Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:44 AM GMT

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)

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

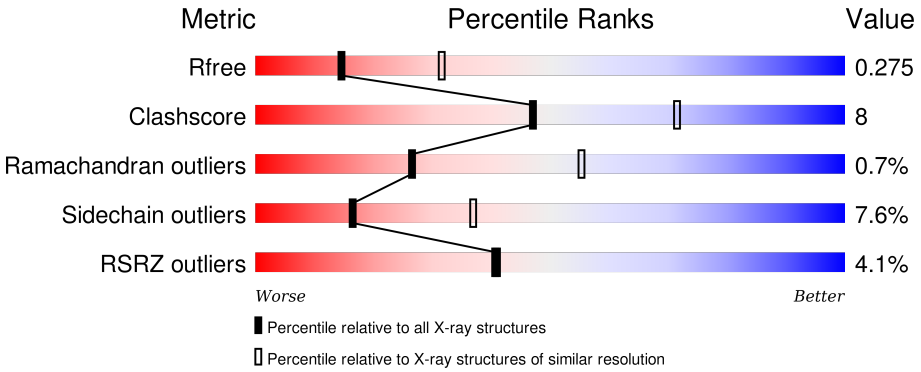
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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. 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% •

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
4	SO4	A	1564	-	-	-	X

2 Entry composition

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	C	N	O	S	0	0	0
			2436	1543	429	449	15			
1	E	325	Total	C	N	O	S	0	0	0
			2513	1584	441	471	17			

- Molecule 2 is a protein called UBIQUITIN.

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

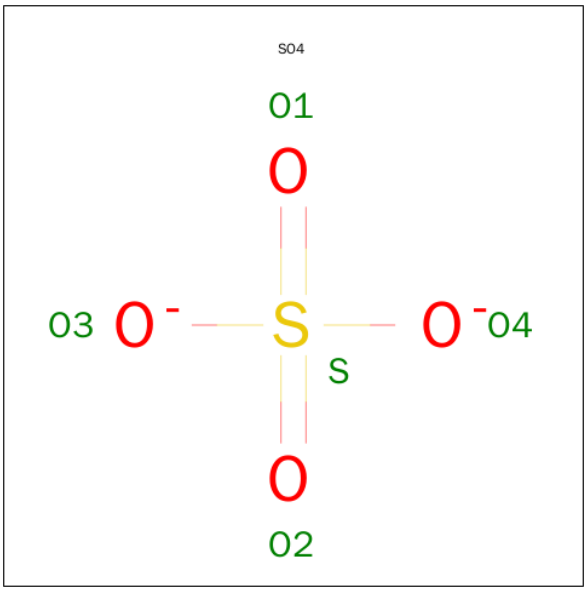
There are 2 discrepancies between the modelled and reference sequences:

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	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		

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



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

- Molecule 5 is water.

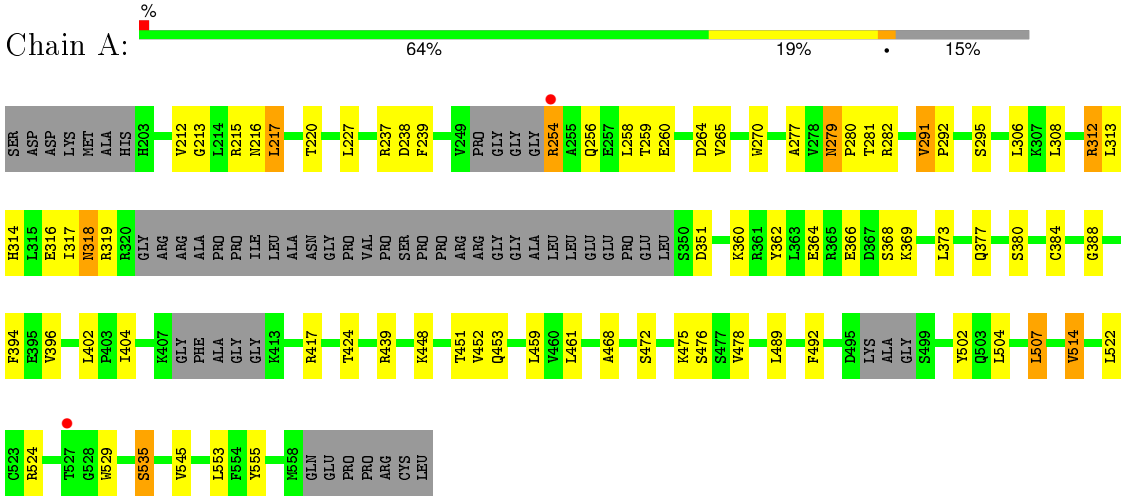
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total O 6 6	0	0
5	B	4	Total O 4 4	0	0
5	E	12	Total O 12 12	0	0
5	F	4	Total O 4 4	0	0

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 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.

