Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 04:46 AM EDT

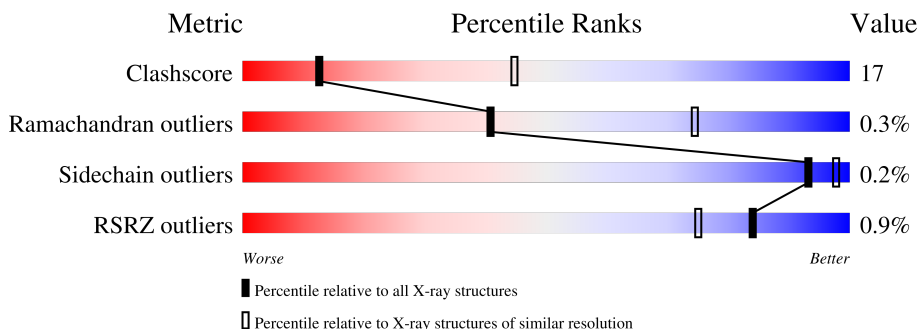|		
PDB ID	:	3KXX
Title	:	Structure of the mutant Fibroblast Growth Factor receptor 1
Authors	:	Bae, J.H.; Boggon, T.J.; Tome, F.; Mandiyan, V.; Lax, I.; Schlessinger, J.
Deposited on	:	2009-12-04
Resolution	:	3.20 Å(reported)

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	Percentile Ranks	Value
Clashscore		17
Ramachandran outliers		0.3%
Sidechain outliers		0.2%
RSRZ outliers		0.9%

Worse　　　　　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	317	68% ... 28% ... •
1	B	317	64% ... 32% ... •
1	C	317	2% / 57% ... 33% ... 10%
1	D	317	.% / 54% ... 37% ... 9%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 9441 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 Basic fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total 2441	C 1549	N 417	O 458	S 17	0	0	0
1	B	305	Total 2438	C 1549	N 417	O 455	S 17	0	0	0
1	C	286	Total 2272	C 1448	N 388	O 419	S 17	0	0	0
1	D	288	Total 2290	C 1459	N 392	O 421	S 18	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	MET	-	expression tag	UNP P11362
A	450	GLY	-	expression tag	UNP P11362
A	451	HIS	-	expression tag	UNP P11362
A	452	HIS	-	expression tag	UNP P11362
A	453	HIS	-	expression tag	UNP P11362
A	454	HIS	-	expression tag	UNP P11362
A	455	HIS	-	expression tag	UNP P11362
A	456	HIS	-	expression tag	UNP P11362
A	457	MET	-	expression tag	UNP P11362
A	488	ALA	CYS	engineered mutation	UNP P11362
A	577	GLU	ARG	engineered mutation	UNP P11362
A	584	SER	CYS	engineered mutation	UNP P11362
B	449	MET	-	expression tag	UNP P11362
B	450	GLY	-	expression tag	UNP P11362
B	451	HIS	-	expression tag	UNP P11362
B	452	HIS	-	expression tag	UNP P11362
B	453	HIS	-	expression tag	UNP P11362
B	454	HIS	-	expression tag	UNP P11362
B	455	HIS	-	expression tag	UNP P11362
B	456	HIS	-	expression tag	UNP P11362
B	457	MET	-	expression tag	UNP P11362

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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| Chain	Residue	Modelled	Actual	Comment	Reference
B	488	ALA	CYS	engineered mutation	UNP P11362
B	577	GLU	ARG	engineered mutation	UNP P11362
B	584	SER	CYS	engineered mutation	UNP P11362
C	449	MET	-	expression tag	UNP P11362
C	450	GLY	-	expression tag	UNP P11362
C	451	HIS	-	expression tag	UNP P11362
C	452	HIS	-	expression tag	UNP P11362
C	453	HIS	-	expression tag	UNP P11362
C	454	HIS	-	expression tag	UNP P11362
C	455	HIS	-	expression tag	UNP P11362
C	456	HIS	-	expression tag	UNP P11362
C	457	MET	-	expression tag	UNP P11362
C	488	ALA	CYS	engineered mutation	UNP P11362
C	577	GLU	ARG	engineered mutation	UNP P11362
C	584	SER	CYS	engineered mutation	UNP P11362
D	449	MET	-	expression tag	UNP P11362
D	450	GLY	-	expression tag	UNP P11362
D	451	HIS	-	expression tag	UNP P11362
D	452	HIS	-	expression tag	UNP P11362
D	453	HIS	-	expression tag	UNP P11362
D	454	HIS	-	expression tag	UNP P11362
D	455	HIS	-	expression tag	UNP P11362
D	456	HIS	-	expression tag	UNP P11362
D	457	MET	-	expression tag	UNP P11362
D	488	ALA	CYS	engineered mutation	UNP P11362
D	577	GLU	ARG	engineered mutation	UNP P11362
D	584	SER	CYS	engineered mutation	UNP P11362

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.

