



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:52 PM GMT

PDB ID : 1CVS  
Title : CRYSTAL STRUCTURE OF A DIMERIC FGF2-FGFR1 COMPLEX  
Authors : Plotnikov, A.N.; Schlessinger, J.; Hubbard, S.R.; Mohammadi, M.  
Deposited on : 1999-08-24  
Resolution : 2.80 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

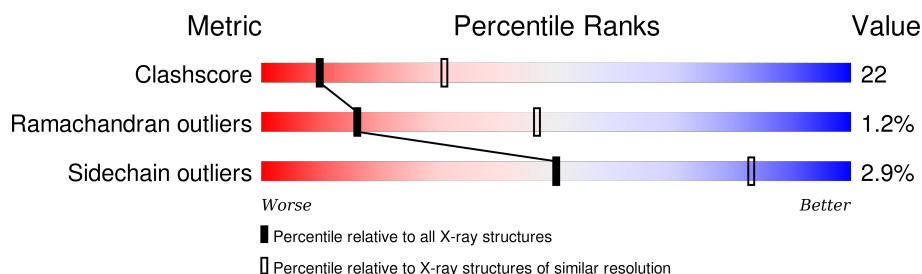
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	132	 61% 36% ..
1	B	132	 60% 36% ..
2	C	225	 55% 36% • 6%
2	D	225	 47% 38% • 13%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5173 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 FIBROBLAST GROWTH FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1040	660	190	186	4			
1	B	129	Total	C	N	O	S	0	0	0
			1040	660	190	186	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	SER	CYS	ENGINEERED MUTATION	UNP P09038
A	87	SER	CYS	ENGINEERED MUTATION	UNP P09038
B	69	SER	CYS	ENGINEERED MUTATION	UNP P09038
B	87	SER	CYS	ENGINEERED MUTATION	UNP P09038

- Molecule 2 is a protein called FIBROBLAST GROWTH FACTOR RECEPTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	211	Total	C	N	O	S	0	0	0
			1588	1015	270	294	9			
2	D	196	Total	C	N	O	S	0	0	0
			1485	951	252	273	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	185	GLN	ASN	ENGINEERED MUTATION	UNP P11362
D	185	GLN	ASN	ENGINEERED MUTATION	UNP P11362

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



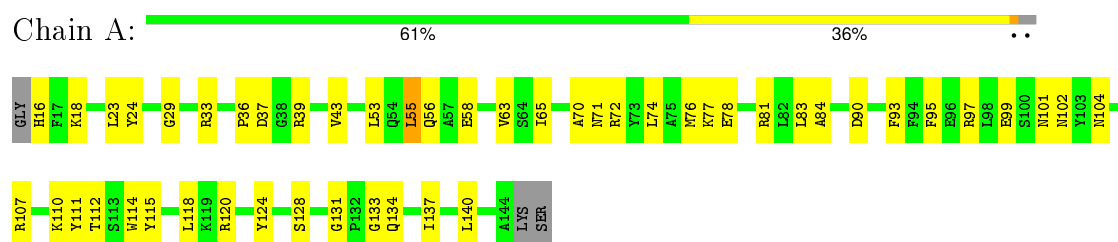
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

### 3 Residue-property plots

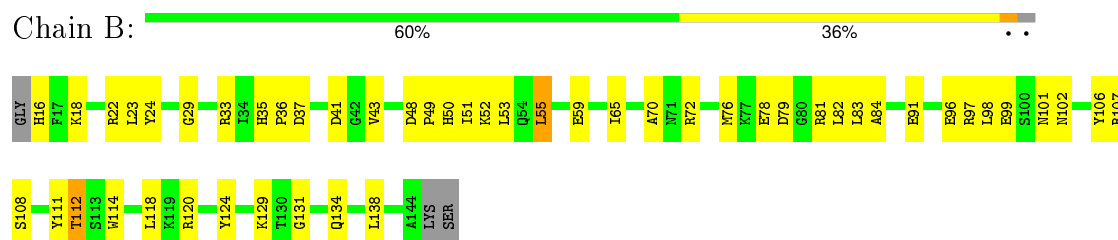
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

