



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 03:03 AM EDT

PDB ID : 1IIL  
Title : CRYSTAL STRUCTURE OF PRO253ARG APERT MUTANT FGF RECEPTOR 2 (FGFR2) IN COMPLEX WITH FGF2  
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Deposited on : 2001-04-23  
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

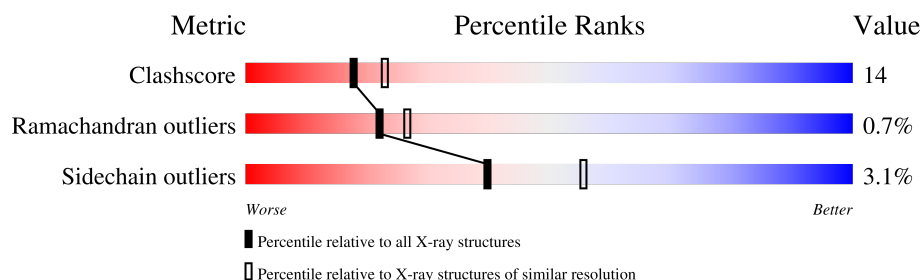
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	155	
1	B	155	
1	C	155	
1	D	155	
2	E	220	
2	F	220	
2	G	220	
2	H	220	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10677 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			1052	670	189	189	4			
1	B	133	Total	C	N	O	S	0	0	0
			1047	667	188	188	4			
1	C	132	Total	C	N	O	S	0	0	0
			1034	657	186	187	4			
1	D	132	Total	C	N	O	S	0	0	0
			1032	656	185	187	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	SER	CYS	engineered mutation	UNP P09038
A	96	SER	CYS	engineered mutation	UNP P09038
B	78	SER	CYS	engineered mutation	UNP P09038
B	96	SER	CYS	engineered mutation	UNP P09038
C	78	SER	CYS	engineered mutation	UNP P09038
C	96	SER	CYS	engineered mutation	UNP P09038
D	78	SER	CYS	engineered mutation	UNP P09038
D	96	SER	CYS	engineered mutation	UNP P09038

- Molecule 2 is a protein called FIBROBLAST GROWTH FACTOR RECEPTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	200	Total	C	N	O	S	0	0	0
			1551	987	278	278	8			
2	F	200	Total	C	N	O	S	0	0	0
			1551	987	278	278	8			
2	G	215	Total	C	N	O	S	0	0	0
			1670	1059	300	303	8			
2	H	215	Total	C	N	O	S	0	0	0
			1663	1055	298	302	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	253	ARG	PRO	engineered mutation	UNP P21802
F	253	ARG	PRO	engineered mutation	UNP P21802
G	253	ARG	PRO	engineered mutation	UNP P21802
H	253	ARG	PRO	engineered mutation	UNP P21802

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total O 6 6	0	0
3	B	9	Total O 9 9	0	0
3	C	7	Total O 7 7	0	0
3	D	9	Total O 9 9	0	0
3	E	9	Total O 9 9	0	0
3	F	12	Total O 12 12	0	0
3	G	15	Total O 15 15	0	0
3	H	10	Total O 10 10	0	0

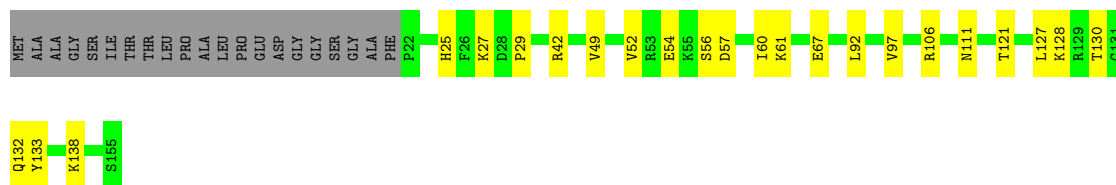
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

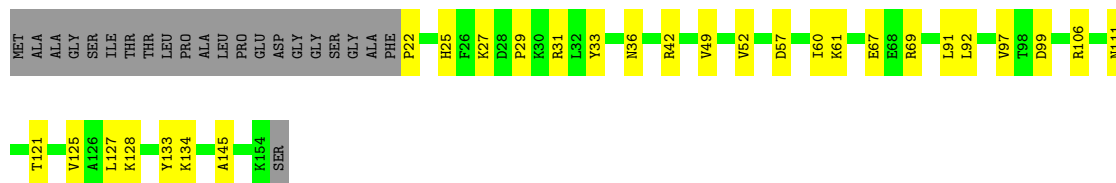
#### • Molecule 1: HEPARIN-BINDING GROWTH FACTOR 2

Chain A: 



