



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:45 AM GMT

PDB ID : 1X9P  
Title : The crystal structure of human adenovirus 2 penton base  
Authors : Zubieta, C.; Schoehn, G.; Chroboczek, J.; Cusack, S.  
Deposited on : 2004-08-24  
Resolution : 3.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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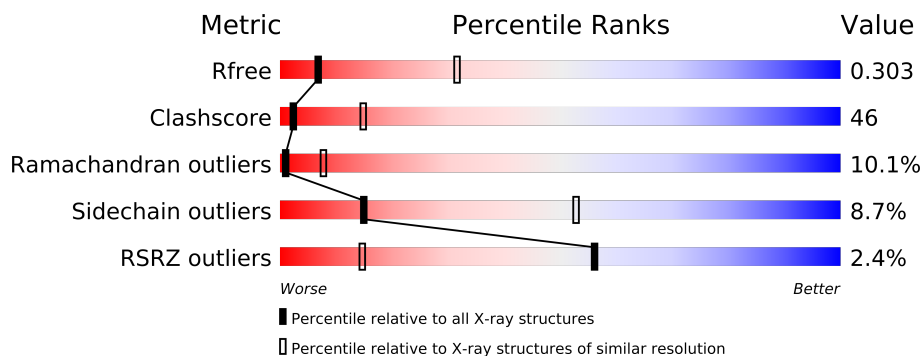
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 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))
$R_{free}$	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	523	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	700	X	X
3	C15	A	998	-	X
3	C15	A	999	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3677 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Penton protein.

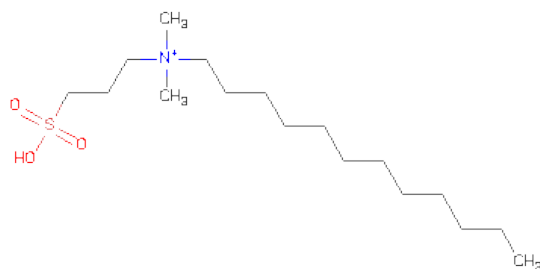
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3632	2294	630	696	12			

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



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

- Molecule 3 is N-DODECYL-N,N-DIMETHYL-3-AMMONIO-1-PROPANESULFONATE (three-letter code: C15) (formula: C<sub>17</sub>H<sub>38</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	15	1	3	1		
3	A	1	Total	C	N	O	S	0	0
			20	15	1	3	1		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	435.98Å 300.17Å 420.62Å 90.00° 104.36° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 19.99 – 3.30	Depositor EDS
% Data completeness (in resolution range)	57.1 (20.00-3.30) 57.2 (19.99-3.30)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	0.21	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 3.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.307 , 0.307 0.303 , 0.303	Depositor DCC
$R_{free}$ test set	22325 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 19.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	1 of 445700 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	3677	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, C15

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	0.57	0/3715	0.82	3/5057 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	GLY	N-CA-C	5.60	127.11	113.10
1	A	153	LEU	CB-CG-CD2	5.36	120.12	111.00
1	A	344	PHE	CA-C-O	5.32	131.28	120.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3632	0	3535	335	0
2	A	5	0	0	0	0
3	A	40	0	64	5	0
All	All	3677	0	3599	337	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 46.