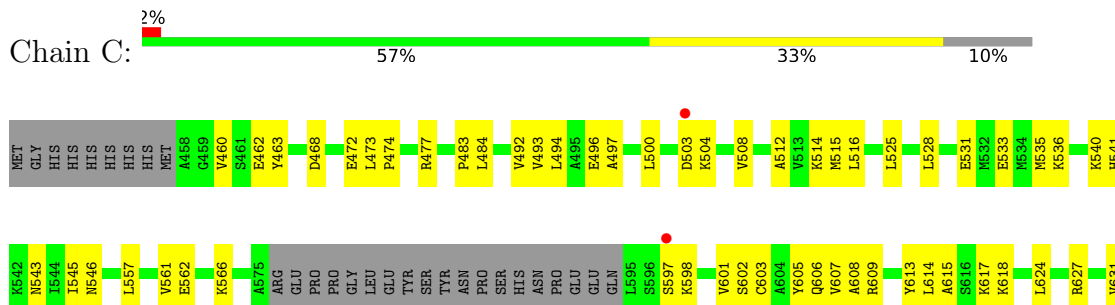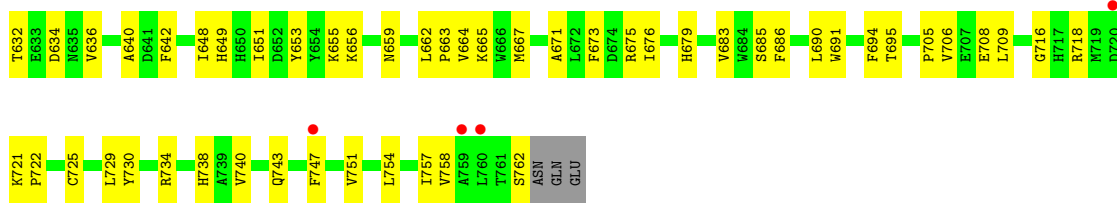- Molecule 1: Basic fibroblast growth factor receptor 1

Chain A:

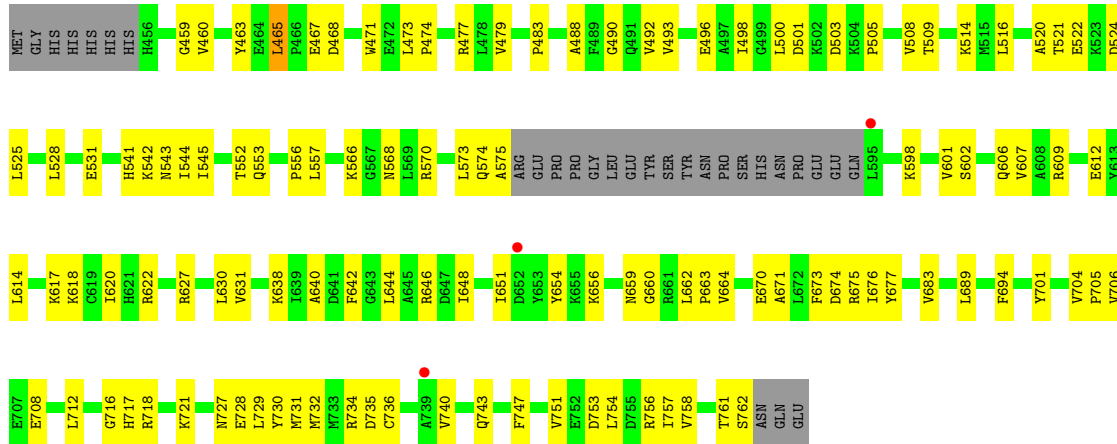- Molecule 1: Basic fibroblast growth factor receptor 1

Chain B:

- Molecule 1: Basic fibroblast growth factor receptor 1

Chain C:

• Molecule 1: Basic fibroblast growth factor receptor 1

Chain D:
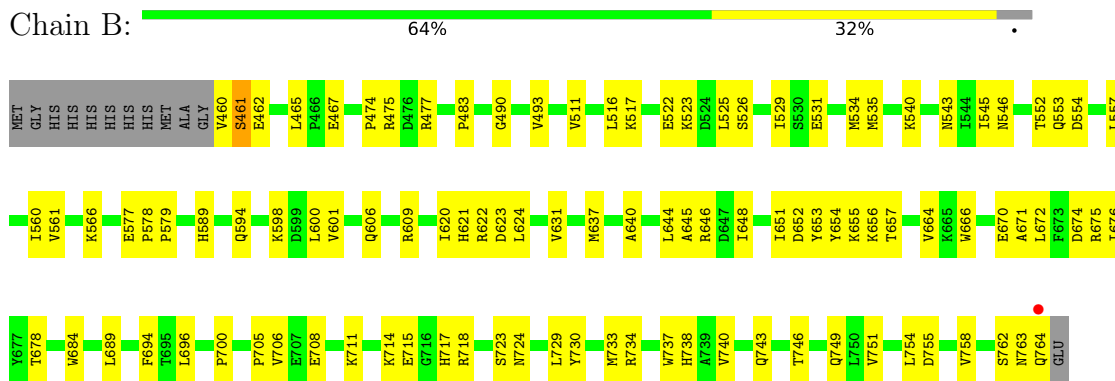
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	186.80Å 74.29Å 135.78Å 90.00° 97.41° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 49.37 – 3.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.20) 95.9 (49.37-3.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.69 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.263 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9441	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.58	0/2496	0.59	0/3376
1	B	0.57	0/2493	0.59	0/3374
1	C	0.39	0/2319	0.51	0/3133
1	D	0.40	0/2338	0.50	0/3158
All	All	0.50	0/9646	0.55	0/13041

