



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:22 PM GMT

PDB ID : 1FCF  
Title : PHOTOSYSTEM II D1 C-TERMINAL PROCESSING PROTEASE  
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Deposited on : 2000-07-18  
Resolution : 2.10 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

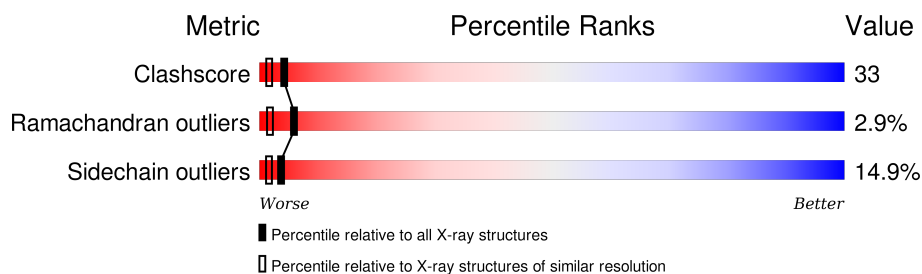
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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	388	

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
2	SO4	A	466	-	X	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3020 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 PHOTOSYSTEM II D1 PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	2861	1791	506	559	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	initiating METHIONINE	UNP O04073

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is water.

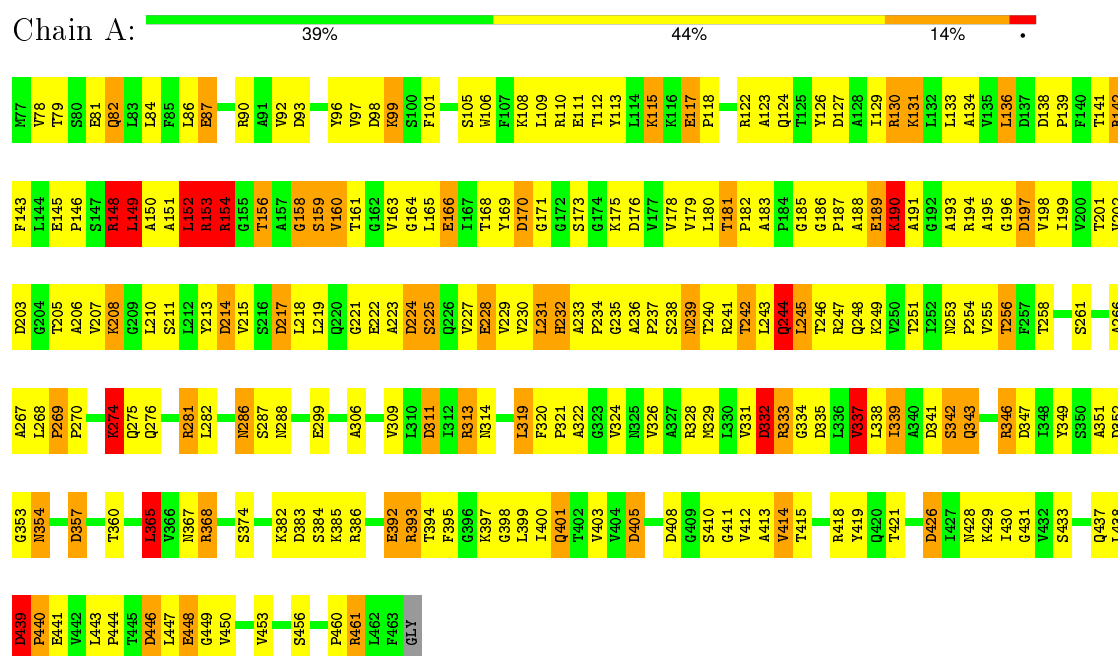
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total 149	O 149	0	0