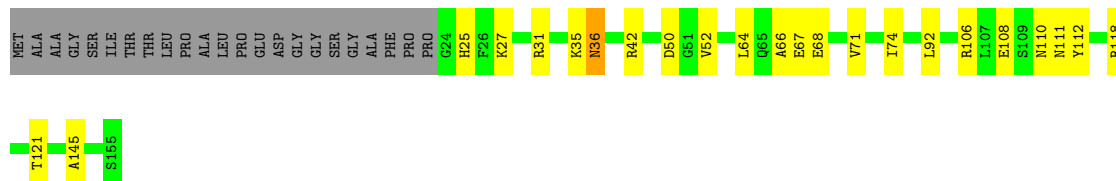
#### • Molecule 1: HEPARIN-BINDING GROWTH FACTOR 2

Chain B: 



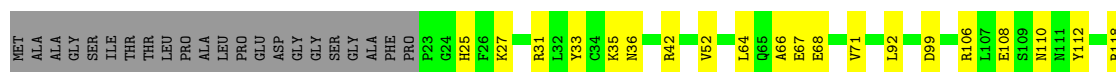
#### • Molecule 1: HEPARIN-BINDING GROWTH FACTOR 2

Chain C: 



#### • Molecule 1: HEPARIN-BINDING GROWTH FACTOR 2

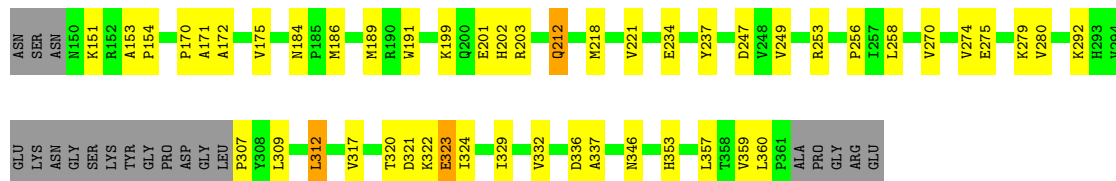
Chain D: 





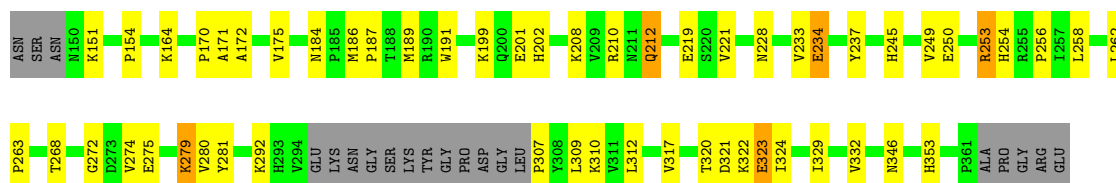
• Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 2

Chain E: 69% 21% 9%



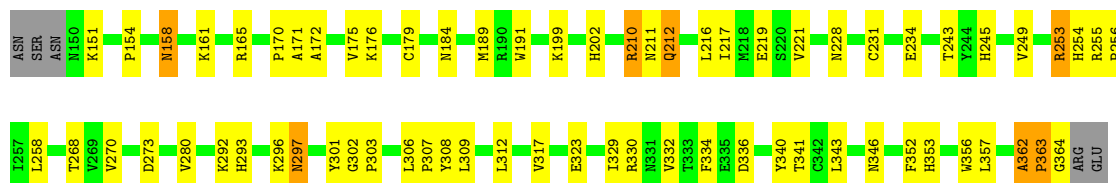
• Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 2

Chain F: 66% 23% 9%



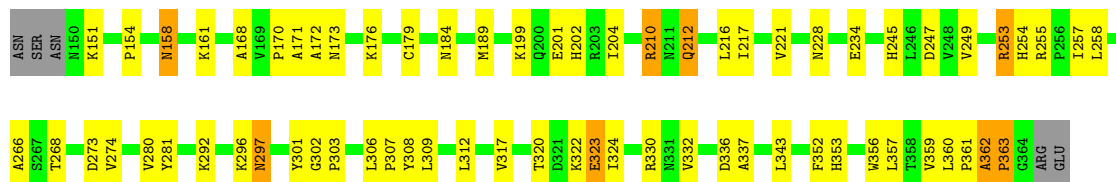
• Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 2

Chain G: 67% 28% 5%



• Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 2

Chain H: 67% 27% 6%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.80 Å   72.49 Å   89.92 Å 90.01°   89.82°   90.00°	Depositor
Resolution (Å)	25.00 – 2.30	Depositor
% Data completeness (in resolution range)	95.1 (25.00-2.30)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.237 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10677	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.41	0/1077	0.68	0/1448
1	B	0.41	0/1072	0.67	0/1441
1	C	0.42	0/1057	0.69	0/1421
1	D	0.40	0/1056	0.69	0/1421
2	E	0.40	0/1592	0.63	0/2166
2	F	0.40	0/1592	0.64	0/2166
2	G	0.41	0/1716	0.67	0/2336
2	H	0.40	0/1709	0.67	0/2328
All	All	0.41	0/10871	0.67	0/14727