All (337) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:68:ARG:HG2	1:A:68:ARG:HH11	1.25	0.99
1:A:295:SER:HB3	1:A:377:PRO:HG3	1.51	0.91
1:A:278:LEU:HD23	1:A:419:ILE:HD12	1.53	0.91
1:A:292:TYR:HA	1:A:377:PRO:CG	2.01	0.90
1:A:68:ARG:HH12	1:A:562:SER:HB3	1.38	0.89
1:A:451:PHE:HD2	1:A:461:PRO:HA	1.38	0.89
1:A:376:LYS:HB3	1:A:377:PRO:HD2	1.54	0.88
1:A:83:ASN:HD22	1:A:91:PHE:HB2	1.40	0.86
1:A:504:ILE:HG22	1:A:505:LEU:HD23	1.57	0.86
1:A:211:ASP:HA	1:A:508:PRO:CG	2.05	0.86
1:A:52:ARG:HB3	1:A:117:SER:OG	1.75	0.86
1:A:193:LEU:HD11	1:A:498:ARG:HH12	1.41	0.85
1:A:58:SER:O	1:A:60:LEU:N	2.09	0.84
1:A:178:THR:HG21	1:A:511:PRO:HD2	1.60	0.84
1:A:49:THR:HG23	1:A:53:ASN:OD1	1.79	0.83
1:A:156:ASP:O	1:A:157:LYS:HG3	1.78	0.83
1:A:468:LEU:HD12	1:A:469:PRO:HD2	1.59	0.82
1:A:544:THR:CG2	1:A:548:ARG:HA	2.10	0.81
1:A:384:GLU:HG2	1:A:390:SER:HA	1.62	0.80
1:A:214:ASN:HD22	1:A:214:ASN:C	1.86	0.78
1:A:237:HIS:CD2	1:A:425:LEU:HD11	2.18	0.78
1:A:154:THR:OG1	1:A:160:GLU:HB2	1.84	0.77
1:A:389:ARG:HD3	1:A:502:ASN:HD22	1.47	0.77
1:A:379:ILE:O	1:A:381:PRO:HD3	1.85	0.76
1:A:403:TYR:CE1	1:A:504:ILE:HG21	2.21	0.76
1:A:211:ASP:HA	1:A:508:PRO:HG3	1.67	0.76
1:A:292:TYR:HA	1:A:377:PRO:HG2	1.67	0.76
1:A:68:ARG:NH1	1:A:562:SER:HB3	2.01	0.75
1:A:475:PHE:O	1:A:513:ILE:HA	1.87	0.74
1:A:295:SER:O	1:A:296:LEU:HB2	1.88	0.74
1:A:451:PHE:CD2	1:A:461:PRO:HA	2.22	0.73
1:A:544:THR:HG22	1:A:548:ARG:HA	1.70	0.73
1:A:249:ASP:C	1:A:249:ASP:OD1	2.26	0.73
1:A:145:ALA:HB3	1:A:168:PHE:HE1	1.53	0.72
1:A:148:MET:HA	1:A:163:TYR:HD2	1.54	0.72
1:A:142:LYS:HG2	1:A:169:THR:HG22	1.70	0.72
1:A:244:PRO:HA	1:A:275:TYR:CD2	2.24	0.72
1:A:197:ARG:HG3	1:A:198:GLN:N	2.05	0.72
1:A:243:LEU:HD21	1:A:403:TYR:CE2	2.23	0.72
1:A:403:TYR:HD1	1:A:504:ILE:HD13	1.52	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:468:LEU:CD1	1:A:469:PRO:HD2	2.19	0.72
1:A:419:ILE:HG22	1:A:423:THR:CG2	2.21	0.71
1:A:160:GLU:OE2	1:A:162:LYS:HE3	1.91	0.70
1:A:243:LEU:HD21	1:A:403:TYR:CD2	2.26	0.70
1:A:249:ASP:HB2	1:A:272:ARG:HG2	1.73	0.70
1:A:68:ARG:NH1	1:A:68:ARG:HG2	1.92	0.69
1:A:215:PHE:CE1	1:A:241:ILE:HD11	2.27	0.69
1:A:444:MET:O	1:A:444:MET:HG2	1.92	0.69
1:A:122:ASP:OD1	1:A:528:THR:HB	1.91	0.69
1:A:142:LYS:HD3	1:A:167:GLU:OE2	1.93	0.69
1:A:217:LEU:HB2	1:A:232:THR:HG21	1.73	0.69
1:A:419:ILE:HG22	1:A:423:THR:HG21	1.75	0.68
1:A:146:ARG:O	1:A:246:CYS:HB2	1.94	0.68
1:A:278:LEU:HD22	1:A:406:TRP:HA	1.76	0.68
1:A:149:VAL:HG23	1:A:195:VAL:HG11	1.76	0.68