### 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: PHOTOSYSTEM II D1 PROTEASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.75Å 148.75Å 100.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.10)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.220 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3020	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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	14/2902 (0.5%)	1.80	72/3948 (1.8%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	GLU	CD-OE2	11.55	1.38	1.25
1	A	166	GLU	CD-OE2	8.42	1.34	1.25
1	A	222	GLU	CD-OE2	8.12	1.34	1.25
1	A	448	GLU	CD-OE2	7.92	1.34	1.25
1	A	228	GLU	CD-OE2	6.92	1.33	1.25
1	A	87	GLU	CD-OE2	6.32	1.32	1.25
1	A	392	GLU	CD-OE2	6.22	1.32	1.25
1	A	111	GLU	CD-OE2	6.04	1.32	1.25
1	A	81	GLU	CD-OE2	5.85	1.32	1.25
1	A	189	GLU	CD-OE2	5.84	1.32	1.25
1	A	299	GLU	CD-OE2	5.62	1.31	1.25
1	A	117	GLU	CD-OE2	5.56	1.31	1.25
1	A	145	GLU	CD-OE2	5.48	1.31	1.25
1	A	117	GLU	CD-OE1	-5.01	1.20	1.25

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ARG	NE-CZ-NH1	12.07	126.33	120.30
1	A	130	ARG	NE-CZ-NH2	-11.49	114.55	120.30
1	A	130	ARG	NE-CZ-NH1	11.47	126.03	120.30
1	A	313	ARG	NE-CZ-NH1	11.19	125.89	120.30
1	A	148	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	A	405	ASP	CB-CG-OD2	-9.82	109.46	118.30
1	A	335	ASP	CB-CG-OD2	-9.34	109.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	ASP	CB-CG-OD1	9.20	126.58	118.30
1	A	217	ASP	CB-CG-OD1	9.16	126.54	118.30
1	A	405	ASP	CB-CG-OD1	8.98	126.38	118.30
1	A	281	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	A	418	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	A	418	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	439	ASP	CB-CG-OD2	-7.86	111.22	118.30
1	A	393	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	386	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	A	194	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	A	281	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	98	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	197	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	A	224	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	217	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	311	ASP	CB-CG-OD2	-7.18	111.83	118.30
1	A	439	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	408	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	127	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	A	346	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	383	ASP	CB-CG-OD1	6.85	124.46	118.30
1	A	426	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	408	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	A	393	ARG	CG-CD-NE	6.61	125.68	111.80
1	A	98	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	332	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	386	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	368	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	110	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	461	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	414	VAL	CB-CA-C	-6.03	99.94	111.40
1	A	152	LEU	CB-CG-CD1	5.99	121.19	111.00
1	A	365	LEU	N-CA-CB	5.97	122.34	110.40
1	A	269	PRO	C-N-CD	-5.95	107.51	120.60
1	A	341	ASP	CB-CG-OD1	5.87	123.59	118.30
1	A	341	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	170	ASP	C-N-CA	5.84	134.56	122.30
1	A	149	LEU	CB-CA-C	5.83	121.28	110.20
1	A	357	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	274	LYS	CB-CA-C	-5.83	98.75	110.40
1	A	153	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	152	LEU	CB-CG-CD2	5.70	120.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	154	ARG	N-CA-CB	5.66	120.79	110.60
1	A	337	VAL	CA-CB-CG2	5.65	119.38	110.90
1	A	335	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	176	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	418	ARG	CD-NE-CZ	5.54	131.36	123.60
1	A	148	ARG	N-CA-CB	5.52	120.53	110.60
1	A	401	GLN	CB-CA-C	-5.50	99.39	110.40
1	A	173	SER	N-CA-CB	5.45	118.68	110.50
1	A	173	SER	CB-CA-C	5.45	120.45	110.10
1	A	244	GLN	CB-CA-C	5.39	121.18	110.40
1	A	148	ARG	CD-NE-CZ	5.38	131.13	123.60
1	A	313	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	346	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	421	THR	CA-CB-CG2	-5.22	105.09	112.40
1	A	214	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	136	LEU	N-CA-CB	-5.14	100.11	110.40
1	A	82	GLN	CA-CB-CG	-5.14	102.09	113.40
1	A	225	SER	N-CA-CB	5.11	118.16	110.50
1	A	149	LEU	N-CA-CB	5.07	120.53	110.40
1	A	93	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	337	VAL	CG1-CB-CG2	5.02	118.93	110.90
1	A	78	VAL	N-CA-C	5.01	124.54	111.00

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	2861	0	2902	193	1
2	A	10	0	0	0	0
3	A	149	0	0	16	1
All	All	3020	0	2902	193	2

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 33.

