



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:01 am GMT

PDB ID : 1SHY  
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](mailto: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.

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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

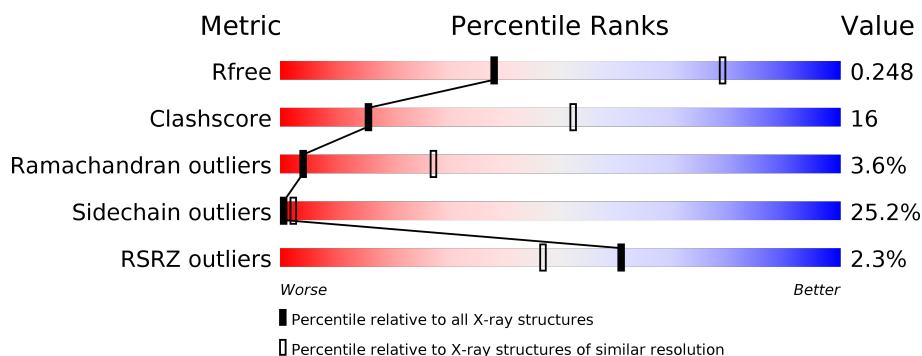
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.22 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))
$R_{free}$	100719	1036 (3.24-3.20)
Clashscore	112137	1161 (3.24-3.20)
Ramachandran outliers	110173	1140 (3.24-3.20)
Sidechain outliers	110143	1139 (3.24-3.20)
RSRZ outliers	101464	1040 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	234	
2	B	551	

## 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	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			

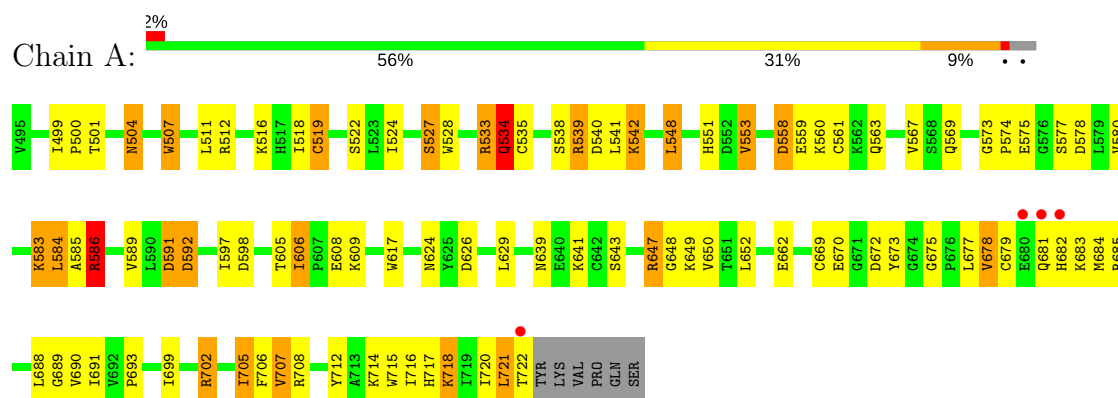
There are 13 discrepancies between the modelled and reference sequences:

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

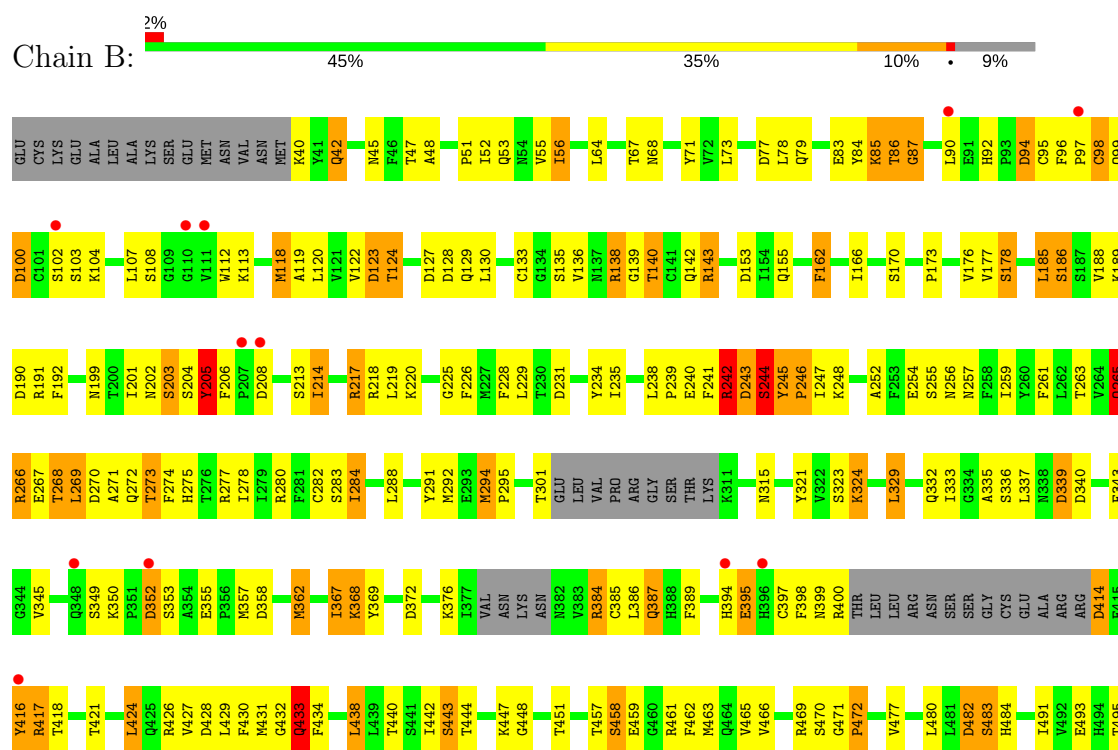
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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, $\alpha$ , $\beta$ , $\gamma$	137.05Å 186.35Å 66.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.22 47.78 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.22) 99.0 (47.78-3.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.209 , 0.270 0.196 , 0.248	Depositor DCC
$R_{free}$ test set	1416 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	103.0	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 86.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.62	0/1815	0.86	3/2459 (0.1%)
2	B	0.56	1/4062 (0.0%)	0.86	18/5515 (0.3%)
All	All	0.58	1/5877 (0.0%)	0.86	21/7974 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	561	CYS	CB-SG	5.54	1.91	1.82

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	543	ASP	CB-CG-OD2	6.80	124.42	118.30
2	B	128	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	558	ASP	CB-CG-OD2	6.34	124.01	118.30
2	B	100	ASP	CB-CG-OD2	6.28	123.95	118.30
2	B	358	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	626	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	592	ASP	CB-CG-OD2	5.87	123.58	118.30
2	B	231	ASP	CB-CG-OD2	5.75	123.48	118.30
2	B	428	ASP	CB-CG-OD2	5.53	123.27	118.30
2	B	190	ASP	CB-CG-OD2	5.50	123.25	118.30
2	B	414	ASP	CB-CG-OD2	5.49	123.24	118.30
2	B	123	ASP	CB-CG-OD2	5.46	123.22	118.30
2	B	77	ASP	CB-CG-OD2	5.46	123.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	352	ASP	CB-CG-OD2	5.44	123.19	118.30
2	B	208	ASP	CB-CG-OD2	5.33	123.10	118.30
2	B	339	ASP	CB-CG-OD2	5.28	123.05	118.30
2	B	243	ASP	CB-CG-OD2	5.17	122.95	118.30
2	B	482	ASP	CB-CG-OD2	5.16	122.94	118.30
2	B	372	ASP	CB-CG-OD2	5.13	122.91	118.30
2	B	127	ASP	CB-CG-OD2	5.11	122.90	118.30
2	B	153	ASP	CB-CG-OD2	5.07	122.86	118.30

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 ⓘ

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	54	0
2	B	3962	0	3806	132	0
All	All	5735	0	5577	186	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 16.