1:A:512:THR:O	1:A:513:ILE:HB	1.93	0.67
1:A:217:LEU:HB2	1:A:232:THR:CG2	2.25	0.66
1:A:227:MET:HB2	1:A:228:PRO:HD3	1.76	0.66
1:A:430:VAL:HG21	1:A:517:SER:N	2.10	0.66
1:A:468:LEU:HD12	1:A:469:PRO:CD	2.26	0.66
1:A:386:SER:O	1:A:387:LYS:HB2	1.94	0.66
1:A:393:LEU:N	1:A:393:LEU:HD12	2.12	0.65
1:A:60:LEU:O	1:A:61:ALA:HB3	1.97	0.65
1:A:193:LEU:HD11	1:A:498:ARG:NH1	2.12	0.65
1:A:83:ASN:N	1:A:83:ASN:OD1	2.26	0.64
1:A:211:ASP:O	1:A:212:THR:HG22	1.97	0.64
1:A:513:ILE:O	1:A:513:ILE:HG22	1.97	0.64
1:A:133:ASN:HB2	1:A:174:ASN:OD1	1.97	0.64
1:A:278:LEU:O	1:A:404:ARG:HD3	1.98	0.63
1:A:422:TRP:CZ3	3:A:999:C15:H1C2	2.34	0.63
1:A:544:THR:HG21	1:A:548:ARG:HD2	1.81	0.63
1:A:493:THR:HG21	1:A:497:ASN:O	1.99	0.62
1:A:499:PHE:N	1:A:500:PRO:HD3	2.13	0.62
1:A:134:VAL:HA	1:A:140:THR:OG1	1.99	0.62
1:A:148:MET:HA	1:A:163:TYR:CD2	2.34	0.62
1:A:178:THR:CG2	1:A:511:PRO:HD2	2.30	0.62
1:A:394:ILE:HG23	1:A:398:SER:HB2	1.82	0.62
1:A:378:VAL:HG12	1:A:379:ILE:N	2.15	0.61
1:A:125:THR:HG23	1:A:524:THR:CG2	2.29	0.61
1:A:220:ASP:OD1	1:A:222:VAL:HG12	2.00	0.61
1:A:125:THR:CG2	1:A:526:HIS:NE2	2.63	0.61
1:A:444:MET:HB2	1:A:539:GLN:OE1	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:LEU:HD23	1:A:419:ILE:CD1	2.30	0.60
1:A:394:ILE:HG23	1:A:395:SER:H	1.67	0.60
1:A:258:LEU:O	1:A:258:LEU:HD12	2.00	0.60
1:A:60:LEU:HG	1:A:60:LEU:O	2.00	0.60
1:A:263:LYS:NZ	1:A:268:GLN:HB2	2.16	0.60
1:A:440:SER:HB3	1:A:461:PRO:O	2.02	0.60
1:A:383:THR:HG22	1:A:384:GLU:HG3	1.83	0.60
1:A:444:MET:HE3	1:A:561:VAL:HG21	1.83	0.60
1:A:125:THR:HG21	1:A:526:HIS:NE2	2.17	0.60
1:A:410:TYR:CD1	1:A:420:ARG:HA	2.37	0.60
1:A:282:ASN:HD21	1:A:404:ARG:HE	1.50	0.59
1:A:278:LEU:CD2	1:A:406:TRP:HA	2.32	0.59
1:A:378:VAL:O	1:A:380:LYS:N	2.35	0.59
1:A:243:LEU:HD11	1:A:403:TYR:HE2	1.67	0.59
1:A:224:GLY:O	1:A:399:THR:HB	2.03	0.59
1:A:389:ARG:NH1	1:A:389:ARG:HG2	2.17	0.59
1:A:243:LEU:CD2	1:A:403:TYR:CD2	2.86	0.59
1:A:220:ASP:HB2	1:A:227:MET:HG2	1.84	0.58
1:A:520:VAL:CG2	1:A:521:PRO:HD2	2.33	0.58
1:A:197:ARG:HG3	1:A:198:GLN:CG	2.33	0.58
1:A:154:THR:HG22	1:A:155:LYS:N	2.18	0.58
1:A:211:ASP:O	1:A:212:THR:CG2	2.52	0.58
1:A:282:ASN:ND2	1:A:404:ARG:HE	2.03	0.57
1:A:287:LEU:C	1:A:287:LEU:HD23	2.24	0.57
1:A:482:TYR:CE1	1:A:486:ILE:HD12	2.40	0.57
1:A:214:ASN:ND2	1:A:214:ASN:C	2.55	0.56
1:A:134:VAL:HG22	1:A:173:GLY:O	2.05	0.56
1:A:125:THR:CG2	1:A:524:THR:HG23	2.35	0.56
1:A:233:ASN:CG	1:A:233:ASN:O	2.43	0.56