All (193) 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:230:VAL:HG22	1:A:242:THR:HG23	1.42	0.98
1:A:286:ASN:ND2	1:A:288:ASN:H	1.62	0.97
1:A:398:GLY:H	1:A:428:ASN:HD22	1.02	0.95
1:A:256:THR:HG23	1:A:447:LEU:HD21	1.51	0.93
1:A:243:LEU:HB3	1:A:245:LEU:HD21	1.50	0.92
1:A:175:LYS:HB3	1:A:208:LYS:HD3	1.57	0.87
1:A:286:ASN:HD21	1:A:288:ASN:HB2	1.40	0.86
1:A:243:LEU:CB	1:A:245:LEU:HD21	2.05	0.85
1:A:161:THR:HG22	1:A:249:LYS:HG3	1.57	0.85
1:A:309:VAL:CG1	1:A:365:LEU:HD21	2.08	0.83
1:A:438:LEU:O	1:A:440:PRO:HD3	1.80	0.81
1:A:186:GLY:O	1:A:190:LYS:HG3	1.80	0.81
1:A:286:ASN:HD22	1:A:288:ASN:H	1.28	0.81
1:A:398:GLY:H	1:A:428:ASN:ND2	1.80	0.79
1:A:365:LEU:HD23	1:A:365:LEU:N	1.98	0.78
1:A:398:GLY:N	1:A:428:ASN:HD22	1.79	0.77
1:A:412:VAL:HG12	1:A:414:VAL:HG22	1.69	0.74
1:A:153:ARG:HH22	1:A:403:VAL:HB	1.53	0.73
1:A:211:SER:O	1:A:215:VAL:HG23	1.88	0.73
1:A:309:VAL:HG12	1:A:365:LEU:HD21	1.71	0.72
1:A:165:LEU:CD2	1:A:179:VAL:HG22	2.20	0.72
1:A:99:LYS:N	1:A:342:SER:OG	2.20	0.72
1:A:208:LYS:HB2	3:A:573:HOH:O	1.90	0.72
1:A:153:ARG:NH2	1:A:403:VAL:HB	2.05	0.70
1:A:202:VAL:HG11	1:A:219:LEU:HD23	1.73	0.70
1:A:196:GLY:O	1:A:234:PRO:HG3	1.93	0.69
1:A:367:ASN:HA	1:A:392:GLU:HG2	1.75	0.69
1:A:202:VAL:HG13	1:A:229:VAL:HG22	1.74	0.68
1:A:238:SER:O	1:A:240:THR:N	2.26	0.68
1:A:165:LEU:HD21	1:A:179:VAL:HG22	1.75	0.68
1:A:235:GLY:C	1:A:237:PRO:HD3	2.13	0.68
1:A:443:LEU:HD23	1:A:453:VAL:HG11	1.74	0.67
1:A:244:GLN:C	1:A:245:LEU:HD23	2.15	0.67
1:A:382:LYS:NZ	1:A:433:SER:O	2.27	0.67
1:A:163:VAL:HG21	1:A:245:LEU:HD12	1.78	0.66
1:A:148:ARG:O	1:A:152:LEU:HB3	1.94	0.66
1:A:334:GLY:N	3:A:505:HOH:O	2.26	0.66
1:A:430:ILE:HG22	1:A:431:GLY:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:C	1:A:191:ALA:H	1.99	0.66
1:A:243:LEU:HB3	1:A:245:LEU:CD2	2.24	0.65
1:A:154:ARG:N	1:A:154:ARG:HD2	2.09	0.65
1:A:365:LEU:H	1:A:365:LEU:HD23	1.60	0.65
1:A:133:LEU:O	1:A:136:LEU:HB2	1.96	0.65
1:A:229:VAL:O	1:A:243:LEU:N	2.28	0.64
1:A:256:THR:CG2	1:A:447:LEU:HD21	2.28	0.63
1:A:337:VAL:HG23	1:A:349:TYR:HB2	1.81	0.63
1:A:148:ARG:HH11	1:A:148:ARG:HG3	1.63	0.63
1:A:229:VAL:HG12	1:A:231:LEU:HD23	1.81	0.62