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 [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	1052	0	1036	24	0
1	B	1047	0	1034	25	0
1	C	1034	0	1010	16	0
1	D	1032	0	1005	17	0
2	E	1551	0	1504	38	0
2	F	1551	0	1504	52	0
2	G	1670	0	1617	63	0
2	H	1663	0	1602	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	0	0	0
3	B	9	0	0	0	0
3	C	7	0	0	0	0
3	D	9	0	0	0	0
3	E	9	0	0	0	0
3	F	12	0	0	0	0
3	G	15	0	0	0	0
3	H	10	0	0	0	0
All	All	10677	0	10312	277	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 14.

All (277) 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:H:362:ALA:HB1	2:H:363:PRO:HD2	1.09	1.06
2:H:362:ALA:CB	2:H:363:PRO:HD2	1.88	1.04
2:E:212:GLN:H	2:E:212:GLN:HE21	1.09	0.99
2:H:362:ALA:HB1	2:H:363:PRO:CD	1.92	0.98
2:H:212:GLN:H	2:H:212:GLN:NE2	1.61	0.97
2:H:212:GLN:H	2:H:212:GLN:HE21	1.06	0.97
2:H:204:ILE:H	2:H:204:ILE:HD12	1.30	0.96
2:G:212:GLN:H	2:G:212:GLN:HE21	1.03	0.94
2:G:212:GLN:H	2:G:212:GLN:NE2	1.66	0.94
2:E:199:LYS:H	2:E:202:HIS:CD2	1.86	0.92
2:F:320:THR:HG22	2:F:322:LYS:H	1.34	0.92
2:F:212:GLN:H	2:F:212:GLN:HE21	1.05	0.91
2:E:212:GLN:H	2:E:212:GLN:NE2	1.65	0.91
1:A:97:VAL:HG21	2:E:317:VAL:HG11	1.51	0.90
2:E:320:THR:HG22	2:E:322:LYS:H	1.36	0.90
2:H:258:LEU:HD22	2:H:280:VAL:HG22	1.54	0.88
2:F:212:GLN:H	2:F:212:GLN:NE2	1.72	0.87
2:H:320:THR:HG22	2:H:322:LYS:H	1.39	0.87
2:F:199:LYS:H	2:F:202:HIS:CD2	1.92	0.86
2:G:258:LEU:HD22	2:G:280:VAL:HG22	1.55	0.86
2:E:258:LEU:HD22	2:E:280:VAL:HG22	1.59	0.84
1:B:97:VAL:HG21	2:F:317:VAL:HG11	1.60	0.83
1:A:25:HIS:CE1	1:A:27:LYS:HG2	2.15	0.82
2:H:151:LYS:HA	2:H:184:ASN:HD22	1.45	0.82
1:B:25:HIS:CD2	1:B:27:LYS:HG2	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:199:LYS:H	2:H:202:HIS:CD2	2.01	0.79
1:C:42:ARG:NH1	1:C:52:VAL:HG11	1.99	0.78
2:H:257:ILE:HG23	2:H:281:TYR:HB3	1.68	0.76
2:E:199:LYS:H	2:E:202:HIS:HD2	1.32	0.75
2:G:151:LYS:HA	2:G:184:ASN:HD22	1.51	0.75
2:F:151:LYS:HD3	2:F:184:ASN:ND2	2.02	0.75
2:F:258:LEU:CD2	2:F:280:VAL:HG22	2.19	0.73
2:G:212:GLN:HE21	2:G:212:GLN:N	1.84	0.72
2:H:176:LYS:HG3	2:H:217:ILE:HD11	1.70	0.72
2:G:228:ASN:OD1	2:G:245:HIS:ND1	2.21	0.72
2:G:256:PRO:HD3	2:G:346:ASN:ND2	2.05	0.71
2:H:258:LEU:CD2	2:H:280:VAL:HG22	2.21	0.71
2:H:212:GLN:NE2	2:H:212:GLN:N	2.38	0.70
2:H:228:ASN:OD1	2:H:245:HIS:ND1	2.24	0.69
2:H:179:CYS:HB2	2:H:189:MET:HE1	1.74	0.69
2:H:343:LEU:HD12	2:H:352:PHE:HB3	1.74	0.68
2:F:307:PRO:O	2:F:309:LEU:HG	1.94	0.68
2:G:212:GLN:NE2	2:G:212:GLN:N	2.40	0.68
2:F:212:GLN:HE21	2:F:212:GLN:N	1.86	0.67
2:G:199:LYS:H	2:G:202:HIS:CD2	2.12	0.67
2:E:307:PRO:O	2:E:309:LEU:HG	1.95	0.66
1:C:42:ARG:CZ	1:C:52:VAL:HG11	2.25	0.66
