Full wwPDB X-ray Structure Validation Report (i)

Jun 14, 2020 – 06:31 pm BST

PDB ID	:	2Y5B
Title	:	Structure of USP21 in complex with linear diubiquitin-aldehyde
Authors	:	Ye, Y.; Akutsu, M.; Reyes-Turcu, F.; Enchev, R.I.; Wilkinson, K.D.; Komander, D.
Deposited on	:	2011-01-12
Resolution	:	2.70 Å(reported)

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

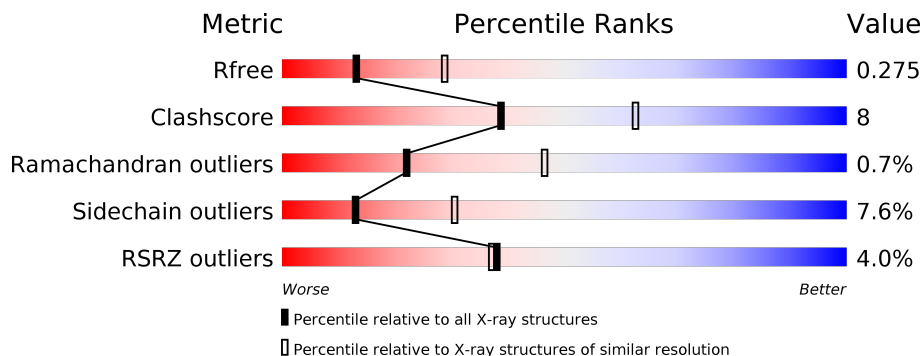|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 >=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	370	64% 19% • 15%
1	E	370	70% 15% • 12%
2	B	152	21% 89% 8% ••
2	F	152	84% 15% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7181 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 UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total 2436	C 1543	N 429	O 449	S 15	0	0	0
1	E	325	Total 2513	C 1584	N 441	O 471	S 17	0	0	0

- Molecule 2 is a protein called UBIQUITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	150	Total 976	C 607	N 179	O 188	S 2	0	0	0
2	F	152	Total 1168	C 736	N 202	O 228	S 2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	HIS	GLY	engineered mutation	UNP P0CG47
F	76	HIS	GLY	engineered mutation	UNP P0CG47

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4
O1

O
‖
O3 O⁻ — S — O⁻ O4
S
‖
O
O2

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

- Molecule 5 is water.

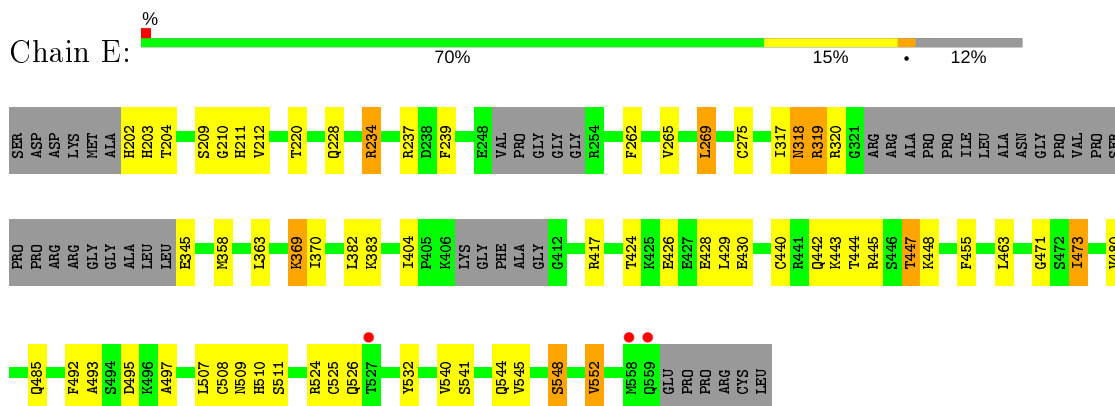| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0
5	B	4	Total 4	O 4	0	0
5	E	12	Total 12	O 12	0	0
5	F	4	Total 4	O 4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