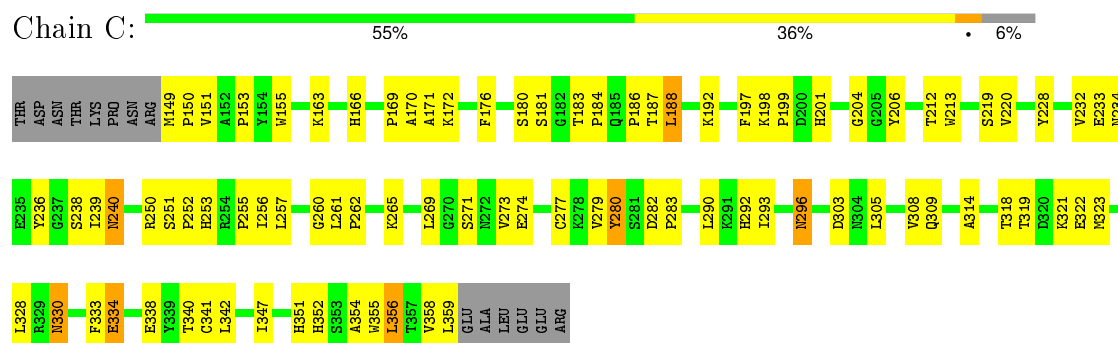
#### • Molecule 1: FIBROBLAST GROWTH FACTOR 2



#### • Molecule 1: FIBROBLAST GROWTH FACTOR 2



#### • Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 1



#### • Molecule 2: FIBROBLAST GROWTH FACTOR RECEPTOR 1



THR	THR
ASP	ASP
ASN	ASN
THR	THR
LYS	LYS
PRO	PRO
ASN	ASN
ARG	ARG
M149	M149
P153	P153
Y154	Y154
H155	H155
T156	T156
M161	M161
E162	E162
K163	K163
K164	K164
L165	L165
H166	H166
A170	A170
A171	A171
K175	K175
C178	C178
P179	P179
S180	S180
S181	S181
G182	G182
T183	T183
P184	P184
Q185	Q185
P186	P186
T187	T187
L188	L188
R189	R189
H190	H190
F197	F197
K198	K198
P199	P199
D200	D200
H201	H201
R202	R202
I203	I203
Y206	Y206
T212	T212
I215	I215
LYS	LYS
I219	I219
GLY	GLY
PRO	PRO
ASP	ASP
ASN	ASN
C230	C230
I231	I231
V232	V232
E233	E233
N234	N234
E235	E235
Y236	Y236
I239	I239
L245	L245
D246	D246
V247	V247
R250	R250
S251	S251
P252	P252
H253	H253
R254	R254
P255	P255
L256	L256
L257	L257
P262	P262
K265	K265
L269	L269
G270	G270
S271	S271
N272	N272
V273	V273
E274	E274
F275	F275
K278	K278
V279	V279
Y280	Y280
S281	S281
D282	D282
P283	P283
Q284	Q284
P285	P285
H286	H286
L287	L287
Q288	Q288
K291	K291
H292	H292
I292	I292
GLU	GLU
VAL	VAL
ASN	ASN
GLY	GLY
SER	SER
LYS	LYS
I299	I299
GLY	GLY
PRO	PRO
ASP	ASP
ASN	ASN
C230	C230
LEU	LEU
PRO	PRO
TYR	TYR
V308	V308
L311	L311
K312	K312
T313	T313
A314	A314
T318	T318
T319	T319
D320	D320
K321	K321
E322	E322
K323	K323
E324	E324
V325	V325
L326	L326
H327	H327
L328	L328
R329	R329
N330	N330
E338	E338
R339	R339
T340	T340
C341	C341
L342	L342
N345	N345
H351	H351
H352	H352
S353	S353
A354	A354
K355	K355
L356	L356
T357	T357
V358	V358
L359	L359
GLU	GLU
ALA	ALA
LEU	LEU
GLU	GLU
GLU	GLU
ARG	ARG

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.45Å 98.45Å 197.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80	Depositor
% Data completeness (in resolution range)	96.9 (25.00-2.80)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.240 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5173	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.45	0/1063	0.69	0/1425
1	B	0.46	0/1063	0.69	0/1425
2	C	0.44	0/1635	0.70	0/2244
2	D	0.42	0/1528	0.68	0/2092
All	All	0.44	0/5289	0.69	0/7186

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	C	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	280	TYR	Sidechain
2	D	280	TYR	Sidechain



## 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	1040	0	1040	37	0
1	B	1040	0	1040	46	0
2	C	1588	0	1499	68	0
2	D	1485	0	1409	84	0
3	A	10	0	0	1	0
3	B	10	0	0	1	0
All	All	5173	0	4988	224	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 22.