1:A:170:ASP:CG	1:A:171:GLY:H	2.03	0.62
1:A:207:VAL:HA	1:A:210:LEU:HD12	1.81	0.62
1:A:179:VAL:HG11	1:A:182:PRO:HD3	1.82	0.61
1:A:148:ARG:NH2	1:A:217:ASP:OD2	2.34	0.61
1:A:149:LEU:HD12	1:A:153:ARG:HE	1.65	0.60
1:A:286:ASN:HD22	1:A:286:ASN:C	2.05	0.60
1:A:354:ASN:H	1:A:354:ASN:HD22	1.49	0.60
1:A:365:LEU:HD11	1:A:443:LEU:HD12	1.83	0.59
1:A:158:GLY:C	1:A:160:VAL:H	2.06	0.59
1:A:141:THR:HA	1:A:413:ALA:O	2.03	0.59
1:A:266:ALA:O	1:A:461:ARG:HA	2.03	0.59
1:A:149:LEU:CD1	1:A:153:ARG:HE	2.15	0.59
1:A:134:ALA:HB3	3:A:561:HOH:O	2.03	0.58
1:A:343:GLN:O	1:A:343:GLN:HG2	2.03	0.58
1:A:286:ASN:ND2	1:A:288:ASN:N	2.42	0.58
1:A:189:GLU:O	1:A:191:ALA:N	2.37	0.58
1:A:426:ASP:OD1	1:A:429:LYS:HG3	2.04	0.57
1:A:351:ALA:HB3	3:A:505:HOH:O	2.05	0.57
1:A:448:GLU:HG2	3:A:603:HOH:O	2.03	0.57
1:A:139:PRO:HB2	1:A:169:TYR:CE1	2.39	0.57
1:A:286:ASN:HD22	1:A:288:ASN:N	1.98	0.56
1:A:236:ALA:HB1	1:A:239:ASN:HB2	1.87	0.56
1:A:178:VAL:HG12	1:A:198:VAL:HG22	1.87	0.56
1:A:232:HIS:HD2	1:A:233:ALA:O	1.89	0.56
1:A:351:ALA:N	3:A:505:HOH:O	2.36	0.56
1:A:210:LEU:HD22	1:A:214:ASP:HB3	1.88	0.56
1:A:384:SER:O	1:A:385:LYS:HB2	2.04	0.56
1:A:397:LYS:HG2	1:A:397:LYS:O	2.06	0.56
1:A:229:VAL:CG1	1:A:231:LEU:HD23	2.36	0.55
1:A:158:GLY:O	1:A:160:VAL:N	2.39	0.54
1:A:339:ILE:HG13	1:A:347:ASP:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ASP:OD1	1:A:354:ASN:ND2	2.41	0.54
1:A:232:HIS:CD2	1:A:233:ALA:O	2.61	0.54
1:A:223:ALA:O	1:A:224:ASP:HB2	2.07	0.54
1:A:229:VAL:HG12	1:A:231:LEU:CD2	2.37	0.54
1:A:130:ARG:HG2	3:A:508:HOH:O	2.06	0.54
1:A:309:VAL:HG13	1:A:365:LEU:HD21	1.88	0.53
1:A:115:LYS:N	1:A:115:LYS:HD3	2.22	0.53
1:A:243:LEU:HB2	1:A:245:LEU:HD21	1.87	0.53
1:A:256:THR:HG21	3:A:528:HOH:O	2.08	0.53
1:A:97:VAL:HG11	1:A:415:THR:HG22	1.91	0.53
1:A:319:LEU:HD23	1:A:321:PRO:HG2	1.90	0.53
1:A:326:VAL:O	1:A:329:MET:HB2	2.09	0.52
1:A:203:ASP:OD2	1:A:227:VAL:HG23	2.09	0.51
1:A:97:VAL:HG11	1:A:415:THR:CG2	2.40	0.51
1:A:324:VAL:O	1:A:328:ARG:HG3	2.10	0.51
1:A:179:VAL:CG1	1:A:182:PRO:HD3	2.40	0.51
1:A:218:LEU:HD23	3:A:607:HOH:O	2.10	0.51
1:A:399:LEU:HB2	3:A:596:HOH:O	2.09	0.51