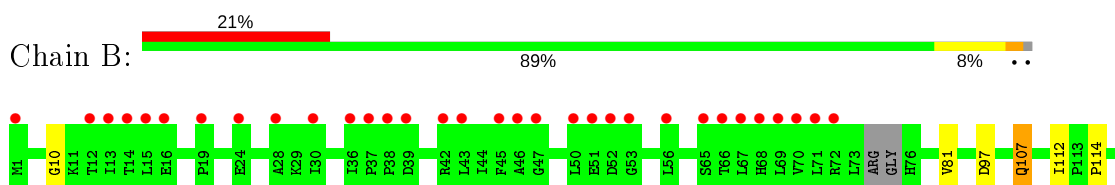- Molecule 1: UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 21

- Molecule 1: UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 21

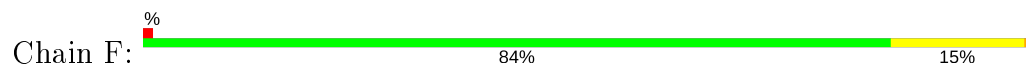- Molecule 2: UBIQUITIN

F121 A122 R130 T131 L132 Q138 L143 L147 R148 L149 G152

• Molecule 2: UBIQUITIN

Chain F:

M1 F4 T22 I36 F45 L50 E51 R54 T55 K63 E64 S65 T66 V70 L71 R72 D97 V102 D108 K109 E110 G111 R118 F121 L126 L132 T142 L143 V146 L149 G152

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.87Å 102.20Å 86.80Å 90.00° 99.82° 90.00°	Depositor
Resolution (Å)	45.00 – 2.70 49.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.3 (45.00-2.70) 90.3 (49.80-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.30 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0098	Depositor
R, R_{free}	0.216 , 0.279 0.216 , 0.275	Depositor DCC
R_{free} test set	1267 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.0	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	7181	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.58% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GLZ, 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	0.38	0/2486	0.54	0/3368
1	E	0.38	0/2564	0.54	0/3472
2	B	0.33	0/981	0.51	0/1338
2	F	0.34	0/1177	0.55	0/1591
All	All	0.36	0/7208	0.54	0/9769

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	2436	0	2302	51	0
1	E	2513	0	2380	35	0
2	B	976	0	808	11	0
2	F	1168	0	1189	14	0
3	A	1	0	0	0	0
3	E	1	0	0	0	0
4	A	35	0	0	0	0
4	B	5	0	0	0	0
4	E	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	5	0	0	0	0
5	A	6	0	0	0	0
5	B	4	0	0	0	0
5	E	12	0	0	0	0
5	F	4	0	0	0	0
All	All	7181	0	6679	104	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 8.

