK 999	UNP P08581
B	568	HIS	-	expression tag	UNP P08581
B	569	HIS	-	expression tag	UNP P08581
B	570	HIS	-	expression tag	UNP P08581
B	571	HIS	-	expression tag	UNP P08581
B	572	HIS	-	expression tag	UNP P08581
B	573	HIS	-	expression tag	UNP P08581
B	574	HIS	-	expression tag	UNP P08581
B	575	HIS	-	expression tag	UNP P08581

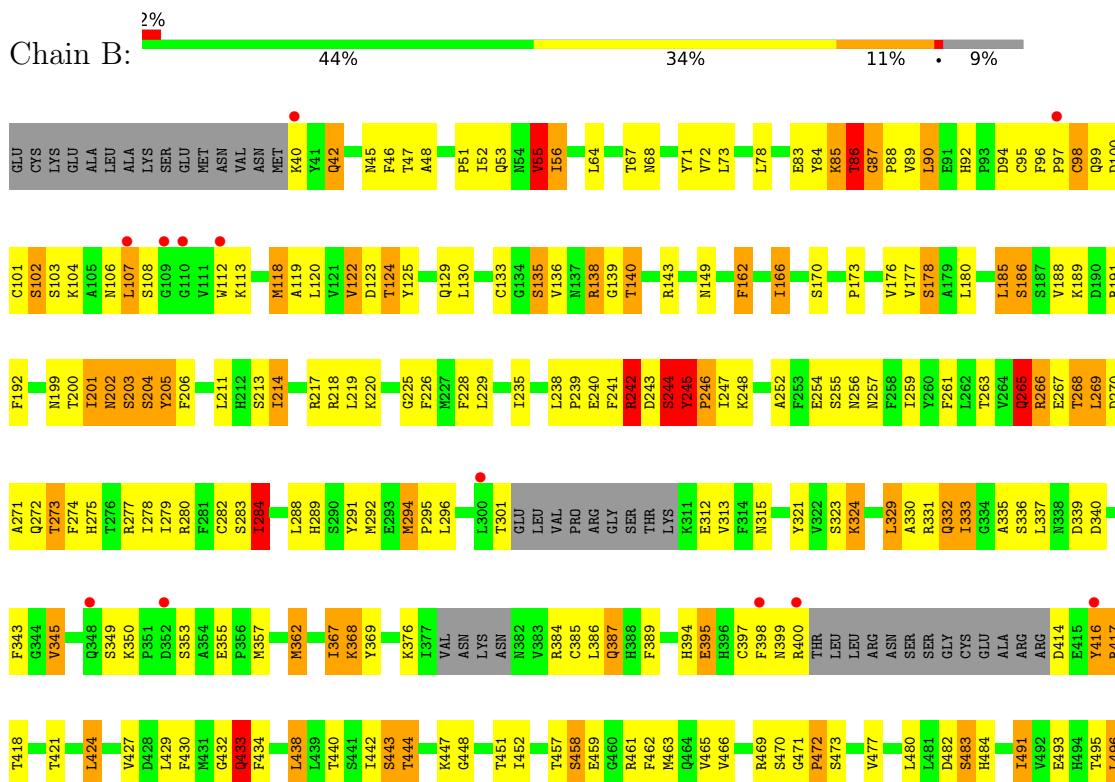
3 Residue-property plots

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: Hepatocyte growth factor



- Molecule 2: Hepatocyte growth factor receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.05Å 186.35Å 66.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.22 30.00 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.22) 99.1 (30.00-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.209 , 0.270 0.197 , 0.248	Depositor DCC
R_{free} test set	1419 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	103.0	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 93.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5735	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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	0.73	1/1815 (0.1%)	1.09	3/2459 (0.1%)
2	B	0.69	2/4062 (0.0%)	1.12	21/5515 (0.4%)
All	All	0.70	3/5877 (0.1%)	1.11	24/7974 (0.3%)