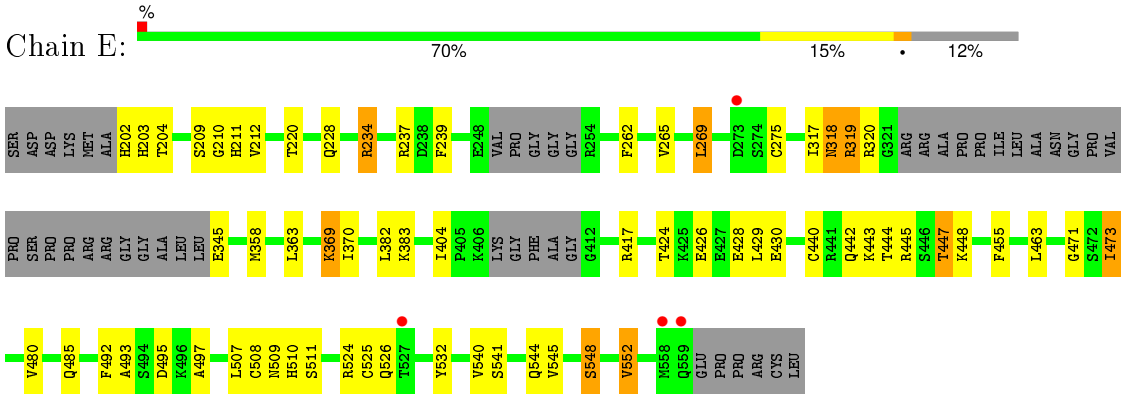
- Molecule 1: UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 21

Chain A:



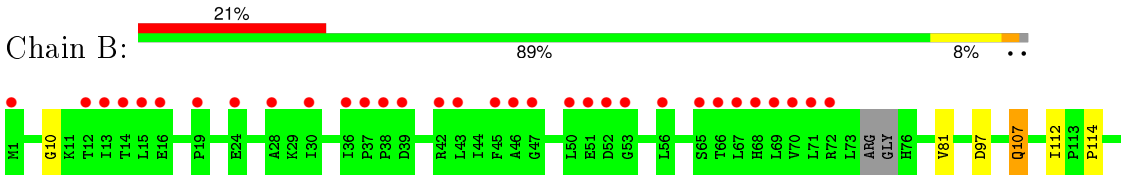
- Molecule 1: UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 21

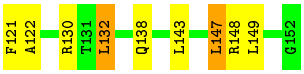
Chain E:



- Molecule 2: UBIQUITIN

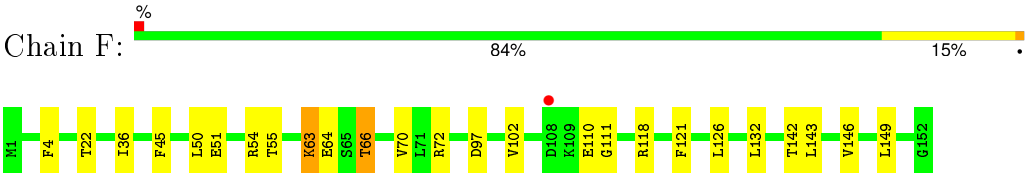
Chain B:





• Molecule 2: UBIQUITIN

Chain F:



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 (5.39%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 24823 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:E:239:PHE:CE1	1:E:369:LYS:HG3	2.46	0.50
1:A:217:LEU:HD21	1:A:281:THR:HA	1.93	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:51:GLU:HB2	2:F:54:ARG:CG	2.36	0.48
2:F:45:PHE:HB3	2:F:50:LEU:HD21	1.96	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

Continued on next page...

Continued from previous page...

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
2:B:97:ASP:HB2	2:B:132:LEU:HD22	1.98	0.45
1:A:514:VAL:HA	2:B:149:LEU:HD12	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
1:E:426:GLU:HG2	1:E:447:THR:HG23	2.02	0.41
2:B:147:LEU:HB3	2:B:148:ARG:H	1.70	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:455:PHE:CE2	1:E:493:ALA:HB2	2.55	0.41
1:E:209:SER:O	1:E:211:HIS:N	2.44	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%)	19	45
1	E	317/370 (86%)	301 (95%)	14 (4%)	2 (1%)	30	59
2	B	146/152 (96%)	139 (95%)	6 (4%)	1 (1%)	26	55
2	F	150/152 (99%)	148 (99%)	2 (1%)	0	100	100
All	All	918/1044 (88%)	870 (95%)	42 (5%)	6 (1%)	26	55

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%)	14	32
1	E	268/322 (83%)	245 (91%)	23 (9%)	13	29
2	B	71/137 (52%)	66 (93%)	5 (7%)	19	42
2	F	128/137 (93%)	122 (95%)	6 (5%)	32	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	724/918 (79%)	669 (92%)	55 (8%)	16 37

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	60	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	0.57	0	0,2,2	0.00	-
2	GLZ	F	152	1,2	3,3,3	0.57	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	0/0/0/0
2	GLZ	F	152	1,2	-	0/0/1/1	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.