All (104) 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:317:ILE:HG23	1:A:368:SER:HB2	1.49	0.95
1:A:254:ARG:CD	1:A:312:ARG:HH22	1.88	0.87
2:F:51:GLU:HB2	2:F:54:ARG:HG3	1.60	0.81
2:F:63:LYS:HD2	2:F:64:GLU:HG2	1.66	0.77
1:A:254:ARG:HD2	1:A:312:ARG:HH22	1.50	0.75
1:A:239:PHE:CE2	1:A:317:ILE:HD11	2.24	0.73
1:A:254:ARG:HD2	1:A:312:ARG:NH2	2.04	0.72
1:A:213:GLY:HA3	1:A:535:SER:HA	1.69	0.72
1:A:254:ARG:HD3	1:A:312:ARG:HH22	1.55	0.68
1:A:277:ALA:HB2	1:A:535:SER:HB2	1.75	0.66
1:E:428:GLU:HG3	1:E:430:GLU:HG3	1.78	0.66
1:E:525:CYS:SG	1:E:526:GLN:N	2.69	0.65
1:E:485:GLN:HE22	1:E:524:ARG:HH22	1.43	0.65
1:E:318:ASN:HD22	1:E:319:ARG:N	1.96	0.63
1:E:318:ASN:ND2	1:E:320:ARG:H	1.96	0.62
1:E:262:PHE:O	1:E:265:VAL:HG22	2.00	0.62
1:A:314:HIS:HA	1:A:317:ILE:HG22	1.83	0.61
1:E:541:SER:H	1:E:544:GLN:NE2	1.99	0.60
2:B:107:GLN:HG3	2:B:114:PRO:HD3	1.82	0.60
1:E:239:PHE:CD1	1:E:369:LYS:HG3	2.37	0.59
1:A:360:LYS:O	1:A:364:GLU:HG3	2.03	0.58
1:A:377:GLN:HE21	1:A:394:PHE:HB3	1.67	0.58
1:E:508:CYS:HB2	1:E:552:VAL:HG13	1.84	0.58
1:A:292:PRO:O	1:A:295:SER:HB2	2.04	0.57
2:F:121:PHE:HB3	2:F:126:LEU:HD21	1.87	0.57
1:A:461:LEU:HB2	1:A:553:LEU:HB2	1.86	0.57
1:A:264:ASP:OD2	1:A:282:ARG:NH2	2.37	0.57
1:E:424:THR:HG21	1:E:492:PHE:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PHE:HE2	1:A:317:ILE:HD11	1.67	0.57
1:E:510:HIS:CE1	2:F:149:LEU:HD22	2.40	0.57
1:A:259:THR:HG22	1:A:316:GLU:OE1	2.05	0.56
1:E:443:LYS:HD2	2:F:36:ILE:HD11	1.88	0.55
1:E:485:GLN:HE22	1:E:524:ARG:NH2	2.03	0.55
1:E:485:GLN:NE2	1:E:524:ARG:HH22	2.03	0.55
1:A:384:CYS:O	1:A:388:GLY:HA2	2.06	0.55
1:A:476:SER:OG	1:A:478:VAL:HG12	2.07	0.54
2:B:107:GLN:CG	2:B:114:PRO:HD3	2.37	0.54
1:A:522:LEU:HD23	1:A:545:VAL:HG22	1.90	0.54
1:E:212:VAL:HG23	1:E:269:LEU:HD12	1.89	0.53
1:A:216:ASN:HD21	1:A:220:THR:H	1.57	0.53
1:A:317:ILE:HG23	1:A:368:SER:CB	2.31	0.52
2:F:121:PHE:HB2	2:F:143:LEU:HD22	1.92	0.51
1:A:317:ILE:CG2	1:A:368:SER:HB2	2.32	0.51
1:A:394:PHE:CE1	1:A:453:GLN:HG3	2.46	0.51
1:A:504:LEU:HD21	1:A:507:LEU:HD22	1.93	0.51
1:E:471:GLY:HA2	2:F:111:GLY:O	2.11	0.51
1:A:237:ARG:NH1	1:A:238:ASP:OD1	2.44	0.50
1:A:217:LEU:HD21	1:A:281:THR:HA	1.93	0.50
1:E:239:PHE:CE1	1:E:369:LYS:HG3	2.46	0.50
2:B:107:GLN:HG2	2:B:112:ILE:O	2.12	0.50
1:A:424:THR:HG21	1:A:492:PHE:HB3	1.93	0.50
1:E:220:THR:CG2	1:E:220:THR:O	2.60	0.50
1:E:545:VAL:O	1:E:548:SER:HB2	2.12	0.49
1:A:239:PHE:CD1	1:A:369:LYS:HG3	2.48	0.49
1:A:254:ARG:CD	1:A:312:ARG:NH2	2.64	0.49
1:E:318:ASN:HD22	1:E:320:ARG:H	1.60	0.49