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
2	B	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	560	ILE	CA-CB	5.76	1.61	1.54
1	A	637	MET	SD-CE	5.66	1.93	1.79
2	B	561	CYS	N-CA	5.23	1.52	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	245	TYR	N-CA-C	10.44	117.61	108.22
2	B	516	ASN	N-CA-C	7.03	121.53	112.12
2	B	102	SER	N-CA-C	-6.55	104.87	112.92
1	A	674	GLY	N-CA-C	-6.53	107.31	115.08
2	B	332	GLN	N-CA-C	6.12	118.04	111.36
2	B	452	ILE	N-CA-C	6.09	116.64	107.75
1	A	616	GLY	N-CA-C	6.04	119.31	110.38
2	B	289	HIS	CA-C-N	-5.69	114.14	122.06
2	B	289	HIS	C-N-CA	-5.69	114.14	122.06
2	B	166	ILE	N-CA-C	5.55	116.78	112.12
2	B	86	THR	N-CA-C	-5.52	106.32	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	46	PHE	N-CA-C	5.45	118.50	109.46
2	B	245	TYR	CB-CA-C	5.43	117.39	110.22
2	B	101	CYS	N-CA-C	5.41	117.03	107.61
2	B	90	LEU	N-CA-C	5.37	117.49	108.73
2	B	135	SER	CA-C-N	-5.22	117.81	123.08
2	B	135	SER	C-N-CA	-5.22	117.81	123.08
2	B	125	TYR	N-CA-C	-5.20	105.52	111.14
2	B	553	SER	N-CA-C	5.12	116.54	110.19
2	B	55	VAL	N-CA-C	5.08	115.23	108.27
1	A	531	THR	N-CA-C	5.08	115.74	108.74
2	B	473	SER	N-CA-C	5.07	117.24	110.35
2	B	202	ASN	N-CA-C	5.05	119.16	112.30
2	B	284	ILE	N-CA-C	5.02	115.50	108.17

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	135	SER	Peptide
2	B	244	SER	Peptide
2	B	265	GLN	Peptide
2	B	274	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	1773	0	1771	60	0
2	B	3962	0	3806	136	0
All	All	5735	0	5577	196	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 17.