1:A:441:LEU:HD12	1:A:445:MET:HE1	1.85	0.56
1:A:263:LYS:HZ3	1:A:268:GLN:HB2	1.70	0.56
1:A:67:THR:O	1:A:68:ARG:HG2	2.06	0.56
1:A:392:ASN:HB3	1:A:402:GLN:NE2	2.21	0.56
1:A:479:GLN:HG2	1:A:479:GLN:O	2.05	0.56
1:A:419:ILE:O	1:A:423:THR:HG22	2.06	0.56
1:A:273:ILE:HG23	1:A:273:ILE:O	2.05	0.56
1:A:428:PRO:O	1:A:429:ASP:HB3	2.06	0.55
1:A:501:GLU:CD	1:A:501:GLU:H	2.10	0.55
1:A:494:HIS:C	1:A:496:PHE:H	2.07	0.55
1:A:68:ARG:NH1	1:A:68:ARG:CG	2.66	0.55
1:A:544:THR:HG21	1:A:548:ARG:HA	1.89	0.55
1:A:283:ILE:O	1:A:401:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:505:LEU:O	1:A:506:ALA:O	2.26	0.54
1:A:211:ASP:CG	1:A:212:THR:H	2.10	0.54
1:A:493:THR:HG22	1:A:494:HIS:N	2.21	0.54
1:A:525:ASP:OD1	1:A:525:ASP:C	2.45	0.54
1:A:389:ARG:HH11	1:A:389:ARG:HG2	1.73	0.54
1:A:440:SER:C	1:A:442:PRO:HD3	2.27	0.54
1:A:197:ARG:HG3	1:A:198:GLN:H	1.71	0.54
1:A:136:GLU:O	1:A:137:PHE:HB2	2.07	0.54
1:A:192:TYR:CZ	1:A:197:ARG:HB3	2.43	0.54
1:A:239:ASP:C	1:A:239:ASP:OD1	2.46	0.54
1:A:385:ASP:O	1:A:386:SER:C	2.45	0.54
1:A:203:GLU:C	1:A:205:ASP:H	2.11	0.53
1:A:478:ASP:C	1:A:480:ALA:H	2.12	0.53
1:A:463:VAL:HB	1:A:529:LEU:CD1	2.38	0.53
1:A:215:PHE:HE1	1:A:241:ILE:HD11	1.71	0.53
1:A:236:PHE:O	1:A:237:HIS:HB3	2.09	0.53
1:A:154:THR:CG2	1:A:155:LYS:N	2.72	0.53
1:A:69:VAL:CG2	1:A:561:VAL:HB	2.39	0.53
1:A:208:VAL:HG23	1:A:208:VAL:O	2.08	0.53
1:A:151:ARG:HG3	1:A:161:LEU:CD2	2.39	0.53
1:A:151:ARG:HG3	1:A:161:LEU:HD21	1.91	0.53
1:A:222:VAL:HG13	1:A:223:THR:N	2.24	0.53
1:A:441:LEU:N	1:A:442:PRO:HD3	2.24	0.52
1:A:386:SER:O	1:A:387:LYS:CB	2.57	0.52
1:A:449:VAL:HG12	1:A:450:THR:N	2.23	0.52
1:A:211:ASP:HA	1:A:508:PRO:HG2	1.89	0.52
1:A:93:THR:HG22	1:A:94:THR:N	2.23	0.52
1:A:53:ASN:O	1:A:54:SER:C	2.48	0.52
1:A:403:TYR:CD1	1:A:504:ILE:HG21	2.45	0.52
1:A:120:GLY:O	1:A:563:PRO:HA	2.10	0.52
1:A:151:ARG:HB3	1:A:200:GLY:O	2.10	0.52
1:A:125:THR:HG22	1:A:524:THR:HG23	1.92	0.51
1:A:138:MET:HB3	1:A:254:ARG:NH1	2.26	0.51
1:A:180:THR:HG21	1:A:258:LEU:CD2	2.40	0.51
1:A:520:VAL:HG23	1:A:521:PRO:HD2	1.92	0.51
1:A:494:HIS:C	1:A:496:PHE:N	2.64	0.51
1:A:403:TYR:CD1	1:A:504:ILE:HD13	2.39	0.51
1:A:425:LEU:HD12	1:A:426:CYS:N	2.26	0.51
1:A:125:THR:CG2	1:A:524:THR:CG2	2.88	0.51
1:A:403:TYR:HD1	1:A:504:ILE:CD1	2.19	0.51
1:A:430:VAL:HG23	1:A:517:SER:HB2	1.93	0.51
1:A:547:ARG:O	1:A:548:ARG:HB2	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:266:PRO:O	1:A:268:GLN:N	2.43	0.50
1:A:295:SER:OG	1:A:377:PRO:HD3	2.10	0.50