2:H:216:LEU:C	2:H:217:ILE:HD12	2.17	0.65
1:D:25:HIS:CE1	1:D:27:LYS:HE2	2.32	0.65
1:B:111:ASN:HD21	2:G:254:HIS:CE1	2.15	0.65
2:F:258:LEU:HD22	2:F:280:VAL:HG22	1.79	0.64
2:G:179:CYS:HB2	2:G:189:MET:HE1	1.79	0.64
2:F:272:GLY:O	2:F:332:VAL:HG22	1.98	0.63
2:G:165:ARG:NH1	2:G:243:THR:O	2.32	0.63
1:B:127:LEU:HD23	1:B:133:TYR:HA	1.81	0.63
2:E:212:GLN:HE21	2:E:212:GLN:N	1.90	0.63
1:A:25:HIS:ND1	1:A:27:LYS:HG2	2.14	0.62
2:H:257:ILE:CG2	2:H:281:TYR:HB3	2.30	0.62
1:D:42:ARG:NH1	1:D:52:VAL:HG11	2.14	0.61
2:H:158:ASN:C	2:H:158:ASN:HD22	2.03	0.61
1:B:42:ARG:CZ	1:B:52:VAL:HG11	2.30	0.60
2:H:302:GLY:HA3	2:H:306:LEU:O	2.01	0.60
2:G:301:TYR:HA	2:G:307:PRO:HA	1.83	0.60
2:H:204:ILE:HD12	2:H:204:ILE:N	2.09	0.59
1:D:68:GLU:OE2	1:D:118:ARG:NH1	2.34	0.59
2:E:151:LYS:HD3	2:E:184:ASN:ND2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:362:ALA:CB	2:G:363:PRO:HD3	2.32	0.59
2:G:176:LYS:HG3	2:G:217:ILE:HD11	1.85	0.59
2:E:212:GLN:NE2	2:E:212:GLN:N	2.45	0.59
2:H:176:LYS:HG3	2:H:217:ILE:CD1	2.32	0.59
2:H:296:LYS:O	2:H:297:ASN:HB2	2.02	0.59
2:H:255:ARG:HG2	2:H:255:ARG:HH11	1.67	0.59
1:A:67:GLU:OE1	2:E:317:VAL:HG23	2.03	0.59
1:B:25:HIS:NE2	1:B:27:LYS:HE2	2.18	0.59
2:H:302:GLY:H	2:H:307:PRO:HA	1.68	0.59
2:F:279:LYS:NZ	2:F:279:LYS:HB3	2.18	0.58
2:G:302:GLY:H	2:G:307:PRO:HA	1.69	0.58
2:G:362:ALA:CB	2:G:363:PRO:CD	2.81	0.58
2:F:228:ASN:OD1	2:F:245:HIS:ND1	2.36	0.58
2:F:312:LEU:N	2:F:312:LEU:HD12	2.18	0.58
1:B:25:HIS:NE2	1:B:27:LYS:HG2	2.18	0.58
1:D:42:ARG:CZ	1:D:52:VAL:HG11	2.33	0.57
1:B:22:PRO:HD2	2:F:281:TYR:OH	2.04	0.57
1:D:106:ARG:NH1	1:D:108:GLU:OE2	2.37	0.57
2:G:268:THR:CG2	2:G:332:VAL:HG21	2.35	0.57
2:H:179:CYS:HB2	2:H:189:MET:CE	2.35	0.57
2:G:216:LEU:C	2:G:217:ILE:HD12	2.25	0.57
1:A:25:HIS:CE1	1:A:27:LYS:NZ	2.73	0.57
2:H:212:GLN:HE21	2:H:212:GLN:N	1.88	0.57
1:C:42:ARG:CZ	1:C:52:VAL:CG1	2.83	0.56
1:B:29:PRO:CG	1:B:61:LYS:HE3	2.36	0.56
2:F:253:ARG:O	2:G:253:ARG:HD3	2.06	0.56
2:E:258:LEU:HB2	2:E:353:HIS:CE1	2.40	0.56
2:H:301:TYR:HA	2:H:307:PRO:HA	1.86	0.56
1:B:106:ARG:HG2	1:B:106:ARG:HH11	1.71	0.56
2:F:154:PRO:HG2	2:F:234:GLU:HA	1.88	0.56
2:H:362:ALA:CB	2:H:363:PRO:CD	2.64	0.55
2:F:329:ILE:N	2:F:329:ILE:HD12	2.21	0.55
1:A:127:LEU:HD23	1:A:133:TYR:HA	1.87	0.55
1:D:68:GLU:HG2	1:D:71:VAL:HB	1.87	0.55
1:A:130:THR:OG1	1:A:132:GLN:HG2	2.07	0.55
2:H:204:ILE:H	2:H:204:ILE:CD1	2.08	0.55
1:B:106:ARG:HG2	1:B:106:ARG:NH1	2.22	0.54
2:G:171:ALA:O	2:G:172:ALA:HB3	2.06	0.54
2:G:362:ALA:HB3	2:G:363:PRO:CD	2.37	0.54
2:E:256:PRO:HD3	2:E:346:ASN:ND2	2.21	0.54
2:H:171:ALA:O	2:H:172:ALA:HB3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:HE3	1:A:132:GLN:HG3	1.89	0.54