All (196) 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:245:TYR:HB2	2:B:246:PRO:HD3	1.36	1.06
2:B:85:LYS:H	2:B:85:LYS:HD2	1.35	0.92
2:B:256:ASN:HD22	2:B:367:ILE:HD11	1.38	0.86
2:B:332:GLN:NE2	2:B:469:ARG:H	1.77	0.83
2:B:269:LEU:H	2:B:269:LEU:CD2	1.92	0.83
2:B:162:PHE:HD2	2:B:162:PHE:C	1.89	0.80
2:B:239:PRO:HA	2:B:242:ARG:HD2	1.64	0.80
1:A:702:ARG:HH11	1:A:702:ARG:HG3	1.47	0.79
2:B:245:TYR:HB2	2:B:246:PRO:CD	2.12	0.79
2:B:315:ASN:HD21	2:B:349:SER:HB2	1.49	0.78
1:A:705:ILE:C	1:A:705:ILE:HD13	2.09	0.78
2:B:129:GLN:HE22	2:B:143:ARG:HE	1.31	0.78
1:A:679:CYS:HB2	1:A:688:LEU:HD22	1.66	0.77
1:A:585:ALA:O	1:A:586:ARG:HB3	1.84	0.77
2:B:332:GLN:HE22	2:B:469:ARG:H	1.35	0.74
1:A:690:VAL:HB	1:A:707:VAL:HG13	1.69	0.73
2:B:162:PHE:C	2:B:162:PHE:CD2	2.63	0.73
2:B:505:ILE:HG13	2:B:510:ILE:HD12	1.70	0.72
2:B:97:PRO:HG2	2:B:162:PHE:HE1	1.56	0.70
2:B:546:VAL:HG22	2:B:547:ARG:N	2.05	0.70
1:A:577:SER:HB3	1:A:712:TYR:CZ	2.27	0.69
2:B:52:ILE:HD13	2:B:64:LEU:HD22	1.71	0.69
1:A:702:ARG:HH11	1:A:702:ARG:CG	2.05	0.69
2:B:275:HIS:CE1	2:B:295:PRO:HB3	2.30	0.67
2:B:245:TYR:CB	2:B:246:PRO:HD3	2.18	0.67
1:A:541:LEU:HD13	1:A:567:VAL:HG12	1.79	0.65
1:A:507:TRP:CZ3	1:A:678:VAL:HG11	2.32	0.64
2:B:269:LEU:H	2:B:269:LEU:HD22	1.63	0.64
2:B:138:ARG:HH11	2:B:138:ARG:HA	1.62	0.64
2:B:457:THR:HG22	2:B:459:GLU:H	1.62	0.64
2:B:482:ASP:HB2	2:B:506:THR:HG21	1.82	0.62
1:A:533:ARG:C	1:A:535:CYS:H	2.09	0.61
2:B:191:ARG:HG2	2:B:191:ARG:HH11	1.66	0.61
2:B:256:ASN:O	2:B:257:ASN:HB2	2.00	0.61
1:A:527:SER:HA	1:A:584:LEU:CD1	2.31	0.60
1:A:534:GLN:NE2	1:A:534:GLN:H	2.00	0.60
2:B:118:MET:HE2	2:B:118:MET:HA	1.84	0.60
2:B:546:VAL:HG21	2:B:550:GLU:HB3	1.83	0.60
2:B:68:ASN:HB3	2:B:87:GLY:HA2	1.84	0.59
2:B:324:LYS:HE3	2:B:340:ASP:OD1	2.03	0.59
2:B:269:LEU:H	2:B:269:LEU:HD23	1.66	0.59
2:B:384:ARG:HD3	2:B:387:GLN:HE22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:SER:C	2:B:284:ILE:HG12	2.26	0.58
2:B:546:VAL:CG2	2:B:550:GLU:HB3	2.34	0.58
2:B:214:ILE:HD13	2:B:214:ILE:N	2.18	0.57
2:B:558:GLN:O	2:B:559:GLN:HG3	2.05	0.57
1:A:705:ILE:HD13	1:A:705:ILE:O	2.04	0.57
2:B:416:TYR:CD1	2:B:416:TYR:N	2.71	0.57
2:B:546:VAL:CG2	2:B:547:ARG:N	2.68	0.57
1:A:501:THR:HG21	1:A:629:LEU:HD23	1.86	0.57
2:B:64:LEU:HD11	2:B:73:LEU:HD11	1.86	0.56
2:B:96:PHE:HB3	2:B:97:PRO:HD3	1.87	0.56
2:B:465:VAL:HG12	2:B:466:VAL:N	2.20	0.56
2:B:124:THR:O	2:B:124:THR:HG23	2.04	0.56
1:A:689:GLY:HA2	1:A:707:VAL:O	2.06	0.56
2:B:98:CYS:SG	2:B:162:PHE:HB3	2.45	0.56
1:A:504:ASN:HB3	1:A:551:HIS:HB2	1.87	0.56
2:B:269:LEU:CD2	2:B:269:LEU:N	2.66	0.56
2:B:530:LEU:HD22	2:B:558:GLN:HA	1.88	0.55
2:B:129:GLN:NE2	2:B:143:ARG:HE	2.01	0.55
2:B:220:LYS:HG3	2:B:225:GLY:O	2.05	0.55
2:B:48:ALA:HB1	2:B:71:TYR:CE1	2.43	0.54
2:B:96:PHE:HB3	2:B:97:PRO:CD	2.37	0.54
1:A:690:VAL:HB	1:A:707:VAL:CG1	2.36	0.54