1:A:233:ASN:OD1	1:A:233:ASN:O	2.30	0.50
1:A:60:LEU:O	1:A:61:ALA:CB	2.59	0.50
1:A:395:SER:C	1:A:397:ASP:H	2.14	0.50
1:A:243:LEU:CD2	1:A:244:PRO:HD3	2.42	0.50
1:A:243:LEU:CD2	1:A:403:TYR:HD2	2.24	0.50
1:A:192:TYR:CD2	1:A:193:LEU:HD23	2.47	0.50
1:A:135:ASN:HA	1:A:172:GLU:HG2	1.94	0.50
1:A:292:TYR:HA	1:A:377:PRO:HG3	1.90	0.50
1:A:197:ARG:HG3	1:A:198:GLN:HG2	1.93	0.50
1:A:132:PRO:HD3	1:A:553:TYR:CE2	2.46	0.50
1:A:178:THR:O	1:A:181:ILE:N	2.45	0.50
1:A:237:HIS:ND1	1:A:238:PRO:O	2.45	0.50
1:A:264:ARG:NH1	1:A:424:LEU:HD13	2.26	0.50
1:A:61:ALA:HB1	1:A:62:PRO:CD	2.42	0.49
1:A:67:THR:OG1	1:A:68:ARG:N	2.45	0.49
1:A:126:ILE:HG23	1:A:523:LEU:HD23	1.94	0.49
1:A:544:THR:HG22	1:A:545:ASP:N	2.27	0.49
1:A:394:ILE:HG22	1:A:400:PHE:O	2.13	0.49
1:A:427:THR:HG23	1:A:428:PRO:HD2	1.94	0.49
1:A:114:ASP:OD1	1:A:115:ASP:N	2.45	0.49
1:A:212:THR:HG23	1:A:508:PRO:HB3	1.94	0.49
1:A:171:PRO:O	1:A:175:TYR:OH	2.25	0.49
1:A:491:SER:O	1:A:492:LEU:O	2.29	0.49
1:A:211:ASP:OD1	1:A:213:ARG:HG2	2.13	0.49
1:A:197:ARG:HG3	1:A:198:GLN:HG3	1.94	0.49
1:A:266:PRO:C	1:A:268:GLN:H	2.15	0.49
3:A:999:C15:H2C1	3:A:999:C15:H131	1.95	0.48
1:A:203:GLU:O	1:A:205:ASP:N	2.46	0.48
1:A:214:ASN:HD21	1:A:216:ARG:HG2	1.78	0.48
1:A:444:MET:CE	1:A:561:VAL:HG21	2.43	0.48
1:A:125:THR:HG22	1:A:526:HIS:NE2	2.28	0.48
1:A:243:LEU:HD22	1:A:244:PRO:CD	2.43	0.48
1:A:476:TYR:HD1	1:A:513:ILE:HD12	1.79	0.48
1:A:129:THR:HG22	1:A:553:TYR:O	2.13	0.48
1:A:449:VAL:HG12	1:A:450:THR:HG23	1.95	0.48
1:A:441:LEU:HB2	1:A:445:MET:HE2	1.96	0.48
1:A:98:ASN:HD22	1:A:99:ASN:N	2.11	0.48
1:A:69:VAL:HG22	1:A:561:VAL:HB	1.95	0.48
1:A:197:ARG:CG	1:A:198:GLN:N	2.72	0.48
1:A:197:ARG:C	1:A:199:ASN:H	2.17	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:THR:HA	1:A:563:PRO:O	2.13	0.48
1:A:243:LEU:HD22	1:A:244:PRO:HD2	1.96	0.48
1:A:451:PHE:HE2	1:A:462:VAL:HG23	1.78	0.48
1:A:545:ASP:OD1	1:A:549:ARG:HG2	2.13	0.48
1:A:430:VAL:CG2	1:A:431:THR:N	2.77	0.47
1:A:410:TYR:O	1:A:420:ARG:HD3	2.14	0.47
1:A:75:LYS:HZ2	1:A:94:THR:HG23	1.79	0.47
1:A:91:PHE:CD2	1:A:91:PHE:N	2.81	0.47
1:A:203:GLU:HA	1:A:206:ILE:HG13	1.96	0.47
1:A:431:THR:O	1:A:432:CYS:HB2	2.14	0.47
1:A:78:ASP:OD1	1:A:94:THR:HG22	2.15	0.47
1:A:216:ARG:O	1:A:216:ARG:HG3	2.15	0.47
1:A:499:PHE:N	1:A:500:PRO:CD	2.77	0.47
1:A:413:GLY:O	1:A:414:ASP:C	2.53	0.47
1:A:149:VAL:CG2	1:A:195:VAL:HG11	2.45	0.47
1:A:131:MET:HA	1:A:553:TYR:CD2	2.50	0.47
1:A:405:SER:HB3	1:A:408:LEU:HB2	1.97	0.47
