



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:29 AM UTC

PDB ID : 1DJS / pdb_00001djs
Title : LIGAND-BINDING PORTION OF FIBROBLAST GROWTH FACTOR RECEPTOR 2 IN COMPLEX WITH FGF1
Authors : Stauber, D.J.; Digabriele, A.D.; Hendrickson, W.A.
Deposited on : 1999-12-03
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

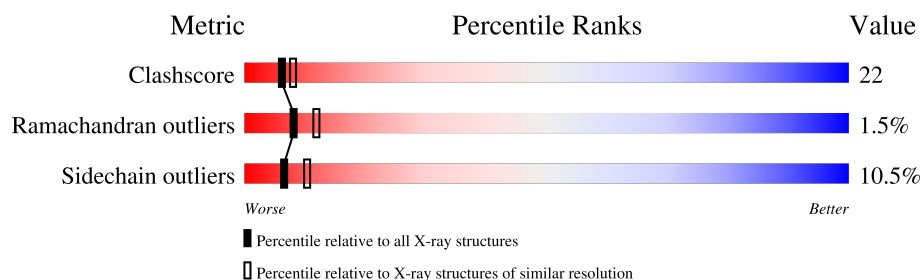
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	216	 53% 29% 11% • 5%
2	B	135	 67% 23% 7% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	403	-	-	X	-
3	SO4	B	409	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3066 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 PROTEIN (FIBROBLAST GROWTH FACTOR RECEPTOR 2).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	Se	0	0	0
			1627	1036	284	299	4	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLY	ARG	engineered mutation	UNP P21802
A	162	MSE	MET	modified residue	UNP P21802
A	186	MSE	MET	modified residue	UNP P21802
A	189	MSE	MET	modified residue	UNP P21802
A	218	MSE	MET	modified residue	UNP P21802

- Molecule 2 is a protein called PROTEIN (FIBROBLAST GROWTH FACTOR 1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	135	Total	C	N	O	S	Se	0	0	0
			1075	677	188	206	3	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MSE	MET	modified residue	UNP P05230

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	189	Total	O	0	0
			189	189		
4	B	130	Total	O	0	0
			130	130		

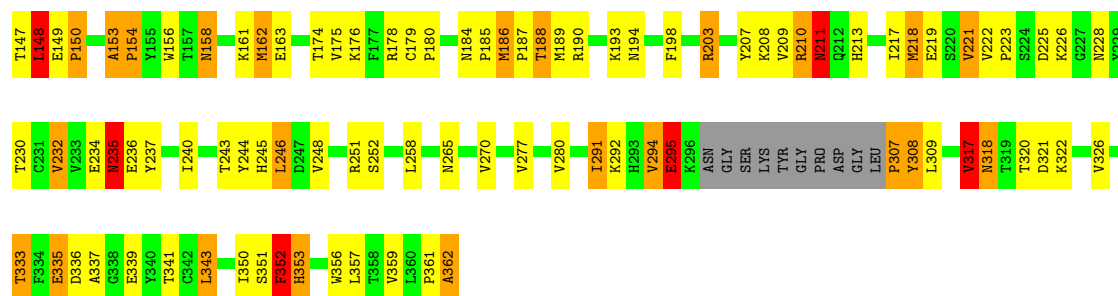
3 Residue-property plots

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. 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.

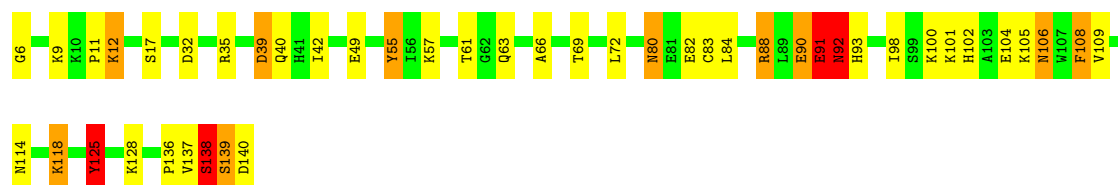
• Molecule 1: PROTEIN (FIBROBLAST GROWTH FACTOR RECEPTOR 2)

Chain A: 



• Molecule 2: PROTEIN (FIBROBLAST GROWTH FACTOR 1)