2:B:368:LYS:HD3	2:B:369:TYR:CE2	2.43	0.54
1:A:606:ILE:HD12	1:A:606:ILE:H	1.72	0.54
2:B:482:ASP:HB2	2:B:506:THR:CG2	2.37	0.54
2:B:482:ASP:O	2:B:484:HIS:N	2.41	0.54
1:A:527:SER:HA	1:A:584:LEU:HD11	1.90	0.54
2:B:96:PHE:CB	2:B:97:PRO:HD3	2.39	0.53
2:B:56:ILE:HD11	2:B:120:LEU:O	2.09	0.53
1:A:585:ALA:O	1:A:586:ARG:CB	2.55	0.52
2:B:315:ASN:ND2	2:B:349:SER:HB2	2.22	0.52
2:B:345:VAL:HG22	2:B:362:MET:HB2	1.92	0.52
2:B:55:VAL:CG2	2:B:64:LEU:HD23	2.40	0.52
1:A:553:VAL:HB	1:A:617:TRP:CD1	2.45	0.51
2:B:235:ILE:HG23	2:B:389:PHE:CD1	2.46	0.51
1:A:681:GLN:HG2	1:A:682:HIS:H	1.74	0.51
2:B:266:ARG:O	2:B:267:GLU:C	2.53	0.51
2:B:288:LEU:O	2:B:417:ARG:NH2	2.44	0.51
1:A:529:VAL:HB	1:A:582:MET:HE2	1.91	0.51
2:B:329:LEU:HD12	2:B:451:THR:HG21	1.93	0.50
1:A:507:TRP:CD1	1:A:507:TRP:N	2.78	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:PHE:CE2	2:B:218:ARG:NH1	2.79	0.50
1:A:681:GLN:HG2	1:A:682:HIS:N	2.26	0.50
1:A:533:ARG:C	1:A:535:CYS:N	2.70	0.49
1:A:673:TYR:HA	1:A:691:ILE:HG22	1.94	0.49
2:B:191:ARG:HG2	2:B:191:ARG:NH1	2.27	0.49
2:B:118:MET:HA	2:B:118:MET:CE	2.42	0.49
2:B:350:LYS:HG3	2:B:357:MET:HG3	1.93	0.49
2:B:269:LEU:HD23	2:B:269:LEU:N	2.27	0.49
2:B:518:LEU:C	2:B:520:CYS:H	2.20	0.49
2:B:86:THR:O	2:B:87:GLY:O	2.30	0.48
1:A:597:ILE:HG13	1:A:598:ASP:N	2.28	0.48
2:B:503:LEU:HB3	2:B:510:ILE:HD11	1.96	0.48
1:A:669:CYS:SG	1:A:670:GLU:N	2.87	0.48
2:B:92:HIS:ND1	2:B:94:ASP:HB2	2.28	0.48
2:B:238:LEU:HD12	2:B:241:PHE:HE1	1.78	0.48
2:B:416:TYR:H	2:B:416:TYR:HD1	1.60	0.48
2:B:329:LEU:O	2:B:333:ILE:HG13	2.14	0.48
2:B:275:HIS:CD2	2:B:277:ARG:HE	2.32	0.48
2:B:55:VAL:HG22	2:B:64:LEU:HD23	1.96	0.47
2:B:51:PRO:HA	2:B:508:LYS:HB3	1.95	0.47
2:B:294:MET:HE3	2:B:424:LEU:HB2	1.97	0.47
1:A:507:TRP:CD1	1:A:507:TRP:H	2.31	0.47
1:A:527:SER:HA	1:A:584:LEU:HD12	1.96	0.47
2:B:173:PRO:O	2:B:226:PHE:HB2	2.14	0.47
2:B:268:THR:O	2:B:271:ALA:HB3	2.15	0.47
2:B:438:LEU:HB3	2:B:458:SER:OG	2.13	0.47
1:A:499:ILE:HB	1:A:500:PRO:HD2	1.97	0.47
2:B:271:ALA:O	2:B:273:THR:N	2.48	0.47
2:B:140:THR:O	2:B:140:THR:CG2	2.62	0.46
1:A:539:ARG:HD3	1:A:539:ARG:HA	1.60	0.46
2:B:185:LEU:HD12	2:B:186:SER:N	2.30	0.46
2:B:555:THR:O	2:B:556:TRP:HB2	2.15	0.46
2:B:84:TYR:CD2	2:B:84:TYR:C	2.93	0.46
1:A:540:ASP:OD1	1:A:542:LYS:HB2	2.15	0.46
2:B:291:TYR:C	2:B:292:MET:HG3	2.41	0.46
1:A:669:CYS:H	1:A:672:ASP:HB2	1.80	0.45
2:B:139:GLY:O	2:B:176:VAL:N	2.46	0.45
2:B:243:ASP:O	2:B:244:SER:C	2.59	0.45
1:A:712:TYR:O	1:A:716:ILE:HG13	2.16	0.45
2:B:119:ALA:HB3	2:B:133:CYS:HB2	1.97	0.45
1:A:534:GLN:H	1:A:534:GLN:HE21	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ASP:O	2:B:245:TYR:HA	2.17	0.45
1:A:597:ILE:HG13	1:A:598:ASP:H	1.82	0.45
2:B:526:CYS:HA	2:B:540:TRP:CE3	2.51	0.45
2:B:491:ILE:O	2:B:502:THR:HA	2.17	0.45
2:B:535:PHE:O	2:B:537:GLN:HG3	2.17	0.44
2:B:64:LEU:HD12	2:B:71:TYR:HB2	1.98	0.44