1:A:146:ARG:NH1	3:A:998:C15:H1C1	2.30	0.46
1:A:130:ASN:HA	1:A:519:ASN:CG	2.36	0.46
1:A:538:VAL:HG23	1:A:538:VAL:O	2.14	0.46
1:A:261:ILE:HD12	1:A:406:TRP:CE3	2.50	0.46
1:A:468:LEU:HA	1:A:469:PRO:HD3	1.76	0.46
1:A:215:PHE:O	1:A:216:ARG:HB3	2.15	0.46
1:A:202:LEU:O	1:A:205:ASP:OD1	2.34	0.46
1:A:244:PRO:HA	1:A:275:TYR:CE2	2.51	0.46
1:A:513:ILE:N	1:A:513:ILE:HD12	2.31	0.46
1:A:146:ARG:HE	1:A:246:CYS:HA	1.80	0.46
3:A:999:C15:H1C1	3:A:999:C15:H151	1.98	0.46
1:A:178:THR:O	1:A:180:THR:N	2.49	0.46
1:A:233:ASN:OD1	1:A:233:ASN:C	2.54	0.46
1:A:493:THR:HG22	1:A:494:HIS:O	2.16	0.45
1:A:151:ARG:NH1	1:A:205:ASP:OD2	2.49	0.45
1:A:51:GLY:HA3	1:A:116:ARG:HH12	1.81	0.45
1:A:211:ASP:C	1:A:212:THR:CG2	2.84	0.45
1:A:225:LEU:HD22	1:A:285:ALA:O	2.16	0.45
1:A:135:ASN:HA	1:A:172:GLU:CG	2.47	0.45
1:A:93:THR:HG22	1:A:94:THR:O	2.17	0.45
1:A:138:MET:HB3	1:A:254:ARG:HH11	1.80	0.45
1:A:544:THR:HG23	1:A:549:ARG:N	2.31	0.45
1:A:146:ARG:HB2	1:A:165:TRP:CD2	2.52	0.45
1:A:243:LEU:CD2	1:A:403:TYR:CE2	2.96	0.45
1:A:135:ASN:HB2	1:A:172:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:180:THR:HG21	1:A:258:LEU:HD23	1.97	0.45
1:A:132:PRO:HD3	1:A:553:TYR:CD2	2.51	0.45
1:A:243:LEU:HD23	1:A:244:PRO:HD3	1.99	0.44
1:A:258:LEU:C	1:A:258:LEU:HD12	2.38	0.44
1:A:446:GLN:O	1:A:448:PRO:HD3	2.17	0.44
1:A:389:ARG:HH11	1:A:389:ARG:CG	2.28	0.44
1:A:558:LEU:HD23	1:A:558:LEU:HA	1.62	0.44
1:A:170:LEU:HB3	1:A:171:PRO:HD2	1.99	0.44
1:A:229:GLY:O	1:A:286:LEU:HD13	2.18	0.44
1:A:493:THR:CG2	1:A:494:HIS:N	2.80	0.44
1:A:420:ARG:HG3	1:A:420:ARG:O	2.17	0.44
1:A:346:THR:C	1:A:348:ALA:H	2.21	0.44
1:A:533:ASN:OD1	1:A:533:ASN:N	2.50	0.44
1:A:250:PHE:O	1:A:252:HIS:N	2.50	0.44
1:A:261:ILE:HD12	1:A:406:TRP:CZ3	2.53	0.44
1:A:272:ARG:HH12	3:A:998:C15:H3C1	1.82	0.44
1:A:74:ASN:ND2	1:A:556:LYS:NZ	2.66	0.44
1:A:476:TYR:HD1	1:A:513:ILE:CD1	2.30	0.44
1:A:195:VAL:HG12	1:A:196:GLY:N	2.32	0.44
1:A:83:ASN:ND2	1:A:92:LEU:O	2.51	0.43
1:A:525:ASP:OD1	1:A:525:ASP:O	2.35	0.43
1:A:225:LEU:HD13	1:A:287:LEU:HA	1.99	0.43
1:A:202:LEU:O	1:A:203:GLU:C	2.55	0.43
1:A:106:ALA:C	1:A:108:THR:N	2.71	0.43
1:A:391:TYR:O	1:A:392:ASN:C	2.57	0.43
1:A:75:LYS:NZ	1:A:94:THR:HG23	2.32	0.43
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.71	0.43
1:A:468:LEU:C	1:A:468:LEU:HD12	2.38	0.43
1:A:524:THR:OG1	1:A:525:ASP:N	2.52	0.43
1:A:106:ALA:C	1:A:108:THR:H	2.22	0.43
1:A:197:ARG:CG	1:A:198:GLN:H	2.30	0.43
1:A:429:ASP:OD1	1:A:432:CYS:N	2.51	0.43
1:A:203:GLU:C	1:A:205:ASP:N	2.70	0.43