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	2441	0	2429	83	0
1	B	2438	0	2432	75	0
1	C	2272	0	2291	82	0
1	D	2290	0	2307	97	0
All	All	9441	0	9459	316	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 (316) 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)
1:D:474:PRO:HB2	1:D:477:ARG:HG2	1.39	0.99
1:D:664:VAL:HG21	1:D:706:VAL:HG13	1.45	0.98
1:B:664:VAL:HG21	1:B:706:VAL:HG13	1.44	0.98
1:A:664:VAL:HG21	1:A:706:VAL:HG13	1.48	0.95
1:C:627:ARG:HH22	1:C:663:PRO:HG3	1.38	0.88
1:D:473:LEU:HD12	1:D:474:PRO:HD2	1.56	0.86
1:D:545:ILE:HD12	1:D:640:ALA:HB2	1.59	0.84
1:C:473:LEU:HD12	1:C:474:PRO:HD2	1.61	0.81
1:C:598:LYS:HB2	1:C:762:SER:HA	1.63	0.79
1:D:545:ILE:HD11	1:D:630:LEU:HD12	1.65	0.77
1:D:627:ARG:NH2	1:D:663:PRO:HG2	1.99	0.77
1:A:474:PRO:HB2	1:A:477:ARG:HG2	1.66	0.77
1:B:648:ILE:O	1:B:648:ILE:HG22	1.85	0.76
1:C:503:ASP:OD1	1:C:504:LYS:HG2	1.87	0.74
1:A:738:HIS:HD2	1:A:740:VAL:H	1.36	0.73
1:C:627:ARG:NH2	1:C:663:PRO:HG3	2.03	0.73
1:C:655:LYS:HG2	1:C:656:LYS:H	1.54	0.72
1:C:545:ILE:HG13	1:C:640:ALA:HB2	1.71	0.71
1:B:738:HIS:HD2	1:B:740:VAL:H	1.38	0.70
1:B:601:VAL:HG12	1:B:758:VAL:HG22	1.73	0.69
1:D:521:THR:HG22	1:D:524:ASP:CG	2.13	0.68
1:C:754:LEU:O	1:C:758:VAL:HG23	1.93	0.68
1:C:460:VAL:HG12	1:C:462:GLU:HG3	1.75	0.68
1:D:528:LEU:HD23	1:D:557:LEU:HD23	1.76	0.67
1:D:656:LYS:HD2	1:D:677:TYR:HE1	1.58	0.67
1:B:474:PRO:HB2	1:B:477:ARG:HG2	1.78	0.64
1:A:678:THR:HG22	1:A:679:HIS:N	2.13	0.64
1:A:618:LYS:HD2	1:A:649:HIS:ND1	2.14	0.63
1:D:566:LYS:HB2	1:D:631:VAL:HB	1.80	0.63
1:C:664:VAL:HG21	1:C:706:VAL:HG13	1.81	0.62
1:A:486:GLU:HB3	1:A:517:LYS:NZ	2.15	0.62
1:C:516:LEU:HD11	1:C:525:LEU:HD13	1.81	0.62
1:D:754:LEU:O	1:D:758:VAL:HG23	1.99	0.61
1:B:705:PRO:HG2	1:B:708:GLU:HB2	1.81	0.61
1:C:730:TYR:O	1:C:734:ARG:HG2	2.01	0.61
1:A:494:LEU:HD12	1:A:495:ALA:H	1.65	0.59
1:A:579:PRO:HG2	1:A:600:LEU:HD11	1.84	0.59
1:A:627:ARG:NH2	1:A:663:PRO:HG2	2.17	0.59
1:B:578:PRO:HG3	1:B:696:LEU:HD13	1.85	0.59
1:C:492:VAL:HG22	1:C:514:LYS:HG2	1.85	0.59
1:B:516:LEU:HD11	1:B:525:LEU:HD13	1.84	0.59
1:A:664:VAL:HG21	1:A:706:VAL:CG1	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:PHE:CZ	1:B:729:LEU:HD13	2.38	0.58
1:D:492:VAL:HG22	1:D:514:LYS:HG3	1.84	0.58
1:B:579:PRO:HG2	1:B:600:LEU:HD11	1.86	0.58
1:D:753:ASP:HA	1:D:756:ARG:HH22	1.68	0.58
1:A:601:VAL:HG12	1:A:758:VAL:HG22	1.86	0.58
1:B:467:GLU:OE1	1:B:553:GLN:HG3	2.04	0.58
1:D:753:ASP:O	1:D:757:ILE:HG13	2.04	0.58
1:B:738:HIS:HD2	1:B:740:VAL:N	2.02	0.57
1:D:473:LEU:HD12	1:D:474:PRO:CD	2.31	0.57
1:A:701:TYR:HB3	1:A:704:VAL:CG2	2.35	0.57
1:A:477:ARG:HA	1:A:477:ARG:NE	2.19	0.57
1:A:694:PHE:CZ	1:A:729:LEU:HD13	2.39	0.57
1:D:730:TYR:O	1:D:734:ARG:HG2	2.04	0.57
1:A:664:VAL:HA	1:A:667:MET:HE2	1.86	0.57
1:D:656:LYS:HB3	1:D:675:ARG:HB3	1.85	0.57
1:A:609:ARG:HG3	1:A:609:ARG:HH11	1.68	0.57
1:B:754:LEU:O	1:B:758:VAL:HG23	2.04	0.57