2:B:263:THR:HG21	2:B:265:GLN:HE21	1.82	0.44
2:B:42:GLN:H	2:B:521:ARG:HH22	1.66	0.44
2:B:87:GLY:O	2:B:88:PRO:C	2.61	0.44
2:B:124:THR:O	2:B:124:THR:CG2	2.65	0.44
1:A:653:ASN:C	1:A:655:SER:H	2.25	0.44
2:B:254:GLU:HG3	2:B:259:ILE:HD13	1.99	0.44
1:A:524:ILE:HD11	1:A:720:ILE:HG21	1.99	0.44
1:A:717:HIS:HD2	1:A:721:LEU:HD13	1.81	0.44
2:B:162:PHE:CD2	2:B:162:PHE:O	2.71	0.44
2:B:201:ILE:HD11	2:B:211:LEU:C	2.43	0.44
2:B:343:PHE:HD2	2:B:362:MET:CE	2.31	0.44
2:B:496:LEU:O	2:B:497:ASN:HB2	2.17	0.44
2:B:294:MET:HA	2:B:295:PRO:HD2	1.76	0.44
2:B:335:ALA:O	2:B:336:SER:HB3	2.16	0.43
2:B:463:MET:HB2	2:B:477:VAL:O	2.18	0.43
1:A:533:ARG:O	1:A:535:CYS:N	2.50	0.43
2:B:330:ALA:O	2:B:331:ARG:C	2.60	0.43
2:B:432:GLY:C	2:B:434:PHE:N	2.74	0.43
1:A:639:ASN:HB3	1:A:652:LEU:HD12	2.00	0.43
2:B:217:ARG:HB3	2:B:228:PHE:CD2	2.54	0.43
2:B:247:ILE:HG23	2:B:265:GLN:HG2	2.00	0.43
2:B:343:PHE:CE1	2:B:444:THR:HG21	2.53	0.43
2:B:557:THR:HB	2:B:559:GLN:H	1.84	0.43
1:A:534:GLN:HG2	1:A:693:PRO:HG2	2.01	0.43
1:A:705:ILE:C	1:A:705:ILE:CD1	2.81	0.43
1:A:706:PHE:N	1:A:706:PHE:CD2	2.87	0.43
2:B:47:THR:HG23	2:B:509:LYS:HG2	2.01	0.43
2:B:53:GLN:HE22	2:B:67:THR:N	2.17	0.43
2:B:178:SER:HB3	2:B:199:ASN:OD1	2.19	0.43
2:B:252:ALA:HB2	2:B:261:PHE:CE2	2.54	0.43
2:B:56:ILE:HD13	2:B:120:LEU:HG	2.01	0.42
2:B:321:TYR:CE2	2:B:323:SER:HB3	2.54	0.42
2:B:239:PRO:HG3	2:B:242:ARG:NH1	2.35	0.42
1:A:718:LYS:O	1:A:718:LYS:HG2	2.19	0.42
2:B:546:VAL:CG2	2:B:547:ARG:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:VAL:HG23	2:B:130:LEU:HD13	2.01	0.42
2:B:430:PHE:O	2:B:433:GLN:HB2	2.19	0.42
1:A:673:TYR:CE1	1:A:693:PRO:HA	2.54	0.42
2:B:203:SER:O	2:B:205:TYR:N	2.52	0.42
2:B:432:GLY:C	2:B:434:PHE:H	2.27	0.42
1:A:528:TRP:CG	1:A:720:ILE:HG22	2.55	0.41
1:A:573:GLY:HA2	1:A:715:TRP:CZ2	2.55	0.41
2:B:438:LEU:O	2:B:440:THR:HG23	2.20	0.41
2:B:92:HIS:HB3	2:B:95:CYS:H	1.85	0.41
2:B:238:LEU:HB2	2:B:241:PHE:CD1	2.55	0.41
2:B:245:TYR:O	2:B:266:ARG:NH1	2.53	0.41
1:A:569:GLN:HB2	1:A:583:LYS:HB2	2.01	0.41
1:A:591:ASP:HB2	1:A:592:ASP:H	1.66	0.41
1:A:697:CYS:O	1:A:698:ALA:C	2.63	0.41
2:B:252:ALA:HB2	2:B:261:PHE:CD2	2.55	0.41
2:B:462:PHE:CE2	2:B:513:ILE:HG21	2.56	0.41
1:A:518:ILE:HG23	1:A:519:CYS:HB2	2.02	0.41
1:A:669:CYS:O	1:A:672:ASP:HB2	2.21	0.41
2:B:513:ILE:HA	2:B:514:PRO:HD2	1.80	0.40
1:A:534:GLN:HE22	1:A:578:ASP:HB3	1.86	0.40
1:A:606:ILE:HD12	1:A:606:ILE:N	2.34	0.40
2:B:92:HIS:CE1	2:B:94:ASP:HB2	2.56	0.40
2:B:442:ILE:CG1	2:B:443:SER:N	2.85	0.40
2:B:506:THR:O	2:B:506:THR:HG22	2.20	0.40
1:A:675:GLY:HA3	1:A:691:ILE:HD12	2.02	0.40
2:B:98:CYS:SG	2:B:162:PHE:CB	3.09	0.40
2:B:106:ASN:C	2:B:107:LEU:HG	2.47	0.40
2:B:471:GLY:HA2	2:B:472:PRO:HD3	1.89	0.40
1:A:548:LEU:HB2	1:A:563:GLN:HB2	2.03	0.40
1:A:647:ARG:C	1:A:649:LYS:H	2.29	0.40
2:B:399:ASN:HB3	2:B:400:ARG:H	1.73	0.40