All (224) 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:B:82:LEU:HD12	1:B:124:TYR:HB2	1.59	0.84
2:C:240:ASN:HD22	2:C:240:ASN:C	1.82	0.82
2:C:293:ILE:HD11	2:C:309:GLN:HB2	1.61	0.82
2:D:342:LEU:HD22	2:D:351:HIS:CB	2.13	0.79
1:A:133:GLY:HA3	2:D:200:ASP:HA	1.65	0.78
2:C:260:GLY:O	2:C:261:LEU:HD23	1.83	0.78
1:A:140:LEU:HD13	2:C:169:PRO:HD3	1.66	0.78
2:D:319:THR:HG22	2:D:321:LYS:H	1.50	0.76
2:D:185:GLN:HA	2:D:185:GLN:NE2	2.03	0.73
2:D:190:TRP:CZ3	2:D:230:CYS:HB3	2.23	0.73
2:D:203:ILE:N	2:D:203:ILE:HD13	2.04	0.73
2:D:342:LEU:HD22	2:D:351:HIS:HB3	1.72	0.70
2:C:172:LYS:O	2:C:220:VAL:HG22	1.92	0.70
2:D:203:ILE:H	2:D:203:ILE:HD13	1.56	0.69
2:C:282:ASP:HB3	2:C:283:PRO:CD	2.22	0.68
2:C:314:ALA:HB2	2:C:323:MET:HG3	1.75	0.68
2:C:233:GLU:HG3	2:C:238:SER:HB3	1.76	0.68
2:D:262:PRO:HG2	2:D:354:ALA:HB2	1.75	0.68
2:D:203:ILE:H	2:D:203:ILE:CD1	2.07	0.67
2:D:282:ASP:HB3	2:D:283:PRO:CD	2.26	0.66
2:D:161:MET:HE1	2:D:178:CYS:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:NH1	1:B:43:VAL:HG11	2.13	0.64
2:D:342:LEU:HD22	2:D:351:HIS:HB2	1.80	0.63
2:D:292:HIS:HD2	2:D:338:GLU:HG2	1.64	0.63
2:C:256:ILE:N	2:C:256:ILE:HD12	2.13	0.63
2:C:253:HIS:CE1	2:C:256:ILE:HD11	2.35	0.62
1:A:72:ARG:HD3	1:A:84:ALA:O	1.99	0.62
1:A:24:TYR:OH	2:C:163:LYS:HE3	2.00	0.62
2:D:257:LEU:CD2	2:D:279:VAL:HG22	2.30	0.61
1:B:98:LEU:HD13	2:D:250:ARG:CZ	2.30	0.61
1:B:131:GLY:N	1:B:134:GLN:NE2	2.48	0.61
1:A:118:LEU:HD23	1:A:124:TYR:HA	1.80	0.61
2:D:225:LYS:HE2	2:D:247:VAL:O	2.00	0.61
2:C:240:ASN:ND2	2:C:240:ASN:C	2.54	0.61
1:B:76:MET:HE1	1:B:114:TRP:HB2	1.82	0.61
1:B:76:MET:CE	1:B:114:TRP:HB2	2.30	0.61
1:B:59:GLU:HA	2:D:286:HIS:ND1	2.16	0.60
2:D:271:SER:O	2:D:330:ASN:HA	2.01	0.60
2:C:340:THR:HG22	2:C:342:LEU:HD12	1.83	0.60
2:D:185:GLN:HA	2:D:185:GLN:HE21	1.67	0.60
1:B:55:LEU:CD1	1:B:65:ILE:HG12	2.31	0.60
2:D:358:VAL:O	2:D:359:LEU:HD23	2.02	0.59
2:C:192:LYS:HE2	2:C:228:TYR:OH	2.03	0.59
2:D:319:THR:HG22	2:D:321:LYS:HG3	1.83	0.59
1:B:138:LEU:HD11	2:C:204:GLY:HA2	1.84	0.59
2:C:153:PRO:HA	2:C:181:SER:O	2.03	0.59
2:D:199:PRO:HA	2:D:206:TYR:CE1	2.38	0.59
2:C:170:ALA:O	2:C:171:ALA:HB3	2.02	0.59
2:C:199:PRO:HA	2:C:206:TYR:CE1	2.39	0.58
2:D:319:THR:HG21	2:D:321:LYS:HE3	1.84	0.58
2:D:170:ALA:O	2:D:171:ALA:HB3	2.03	0.58
2:C:257:LEU:HD13	2:C:277:CYS:SG	2.44	0.58
2:D:319:THR:CG2	2:D:321:LYS:HG3	2.34	0.57
1:B:79:ASP:CG	1:B:81:ARG:HH11	2.07	0.57
2:C:273:VAL:HG13	2:C:328:LEU:HB2	1.86	0.57
2:C:319:THR:HG22	2:C:321:LYS:HG3	1.86	0.57