1:C:541:HIS:H	1:C:546:ASN:HD21	1.51	0.56
1:D:701:TYR:O	1:D:704:VAL:HG22	2.04	0.56
1:D:543:ASN:ND2	1:D:606:GLN:HB3	2.21	0.56
1:D:503:ASP:O	1:D:505:PRO:HD3	2.06	0.56
1:D:717:HIS:O	1:D:718:ARG:HD2	2.04	0.56
1:A:606:GLN:HB3	1:A:637:MET:HB2	1.88	0.56
1:C:540:LYS:HA	1:C:546:ASN:ND2	2.21	0.56
1:B:462:GLU:HG2	1:C:673:PHE:HD1	1.72	0.55
1:A:477:ARG:HA	1:A:477:ARG:HE	1.69	0.55
1:C:709:LEU:HD23	1:C:709:LEU:O	2.06	0.55
1:A:756:ARG:O	1:A:760:LEU:HG	2.05	0.55
1:A:590:ASN:ND2	1:A:593:GLU:HB3	2.22	0.55
1:C:694:PHE:CZ	1:C:729:LEU:HD13	2.41	0.55
1:D:598:LYS:NZ	1:D:761:THR:HB	2.22	0.55
1:B:526:SER:HB3	1:C:659:ASN:HD22	1.70	0.55
1:D:730:TYR:CZ	1:D:734:ARG:HD3	2.42	0.55
1:A:622:ARG:O	1:A:662:LEU:HD22	2.06	0.55
1:B:545:ILE:HG22	1:B:561:VAL:HB	1.89	0.54
1:A:522:GLU:HB2	1:D:660:GLY:O	2.07	0.54
1:C:533:GLU:OE1	1:C:536:LYS:HE2	2.06	0.54
1:D:474:PRO:HB2	1:D:477:ARG:CG	2.26	0.54
1:A:461:SER:HB3	1:D:659:ASN:HB3	1.88	0.54
1:B:598:LYS:HZ1	1:B:762:SER:HB2	1.73	0.54
1:A:545:ILE:CG1	1:A:640:ALA:HB2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:LYS:HE3	1:C:659:ASN:O	2.06	0.54
1:C:738:HIS:CD2	1:C:743:GLN:HB2	2.42	0.54
1:B:648:ILE:HG23	1:B:651:ILE:HB	1.89	0.54
1:A:488:ALA:HB2	1:D:488:ALA:HB2	1.90	0.54
1:D:701:TYR:HB3	1:D:704:VAL:HG21	1.90	0.54
1:C:566:LYS:HB2	1:C:631:VAL:O	2.07	0.53
1:C:614:LEU:HD21	1:C:642:PHE:HE1	1.73	0.53
1:C:531:GLU:O	1:C:535:MET:HG2	2.08	0.53
1:D:701:TYR:HB3	1:D:704:VAL:CG2	2.38	0.53
1:C:632:THR:HG22	1:C:636:VAL:H	1.74	0.53
1:A:511:VAL:HG21	1:A:560:ILE:HG23	1.91	0.53
1:B:746:THR:OG1	1:B:749:GLN:HG3	2.09	0.53
1:A:470:ARG:HE	1:A:470:ARG:HA	1.75	0.52
1:A:620:ILE:HD11	1:A:648:ILE:HD11	1.90	0.52
1:C:605:TYR:CZ	1:C:609:ARG:HD2	2.43	0.52
1:A:541:HIS:HB3	1:A:544:ILE:HG12	1.92	0.52
1:B:738:HIS:CD2	1:B:740:VAL:H	2.24	0.52
1:B:511:VAL:HG21	1:B:560:ILE:HG23	1.91	0.52
1:D:648:ILE:HB	1:D:651:ILE:O	2.10	0.52
1:A:578:PRO:HG3	1:A:696:LEU:HD22	1.92	0.52
1:C:601:VAL:HG11	1:C:757:ILE:HG22	1.91	0.52
1:D:566:LYS:HB2	1:D:631:VAL:O	2.09	0.52
1:D:671:ALA:HA	1:D:676:ILE:H	1.74	0.51
1:D:479:VAL:HB	1:D:496:GLU:HB2	1.93	0.51
1:D:500:LEU:HD12	1:D:509:THR:HB	1.92	0.51
1:A:474:PRO:HB2	1:A:477:ARG:CG	2.38	0.51
1:D:598:LYS:HE3	1:D:762:SER:HA	1.92	0.51
1:D:543:ASN:HD22	1:D:606:GLN:HB3	1.76	0.51
1:D:716:GLY:HA2	1:D:718:ARG:NH1	2.26	0.51
1:B:534:MET:HG2	1:B:645:ALA:HB3	1.93	0.51
1:A:648:ILE:O	1:A:648:ILE:CG2	2.58	0.51
1:C:738:HIS:CD2	1:C:740:VAL:H	2.27	0.51
1:D:467:GLU:HG2	1:D:553:GLN:NE2	2.26	0.50
1:D:747:PHE:O	1:D:751:VAL:HG23	2.10	0.50
1:A:706:VAL:HG21	1:D:520:ALA:HB3	1.94	0.50
1:B:465:LEU:HD21	1:B:529:ILE:HG12	1.93	0.50
1:B:730:TYR:HA	1:B:733:MET:HG3	1.93	0.50
1:C:503:ASP:O	1:C:504:LYS:HD3	2.11	0.50
1:A:738:HIS:CD2	1:A:740:VAL:H	2.25	0.50
1:C:603:CYS:O	1:C:607:VAL:HG23	2.12	0.50
1:A:707:GLU:OE1	1:D:556:PRO:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:721:LYS:HZ2	1:C:725:CYS:HB3	1.75	0.50