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	129.97Å 129.97Å 129.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.221 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3066	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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	1.20	5/1667 (0.3%)	1.72	34/2260 (1.5%)
2	B	0.75	0/1098	1.85	30/1479 (2.0%)
All	All	1.05	5/2765 (0.2%)	1.77	64/3739 (1.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	MSE	SE-CE	32.23	2.92	1.95
1	A	162	MSE	CG-SE	16.19	2.44	1.95
1	A	218	MSE	CG-SE	10.10	2.25	1.95
1	A	218	MSE	SE-CE	7.85	2.19	1.95
1	A	189	MSE	SE-CE	-5.50	1.78	1.95

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	MSE	CG-SE-CE	-15.45	64.94	98.92
2	B	91	GLU	CB-CG-CD	14.69	137.57	112.60
1	A	153	ALA	CA-C-O	-14.45	104.97	120.87
2	B	92	ASN	CA-C-N	11.32	139.04	122.74
2	B	92	ASN	C-N-CA	11.32	139.04	122.74
2	B	91	GLU	CA-C-N	11.17	143.29	121.18
2	B	91	GLU	C-N-CA	11.17	143.29	121.18
2	B	91	GLU	CA-CB-CG	10.55	135.20	114.10
1	A	162	MSE	CG-SE-CE	-10.24	76.39	98.92
1	A	218	MSE	CG-SE-CE	-10.24	76.40	98.92
2	B	92	ASN	CA-CB-CG	10.23	122.83	112.60
2	B	92	ASN	CA-C-O	10.00	132.05	119.05
2	B	88	ARG	CD-NE-CZ	9.54	137.76	124.40
2	B	90	GLU	O-C-N	-9.45	112.26	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	91	GLU	O-C-N	-9.35	110.16	122.59
1	A	352	PHE	CA-CB-CG	8.81	122.61	113.80
1	A	162	MSE	CB-CG-SE	-8.17	88.18	112.70
1	A	218	MSE	CB-CG-SE	-8.03	88.60	112.70
1	A	309	LEU	N-CA-C	7.84	122.22	109.59
2	B	91	GLU	CA-C-O	7.72	131.55	120.51
1	A	251	ARG	CD-NE-CZ	7.65	135.11	124.40
1	A	308	TYR	N-CA-C	7.54	126.86	110.80
2	B	92	ASN	N-CA-C	-7.50	104.00	113.01
1	A	153	ALA	O-C-N	7.10	129.12	121.60
1	A	294	VAL	CA-C-N	6.97	134.85	121.54
1	A	294	VAL	C-N-CA	6.97	134.85	121.54
1	A	211	ASN	CA-C-N	6.92	134.75	121.54
1	A	211	ASN	C-N-CA	6.92	134.75	121.54
1	A	235	ASN	CA-CB-CG	6.79	119.39	112.60
1	A	154	PRO	CA-N-CD	-6.67	102.66	112.00
1	A	210	ARG	CD-NE-CZ	6.62	133.66	124.40
1	A	307	PRO	CA-C-N	6.53	134.02	121.54
1	A	307	PRO	C-N-CA	6.53	134.02	121.54
2	B	88	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	A	317	VAL	CB-CA-C	-6.46	103.58	112.04
2	B	138	SER	O-C-N	-6.24	116.45	123.13
1	A	294	VAL	CA-C-O	6.22	128.56	120.78
1	A	234	GLU	N-CA-C	6.14	118.41	109.07
1	A	154	PRO	N-CA-CB	6.05	111.41	103.42
2	B	39	ASP	CA-CB-CG	5.96	118.56	112.60
2	B	32	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	353	HIS	CA-CB-CG	5.93	119.73	113.80
1	A	234	GLU	CA-C-O	5.82	127.61	121.33
2	B	109	VAL	N-CA-C	-5.81	102.04	109.30
1	A	150	PRO	N-CA-C	5.68	120.14	111.34
2	B	138	SER	CA-C-O	5.53	125.22	119.91
2	B	55	TYR	N-CA-CB	5.51	119.55	110.69
1	A	280	VAL	CA-C-O	5.47	127.08	120.67
1	A	307	PRO	CA-N-CD	-5.43	104.40	112.00
2	B	92	ASN	N-CA-CB	5.37	119.79	110.39
1	A	174	THR	N-CA-CB	5.37	119.16	110.41
1	A	188	THR	CB-CA-C	5.33	118.52	109.50
1	A	362	ALA	CA-C-O	-5.27	111.84	120.80
2	B	114	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	198	PHE	CA-CB-CG	5.21	119.01	113.80
2	B	40	GLN	CB-CG-CD	5.14	121.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	258	LEU	CB-CA-C	5.11	117.96	109.53
2	B	125	TYR	N-CA-C	5.06	117.69	111.82
2	B	90	GLU	CA-C-N	5.05	131.19	121.54
2	B	90	GLU	C-N-CA	5.05	131.19	121.54
2	B	49	GLU	N-CA-C	-5.05	107.25	113.41
2	B	106	ASN	OD1-CG-ND2	5.04	127.64	122.60
2	B	138	SER	N-CA-C	5.02	116.36	109.29