1:A:149:LEU:HD22	1:A:411:GLY:HA3	1.92	0.51
1:A:163:VAL:O	1:A:188:ALA:HB2	2.11	0.50
1:A:149:LEU:O	1:A:149:LEU:HG	2.11	0.50
1:A:229:VAL:CG1	1:A:231:LEU:CD2	2.89	0.50
1:A:139:PRO:HB2	1:A:169:TYR:CD1	2.47	0.50
1:A:255:VAL:HA	1:A:281:ARG:O	2.11	0.50
1:A:320:PHE:N	1:A:321:PRO:HD2	2.27	0.49
1:A:130:ARG:HH11	1:A:143:PHE:HD2	1.61	0.49
1:A:253:ASN:OD1	1:A:254:PRO:HD2	2.13	0.49
1:A:365:LEU:CD2	1:A:365:LEU:N	2.74	0.48
1:A:246:THR:O	1:A:248:GLN:HG3	2.12	0.48
1:A:163:VAL:HG23	1:A:163:VAL:O	2.14	0.48
1:A:149:LEU:HD13	1:A:403:VAL:HG11	1.94	0.48
1:A:365:LEU:CD1	1:A:443:LEU:HD12	2.43	0.48
1:A:113:TYR:HE2	1:A:131:LYS:HB3	1.78	0.48
1:A:96:TYR:O	1:A:99:LYS:HE3	2.14	0.48
1:A:138:ASP:OD2	1:A:415:THR:OG1	2.23	0.47
1:A:146:PRO:HD3	1:A:410:SER:HB3	1.95	0.47
1:A:84:LEU:HD22	1:A:122:ARG:HD2	1.97	0.47
1:A:84:LEU:O	1:A:87:GLU:HB2	2.15	0.47
1:A:101:PHE:CD1	1:A:106:TRP:HB2	2.50	0.47
1:A:367:ASN:O	1:A:394:THR:HA	2.13	0.47
1:A:148:ARG:C	1:A:150:ALA:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LYS:HE3	3:A:514:HOH:O	2.15	0.47
1:A:395:PHE:HD2	1:A:397:LYS:HB2	1.80	0.47
1:A:207:VAL:O	1:A:210:LEU:HB2	2.15	0.47
1:A:446:ASP:O	1:A:450:VAL:HG23	2.14	0.47
1:A:113:TYR:CE2	1:A:131:LYS:HD3	2.50	0.46
1:A:267:ALA:HB2	1:A:460:PRO:O	2.15	0.46
1:A:105:SER:HB3	1:A:108:LYS:HB3	1.98	0.46
1:A:444:PRO:O	1:A:450:VAL:HG22	2.14	0.46
1:A:197:ASP:HA	1:A:234:PRO:HD3	1.97	0.46
1:A:368:ARG:HB3	3:A:564:HOH:O	2.16	0.46
1:A:213:TYR:O	1:A:217:ASP:OD2	2.34	0.46
1:A:225:SER:OG	1:A:247:ARG:HD2	2.16	0.46
1:A:198:VAL:CG1	1:A:199:ILE:N	2.80	0.45
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.56	0.45
1:A:401:GLN:HA	1:A:415:THR:HA	1.97	0.45
1:A:258:THR:HG22	1:A:447:LEU:HD22	1.99	0.45
1:A:236:ALA:HB1	1:A:239:ASN:CB	2.46	0.45
1:A:97:VAL:CG1	1:A:415:THR:HG22	2.47	0.45
1:A:118:PRO:O	1:A:124:GLN:HB3	2.16	0.45
1:A:405:ASP:HB3	3:A:566:HOH:O	2.17	0.45
1:A:446:ASP:OD2	1:A:449:GLY:N	2.44	0.45
1:A:195:ALA:HB2	1:A:314:ASN:HD21	1.82	0.44
1:A:139:PRO:HD2	3:A:540:HOH:O	2.17	0.44
1:A:242:THR:O	1:A:243:LEU:HD23	2.17	0.44
1:A:159:SER:HA	1:A:249:LYS:NZ	2.33	0.44
1:A:268:LEU:HA	1:A:268:LEU:HD23	1.74	0.44