1:C:747:PHE:O	1:C:751:VAL:HG23	2.12	0.50
1:A:544:ILE:HG22	1:A:639:ILE:HB	1.94	0.49
1:A:598:LYS:NZ	1:A:762:SER:HB2	2.27	0.49
1:C:662:LEU:HD11	1:C:667:MET:HG2	1.94	0.49
1:D:545:ILE:CD1	1:D:630:LEU:HD12	2.39	0.49
1:D:753:ASP:HA	1:D:756:ARG:NH2	2.27	0.49
1:A:494:LEU:HD12	1:A:511:VAL:O	2.12	0.49
1:A:701:TYR:HB3	1:A:704:VAL:HG21	1.95	0.49
1:A:727:ASN:O	1:A:731:MET:HG3	2.13	0.49
1:B:651:ILE:HG22	1:B:652:ASP:N	2.28	0.49
1:D:602:SER:O	1:D:606:GLN:HG3	2.12	0.49
1:B:545:ILE:HG13	1:B:640:ALA:HB2	1.95	0.49
1:D:758:VAL:O	1:D:762:SER:HB2	2.12	0.49
1:B:531:GLU:HG2	1:B:535:MET:HE1	1.94	0.49
1:D:465:LEU:O	1:D:465:LEU:HD12	2.12	0.49
1:A:494:LEU:HD11	1:A:510:LYS:HG3	1.95	0.48
1:B:461:SER:O	1:B:462:GLU:HB3	2.13	0.48
1:B:589:HIS:HE1	1:B:594:GLN:NE2	2.12	0.48
1:B:670:GLU:HG2	1:B:671:ALA:N	2.27	0.48
1:C:632:THR:HG23	1:C:634:ASP:H	1.78	0.48
1:D:490:GLY:HA2	1:D:516:LEU:HA	1.95	0.48
1:A:747:PHE:O	1:A:751:VAL:HG23	2.13	0.48
1:A:598:LYS:HZ1	1:A:762:SER:HB2	1.78	0.48
1:A:678:THR:HG22	1:A:679:HIS:H	1.78	0.48
1:C:540:LYS:HA	1:C:546:ASN:HD22	1.77	0.48
1:B:674:ASP:O	1:B:676:ILE:HG13	2.14	0.48
1:B:684:TRP:CE3	1:B:737:TRP:HA	2.48	0.48
1:B:490:GLY:HA2	1:B:517:LYS:HG3	1.95	0.47
1:D:483:PRO:HA	1:D:493:VAL:HG12	1.96	0.47
1:C:545:ILE:HA	1:C:562:GLU:OE1	2.14	0.47
1:C:602:SER:O	1:C:606:GLN:HG3	2.14	0.47
1:C:632:THR:CG2	1:C:636:VAL:HB	2.44	0.47
1:A:627:ARG:HH22	1:A:663:PRO:HG2	1.79	0.47
1:B:566:LYS:HB2	1:B:631:VAL:O	2.14	0.47
1:A:461:SER:CB	1:D:659:ASN:HB3	2.45	0.47
1:B:483:PRO:HA	1:B:493:VAL:HA	1.96	0.47
1:C:497:ALA:CB	1:C:500:LEU:HG	2.44	0.47
1:B:656:LYS:HE2	1:B:675:ARG:HA	1.95	0.47
1:B:477:ARG:HA	1:B:477:ARG:NE	2.29	0.47
1:B:672:LEU:HG	1:C:462:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:THR:HG22	1:B:557:LEU:CD1	2.44	0.47
1:B:714:LYS:HE3	1:C:463:TYR:CE1	2.50	0.46
1:D:541:HIS:HB3	1:D:544:ILE:HD12	1.97	0.46
1:D:570:ARG:O	1:D:574:GLN:HG3	2.15	0.46
1:A:486:GLU:HB3	1:A:517:LYS:HZ1	1.80	0.46
1:A:609:ARG:HG3	1:A:609:ARG:NH1	2.30	0.46
1:B:460:VAL:HA	1:C:659:ASN:OD1	2.15	0.46
1:C:663:PRO:O	1:C:667:MET:HG3	2.16	0.46
1:A:662:LEU:HD13	1:A:677:TYR:OH	2.16	0.46
1:A:656:LYS:HG3	1:A:657:THR:O	2.16	0.46
1:A:656:LYS:HG2	1:A:675:ARG:HA	1.97	0.46
1:D:531:GLU:HG3	1:D:642:PHE:HB2	1.98	0.46
1:D:712:LEU:HD13	1:D:717:HIS:ND1	2.30	0.46
1:B:543:ASN:ND2	1:B:606:GLN:HB3	2.31	0.46
1:D:542:LYS:HZ1	1:D:609:ARG:NH1	2.14	0.46
1:B:711:LYS:O	1:B:715:GLU:HG2	2.15	0.46
1:C:566:LYS:HB2	1:C:631:VAL:HB	1.98	0.46
1:D:607:VAL:HG11	1:D:689:LEU:HD21	1.97	0.46
1:D:727:ASN:O	1:D:731:MET:HG2	2.15	0.46
1:B:531:GLU:HG2	1:B:535:MET:CE	2.46	0.46
1:B:577:GLU:HA	1:B:578:PRO:HD3	1.87	0.46
1:B:671:ALA:HA	1:B:676:ILE:H	1.80	0.46
1:B:475:ARG:NH2	1:B:554:ASP:O	2.49	0.45
1:C:493:VAL:HG22	1:C:515:MET:HE3	1.98	0.45
1:C:543:ASN:HD22	1:C:606:GLN:HB3	1.81	0.45
1:D:501:ASP:OD1	1:D:503:ASP:HB2	2.15	0.45
1:A:543:ASN:ND2	1:A:606:GLN:HB3	2.32	0.45
1:B:609:ARG:HG2	1:B:609:ARG:HH11	1.81	0.45