1:A:444:MET:HB2	1:A:539:GLN:CD	2.39	0.43
1:A:128:HIS:HD2	1:A:555:TYR:HD2	1.66	0.43
1:A:436:GLN:N	1:A:436:GLN:OE1	2.39	0.43
1:A:145:ALA:HB3	1:A:168:PHE:CE1	2.44	0.43
1:A:264:ARG:HG3	1:A:264:ARG:O	2.18	0.43
1:A:295:SER:HB3	1:A:377:PRO:CG	2.33	0.43
1:A:419:ILE:O	1:A:421:SER:N	2.52	0.43
1:A:389:ARG:CD	1:A:502:ASN:HD22	2.23	0.43
1:A:463:VAL:HB	1:A:529:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:LEU:HD12	1:A:63:LEU:HA	1.82	0.43
1:A:430:VAL:O	1:A:432:CYS:N	2.53	0.42
1:A:275:TYR:CE1	1:A:404:ARG:HD2	2.54	0.42
1:A:217:LEU:CB	1:A:232:THR:HG21	2.46	0.42
1:A:393:LEU:N	1:A:393:LEU:CD1	2.81	0.42
1:A:427:THR:HA	1:A:428:PRO:HD3	1.75	0.42
1:A:497:ASN:O	1:A:500:PRO:HD3	2.19	0.42
1:A:395:SER:C	1:A:397:ASP:N	2.71	0.42
1:A:502:ASN:C	1:A:504:ILE:H	2.23	0.42
1:A:135:ASN:N	1:A:140:THR:OG1	2.47	0.42
1:A:237:HIS:CD2	1:A:425:LEU:CD1	2.97	0.42
1:A:178:THR:C	1:A:180:THR:N	2.73	0.42
1:A:180:THR:O	1:A:181:ILE:C	2.58	0.42
1:A:237:HIS:NE2	1:A:425:LEU:CD1	2.83	0.42
1:A:478:ASP:C	1:A:480:ALA:N	2.73	0.42
1:A:194:LYS:HG2	1:A:194:LYS:O	2.19	0.42
1:A:68:ARG:NH1	1:A:562:SER:CB	2.79	0.41
1:A:93:THR:CG2	1:A:94:THR:N	2.83	0.41
1:A:65:ASP:O	1:A:66:THR:C	2.57	0.41
1:A:406:TRP:HE1	1:A:419:ILE:HG21	1.85	0.41
1:A:149:VAL:O	1:A:149:VAL:HG22	2.21	0.41
1:A:230:VAL:HG13	1:A:503:GLN:NE2	2.35	0.41
1:A:475:PHE:N	1:A:475:PHE:CD1	2.88	0.41
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.75	0.41
1:A:441:LEU:HD12	1:A:445:MET:CE	2.48	0.41
1:A:513:ILE:O	1:A:513:ILE:CG2	2.68	0.41
1:A:501:GLU:O	1:A:501:GLU:HG2	2.20	0.41
1:A:88:HIS:CD2	1:A:555:TYR:O	2.74	0.41
1:A:279:GLU:O	1:A:280:GLY:O	2.38	0.41
1:A:481:VAL:O	1:A:482:TYR:C	2.57	0.41
1:A:381:PRO:HG2	1:A:381:PRO:O	2.21	0.41
1:A:265:GLN:NE2	1:A:268:GLN:NE2	2.68	0.41
1:A:53:ASN:O	1:A:54:SER:O	2.38	0.41
1:A:134:VAL:HG21	1:A:175:TYR:CE2	2.56	0.41
1:A:287:LEU:HD23	1:A:288:ASP:C	2.41	0.41
1:A:467:LEU:HD12	1:A:467:LEU:HA	1.83	0.41
1:A:383:THR:C	1:A:384:GLU:HG3	2.41	0.41
1:A:419:ILE:C	1:A:421:SER:N	2.72	0.40
1:A:96:ILE:HG22	1:A:98:ASN:H	1.86	0.40
1:A:211:ASP:C	1:A:212:THR:HG23	2.41	0.40
1:A:129:THR:HB	1:A:130:ASN:H	1.65	0.40
1:A:153:LEU:HD23	1:A:159:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:542:THR:HG22	1:A:542:THR:O	2.21	0.40
1:A:481:VAL:HG13	1:A:482:TYR:N	2.37	0.40
1:A:78:ASP:OD1	1:A:94:THR:CG2	2.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	454/523 (87%)	332 (73%)	76 (17%)	46 (10%)	<b>1</b> <b>8</b>