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	1627	0	1593	78	0
2	B	1075	0	1052	48	0
3	A	20	0	0	3	0
3	B	25	0	0	5	0
4	A	189	0	0	8	0
4	B	130	0	0	12	0
All	All	3066	0	2645	121	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 (121) 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:A:218:MSE:CE	1:A:218:MSE:SE	2.19	1.41
1:A:218:MSE:SE	1:A:218:MSE:CG	2.25	1.34
1:A:162:MSE:SE	1:A:162:MSE:CG	2.44	1.16
1:A:218:MSE:SE	1:A:218:MSE:CB	2.68	0.90
2:B:6:GLY:HA3	3:B:409:SO4:O3	1.74	0.87
2:B:136:PRO:HG3	2:B:140:ASP:HA	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:MSE:HG2	1:A:186:MSE:CE	2.09	0.82
2:B:88:ARG:NH1	2:B:98:ILE:HG13	1.95	0.81
1:A:230:THR:OG1	1:A:243:THR:HG22	1.83	0.77
1:A:162:MSE:SE	1:A:162:MSE:CB	2.82	0.77
2:B:92:ASN:N	4:B:410:HOH:O	2.18	0.75
2:B:84:LEU:HD23	2:B:100:LYS:HD2	1.69	0.74
1:A:333:THR:HG22	1:A:335:GLU:H	1.55	0.72
2:B:80:ASN:HD22	2:B:82:GLU:H	1.37	0.70
1:A:222:VAL:HB	1:A:223:PRO:HD2	1.76	0.68
1:A:186:MSE:CE	1:A:186:MSE:SE	2.92	0.68
1:A:218:MSE:SE	1:A:218:MSE:HB3	2.43	0.68
1:A:158:ASN:HD21	1:A:161:LYS:H	1.42	0.67
1:A:190:ARG:HB3	1:A:232:VAL:HG22	1.77	0.67
1:A:318:ASN:HD21	2:B:57:LYS:NZ	1.93	0.65
1:A:186:MSE:CE	1:A:186:MSE:CG	2.74	0.65
1:A:218:MSE:CE	1:A:218:MSE:CG	2.75	0.65
1:A:333:THR:HG22	1:A:335:GLU:N	2.11	0.65
2:B:98:ILE:HD11	2:B:108:PHE:CZ	2.32	0.63
1:A:190:ARG:NH2	1:A:232:VAL:HG21	2.13	0.63
1:A:158:ASN:ND2	1:A:161:LYS:H	1.96	0.63
1:A:162:MSE:CG	1:A:162:MSE:CE	2.76	0.62
2:B:72:LEU:HA	4:B:433:HOH:O	2.01	0.61
2:B:91:GLU:CA	4:B:410:HOH:O	2.47	0.61
2:B:101:LYS:HD3	4:B:428:HOH:O	2.01	0.60
2:B:91:GLU:N	4:B:410:HOH:O	2.36	0.58
2:B:88:ARG:HH11	2:B:98:ILE:HG13	1.69	0.58
1:A:336:ASP:O	1:A:357:LEU:HD23	2.03	0.57
1:A:339:GLU:HG3	3:A:403:SO4:O2	2.03	0.57
1:A:221:VAL:HG13	1:A:248:VAL:HG22	1.86	0.57
1:A:184:ASN:HA	1:A:185:PRO:C	2.29	0.57
2:B:98:ILE:HD11	2:B:108:PHE:CE2	2.39	0.57
1:A:203:ARG:NH2	1:A:219:GLU:O	2.38	0.57
1:A:337:ALA:HB2	1:A:359:VAL:HG23	1.87	0.56
2:B:91:GLU:C	4:B:410:HOH:O	2.47	0.56
2:B:102:HIS:HA	2:B:104:GLU:OE2	2.05	0.56
1:A:318:ASN:HD21	2:B:57:LYS:HZ2	1.54	0.56
2:B:139:SER:O	2:B:140:ASP:HB2	2.06	0.56
2:B:136:PRO:CG	2:B:140:ASP:HA	2.33	0.54
1:A:265:ASN:ND2	1:A:356:TRP:H	2.06	0.54
1:A:156:TRP:CE2	1:A:240:ILE:HD12	2.42	0.54
1:A:317:VAL:HG23	4:B:438:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:GLU:HB2	4:B:533:HOH:O	2.06	0.54
1:A:321:ASP:OD1	2:B:9:LYS:HG2	2.07	0.53
2:B:137:VAL:HB	3:B:405:SO4:O3	2.08	0.53
1:A:149:GLU:CB	1:A:150:PRO:HD2	2.38	0.53
1:A:190:ARG:HD2	4:A:555:HOH:O	2.08	0.53
2:B:80:ASN:ND2	2:B:82:GLU:H	2.06	0.53
1:A:162:MSE:SE	1:A:162:MSE:HB2	2.59	0.53
1:A:194:ASN:ND2	1:A:228:ASN:H	2.07	0.52
1:A:208:LYS:CD	1:A:210:ARG:HE	2.22	0.52
2:B:11:PRO:HD2	4:B:490:HOH:O	2.10	0.52
1:A:277:VAL:HG22	1:A:326:VAL:HG22	1.92	0.51
2:B:138:SER:O	2:B:140:ASP:N	2.44	0.51
1:A:154:PRO:HG2	1:A:240:ILE:HG12	1.94	0.50