1:A:741:PRO:HG2	1:B:652:ASP:OD2	2.16	0.45
1:B:651:ILE:HG22	1:B:653:TYR:H	1.81	0.45
1:D:460:VAL:HG11	1:D:525:LEU:HG	1.99	0.45
1:D:721:LYS:HG3	1:D:730:TYR:HB2	1.99	0.45
1:A:701:TYR:O	1:A:704:VAL:HG22	2.16	0.45
1:D:670:GLU:O	1:D:674:ASP:HB2	2.16	0.45
1:A:611:MET:SD	1:A:614:LEU:HD12	2.57	0.45
1:D:566:LYS:HG3	1:D:631:VAL:HG12	1.99	0.45
1:D:683:VAL:HG12	1:D:736:CYS:HB3	1.97	0.45
1:A:674:ASP:OD1	1:B:655:LYS:HD2	2.17	0.45
1:B:646:ARG:HG3	1:B:654:TYR:CZ	2.52	0.45
1:D:705:PRO:HB2	1:D:708:GLU:HG3	1.98	0.45
1:B:522:GLU:HB2	1:C:659:ASN:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ILE:HG12	1:A:640:ALA:HB2	1.98	0.45
1:A:656:LYS:HE2	1:D:522:GLU:OE2	2.16	0.45
1:C:605:TYR:O	1:C:608:ALA:HB3	2.17	0.45
1:A:603:CYS:O	1:A:607:VAL:HG23	2.17	0.45
1:B:672:LEU:C	1:C:462:GLU:OE2	2.55	0.45
1:C:512:ALA:HB3	1:C:561:VAL:HG23	1.99	0.45
1:C:648:ILE:HD11	1:C:679:HIS:NE2	2.31	0.45
1:C:705:PRO:HG2	1:C:708:GLU:HB2	1.98	0.45
1:D:516:LEU:HG	1:D:528:LEU:HD22	1.98	0.45
1:D:644:LEU:HD13	1:D:662:LEU:HD21	1.98	0.45
1:D:656:LYS:HD3	1:D:675:ARG:HA	1.98	0.45
1:A:678:THR:CG2	1:A:679:HIS:N	2.80	0.44
1:B:620:ILE:HD11	1:B:678:THR:HA	1.99	0.44
1:D:704:VAL:O	1:D:704:VAL:HG23	2.17	0.44
1:A:618:LYS:HD2	1:A:649:HIS:CE1	2.52	0.44
1:B:763:ASN:O	1:B:764:GLN:HB2	2.17	0.44
1:D:646:ARG:HG3	1:D:654:TYR:CE1	2.52	0.44
1:D:728:GLU:HG3	1:D:729:LEU:N	2.33	0.44
1:A:462:GLU:OE1	1:D:673:PHE:HA	2.17	0.44
1:D:477:ARG:HB3	1:D:498:ILE:O	2.16	0.44
1:D:717:HIS:C	1:D:718:ARG:HD2	2.38	0.44
1:B:738:HIS:CD2	1:B:743:GLN:HB2	2.53	0.44
1:D:671:ALA:HA	1:D:676:ILE:N	2.33	0.44
1:A:578:PRO:HA	1:A:696:LEU:HD21	2.00	0.44
1:B:730:TYR:CZ	1:B:734:ARG:HD3	2.52	0.44
1:C:496:GLU:HB3	1:C:508:VAL:CG1	2.48	0.44
1:D:732:MET:HA	1:D:735:ASP:OD2	2.18	0.44
1:D:459:GLY:O	1:D:463:TYR:HB2	2.17	0.44
1:C:484:LEU:HD21	1:C:494:LEU:HB2	2.00	0.44
1:A:578:PRO:HA	1:A:579:PRO:HD3	1.83	0.43
1:C:614:LEU:HD21	1:C:642:PHE:CE1	2.52	0.43
1:D:498:ILE:HG13	1:D:508:VAL:HG22	2.00	0.43
1:B:651:ILE:HG22	1:B:652:ASP:H	1.83	0.43
1:C:656:LYS:HA	1:C:675:ARG:HH21	1.83	0.43
1:C:716:GLY:HA2	1:C:718:ARG:NH1	2.33	0.43
1:D:740:VAL:HB	1:D:743:GLN:HG2	2.00	0.43
1:B:540:LYS:HB2	1:B:546:ASN:ND2	2.32	0.43
1:C:528:LEU:HD23	1:C:557:LEU:HD23	2.00	0.43
1:D:545:ILE:HG13	1:D:638:LYS:HB3	2.00	0.43
1:A:666:TRP:CZ2	1:A:700:PRO:HG2	2.54	0.43
1:C:632:THR:CG2	1:C:636:VAL:H	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:THR:HG22	1:A:557:LEU:CD1	2.49	0.43
1:B:578:PRO:HG3	1:B:696:LEU:CD1	2.47	0.43
1:C:721:LYS:HA	1:C:722:PRO:HD3	1.85	0.43
1:D:740:VAL:HB	1:D:743:GLN:CG	2.49	0.43
1:A:551:CYS:HB2	1:A:558:TYR:HB2	2.01	0.43
1:B:751:VAL:O	1:B:755:ASP:HB2	2.19	0.42
1:C:721:LYS:NZ	1:C:725:CYS:HB3	2.34	0.42
1:D:694:PHE:CZ	1:D:729:LEU:HD13	2.53	0.42
1:C:683:VAL:O	1:C:686:PHE:HB3	2.19	0.42
1:D:656:LYS:HD2	1:D:677:TYR:CE1	2.46	0.42
1:A:704:VAL:O	1:A:704:VAL:HG23	2.19	0.42