1:A:239:PHE:CE1	1:A:369:LYS:HG3	2.48	0.48
2:F:45:PHE:HB3	2:F:50:LEU:HD21	1.96	0.48
2:F:51:GLU:HB2	2:F:54:ARG:CG	2.36	0.48
1:E:234:ARG:HD2	1:E:237:ARG:NH2	2.28	0.48
2:F:102:VAL:HG21	2:F:132:LEU:HD21	1.96	0.48
1:E:228:GLN:HG2	1:E:532:TYR:CG	2.48	0.48
1:A:502:TYR:HB3	1:A:555:TYR:HB3	1.95	0.48
1:E:202:HIS:N	1:E:203:HIS:HA	2.29	0.47
2:F:118:ARG:HB2	2:F:146:VAL:HG23	1.96	0.47
1:E:541:SER:H	1:E:544:GLN:HE21	1.62	0.46
1:E:473:ILE:H	1:E:473:ILE:HD13	1.81	0.45
1:E:440:CYS:SG	1:E:442:GLN:HG2	2.57	0.45
1:A:256:GLN:O	1:A:260:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:448:LYS:HZ1	2:F:142:THR:HG1	1.56	0.45
2:F:4:PHE:HB2	2:F:66:THR:HB	1.99	0.45
1:A:256:GLN:HB3	1:A:259:THR:HG23	1.99	0.45
1:A:216:ASN:ND2	1:A:220:THR:H	2.14	0.45
1:A:514:VAL:HA	2:B:149:LEU:HD12	1.98	0.45
2:B:97:ASP:HB2	2:B:132:LEU:HD22	1.98	0.45
1:A:362:TYR:CE1	1:A:366:GLU:HG3	2.51	0.44
2:B:81:VAL:HG22	2:B:143:LEU:HB2	2.00	0.44
1:A:237:ARG:HD2	1:A:270:TRP:CE2	2.52	0.44
1:A:396:VAL:O	2:B:122:ALA:HA	2.17	0.44
2:F:22:THR:HA	2:F:55:THR:HA	1.99	0.44
1:A:256:GLN:HB3	1:A:259:THR:CG2	2.48	0.44
1:A:475:LYS:HD2	2:B:149:LEU:HD11	1.99	0.43
1:E:404:ILE:HD12	1:E:480:VAL:HG21	2.00	0.43
1:A:524:ARG:HB2	1:A:529:TRP:CE2	2.53	0.43
1:A:291:VAL:HA	1:A:292:PRO:HD3	1.78	0.43
1:A:380:SER:OG	1:A:448:LYS:NZ	2.52	0.43
1:A:258:LEU:HD23	1:A:312:ARG:HB3	2.01	0.42
1:E:455:PHE:HE2	1:E:493:ALA:HB2	1.84	0.42
1:A:394:PHE:HE1	1:A:453:GLN:HG3	1.84	0.42
2:B:149:LEU:HA	2:B:149:LEU:HD12	1.88	0.42
1:E:429:LEU:O	1:E:445:ARG:HA	2.18	0.42
1:A:227:LEU:HD13	1:A:265:VAL:HG11	2.02	0.41
1:A:318:ASN:HD22	1:A:319:ARG:N	2.17	0.41
2:B:147:LEU:HB3	2:B:148:ARG:H	1.70	0.41
1:E:426:GLU:HG2	1:E:447:THR:HG23	2.02	0.41
1:A:312:ARG:NH1	1:A:316:GLU:OE2	2.48	0.41
1:A:468:ALA:HA	1:A:472:SER:O	2.20	0.41
1:A:217:LEU:HD11	1:A:279:ASN:HD21	1.86	0.41
1:E:209:SER:O	1:E:211:HIS:N	2.44	0.41
1:E:455:PHE:CE2	1:E:493:ALA:HB2	2.55	0.41
2:B:121:PHE:HB2	2:B:143:LEU:HD22	2.03	0.41
1:E:317:ILE:HD11	1:E:370:ILE:HG12	2.02	0.41
1:A:404:ILE:HG21	1:A:478:VAL:HG13	2.04	0.40
1:E:493:ALA:HB1	1:E:497:ALA:HB3	2.04	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	305/370 (82%)	282 (92%)	20 (7%)	3 (1%)	15	37
1	E	317/370 (86%)	301 (95%)	14 (4%)	2 (1%)	25	50
2	B	146/152 (96%)	139 (95%)	6 (4%)	1 (1%)	22	46
2	F	150/152 (99%)	148 (99%)	2 (1%)	0	100	100
All	All	918/1044 (88%)	870 (95%)	42 (5%)	6 (1%)	22	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	210	GLY
1	E	275	CYS
1	A	351	ASP
1	A	535	SER
1	A	280	PRO
2	B	10	GLY