2:E:332:VAL:HG13	2:E:336:ASP:HB2	1.89	0.54
2:H:268:THR:CG2	2:H:332:VAL:HG21	2.38	0.54
2:G:363:PRO:HG2	2:G:364:GLY:H	1.73	0.54
2:H:154:PRO:HG2	2:H:234:GLU:HA	1.90	0.54
1:C:68:GLU:OE2	1:C:118:ARG:NH1	2.41	0.54
1:B:29:PRO:HG3	1:B:61:LYS:HE3	1.90	0.54
2:F:151:LYS:HB3	2:F:237:TYR:HE1	1.72	0.53
2:G:268:THR:HG21	2:G:332:VAL:HG21	1.90	0.53
2:G:292:LYS:HB2	2:G:312:LEU:HD11	1.91	0.53
2:H:151:LYS:HA	2:H:184:ASN:ND2	2.21	0.53
2:E:256:PRO:HD3	2:E:346:ASN:CG	2.28	0.53
1:B:42:ARG:NH1	1:B:52:VAL:HG11	2.24	0.53
2:F:199:LYS:H	2:F:202:HIS:HD2	1.53	0.53
2:G:296:LYS:O	2:G:297:ASN:HB2	2.09	0.53
2:G:176:LYS:HG3	2:G:217:ILE:CD1	2.38	0.52
1:D:42:ARG:CZ	1:D:52:VAL:CG1	2.87	0.52
1:D:99:ASP:OD2	2:F:199:LYS:HE3	2.09	0.52
1:C:31:ARG:HG2	1:C:31:ARG:HH11	1.74	0.52
1:D:35:LYS:HD2	1:D:112:TYR:CZ	2.45	0.52
2:F:151:LYS:HB3	2:F:237:TYR:CE1	2.45	0.52
2:G:154:PRO:HG2	2:G:234:GLU:HA	1.91	0.52
2:H:151:LYS:CA	2:H:184:ASN:HD22	2.20	0.52
2:F:212:GLN:NE2	2:F:212:GLN:N	2.48	0.52
2:G:151:LYS:CA	2:G:184:ASN:HD22	2.22	0.52
1:C:64:LEU:HD13	1:C:74:ILE:HG12	1.92	0.52
2:G:158:ASN:C	2:G:158:ASN:HD22	2.11	0.52
2:F:321:ASP:HA	2:F:324:ILE:HG22	1.91	0.51
1:B:128:LYS:HE3	1:B:134:LYS:HA	1.92	0.51
2:G:151:LYS:HA	2:G:184:ASN:ND2	2.20	0.51
2:E:292:LYS:HB3	2:E:312:LEU:HD21	1.91	0.51
2:F:171:ALA:O	2:F:172:ALA:HB3	2.10	0.51
2:G:307:PRO:O	2:G:309:LEU:HG	2.10	0.51
2:E:253:ARG:O	2:H:253:ARG:HD3	2.11	0.50
2:H:337:ALA:HB2	2:H:359:VAL:HG23	1.94	0.50
2:G:210:ARG:HA	2:G:210:ARG:HH11	1.76	0.50
1:B:42:ARG:CZ	1:B:52:VAL:CG1	2.90	0.50
2:G:256:PRO:HD3	2:G:346:ASN:CG	2.32	0.50
2:G:302:GLY:HA3	2:G:306:LEU:O	2.11	0.49
1:C:68:GLU:HG2	1:C:71:VAL:HB	1.92	0.49
2:F:268:THR:CG2	2:F:332:VAL:HG21	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:268:THR:HG21	2:F:332:VAL:HG21	1.94	0.49
2:F:256:PRO:HD3	2:F:346:ASN:ND2	2.27	0.49
2:F:256:PRO:HD3	2:F:346:ASN:CG	2.32	0.49
2:G:362:ALA:HB1	2:G:363:PRO:HD3	1.93	0.49
2:H:307:PRO:O	2:H:309:LEU:HG	2.13	0.49
2:H:158:ASN:OD1	2:H:161:LYS:HE3	2.13	0.49
1:C:36:ASN:HB2	1:C:145:ALA:HA	1.95	0.49
2:E:292:LYS:NZ	2:E:336:ASP:O	2.45	0.49
2:E:323:GLU:O	2:E:323:GLU:HG2	2.11	0.49
2:E:321:ASP:HA	2:E:324:ILE:HG22	1.95	0.49
2:F:310:LYS:O	2:F:312:LEU:HD12	2.12	0.49
2:E:153:ALA:HB1	2:E:154:PRO:HD2	1.94	0.49
2:E:171:ALA:O	2:E:172:ALA:HB3	2.13	0.49
2:F:199:LYS:HB3	2:F:201:GLU:OE1	2.13	0.48
1:A:29:PRO:CG	1:A:61:LYS:HE3	2.43	0.48
1:A:42:ARG:NH1	1:A:52:VAL:HG11	2.29	0.48
1:B:49:VAL:HG23	1:B:92:LEU:HA	1.95	0.48
1:D:67:GLU:OE1	2:H:317:VAL:HG13	2.14	0.48
1:D:92:LEU:C	1:D:92:LEU:HD12	2.34	0.48
1:A:138:LYS:O	1:A:138:LYS:HG2	2.13	0.48
2:H:303:PRO:HD3	2:H:308:TYR:OH	2.13	0.48