2:C:265:LYS:HB2	2:C:356:LEU:HD23	1.87	0.57
1:B:96:GLU:HG3	1:B:106:TYR:CE1	2.40	0.57
1:A:83:LEU:C	1:A:83:LEU:HD12	2.26	0.56
2:C:338:GLU:HB2	2:C:355:TRP:CZ3	2.40	0.56
2:D:251:SER:HB2	2:D:282:ASP:HB2	1.88	0.56
2:C:197:PHE:O	2:C:206:TYR:OH	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:257:LEU:HB2	2:C:352:HIS:CE1	2.40	0.56
2:D:312:LYS:HG2	2:D:323:MET:SD	2.46	0.56
2:D:203:ILE:N	2:D:203:ILE:CD1	2.68	0.56
1:A:78:GLU:HA	1:A:111:TYR:CZ	2.41	0.56
2:C:180:SER:OG	2:C:232:VAL:HG11	2.06	0.56
2:D:282:ASP:HB3	2:D:283:PRO:HD3	1.87	0.55
2:D:163:LYS:HE2	2:D:166:HIS:CD2	2.40	0.55
1:A:71:ASN:O	1:A:71:ASN:ND2	2.40	0.55
2:C:303:ASP:OD2	2:C:305:LEU:HB2	2.07	0.55
2:D:340:THR:HG22	2:D:342:LEU:HD23	1.88	0.55
2:D:153:PRO:HA	2:D:181:SER:O	2.07	0.55
2:D:185:GLN:CA	2:D:185:GLN:HE21	2.18	0.55
2:D:292:HIS:CD2	2:D:338:GLU:HG2	2.41	0.54
1:B:98:LEU:HD13	2:D:250:ARG:NH2	2.22	0.54
2:D:189:ARG:HG3	2:D:231:ILE:HB	1.90	0.54
2:D:161:MET:CE	2:D:178:CYS:HA	2.37	0.54
1:A:134:GLN:O	1:A:137:ILE:HG12	2.07	0.54
2:D:314:ALA:HB2	2:D:323:MET:HG3	1.88	0.54
1:B:23:LEU:HG	1:B:53:LEU:HD12	1.90	0.54
1:A:78:GLU:HA	1:A:111:TYR:CE1	2.42	0.54
1:B:55:LEU:N	1:B:55:LEU:HD22	2.22	0.53
2:D:279:VAL:HG12	2:D:280:TYR:N	2.22	0.53
2:D:165:LEU:HD12	2:D:166:HIS:N	2.22	0.53
1:B:76:MET:HE2	1:B:108:SER:HB2	1.90	0.53
2:D:342:LEU:CD2	2:D:351:HIS:HB2	2.39	0.52
2:C:282:ASP:HB3	2:C:283:PRO:HD3	1.92	0.52
2:C:255:PRO:C	2:C:256:ILE:HD12	2.28	0.52
1:A:104:ASN:OD1	2:C:250:ARG:NH2	2.37	0.52
1:A:101:ASN:O	1:A:102:ASN:HB2	2.10	0.52
1:A:33:ARG:CZ	1:A:43:VAL:HG11	2.40	0.51
1:B:101:ASN:O	1:B:102:ASN:HB2	2.09	0.51
2:C:150:PRO:HB3	2:C:236:TYR:CZ	2.45	0.51
1:B:76:MET:HE1	1:B:114:TRP:CB	2.40	0.51
1:B:59:GLU:HA	2:D:286:HIS:CE1	2.46	0.51
2:C:149:MET:HG3	2:C:149:MET:O	2.11	0.51
2:C:166:HIS:CG	2:C:176:PHE:HE1	2.29	0.51
2:C:319:THR:CG2	2:C:321:LYS:HG3	2.42	0.50
2:D:325:VAL:O	2:D:325:VAL:HG13	2.11	0.50
1:B:79:ASP:OD2	1:B:81:ARG:HG2	2.12	0.50
1:B:107:ARG:HD2	1:B:112:THR:O	2.13	0.49
2:C:319:THR:HG21	2:C:321:LYS:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:318:THR:HG22	2:D:323:MET:SD	2.52	0.49
2:C:293:ILE:CD1	2:C:309:GLN:HB2	2.38	0.49
2:C:338:GLU:HB2	2:C:355:TRP:CE3	2.47	0.49
2:C:155:TRP:CE2	2:C:239:ILE:HD12	2.48	0.49
1:A:90:ASP:OD2	1:A:110:LYS:HD2	2.12	0.49
2:C:358:VAL:O	2:C:359:LEU:HD23	2.13	0.49
2:D:197:PHE:O	2:D:206:TYR:OH	2.23	0.49
2:C:290:LEU:HD23	2:C:308:VAL:HG11	1.95	0.49
2:C:262:PRO:HG2	2:C:354:ALA:HB2	1.95	0.48
2:C:296:ASN:OD1	2:C:296:ASN:N	2.45	0.48
2:C:261:LEU:HA	2:C:262:PRO:C	2.33	0.48