1:A:92:VAL:HG13	1:A:96:TYR:HB2	2.00	0.44
1:A:244:GLN:O	1:A:245:LEU:HD23	2.18	0.43
1:A:202:VAL:HG13	1:A:229:VAL:CG2	2.46	0.43
1:A:332:ASP:O	1:A:353:GLY:HA2	2.18	0.43
1:A:195:ALA:HB2	1:A:314:ASN:ND2	2.33	0.43
1:A:245:LEU:HD23	1:A:245:LEU:N	2.32	0.43
1:A:205:THR:HG22	1:A:206:ALA:O	2.19	0.43
1:A:196:GLY:C	1:A:234:PRO:HG3	2.39	0.43
1:A:286:ASN:C	1:A:319:LEU:HD13	2.39	0.43
1:A:187:PRO:HB3	3:A:576:HOH:O	2.19	0.42
1:A:170:ASP:CG	1:A:171:GLY:N	2.71	0.42
1:A:412:VAL:CG1	1:A:414:VAL:HG22	2.43	0.42
1:A:185:GLY:N	1:A:189:GLU:OE1	2.27	0.42
1:A:164:GLY:HA3	1:A:183:ALA:HB3	2.01	0.42
1:A:333:ARG:NH2	3:A:594:HOH:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:NH2	1:A:403:VAL:CB	2.78	0.42
1:A:79:THR:OG1	1:A:82:GLN:HG3	2.20	0.42
1:A:221:GLY:CA	1:A:247:ARG:CD	2.97	0.42
1:A:400:ILE:HD11	1:A:419:TYR:CE2	2.54	0.42
1:A:331:VAL:O	1:A:351:ALA:HB1	2.21	0.41
1:A:106:TRP:CE3	1:A:106:TRP:HA	2.55	0.41
1:A:221:GLY:HA3	1:A:247:ARG:CD	2.49	0.41
1:A:123:ALA:O	1:A:126:TYR:HB2	2.20	0.41
1:A:392:GLU:HB3	1:A:440:PRO:HG3	2.02	0.41
1:A:313:ARG:NH1	1:A:443:LEU:O	2.46	0.41
1:A:166:GLU:OE2	1:A:181:THR:HG22	2.20	0.41
1:A:168:THR:HG23	1:A:169:TYR:N	2.34	0.41
1:A:86:LEU:O	1:A:90:ARG:HB2	2.20	0.41
1:A:105:SER:O	1:A:109:LEU:HD13	2.20	0.41
1:A:190:LYS:HE2	1:A:190:LYS:HB2	1.59	0.41
1:A:429:LYS:HB2	1:A:430:ILE:H	1.37	0.41
1:A:354:ASN:HD22	1:A:354:ASN:N	2.11	0.41
1:A:311:ASP:OD1	1:A:313:ARG:HG3	2.21	0.40
1:A:142:ARG:N	1:A:413:ALA:O	2.47	0.40
1:A:357:ASP:OD2	1:A:360:THR:OG1	2.28	0.40
1:A:148:ARG:HA	1:A:151:ALA:HB3	2.03	0.40
1:A:276:GLN:O	1:A:306:ALA:HB3	2.21	0.40
1:A:188:ALA:O	1:A:193:ALA:HB3	2.22	0.40
1:A:189:GLU:C	1:A:191:ALA:N	2.65	0.40
1:A:129:ILE:O	1:A:133:LEU:HG	2.22	0.40
1:A:395:PHE:CD2	1:A:397:LYS:HB2	2.56	0.40
1:A:221:GLY:N	1:A:247:ARG:NE	2.70	0.40
1:A:117:GLU:HA	1:A:118:PRO:HD3	1.92	0.40
1:A:453:VAL:O	1:A:456:SER:OG	2.28	0.40
1:A:322:ALA:O	1:A:326:VAL:HG23	2.21	0.40
1:A:219:LEU:HA	1:A:219:LEU:HD23	1.72	0.40
1:A:165:LEU:HD22	1:A:179:VAL:HG22	1.98	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:513:HOH:O	3:A:513:HOH:O[5_555]	1.84	0.36
1:A:439:ASP:OD1	1:A:439:ASP:OD1[10_545]	1.89	0.31