1:A:162:MSE:HG3	1:A:244:TYR:OH	2.11	0.50
1:A:163:GLU:HG3	2:B:35:ARG:NH1	2.26	0.50
2:B:84:LEU:HD23	2:B:100:LYS:CD	2.41	0.50
1:A:333:THR:CG2	1:A:335:GLU:H	2.22	0.50
1:A:176:LYS:HE2	1:A:178:ARG:NH1	2.26	0.50
1:A:356:TRP:HB2	3:A:403:SO4:O4	2.13	0.49
1:A:353:HIS:HB3	4:A:459:HOH:O	2.12	0.49
2:B:80:ASN:HD22	2:B:82:GLU:N	2.09	0.49
1:A:245:HIS:HB3	4:A:505:HOH:O	2.13	0.49
2:B:118:LYS:HE3	3:B:402:SO4:O1	2.13	0.49
2:B:102:HIS:HB3	2:B:105:LYS:HE3	1.94	0.48
1:A:235:ASN:C	1:A:235:ASN:HD22	2.21	0.48
1:A:149:GLU:HB3	1:A:150:PRO:HD2	1.95	0.47
1:A:203:ARG:NH1	1:A:225:ASP:OD2	2.47	0.47
2:B:90:GLU:O	2:B:92:ASN:N	2.48	0.47
1:A:221:VAL:HG13	1:A:248:VAL:CG2	2.44	0.47
1:A:235:ASN:ND2	1:A:237:TYR:H	2.13	0.47
1:A:208:LYS:HD3	1:A:210:ARG:HE	1.80	0.46
1:A:294:VAL:HB	1:A:295:GLU:CD	2.40	0.46
2:B:72:LEU:HD23	4:B:433:HOH:O	2.15	0.46
2:B:104:GLU:H	2:B:104:GLU:CD	2.23	0.46
2:B:69:THR:HG23	4:B:520:HOH:O	2.15	0.45
2:B:88:ARG:NH2	2:B:125:TYR:OH	2.49	0.45
1:A:158:ASN:HD21	1:A:161:LYS:N	2.12	0.45
1:A:252:SER:HB3	4:A:466:HOH:O	2.16	0.45
2:B:61:THR:OG1	2:B:63:GLN:HG3	2.16	0.45
2:B:39:ASP:O	2:B:42:ILE:HG12	2.17	0.45
2:B:128:LYS:NZ	3:B:408:SO4:O2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:THR:HG21	1:A:335:GLU:OE1	2.17	0.44
2:B:136:PRO:HD2	2:B:140:ASP:OD2	2.17	0.44
1:A:176:LYS:NZ	3:A:406:SO4:O4	2.51	0.44
1:A:203:ARG:NH1	1:A:225:ASP:OD1	2.50	0.44
1:A:226:LYS:HE2	4:A:573:HOH:O	2.18	0.44
1:A:320:THR:HB	4:A:563:HOH:O	2.17	0.43
1:A:211:ASN:HB2	4:A:593:HOH:O	2.18	0.43
1:A:350:ILE:O	1:A:350:ILE:HG13	2.18	0.43
1:A:153:ALA:HA	1:A:235:ASN:HD21	1.84	0.43
1:A:207:TYR:CE2	1:A:209:VAL:HG23	2.53	0.43
1:A:176:LYS:HD2	1:A:217:ILE:HD11	2.00	0.43
1:A:186:MSE:HA	1:A:187:PRO:HD3	1.84	0.43
1:A:291:ILE:HG12	1:A:341:THR:HB	2.00	0.43
2:B:55:TYR:CZ	2:B:84:LEU:HD13	2.54	0.43
1:A:317:VAL:HG13	2:B:55:TYR:CD2	2.53	0.43
1:A:193:LYS:O	1:A:194:ASN:C	2.62	0.42
1:A:361:PRO:O	1:A:362:ALA:CB	2.67	0.42
2:B:91:GLU:HG3	4:B:482:HOH:O	2.18	0.42
1:A:322:LYS:HG3	4:A:471:HOH:O	2.19	0.42
2:B:80:ASN:O	2:B:83:CYS:HB2	2.19	0.42
2:B:80:ASN:HD22	2:B:80:ASN:C	2.28	0.42
2:B:91:GLU:O	2:B:93:HIS:CE1	2.72	0.42
2:B:66:ALA:HB2	2:B:83:CYS:SG	2.60	0.41
2:B:105:LYS:O	2:B:106:ASN:HB2	2.20	0.41
1:A:295:GLU:CD	1:A:295:GLU:H	2.29	0.41
1:A:147:THR:O	1:A:148:LEU:C	2.63	0.41
1:A:236:GLU:HG3	1:A:237:TYR:CE2	2.56	0.41
1:A:343:LEU:HD23	1:A:352:PHE:HB3	2.03	0.40
1:A:246:LEU:HD13	1:A:248:VAL:HG23	2.02	0.40
2:B:12:LYS:HD3	3:B:409:SO4:O2	2.22	0.40
1:A:179:CYS:N	1:A:180:PRO:CD	2.85	0.40
1:A:184:ASN:OD1	1:A:185:PRO:HA	2.22	0.40
1:A:333:THR:HG21	1:A:335:GLU:CD	2.47	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	202/216 (94%)	190 (94%)	9 (4%)	3 (2%)	8	12
2	B	133/135 (98%)	123 (92%)	8 (6%)	2 (2%)	8	12
All	All	335/351 (95%)	313 (93%)	17 (5%)	5 (2%)	8	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	TYR
2	B	91	GLU
2	B	139	SER
1	A	295	GLU
1	A	148	LEU