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	1559	-	4,4,4	0.35	0	6,6,6	0.18	0
4	SO4	A	1560	-	4,4,4	0.38	0	6,6,6	0.21	0
4	SO4	A	1561	-	4,4,4	0.37	0	6,6,6	0.07	0
4	SO4	A	1562	-	4,4,4	0.39	0	6,6,6	0.17	0
4	SO4	A	1563	-	4,4,4	0.39	0	6,6,6	0.13	0
4	SO4	A	1564	-	4,4,4	0.44	0	6,6,6	0.10	0
4	SO4	A	1565	-	4,4,4	0.40	0	6,6,6	0.18	0
4	SO4	B	1152	-	4,4,4	0.44	0	6,6,6	0.14	0
4	SO4	E	1560	-	4,4,4	0.39	0	6,6,6	0.20	0
4	SO4	E	1561	-	4,4,4	0.38	0	6,6,6	0.09	0
4	SO4	E	1562	-	4,4,4	0.36	0	6,6,6	0.19	0
4	SO4	F	1152	-	4,4,4	0.49	0	6,6,6	0.09	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
4	SO4	A	1559	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1560	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1561	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1562	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1563	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1564	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1565	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1152	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	E	1560	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1561	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1562	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1152	-	-	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.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.20	2 (0%) 90 91	12, 19, 34, 46	0
1	E	325/370 (87%)	-0.16	4 (1%) 81 81	10, 18, 31, 39	0
2	B	149/152 (98%)	0.81	32 (21%) 1 1	12, 25, 61, 67	0
2	F	151/152 (99%)	-0.18	1 (0%) 89 90	12, 20, 28, 36	0
All	All	940/1044 (90%)	-0.02	39 (4%) 41 41	10, 19, 49, 67	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	37	PRO	5.3
2	B	47	GLY	4.8
2	B	15	LEU	4.7
2	B	51	GLU	4.5
2	B	52	ASP	4.4
2	B	14	THR	4.0
2	B	53	GLY	3.9
1	A	254	ARG	3.4
1	A	527	THR	3.4
2	B	30	ILE	3.4
2	B	50	LEU	3.1
2	B	13	ILE	3.1
2	B	12	THR	3.0
2	B	42	ARG	2.9
2	B	65	SER	2.8
1	E	559	GLN	2.8
2	B	19	PRO	2.8
2	B	69	LEU	2.7
2	B	70	VAL	2.7
2	B	46	ALA	2.7
2	B	45	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	66	THR	2.6
2	B	72	ARG	2.6
2	B	68	HIS	2.5
2	B	36	ILE	2.5
2	F	108	ASP	2.5
2	B	56	LEU	2.4
2	B	71	LEU	2.4
2	B	28	ALA	2.3
1	E	527	THR	2.3
2	B	67	LEU	2.3
2	B	39	ASP	2.2
2	B	24	GLU	2.2
2	B	43	LEU	2.2
2	B	16	GLU	2.2
2	B	1	MET	2.2
2	B	38	PRO	2.2
1	E	558	MET	2.1
1	E	273	ASP	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	A	1564	5/5	0.93	0.16	2.00	48,49,50,51	0
4	SO4	A	1565	5/5	0.96	0.15	-0.29	29,29,29,30	0
4	SO4	E	1561	5/5	0.97	0.14	-0.63	42,43,44,44	0
4	SO4	A	1563	5/5	0.96	0.15	-0.67	38,39,39,40	0
3	ZN	A	1000	1/1	0.99	0.09	-1.24	18,18,18,18	0
4	SO4	A	1559	5/5	0.97	0.14	-1.65	23,23,23,23	0
4	SO4	A	1560	5/5	0.98	0.11	-1.81	31,31,31,32	0
3	ZN	E	1000	1/1	1.00	0.05	-2.79	19,19,19,19	0
4	SO4	A	1561	5/5	0.97	0.11	-	38,39,39,40	0
4	SO4	F	1152	5/5	0.95	0.23	-	37,38,40,40	0
4	SO4	A	1562	5/5	0.92	0.17	-	41,41,42,42	0
4	SO4	E	1562	5/5	0.91	0.27	-	51,52,53,54	0
4	SO4	E	1560	5/5	0.97	0.10	-	30,30,31,31	0
4	SO4	B	1152	5/5	0.90	0.19	-	52,53,54,55	0

6.5 Other polymers (i)

There are no such residues in this entry.