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	59	GLU
1	A	130	ASN
1	A	137	PHE
1	A	296	LEU
1	A	375	LYS
1	A	378	VAL
1	A	379	ILE
1	A	449	VAL
1	A	469	PRO
1	A	492	LEU
1	A	506	ALA
1	A	50	GLY
1	A	79	VAL
1	A	157	LYS
1	A	196	GLY
1	A	204	SER
1	A	212	THR
1	A	216	ARG
1	A	251	THR

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Mol	Chain	Res	Type
1	A	267	PHE
1	A	280	GLY
1	A	386	SER
1	A	527	GLY
1	A	66	THR
1	A	74	ASN
1	A	198	GLN
1	A	199	ASN
1	A	215	PHE
1	A	233	ASN
1	A	392	ASN
1	A	414	ASP
1	A	428	PRO
1	A	431	THR
1	A	479	GLN
1	A	388	LYS
1	A	155	LYS
1	A	179	MET
1	A	232	THR
1	A	490	THR
1	A	513	ILE
1	A	61	ALA
1	A	237	HIS
1	A	266	PRO
1	A	486	ILE
1	A	195	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	404/451 (90%)	369 (91%)	35 (9%)	15 53

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	76	SER

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Mol	Chain	Res	Type
1	A	83	ASN
1	A	98	ASN
1	A	100	ASP
1	A	102	SER
1	A	146	ARG
1	A	153	LEU
1	A	166	VAL
1	A	214	ASN
1	A	223	THR
1	A	232	THR
1	A	233	ASN
1	A	238	PRO
1	A	249	ASP
1	A	256	SER
1	A	258	LEU
1	A	271	PHE
1	A	287	LEU
1	A	401	THR
1	A	420	ARG
1	A	429	ASP
1	A	440	SER
1	A	446	GLN
1	A	459	ASN
1	A	468	LEU
1	A	482	TYR
1	A	501	GLU
1	A	512	THR
1	A	525	ASP
1	A	528	THR
1	A	531	LEU
1	A	533	ASN
1	A	534	SER
1	A	562	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	86	ASN
1	A	88	HIS
1	A	98	ASN
1	A	128	HIS

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Mol	Chain	Res	Type
1	A	199	ASN
1	A	214	ASN
1	A	265	GLN
1	A	282	ASN
1	A	402	GLN
1	A	459	ASN
1	A	471	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

3 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	700	-	4,4,4	3.35	2 (50%)	6,6,6	2.93	4 (66%)
3	C15	A	998	-	19,19,21	3.05	2 (10%)	21,21,26	2.18	7 (33%)
3	C15	A	999	-	19,19,21	2.92	2 (10%)	21,21,26	2.26	6 (28%)

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	700	-	-	0/0/0/0	0/0/0/0
3	C15	A	998	-	-	0/17/17/21	0/0/0/0
3	C15	A	999	-	-	0/17/17/21	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	998	C15	O3S-S1	12.64	1.77	1.46
3	A	999	C15	O3S-S1	12.19	1.76	1.46
2	A	700	SO4	O1-S	5.00	1.63	1.47
2	A	700	SO4	O3-S	-4.44	1.32	1.47
3	A	998	C15	C1-S1	3.60	1.83	1.77
3	A	999	C15	C1-S1	2.95	1.82	1.77

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	998	C15	O2S-S1-C1	6.28	112.19	106.81
3	A	999	C15	O2S-S1-C1	5.47	111.49	106.81
3	A	999	C15	C2-C3-N1	4.98	115.15	111.63
2	A	700	SO4	O4-S-O3	-4.34	90.73	109.08
3	A	999	C15	O3S-S1-C1	4.10	111.13	105.93
2	A	700	SO4	O4-S-O1	-3.57	77.68	110.12
3	A	998	C15	O3S-S1-C1	3.13	109.89	105.93
2	A	700	SO4	O2-S-O1	3.09	119.76	109.53
3	A	999	C15	C16-N1-C3	3.08	118.34	113.00
2	A	700	SO4	O4-S-O2	-2.93	83.46	110.12
3	A	998	C15	C16-N1-C3	2.81	117.87	113.00
3	A	998	C15	O3S-S1-O1S	-2.79	105.76	111.78
3	A	998	C15	C2-C1-S1	2.70	116.73	113.24
3	A	999	C15	C2-C1-S1	2.68	116.69	113.24
3	A	999	C15	O3S-S1-O1S	-2.67	106.02	111.78
3	A	998	C15	C2-C3-N1	2.65	113.51	111.63
3	A	998	C15	C15-C16-N1	2.47	113.38	111.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	460/523 (87%)	0.03	11 (2%) 56 15	30, 54, 150, 186	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	ARG	7.7
1	A	356	GLU	6.4
1	A	353	ALA	6.4
1	A	297	LYS	4.1
1	A	355	ALA	3.7
1	A	351	LYS	2.9
1	A	345	ALA	2.8
1	A	158	GLN	2.8
1	A	344	PHE	2.5
1	A	373	PRO	2.4
1	A	486	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	700	5/5	0.40	6.56	166,166,166,166	0
3	C15	A	998	20/22	0.45	4.48	91,95,113,114	0
3	C15	A	999	20/22	0.35	2.70	70,83,94,94	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.