1:A:467:GLU:O	1:A:469:PRO:HD3	2.18	0.42
1:D:601:VAL:HG12	1:D:758:VAL:HG22	2.02	0.42
1:A:764:GLN:O	1:A:765:GLU:HG2	2.18	0.42
1:C:615:ALA:HA	1:C:679:HIS:CE1	2.55	0.42
1:C:686:PHE:CE2	1:C:690:LEU:HD11	2.55	0.42
1:D:620:ILE:HD11	1:D:648:ILE:HD13	2.01	0.42
1:C:618:LYS:HB2	1:C:649:HIS:CE1	2.55	0.42
1:A:659:ASN:OD1	1:D:460:VAL:HG23	2.20	0.42
1:B:666:TRP:CZ2	1:B:700:PRO:HG2	2.54	0.42
1:D:468:ASP:OD2	1:D:471:TRP:HD1	2.02	0.42
1:B:644:LEU:N	1:B:644:LEU:HD12	2.35	0.42
1:C:624:LEU:HB3	1:C:685:SER:HB3	2.02	0.42
1:D:568:ASN:HA	1:D:630:LEU:HA	2.02	0.42
1:D:612:GLU:OE1	1:D:751:VAL:HG21	2.20	0.42
1:D:617:LYS:O	1:D:618:LYS:HB2	2.20	0.42
1:A:462:GLU:O	1:A:462:GLU:HG3	2.20	0.41
1:B:624:LEU:HG	1:B:689:LEU:HD12	2.02	0.41
1:C:651:ILE:HG13	1:C:653:TYR:H	1.85	0.41
1:A:477:ARG:HE	1:A:477:ARG:CA	2.33	0.41
1:A:488:ALA:HB2	1:D:488:ALA:CB	2.49	0.41
1:B:664:VAL:HG21	1:B:706:VAL:CG1	2.32	0.41
1:C:671:ALA:HA	1:C:676:ILE:H	1.85	0.41
1:A:622:ARG:NH1	1:A:654:TYR:HE1	2.18	0.41
1:B:631:VAL:HG13	1:B:637:MET:CE	2.51	0.41
1:C:597:SER:O	1:C:601:VAL:HG23	2.21	0.41
1:A:545:ILE:HG13	1:A:640:ALA:HB2	2.01	0.41
1:B:540:LYS:HB2	1:B:546:ASN:HD22	1.86	0.41
1:C:691:TRP:O	1:C:695:THR:HG23	2.20	0.41
1:D:465:LEU:H	1:D:465:LEU:HG	1.70	0.41
1:A:738:HIS:HD2	1:A:740:VAL:N	2.10	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:HIS:O	1:B:718:ARG:NH1	2.47	0.41
1:B:723:SER:O	1:B:724:ASN:HB3	2.21	0.41
1:C:497:ALA:HB1	1:C:500:LEU:HG	2.01	0.41
1:A:670:GLU:O	1:A:674:ASP:HB2	2.21	0.41
1:C:483:PRO:HA	1:C:493:VAL:HA	2.03	0.41
1:D:465:LEU:HD13	1:D:552:THR:O	2.21	0.41
1:B:672:LEU:O	1:C:462:GLU:OE2	2.39	0.41
1:C:474:PRO:HG2	1:C:477:ARG:HB2	2.03	0.41
1:C:609:ARG:HH11	1:C:609:ARG:HG2	1.86	0.41
1:C:705:PRO:HG2	1:C:708:GLU:CB	2.51	0.41
1:D:573:LEU:C	1:D:575:ALA:H	2.23	0.41
1:D:614:LEU:HD21	1:D:642:PHE:HE1	1.85	0.41
1:D:664:VAL:HG21	1:D:706:VAL:CG1	2.33	0.41
1:B:656:LYS:HG2	1:B:657:THR:N	2.35	0.41
1:D:521:THR:HG22	1:D:524:ASP:OD2	2.21	0.41
1:A:623:ASP:HB2	1:A:662:LEU:CD2	2.51	0.40
1:A:501:ASP:OD1	1:A:503:ASP:HB3	2.21	0.40
1:A:576:ARG:HG3	1:A:576:ARG:HH11	1.87	0.40
1:C:632:THR:HG21	1:C:636:VAL:HB	2.03	0.40
1:D:543:ASN:C	1:D:544:ILE:HG13	2.42	0.40
1:A:577:GLU:HA	1:A:578:PRO:HD3	1.91	0.40
1:C:468:ASP:O	1:C:472:GLU:HB2	2.20	0.40
1:C:601:VAL:HG12	1:C:758:VAL:HG22	2.02	0.40
1:C:613:TYR:O	1:C:617:LYS:HG2	2.22	0.40
1:A:736:CYS:O	1:A:744:ARG:HD3	2.20	0.40
1:B:467:GLU:HG3	1:B:553:GLN:HG2	2.03	0.40
1:B:621:HIS:O	1:B:623:ASP:N	2.54	0.40
1:C:664:VAL:HG23	1:C:665:LYS:N	2.36	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	303/317 (96%)	288 (95%)	14 (5%)	1 (0%)	41	74
1	B	303/317 (96%)	287 (95%)	14 (5%)	2 (1%)	22	61
1	C	282/317 (89%)	254 (90%)	28 (10%)	0	100	100
1	D	284/317 (90%)	270 (95%)	13 (5%)	1 (0%)	34	69
All	All	1172/1268 (92%)	1099 (94%)	69 (6%)	4 (0%)	41	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	622	ARG
1	A	622	ARG
1	B	461	SER
1	D	622	ARG