1:A:58:GLU:HG2	1:A:93:PHE:CE1	2.49	0.48
1:A:33:ARG:CZ	1:A:43:VAL:CG1	2.92	0.48
1:A:36:PRO:HA	1:A:70:ALA:CB	2.44	0.48
1:B:48:ASP:HB3	1:B:51:ILE:HG23	1.96	0.48
1:B:120:ARG:HG3	3:B:2:SO4:O2	2.14	0.47
1:A:55:LEU:CD2	1:A:55:LEU:N	2.77	0.47
2:D:170:ALA:O	2:D:171:ALA:CB	2.63	0.47
2:C:257:LEU:HD12	2:C:352:HIS:HB2	1.97	0.47
2:C:198:LYS:H	2:C:201:HIS:CE1	2.32	0.47
2:C:234:ASN:C	2:C:234:ASN:OD1	2.53	0.47
1:A:65:ILE:HD12	1:A:74:LEU:HD23	1.97	0.47
2:C:271:SER:O	2:C:330:ASN:HA	2.15	0.47
1:A:81:ARG:HB2	1:A:124:TYR:OH	2.16	0.46
1:B:37:ASP:OD1	1:B:37:ASP:C	2.54	0.46
2:D:269:LEU:HD23	2:D:270:GLY:N	2.31	0.46
1:B:131:GLY:H	1:B:134:GLN:NE2	2.13	0.46
2:D:178:CYS:N	2:D:179:PRO:HD3	2.31	0.46
2:C:253:HIS:CE1	2:C:256:ILE:CD1	2.98	0.46
2:D:155:TRP:CZ3	2:D:178:CYS:HB3	2.50	0.46
2:D:189:ARG:CG	2:D:231:ILE:HB	2.45	0.46
2:D:291:LYS:HB2	2:D:311:LEU:HD11	1.96	0.46
2:D:273:VAL:HG13	2:D:328:LEU:HB2	1.97	0.46
1:B:82:LEU:HD12	1:B:124:TYR:CB	2.37	0.46
2:D:255:PRO:HD3	2:D:345:ASN:ND2	2.31	0.46
2:D:212:THR:HG22	2:D:212:THR:O	2.16	0.46
2:C:233:GLU:HG3	2:C:238:SER:CB	2.45	0.45
2:D:287:ILE:HG22	2:D:288:GLN:N	2.30	0.45
1:B:36:PRO:HA	1:B:70:ALA:CB	2.46	0.45
1:A:97:ARG:HD3	1:A:99:GLU:OE1	2.16	0.45
2:D:356:LEU:HD23	2:D:357:THR:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:ALA:O	2:C:171:ALA:CB	2.64	0.45
2:D:272:ASN:OD1	2:D:329:ARG:HA	2.17	0.45
1:B:16:HIS:CE1	1:B:18:LYS:CB	3.00	0.45
2:C:233:GLU:CG	2:C:238:SER:HB3	2.46	0.45
2:D:184:PRO:HD2	2:D:236:TYR:HE1	1.81	0.45
2:D:265:LYS:HG2	2:D:275:PHE:CE1	2.51	0.45
1:B:48:ASP:OD2	1:B:49:PRO:HD2	2.16	0.45
2:D:318:THR:HG23	2:D:322:GLU:HG3	1.97	0.45
1:B:76:MET:O	1:B:91:GLU:HB3	2.17	0.45
1:B:24:TYR:CZ	1:B:29:GLY:HA2	2.52	0.45
1:A:115:TYR:HB2	1:A:137:ILE:HG22	1.99	0.45
1:B:59:GLU:HA	2:D:286:HIS:CG	2.52	0.44
2:C:319:THR:HG22	2:C:321:LYS:H	1.82	0.44
2:D:190:TRP:CH2	2:D:230:CYS:HB3	2.53	0.44
2:D:163:LYS:HE2	2:D:166:HIS:CG	2.52	0.44
2:C:334:GLU:HG3	2:C:334:GLU:H	1.52	0.44
2:D:318:THR:CG2	2:D:323:MET:SD	3.05	0.44
2:D:163:LYS:HG2	2:D:163:LYS:O	2.17	0.44
2:D:281:SER:HB3	2:D:285:PRO:HD3	2.00	0.44
2:C:279:VAL:HG12	2:C:280:TYR:N	2.31	0.44
1:B:81:ARG:HB2	1:B:124:TYR:OH	2.16	0.44
2:D:187:THR:O	2:D:232:VAL:HA	2.18	0.44
1:A:33:ARG:NH1	1:A:43:VAL:HG11	2.33	0.44
2:C:187:THR:O	2:C:232:VAL:HA	2.18	0.43
1:A:55:LEU:HD22	1:A:55:LEU:N	2.33	0.43
1:B:48:ASP:CG	1:B:49:PRO:HD2	2.38	0.43
2:D:183:THR:HA	2:D:184:PRO:C	2.37	0.43
2:D:327:HIS:O	2:D:328:LEU:HD23	2.19	0.43
2:D:234:ASN:OD1	2:D:234:ASN:C	2.57	0.43