## 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	385/388 (99%)	350 (91%)	24 (6%)	11 (3%)	<b>6</b> <b>2</b>

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	THR
1	A	159	SER
1	A	190	LYS
1	A	239	ASN
1	A	274	LYS
1	A	440	PRO
1	A	439	ASP
1	A	99	LYS
1	A	270	PRO
1	A	158	GLY
1	A	269	PRO

### 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	303/303 (100%)	258 (85%)	45 (15%)	<b>4</b> <b>1</b>

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	A	115	LYS
1	A	131	LYS
1	A	142	ARG
1	A	148	ARG
1	A	149	LEU
1	A	152	LEU
1	A	153	ARG
1	A	154	ARG
1	A	156	THR
1	A	160	VAL
1	A	180	LEU
1	A	181	THR
1	A	190	LYS
1	A	201	THR
1	A	208	LYS
1	A	228	GLU
1	A	231	LEU
1	A	232	HIS
1	A	241	ARG
1	A	242	THR
1	A	244	GLN
1	A	245	LEU
1	A	251	THR
1	A	256	THR
1	A	261	SER
1	A	274	LYS
1	A	275	GLN
1	A	282	LEU
1	A	286	ASN
1	A	287	SER
1	A	319	LEU
1	A	332	ASP
1	A	333	ARG
1	A	337	VAL
1	A	338	LEU
1	A	339	ILE
1	A	342	SER
1	A	343	GLN
1	A	346	ARG
1	A	354	ASN
1	A	365	LEU
1	A	374	SER

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Mol	Chain	Res	Type
1	A	393	ARG
1	A	437	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	HIS
1	A	286	ASN
1	A	303	GLN
1	A	354	ASN
1	A	428	ASN
1	A	437	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
2	SO4	A	465	-	4,4,4	1.24	1 (25%)	6,6,6	1.71	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	466	-	4,4,4	1.86	2 (50%)	6,6,6	1.57	2 (33%)

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	SO4	A	465	-	-	0/0/0/0	0/0/0/0
2	SO4	A	466	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	465	SO4	O2-S	2.16	1.54	1.47
2	A	466	SO4	O2-S	2.17	1.54	1.47
2	A	466	SO4	O1-S	2.62	1.56	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	465	SO4	O2-S-O1	-3.19	99.39	109.50
2	A	466	SO4	O2-S-O1	-2.80	100.62	109.50
2	A	466	SO4	O4-S-O3	2.61	119.59	108.98
2	A	465	SO4	O4-S-O3	2.69	119.94	108.98

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 ⓘ

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.