All (186) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:239:PRO:HA	2:B:242:ARG:HD2	1.64	0.80
1:A:702:ARG:HG3	1:A:702:ARG:HH11	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
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:162:PHE:HD2	2:B:162:PHE:C	1.89	0.76
2:B:332:GLN:HE22	2:B:469:ARG:H	1.35	0.74
1:A:705:ILE:C	1:A:705:ILE:HD13	2.09	0.73
1:A:690:VAL:HB	1:A:707:VAL:HG13	1.69	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:CG	1:A:702:ARG:HH11	2.05	0.69
2:B:162:PHE:C	2:B:162:PHE:CD2	2.63	0.68
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:HA	2:B:138:ARG:HH11	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
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:H	1:A:534:GLN:NE2	2.00	0.60
2:B:546:VAL:HG21	2:B:550:GLU:HB3	1.83	0.60
2:B:324:LYS:HE3	2:B:340:ASP:OD1	2.03	0.59
2:B:68:ASN:HB3	2:B:87:GLY:HA2	1.84	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
1:A:705:ILE:O	1:A:705:ILE:HD13	2.04	0.58
2:B:546:VAL:CG2	2:B:550:GLU:HB3	2.34	0.58
2:B:214:ILE:N	2:B:214:ILE:HD13	2.18	0.57
2:B:558:GLN:O	2:B:559:GLN:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:TYR:N	2:B:416:TYR:CD1	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
1:A:533:ARG:C	1:A:535:CYS:H	2.09	0.56
2:B:124:THR:HG23	2:B:124:THR:O	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:H	1:A:606:ILE:HD12	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
2:B:283:SER:C	2:B:284:ILE:HG12	2.26	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:288:LEU:O	2:B:417:ARG:NH2	2.44	0.51
2:B:329:LEU:HD12	2:B:451:THR:HG21	1.93	0.50
1:A:507:TRP:N	1:A:507:TRP:CD1	2.78	0.50
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:238:LEU:HD12	2:B:241:PHE:HE1	1.78	0.48
2:B:92:HIS:ND1	2:B:94:ASP:HB2	2.28	0.48
2:B:416:TYR:HD1	2:B:416:TYR:H	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: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:HA	1:A:539:ARG:HD3	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:266:ARG:O	2:B:267:GLU:C	2.53	0.46
1:A:540:ASP:OD1	1:A:542:LYS:HB2	2.15	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:335:ALA:O	2:B:336:SER:HB3	2.16	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:HE21	1:A:534:GLN:H	1.64	0.45
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
1:A:533:ARG:C	1:A:535:CYS:N	2.70	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:263:THR:HG21	2:B:265:GLN:HE21	1.82	0.44
2:B:64:LEU:HD12	2:B:71:TYR:HB2	1.98	0.44
2:B:124:THR:CG2	2:B:124:THR:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:GLN:H	2:B:521:ARG:HH22	1.66	0.44
2:B:254:GLU:HG3	2:B:259:ILE:HD13	1.99	0.44
1:A:717:HIS:HD2	1:A:721:LEU:HD13	1.81	0.44
1:A:524:ILE:HD11	1:A:720:ILE:HG21	1.99	0.44
2:B:518:LEU:C	2:B:520:CYS:H	2.20	0.44
2:B:162:PHE:O	2:B:162:PHE:CD2	2.71	0.44
2:B:343:PHE:HD2	2:B:362:MET:HE1	1.82	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: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
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:706:PHE:CD2	1:A:706:PHE:N	2.87	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: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: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:HG2	1:A:718:LYS:O	2.19	0.42
2:B:546:VAL:CG2	2:B:547:ARG:H	2.32	0.42
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
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
2:B:84:TYR:CD2	2:B:84:TYR:C	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:ALA:HB2	2:B:261:PHE:CD2	2.55	0.41
2:B:291:TYR:C	2:B:292:MET:HG3	2.41	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:243:ASP:O	2:B:244:SER:C	2.59	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:N	1:A:606:ILE:HD12	2.34	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
2:B:92:HIS:CE1	2:B:94:ASP:HB2	2.56	0.40
1:A:675:GLY:HA3	1:A:691:ILE:HD12	2.02	0.40
2:B:432:GLY:C	2:B:434:PHE:N	2.74	0.40
2:B:471:GLY:HA2	2:B:472:PRO:HD3	1.89	0.40
2:B:98:CYS:SG	2:B:162:PHE:CB	3.09	0.40
1:A:548:LEU:HB2	1:A:563:GLN:HB2	2.03	0.40
2:B:118:MET:HE3	2:B:118:MET:HA	2.04	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%)	5	31
2	B	491/551 (89%)	415 (84%)	57 (12%)	19 (4%)	3	25
All	All	717/785 (91%)	618 (86%)	73 (10%)	26 (4%)	4	27