1:B:35:HIS:HE2	1:B:41:ASP:CG	2.20	0.43
2:D:288:GLN:HG3	2:D:312:LYS:O	2.18	0.43
2:C:188:LEU:HD12	2:C:213:TRP:HA	2.00	0.43
1:A:120:ARG:HG3	3:A:3:SO4:O2	2.19	0.43
1:A:55:LEU:HD13	1:A:65:ILE:HG12	2.00	0.43
1:B:22:ARG:HH12	1:B:52:LYS:HE2	1.84	0.43
1:B:99:GLU:HB2	1:B:101:ASN:OD1	2.19	0.43
2:D:156:THR:HG23	2:D:180:SER:C	2.38	0.43
1:B:72:ARG:HB3	1:B:84:ALA:HB1	2.00	0.43
1:A:23:LEU:HG	1:A:53:LEU:HD12	2.01	0.43
2:D:175:LYS:HA	2:D:215:ILE:O	2.19	0.43
1:B:83:LEU:C	1:B:83:LEU:HD12	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:183:THR:HA	2:C:184:PRO:C	2.38	0.42
2:C:314:ALA:CB	2:C:323:MET:HG3	2.48	0.42
1:B:78:GLU:HA	1:B:111:TYR:CZ	2.55	0.42
2:D:257:LEU:HB2	2:D:352:HIS:CE1	2.54	0.42
1:B:36:PRO:HA	1:B:70:ALA:HB1	2.02	0.42
1:A:95:PHE:HD1	1:A:107:ARG:CZ	2.33	0.42
2:C:282:ASP:HB3	2:C:283:PRO:HD2	2.02	0.42
1:A:36:PRO:HA	1:A:70:ALA:HB1	2.00	0.42
1:B:49:PRO:HG2	1:B:50:HIS:CD2	2.54	0.42
2:C:269:LEU:HD12	2:C:333:PHE:CD2	2.55	0.42
2:C:250:ARG:HB3	2:C:282:ASP:OD1	2.20	0.42
2:D:279:VAL:CG1	2:D:280:TYR:N	2.83	0.42
2:C:341:CYS:O	2:C:351:HIS:HA	2.20	0.42
1:B:97:ARG:HD3	1:B:99:GLU:OE1	2.20	0.41
1:A:16:HIS:CE1	1:A:18:LYS:CB	3.03	0.41
2:C:273:VAL:HG22	2:C:274:GLU:N	2.35	0.41
1:A:37:ASP:OD2	1:A:39:ARG:NE	2.53	0.41
1:A:24:TYR:CZ	1:A:29:GLY:HA2	2.55	0.41
2:D:257:LEU:HD23	2:D:279:VAL:HG22	2.01	0.41
2:C:155:TRP:CD2	2:C:239:ILE:HD12	2.55	0.41
1:B:124:TYR:C	1:B:124:TYR:CD1	2.94	0.41
1:A:77:LYS:HG2	1:A:81:ARG:O	2.21	0.41
2:D:188:LEU:HD22	2:D:189:ARG:N	2.36	0.41
2:D:189:ARG:HE	2:D:231:ILE:HG21	1.86	0.41
1:A:56:GLN:O	1:A:63:VAL:HA	2.21	0.41
2:C:292:HIS:CD2	2:C:338:GLU:HG2	2.55	0.41
1:A:76:MET:HE3	1:A:114:TRP:HB2	2.02	0.41
1:B:129:LYS:HE3	1:B:129:LYS:HB2	1.91	0.41
2:D:155:TRP:HZ3	2:D:178:CYS:HB3	1.86	0.41
1:B:55:LEU:HD12	1:B:65:ILE:HG12	1.99	0.41
2:C:186:PRO:HB2	2:C:232:VAL:HG12	2.03	0.41
1:A:131:GLY:O	1:A:137:ILE:HD13	2.21	0.41
2:D:254:ARG:HG2	2:D:254:ARG:HH11	1.84	0.41
2:C:252:PRO:C	2:C:347:ILE:HD13	2.41	0.41
1:B:118:LEU:HD23	1:B:124:TYR:HA	2.02	0.41
2:C:149:MET:O	2:C:151:VAL:HG23	2.21	0.41
2:D:253:HIS:CE1	2:D:256:ILE:HD13	2.55	0.40
1:A:133:GLY:HA2	2:D:202:ARG:O	2.21	0.40
2:D:166:HIS:O	2:D:245:LEU:HD12	2.22	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	127/132 (96%)	121 (95%)	5 (4%)	1 (1%)	24	58
1	B	127/132 (96%)	121 (95%)	5 (4%)	1 (1%)	24	58
2	C	209/225 (93%)	195 (93%)	10 (5%)	4 (2%)	10	32
2	D	192/225 (85%)	183 (95%)	7 (4%)	2 (1%)	19	52
All	All	655/714 (92%)	620 (95%)	27 (4%)	8 (1%)	16	47