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	257/322 (80%)	236 (92%)	21 (8%)	11	26
1	E	268/322 (83%)	245 (91%)	23 (9%)	10	24
2	B	71/137 (52%)	66 (93%)	5 (7%)	15	35
2	F	128/137 (93%)	122 (95%)	6 (5%)	26	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	724/918 (79%)	669 (92%)	55 (8%)	13 30

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	VAL
1	A	215	ARG
1	A	217	LEU
1	A	254	ARG
1	A	279	ASN
1	A	291	VAL
1	A	306	LEU
1	A	308	LEU
1	A	312	ARG
1	A	313	LEU
1	A	318	ASN
1	A	373	LEU
1	A	402	LEU
1	A	417	ARG
1	A	439	ARG
1	A	451	THR
1	A	452	VAL
1	A	459	LEU
1	A	489	LEU
1	A	507	LEU
1	A	514	VAL
2	B	107	GLN
2	B	130	ARG
2	B	132	LEU
2	B	138	GLN
2	B	147	LEU
1	E	204	THR
1	E	234	ARG
1	E	269	LEU
1	E	318	ASN
1	E	319	ARG
1	E	345	GLU
1	E	358	MET
1	E	363	LEU
1	E	369	LYS
1	E	382	LEU
1	E	383	LYS

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Mol	Chain	Res	Type
1	E	417	ARG
1	E	444	THR
1	E	447	THR
1	E	463	LEU
1	E	473	ILE
1	E	495	ASP
1	E	507	LEU
1	E	509	ASN
1	E	511	SER
1	E	540	VAL
1	E	548	SER
1	E	552	VAL
2	F	63	LYS
2	F	66	THR
2	F	70	VAL
2	F	72	ARG
2	F	97	ASP
2	F	110	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	HIS
1	A	216	ASN
1	A	219	ASN
1	A	256	GLN
1	A	279	ASN
1	A	318	ASN
1	A	377	GLN
1	A	453	GLN
1	A	530	HIS
1	A	543	ASN
2	B	136	ASN
1	E	219	ASN
1	E	288	GLN
1	E	318	ASN
1	E	433	ASN
1	E	442	GLN
1	E	485	GLN
1	E	543	ASN
1	E	544	GLN
2	F	2	GLN

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Mol	Chain	Res	Type
2	F	60	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)

2 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
2	GLZ	B	152	1,2	3,3,3	0.53	0	0,2,2	0.00	-
2	GLZ	F	152	1,2	3,3,3	0.53	0	0,2,2	0.00	-

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
2	GLZ	B	152	1,2	-	0/0/1/1	-
2	GLZ	F	152	1,2	-	0/0/1/1	-