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%)	143 (74%)	49 (26%)	0	2
2	B	450/498 (90%)	337 (75%)	113 (25%)	0	2
All	All	642/696 (92%)	480 (75%)	162 (25%)	0	2

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	504	ASN
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	605	THR
1	A	606	ILE
1	A	608	GLU
1	A	609	LYS
1	A	624	ASN
1	A	641	LYS
1	A	643	SER
1	A	647	ARG
1	A	649	LYS
1	A	650	VAL
1	A	662	GLU
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

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Mol	Chain	Res	Type
1	A	707	VAL
1	A	708	ARG
1	A	714	LYS
1	A	718	LYS
1	A	721	LEU
1	A	722	THR
2	B	40	LYS
2	B	42	GLN
2	B	45	ASN
2	B	56	ILE
2	B	78	LEU
2	B	79	GLN
2	B	83	GLU
2	B	85	LYS
2	B	86	THR
2	B	90	LEU
2	B	94	ASP
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
2	B	118	MET
2	B	123	ASP
2	B	124	THR
2	B	136	VAL
2	B	138	ARG
2	B	140	THR
2	B	142	GLN
2	B	143	ARG
2	B	155	GLN
2	B	162	PHE
2	B	166	ILE
2	B	170	SER
2	B	177	VAL
2	B	178	SER
2	B	185	LEU
2	B	186	SER

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Mol	Chain	Res	Type
2	B	188	VAL
2	B	189	LYS
2	B	201	ILE
2	B	202	ASN
2	B	203	SER
2	B	205	TYR
2	B	206	PHE
2	B	213	SER
2	B	214	ILE
2	B	217	ARG
2	B	219	LEU
2	B	229	LEU
2	B	234	TYR
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	280	ARG
2	B	282	CYS
2	B	284	ILE
2	B	294	MET
2	B	301	THR
2	B	324	LYS
2	B	329	LEU
2	B	337	LEU
2	B	339	ASP
2	B	352	ASP
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	384	ARG
2	B	385	CYS
2	B	386	LEU

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Mol	Chain	Res	Type
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	426	ARG
2	B	427	VAL
2	B	429	LEU
2	B	431	MET
2	B	433	GLN
2	B	438	LEU
2	B	443	SER
2	B	447	LYS
2	B	458	SER
2	B	461	ARG
2	B	470	SER
2	B	480	LEU
2	B	483	SER
2	B	493	GLU
2	B	495	THR
2	B	496	LEU
2	B	506	THR
2	B	508	LYS
2	B	511	THR
2	B	524	GLN
2	B	528	GLN
2	B	531	SER
2	B	547	ARG
2	B	557	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	534	GLN
1	A	624	ASN
1	A	717	HIS

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Mol	Chain	Res	Type
2	B	53	GLN
2	B	61	HIS
2	B	129	GLN
2	B	256	ASN
2	B	275	HIS
2	B	318	GLN
2	B	332	GLN
2	B	387	GLN
2	B	476	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	228/234 (97%)	-0.20	4 (1%) 69 55	23, 44, 92, 126	0
2	B	499/551 (90%)	0.04	13 (2%) 56 42	6, 52, 111, 135	0
All	All	727/785 (92%)	-0.04	17 (2%) 61 47	6, 49, 105, 135	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	680	GLU	3.6
2	B	207	PRO	3.3
2	B	416	TYR	2.8
1	A	722	THR	2.8
2	B	111	VAL	2.6
1	A	682	HIS	2.5
2	B	110	GLY	2.5
2	B	348	GLN	2.5
2	B	394	HIS	2.4
2	B	90	LEU	2.4
2	B	524	GLN	2.4
1	A	681	GLN	2.3
2	B	102	SER	2.3
2	B	208	ASP	2.3
2	B	396	HIS	2.1
2	B	352	ASP	2.1
2	B	97	PRO	2.0

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

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

### 6.3 Carbohydrates [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.