5.3.2 Protein sidechains [i](#)

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	176/179 (98%)	153 (87%)	23 (13%)	4	5
2	B	118/117 (101%)	110 (93%)	8 (7%)	14	25
All	All	294/296 (99%)	263 (90%)	31 (10%)	6	10

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU

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Mol	Chain	Res	Type
1	A	158	ASN
1	A	175	VAL
1	A	188	THR
1	A	203	ARG
1	A	211	ASN
1	A	213	HIS
1	A	221	VAL
1	A	232	VAL
1	A	235	ASN
1	A	246	LEU
1	A	270	VAL
1	A	291	ILE
1	A	292	LYS
1	A	295	GLU
1	A	307	PRO
1	A	317	VAL
1	A	318	ASN
1	A	333	THR
1	A	335	GLU
1	A	343	LEU
1	A	351	SER
1	A	352	PHE
2	B	12	LYS
2	B	17	SER
2	B	80	ASN
2	B	91	GLU
2	B	92	ASN
2	B	118	LYS
2	B	125	TYR
2	B	138	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	194	ASN
1	A	235	ASN
1	A	242	HIS
1	A	265	ASN
1	A	318	ASN
2	B	80	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	B	408	-	4,4,4	0.67	0	6,6,6	0.29	0
3	SO4	A	404	-	4,4,4	0.61	0	6,6,6	0.30	0
3	SO4	B	405	-	4,4,4	0.61	0	6,6,6	0.33	0
3	SO4	A	406	-	4,4,4	0.68	0	6,6,6	0.17	0
3	SO4	A	407	-	4,4,4	0.64	0	6,6,6	0.22	0
3	SO4	B	409	-	4,4,4	0.34	0	6,6,6	0.76	0
3	SO4	B	402	-	4,4,4	0.61	0	6,6,6	0.27	0
3	SO4	B	401	-	4,4,4	0.53	0	6,6,6	0.37	0
3	SO4	A	403	-	4,4,4	0.47	0	6,6,6	0.22	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.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	408	SO4	1	0
3	B	405	SO4	1	0
3	A	406	SO4	1	0
3	B	409	SO4	2	0
3	B	402	SO4	1	0
3	A	403	SO4	2	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 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.