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.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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	#$|Z| > 2$
4	SO4	A	1561	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	A	1559	-	4,4,4	0.34	0	6,6,6	0.19	0
4	SO4	A	1565	-	4,4,4	0.37	0	6,6,6	0.14	0
4	SO4	A	1564	-	4,4,4	0.37	0	6,6,6	0.07	0
4	SO4	E	1560	-	4,4,4	0.34	0	6,6,6	0.20	0
4	SO4	A	1563	-	4,4,4	0.34	0	6,6,6	0.19	0
4	SO4	E	1561	-	4,4,4	0.35	0	6,6,6	0.06	0
4	SO4	A	1560	-	4,4,4	0.34	0	6,6,6	0.18	0
4	SO4	F	1152	-	4,4,4	0.39	0	6,6,6	0.09	0
4	SO4	A	1562	-	4,4,4	0.35	0	6,6,6	0.17	0
4	SO4	E	1562	-	4,4,4	0.32	0	6,6,6	0.16	0
4	SO4	B	1152	-	4,4,4	0.37	0	6,6,6	0.12	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.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	315/370 (85%)	-0.24	2 (0%)	89	91	12, 19, 34, 46	0
1	E	325/370 (87%)	-0.19	3 (0%)	84	85	10, 18, 31, 39	0
2	B	149/152 (98%)	0.77	32 (21%)	0	0	12, 25, 61, 67	0
2	F	151/152 (99%)	-0.22	1 (0%)	87	89	12, 20, 28, 36	0
All	All	940/1044 (90%)	-0.06	38 (4%)	38	37	10, 19, 49, 67	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	37	PRO	5.2
2	B	15	LEU	4.7
2	B	47	GLY	4.7
2	B	51	GLU	4.4
2	B	52	ASP	4.3
2	B	14	THR	3.9
2	B	53	GLY	3.8
1	A	254	ARG	3.4
2	B	30	ILE	3.4
1	A	527	THR	3.3
2	B	13	ILE	3.1
2	B	50	LEU	3.1
2	B	12	THR	2.9
2	B	42	ARG	2.8
1	E	559	GLN	2.7
2	B	65	SER	2.7
2	B	69	LEU	2.7
2	B	19	PRO	2.7
2	B	70	VAL	2.6
2	B	45	PHE	2.6
2	B	46	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	66	THR	2.5
2	B	72	ARG	2.5
2	B	36	ILE	2.5
2	B	68	HIS	2.4
2	B	56	LEU	2.4
2	B	71	LEU	2.4
2	F	108	ASP	2.3
2	B	28	ALA	2.3
2	B	67	LEU	2.2
1	E	527	THR	2.2
2	B	43	LEU	2.2
2	B	16	GLU	2.1
2	B	38	PRO	2.1
2	B	24	GLU	2.1
2	B	39	ASP	2.1
2	B	1	MET	2.1
1	E	558	MET	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLZ	B	152	4/4	0.99	0.08	12,12,12,13	0
2	GLZ	F	152	4/4	0.99	0.13	10,10,11,11	0

6.3　Carbohydrates (i)

There are no carbohydrates in this entry.

6.4　Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	B	1152	5/5	0.90	0.19	52,53,54,55	0
4	SO4	E	1562	5/5	0.91	0.27	51,52,53,54	0
4	SO4	A	1562	5/5	0.92	0.17	41,41,42,42	0
4	SO4	A	1564	5/5	0.93	0.16	48,49,50,51	0
4	SO4	F	1152	5/5	0.95	0.23	37,38,40,40	0
4	SO4	A	1565	5/5	0.96	0.15	29,29,29,30	0
4	SO4	A	1563	5/5	0.96	0.15	38,39,39,40	0
4	SO4	E	1561	5/5	0.97	0.14	42,43,44,44	0
4	SO4	E	1560	5/5	0.97	0.10	30,30,31,31	0
4	SO4	A	1561	5/5	0.97	0.11	38,39,39,40	0
4	SO4	A	1559	5/5	0.97	0.14	23,23,23,23	0
4	SO4	A	1560	5/5	0.98	0.11	31,31,31,32	0
3	ZN	A	1000	1/1	0.99	0.09	18,18,18,18	0
3	ZN	E	1000	1/1	1.00	0.05	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.