1:A:49:VAL:HG23	1:A:92:LEU:HA	1.96	0.47
1:C:92:LEU:HD12	1:C:92:LEU:C	2.34	0.47
2:F:321:ASP:HA	2:F:324:ILE:CG2	2.44	0.47
2:G:293:HIS:HE1	2:G:341:THR:OG1	1.96	0.47
2:H:268:THR:HG21	2:H:332:VAL:HG21	1.95	0.47
1:B:111:ASN:HD21	2:G:254:HIS:HE1	1.62	0.47
1:D:31:ARG:HG2	1:D:31:ARG:HH11	1.79	0.47
2:F:258:LEU:HB2	2:F:353:HIS:CE1	2.50	0.47
2:E:329:ILE:HD12	2:E:329:ILE:N	2.29	0.47
2:G:254:HIS:HD2	2:G:255:ARG:O	1.98	0.47
1:D:36:ASN:HB2	1:D:145:ALA:HA	1.97	0.47
2:H:254:HIS:HD2	2:H:255:ARG:O	1.98	0.47
2:G:301:TYR:HA	2:G:307:PRO:CA	2.45	0.47
2:H:210:ARG:HH11	2:H:210:ARG:HA	1.80	0.46
2:H:336:ASP:O	2:H:357:LEU:HD23	2.16	0.46
1:B:22:PRO:HB3	2:F:250:GLU:HB2	1.98	0.46
2:F:151:LYS:HD3	2:F:184:ASN:CG	2.35	0.46
2:G:303:PRO:HD3	2:G:308:TYR:OH	2.15	0.46
1:A:54:GLU:OE2	1:A:56:SER:HB3	2.14	0.46
1:A:106:ARG:HG2	1:A:106:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:GLU:HB2	1:D:110:ASN:OD1	2.15	0.46
2:G:158:ASN:OD1	2:G:161:LYS:HE3	2.16	0.46
2:G:170:PRO:HA	2:G:249:VAL:O	2.17	0.45
2:H:306:LEU:N	2:H:306:LEU:HD22	2.32	0.45
2:H:323:GLU:O	2:H:323:GLU:HG2	2.15	0.45
1:C:111:ASN:HD21	2:F:254:HIS:CE1	2.34	0.45
2:E:274:VAL:HG22	2:E:275:GLU:N	2.32	0.45
1:A:25:HIS:CE1	1:A:27:LYS:HZ2	2.35	0.45
1:A:106:ARG:HG2	1:A:106:ARG:NH1	2.32	0.45
1:C:67:GLU:OE1	2:G:317:VAL:HG13	2.16	0.45
2:H:301:TYR:HA	2:H:307:PRO:CA	2.47	0.44
2:E:189:MET:CE	2:E:191:TRP:HE1	2.31	0.44
2:G:343:LEU:HD12	2:G:352:PHE:HB3	1.99	0.44
2:H:258:LEU:HB2	2:H:353:HIS:CE1	2.53	0.44
2:H:273:ASP:OD1	2:H:330:ARG:HA	2.18	0.44
1:A:130:THR:OG1	1:A:132:GLN:CG	2.64	0.44
1:B:91:LEU:HD21	1:B:125:VAL:HG13	1.99	0.44
2:F:208:LYS:NZ	2:F:219:GLU:OE1	2.51	0.44
1:C:42:ARG:HB3	1:C:50:ASP:OD2	2.18	0.44
1:C:108:GLU:HB2	1:C:110:ASN:OD1	2.18	0.44
2:F:170:PRO:HA	2:F:249:VAL:O	2.18	0.44
1:B:33:TYR:OH	2:F:164:LYS:HE3	2.17	0.43
1:A:25:HIS:CE1	1:A:27:LYS:HZ3	2.36	0.43
2:G:191:TRP:CH2	2:G:231:CYS:HB3	2.53	0.43
1:A:29:PRO:HG3	1:A:61:LYS:HE3	2.00	0.43
1:A:111:ASN:HD21	2:H:254:HIS:CE1	2.37	0.43
1:B:31:ARG:HD3	1:B:60:ILE:HD12	2.00	0.43
2:G:258:LEU:HB2	2:G:353:HIS:CE1	2.53	0.43
1:A:25:HIS:HE1	1:A:27:LYS:HZ2	1.65	0.43
2:E:170:PRO:HA	2:E:249:VAL:O	2.18	0.43
2:E:279:LYS:NZ	2:E:279:LYS:HB3	2.34	0.43
2:F:187:PRO:HB2	2:F:233:VAL:HG12	1.99	0.43
2:E:321:ASP:HA	2:E:324:ILE:CG2	2.49	0.43
2:H:292:LYS:HB2	2:H:312:LEU:HD11	1.99	0.43
2:H:173:ASN:O	2:H:221:VAL:HG22	2.19	0.43
2:E:253:ARG:HD3	2:H:253:ARG:O	2.19	0.43
2:H:158:ASN:C	2:H:158:ASN:ND2	2.70	0.43
2:E:151:LYS:HB3	2:E:237:TYR:CE1	2.54	0.43
2:G:329:ILE:HG22	2:G:332:VAL:HG12	2.01	0.43
2:H:255:ARG:HH11	2:H:255:ARG:CG	2.32	0.43