There are no symmetry-related clashes.

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	226/234 (97%)	203 (90%)	16 (7%)	7 (3%)	3	21
2	B	491/551 (89%)	415 (84%)	57 (12%)	19 (4%)	2	17
All	All	717/785 (91%)	618 (86%)	73 (10%)	26 (4%)	2	18

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	586	ARG
2	B	87	GLY
2	B	270	ASP
2	B	272	GLN
2	B	483	SER
1	A	534	GLN
2	B	107	LEU
2	B	204	SER
2	B	205	TYR
2	B	266	ARG
2	B	556	TRP
1	A	574	PRO
2	B	244	SER
2	B	395	GLU
2	B	433	GLN
2	B	552	LEU
1	A	683	LYS
2	B	448	GLY
2	B	507	GLY
1	A	647	ARG
1	A	648	GLY
2	B	242	ARG
2	B	563	PRO
2	B	246	PRO
1	A	553	VAL
2	B	472	PRO

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	192/198 (97%)	138 (72%)	54 (28%)	0	2
2	B	450/498 (90%)	329 (73%)	121 (27%)	0	2
All	All	642/696 (92%)	467 (73%)	175 (27%)	0	2

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	505	ILE
1	A	507	TRP
1	A	511	LEU
1	A	512	ARG
1	A	516	LYS
1	A	519	CYS
1	A	522	SER
1	A	527	SER
1	A	533	ARG
1	A	534	GLN
1	A	538	SER
1	A	539	ARG
1	A	542	LYS
1	A	548	LEU
1	A	558	ASP
1	A	559	GLU
1	A	560	LYS
1	A	561	CYS
1	A	575	GLU
1	A	580	VAL
1	A	583	LYS
1	A	584	LEU
1	A	586	ARG
1	A	589	VAL
1	A	591	ASP
1	A	597	ILE
1	A	605	THR
1	A	606	ILE
1	A	608	GLU
1	A	609	LYS
1	A	624	ASN
1	A	634	LEU
1	A	641	LYS

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Mol	Chain	Res	Type
1	A	643	SER
1	A	647	ARG
1	A	649	LYS
1	A	650	VAL
1	A	657	ILE
1	A	662	GLU
1	A	663	LYS
1	A	677	LEU
1	A	678	VAL
1	A	684	MET
1	A	685	ARG
1	A	699	ILE
1	A	702	ARG
1	A	705	ILE
1	A	707	VAL
1	A	708	ARG
1	A	714	LYS
1	A	718	LYS
1	A	720	ILE
1	A	721	LEU
1	A	722	THR
2	B	40	LYS
2	B	42	GLN
2	B	45	ASN
2	B	55	VAL
2	B	56	ILE
2	B	72	VAL
2	B	78	LEU
2	B	83	GLU
2	B	85	LYS
2	B	86	THR
2	B	89	VAL
2	B	90	LEU
2	B	98	CYS
2	B	99	GLN
2	B	100	ASP
2	B	102	SER
2	B	103	SER
2	B	104	LYS
2	B	108	SER
2	B	112	TRP
2	B	113	LYS