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	B	112	THR
2	C	330	ASN
2	D	330	ASN
2	C	296	ASN
2	D	219	SER
2	C	219	SER
2	C	251	SER

### 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	110/113 (97%)	108 (98%)	2 (2%)	66	91
1	B	110/113 (97%)	109 (99%)	1 (1%)	84	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	168/198 (85%)	161 (96%)	7 (4%)	36	71
2	D	158/198 (80%)	152 (96%)	6 (4%)	40	74
All	All	546/622 (88%)	530 (97%)	16 (3%)	50	83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	128	SER
1	B	55	LEU
2	C	188	LEU
2	C	212	THR
2	C	240	ASN
2	C	318	THR
2	C	322	GLU
2	C	334	GLU
2	C	356	LEU
2	D	188	LEU
2	D	203	ILE
2	D	239	ILE
2	D	278	LYS
2	D	355	TRP
2	D	356	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	185	GLN
2	C	240	ASN
2	C	241	HIS
2	C	288	GLN
2	C	317	ASN
2	D	166	HIS
2	D	185	GLN
2	D	241	HIS
2	D	284	GLN
2	D	317	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	A	3	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SO4	A	4	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	B	1	-	4,4,4	0.18	0	6,6,6	0.05	0
3	SO4	B	2	-	4,4,4	0.26	0	6,6,6	0.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	3	-	-	0/0/0/0	0/0/0/0
3	SO4	A	4	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	SO4	1	0
3	B	2	SO4	1	0

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.