2:E:203:ARG:HD2	2:E:218:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:170:PRO:HA	2:H:249:VAL:O	2.19	0.42
1:B:67:GLU:OE1	2:F:317:VAL:HG23	2.19	0.42
2:E:336:ASP:O	2:E:357:LEU:HD23	2.19	0.42
2:G:179:CYS:HB2	2:G:189:MET:CE	2.46	0.42
2:G:306:LEU:HA	2:G:307:PRO:HD2	1.62	0.42
2:F:274:VAL:HG22	2:F:275:GLU:N	2.34	0.42
2:G:329:ILE:HD11	2:G:340:TYR:CE2	2.54	0.42
2:G:175:VAL:CG2	2:G:221:VAL:HG11	2.49	0.42
1:D:66:ALA:HA	1:D:71:VAL:O	2.20	0.42
2:E:337:ALA:HB2	2:E:359:VAL:HG23	2.02	0.42
2:G:273:ASP:OD1	2:G:330:ARG:HA	2.19	0.42
1:A:57:ASP:O	1:A:60:ILE:HG12	2.19	0.42
2:F:292:LYS:N	2:F:312:LEU:HD11	2.35	0.42
2:G:210:ARG:CZ	2:G:212:GLN:NE2	2.83	0.42
2:G:270:VAL:HG11	2:G:334:PHE:CE1	2.55	0.42
2:G:296:LYS:O	2:G:297:ASN:CB	2.68	0.42
2:H:171:ALA:O	2:H:172:ALA:CB	2.68	0.41
2:F:151:LYS:HA	2:F:184:ASN:ND2	2.34	0.41
2:F:353:HIS:CE1	2:G:219:GLU:HB3	2.55	0.41
2:H:296:LYS:O	2:H:297:ASN:CB	2.65	0.41
1:C:66:ALA:HA	1:C:71:VAL:O	2.20	0.41
2:G:171:ALA:O	2:G:172:ALA:CB	2.68	0.41
2:H:360:LEU:HA	2:H:361:PRO:HD3	1.84	0.41
1:B:111:ASN:ND2	2:G:254:HIS:CE1	2.87	0.41
1:A:25:HIS:HE1	1:A:27:LYS:HG2	1.78	0.41
2:E:175:VAL:CG2	2:E:221:VAL:HG11	2.50	0.41
2:F:253:ARG:HD3	2:G:253:ARG:O	2.20	0.41
2:F:279:LYS:HB3	2:F:279:LYS:HZ2	1.82	0.41
1:C:35:LYS:HD2	1:C:112:TYR:CZ	2.55	0.41
1:D:33:TYR:CE1	2:H:168:ALA:HB3	2.55	0.41
2:G:158:ASN:C	2:G:158:ASN:ND2	2.73	0.41
1:B:36:ASN:HB2	1:B:145:ALA:HA	2.03	0.41
2:E:258:LEU:CD2	2:E:280:VAL:HG22	2.41	0.41
2:E:270:VAL:HG23	2:E:360:LEU:O	2.21	0.41
2:F:175:VAL:CG2	2:F:221:VAL:HG11	2.51	0.41
2:F:189:MET:CE	2:F:191:TRP:HE1	2.34	0.41
2:F:262:LEU:HA	2:F:263:PRO:C	2.40	0.41
2:H:266:ALA:HB1	2:H:274:VAL:HG21	2.02	0.41
1:C:25:HIS:NE2	1:C:27:LYS:HE3	2.36	0.41
1:D:25:HIS:HE1	1:D:27:LYS:HE2	1.83	0.41
1:B:57:ASP:O	1:B:60:ILE:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:199:LYS:HB3	2:E:201:GLU:OE1	2.21	0.40
2:F:175:VAL:HG23	2:F:221:VAL:HG11	2.03	0.40
2:G:255:ARG:HB2	2:G:256:PRO:HD2	2.02	0.40
2:G:336:ASP:O	2:G:357:LEU:HD23	2.21	0.40
1:A:42:ARG:CZ	1:A:52:VAL:HG11	2.51	0.40
2:F:320:THR:O	2:F:323:GLU:OE2	2.40	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	132/155 (85%)	129 (98%)	2 (2%)	1 (1%)	19	23
1	B	131/155 (84%)	128 (98%)	2 (2%)	1 (1%)	19	23
1	C	130/155 (84%)	127 (98%)	2 (2%)	1 (1%)	19	23
1	D	130/155 (84%)	127 (98%)	2 (2%)	1 (1%)	19	23
2	E	196/220 (89%)	187 (95%)	9 (5%)	0	100	100
2	F	196/220 (89%)	187 (95%)	9 (5%)	0	100	100
2	G	213/220 (97%)	197 (92%)	13 (6%)	3 (1%)	11	11
2	H	213/220 (97%)	196 (92%)	14 (7%)	3 (1%)	11	11
All	All	1341/1500 (89%)	1278 (95%)	53 (4%)	10 (1%)	22	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	297	ASN
2	G	362	ALA
2	G	363	PRO
2	H	297	ASN