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	268/277 (97%)	267 (100%)	1 (0%)	91	95
1	B	268/277 (97%)	268 (100%)	0	100	100
1	C	248/277 (90%)	248 (100%)	0	100	100
1	D	250/277 (90%)	249 (100%)	1 (0%)	91	95
All	All	1034/1108 (93%)	1032 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	ASP
1	D	465	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	491	GLN
1	A	738	HIS
1	B	553	GLN
1	B	589	HIS
1	B	594	GLN
1	B	724	ASN
1	B	738	HIS
1	C	546	ASN
1	C	738	HIS
1	C	749	GLN
1	D	546	ASN
1	D	628	ASN
1	D	649	HIS
1	D	659	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	305/317 (96%)	-0.27	1 (0%) 94	92	12, 39, 83, 97	0
1	B	305/317 (96%)	-0.24	1 (0%) 94	92	14, 39, 84, 98	0
1	C	286/317 (90%)	0.26	6 (2%) 63	49	29, 80, 115, 125	0
1	D	288/317 (90%)	0.14	3 (1%) 82	72	28, 74, 111, 122	0
All	All	1184/1268 (93%)	-0.04	11 (0%) 84	75	12, 58, 106, 125	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	765	GLU	3.4
1	B	764	GLN	2.8
1	C	760	LEU	2.8
1	C	720	ASP	2.8
1	D	652	ASP	2.4
1	D	739	ALA	2.4
1	C	503	ASP	2.3
1	C	759	ALA	2.3
1	D	595	LEU	2.2
1	C	597	SER	2.0
1	C	747	PHE	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.