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Mol	Chain	Res	Type
2	B	118	MET
2	B	122	VAL
2	B	123	ASP
2	B	124	THR
2	B	136	VAL
2	B	138	ARG
2	B	140	THR
2	B	149	ASN
2	B	162	PHE
2	B	166	ILE
2	B	170	SER
2	B	177	VAL
2	B	178	SER
2	B	180	LEU
2	B	185	LEU
2	B	186	SER
2	B	188	VAL
2	B	189	LYS
2	B	200	THR
2	B	201	ILE
2	B	202	ASN
2	B	203	SER
2	B	204	SER
2	B	206	PHE
2	B	213	SER
2	B	214	ILE
2	B	219	LEU
2	B	229	LEU
2	B	240	GLU
2	B	242	ARG
2	B	245	TYR
2	B	248	LYS
2	B	255	SER
2	B	265	GLN
2	B	268	THR
2	B	269	LEU
2	B	273	THR
2	B	278	ILE
2	B	279	ILE
2	B	280	ARG
2	B	282	CYS
2	B	284	ILE

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Mol	Chain	Res	Type
2	B	294	MET
2	B	296	LEU
2	B	301	THR
2	B	312	GLU
2	B	313	VAL
2	B	324	LYS
2	B	329	LEU
2	B	333	ILE
2	B	337	LEU
2	B	339	ASP
2	B	345	VAL
2	B	353	SER
2	B	355	GLU
2	B	362	MET
2	B	367	ILE
2	B	368	LYS
2	B	376	LYS
2	B	385	CYS
2	B	386	LEU
2	B	387	GLN
2	B	394	HIS
2	B	395	GLU
2	B	397	CYS
2	B	398	PHE
2	B	414	ASP
2	B	416	TYR
2	B	417	ARG
2	B	418	THR
2	B	421	THR
2	B	424	LEU
2	B	427	VAL
2	B	429	LEU
2	B	433	GLN
2	B	438	LEU
2	B	443	SER
2	B	444	THR
2	B	447	LYS
2	B	458	SER
2	B	461	ARG
2	B	470	SER
2	B	480	LEU
2	B	483	SER

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Mol	Chain	Res	Type
2	B	491	ILE
2	B	493	GLU
2	B	495	THR
2	B	496	LEU
2	B	506	THR
2	B	508	LYS
2	B	510	ILE
2	B	511	THR
2	B	518	LEU
2	B	524	GLN
2	B	528	GLN
2	B	531	SER
2	B	547	ARG
2	B	557	THR
2	B	558	GLN
2	B	560	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	504	ASN
1	A	534	GLN
1	A	624	ASN
1	A	717	HIS
2	B	53	GLN
2	B	61	HIS
2	B	129	GLN
2	B	142	GLN
2	B	148	HIS
2	B	256	ASN
2	B	275	HIS
2	B	332	GLN
2	B	387	GLN
2	B	425	GLN
2	B	476	HIS
2	B	497	ASN

5.3.3 RNA ⓘ

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, 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	228/234 (97%)	0.50	12 (5%) 32 20	23, 44, 92, 126	0
2	B	499/551 (90%)	0.14	13 (2%) 57 38	6, 52, 111, 135	0
All	All	727/785 (92%)	0.25	25 (3%) 48 30	6, 49, 105, 135	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	680	GLU	4.7
2	B	110	GLY	4.4
2	B	348	GLN	3.9
1	A	545	GLU	3.8
2	B	109	GLY	3.4
1	A	616	GLY	3.2
2	B	400	ARG	3.0
1	A	722	THR	3.0
2	B	97	PRO	2.8
2	B	416	TYR	2.7
1	A	645	HIS	2.7
2	B	398	PHE	2.7
1	A	682	HIS	2.7
1	A	595	SER	2.6
2	B	112	TRP	2.5
1	A	681	GLN	2.5
2	B	40	LYS	2.4
2	B	107	LEU	2.3
2	B	352	ASP	2.3
1	A	507	TRP	2.3
1	A	549	GLY	2.1
2	B	562	LEU	2.1
2	B	300	LEU	2.1
1	A	654	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	649	LYS	2.1

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 oligosaccharides 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.