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Mol	Chain	Res	Type
2	H	362	ALA
2	H	363	PRO
1	A	121	THR
1	B	121	THR
1	C	121	THR
1	D	121	THR

### 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	109/128 (85%)	109 (100%)	0	100	100
1	B	109/128 (85%)	107 (98%)	2 (2%)	59	75
1	C	106/128 (83%)	104 (98%)	2 (2%)	57	73
1	D	106/128 (83%)	105 (99%)	1 (1%)	78	89
2	E	162/187 (87%)	156 (96%)	6 (4%)	34	48
2	F	162/187 (87%)	155 (96%)	7 (4%)	29	40
2	G	175/187 (94%)	168 (96%)	7 (4%)	31	44
2	H	173/187 (92%)	164 (95%)	9 (5%)	23	32
All	All	1102/1260 (88%)	1068 (97%)	34 (3%)	40	55

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	69	ARG
1	B	99	ASP
1	C	36	ASN
1	C	106	ARG
1	D	64	LEU
2	E	186	MET
2	E	212	GLN
2	E	234	GLU
2	E	247	ASP

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Mol	Chain	Res	Type
2	E	312	LEU
2	E	323	GLU
2	F	186	MET
2	F	210	ARG
2	F	212	GLN
2	F	234	GLU
2	F	253	ARG
2	F	279	LYS
2	F	323	GLU
2	G	158	ASN
2	G	210	ARG
2	G	211	ASN
2	G	212	GLN
2	G	253	ARG
2	G	323	GLU
2	G	356	TRP
2	H	158	ASN
2	H	201	GLU
2	H	210	ARG
2	H	212	GLN
2	H	247	ASP
2	H	253	ARG
2	H	323	GLU
2	H	324	ILE
2	H	356	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	36	ASN
1	B	36	ASN
1	C	36	ASN
1	D	36	ASN
1	D	59	HIS
2	E	184	ASN
2	E	202	HIS
2	E	212	GLN
2	E	213	HIS
2	E	318	ASN
2	E	353	HIS
2	F	158	ASN

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Mol	Chain	Res	Type
2	F	184	ASN
2	F	202	HIS
2	F	212	GLN
2	F	254	HIS
2	F	293	HIS
2	F	318	ASN
2	G	150	ASN
2	G	158	ASN
2	G	167	HIS
2	G	184	ASN
2	G	202	HIS
2	G	211	ASN
2	G	212	GLN
2	G	254	HIS
2	G	293	HIS
2	H	158	ASN
2	H	184	ASN
2	H	202	HIS
2	H	212	GLN
2	H	213	HIS
2	H	254	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 monosaccharides in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.