



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:28 PM 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 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

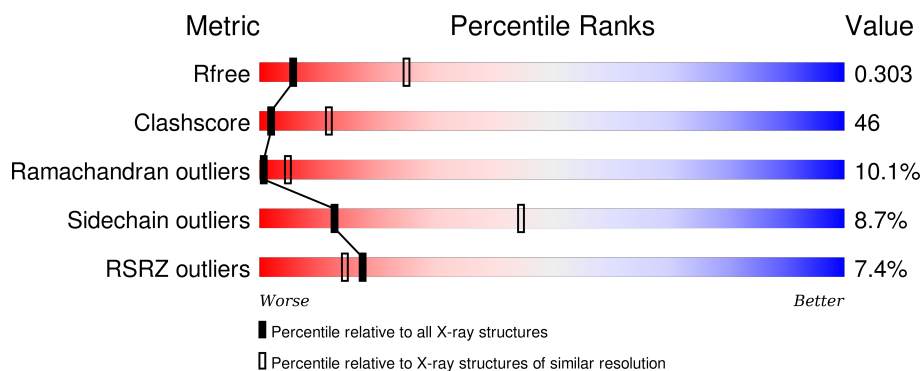
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	523	

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	700	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	C15	A	999	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3677 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 Penton protein.

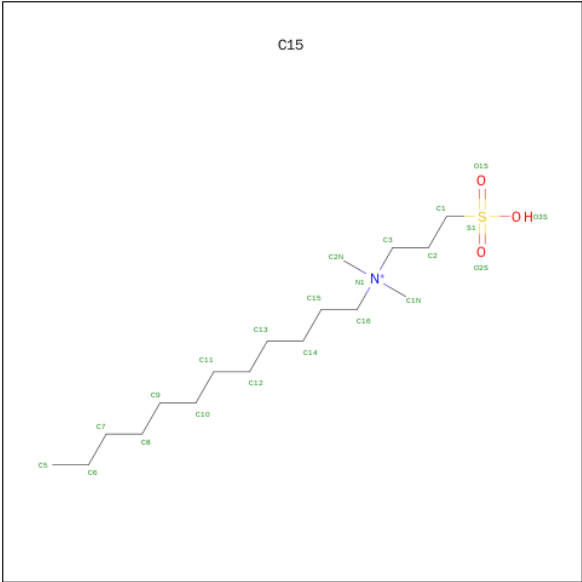
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	460	3632	2294	630	696	12	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is N-DODECYL-N,N-DIMETHYL-3-AMMONIO-1-PROPANESULFONATE (three-letter code: C15) (formula: C₁₇H₃₈NO₃S).

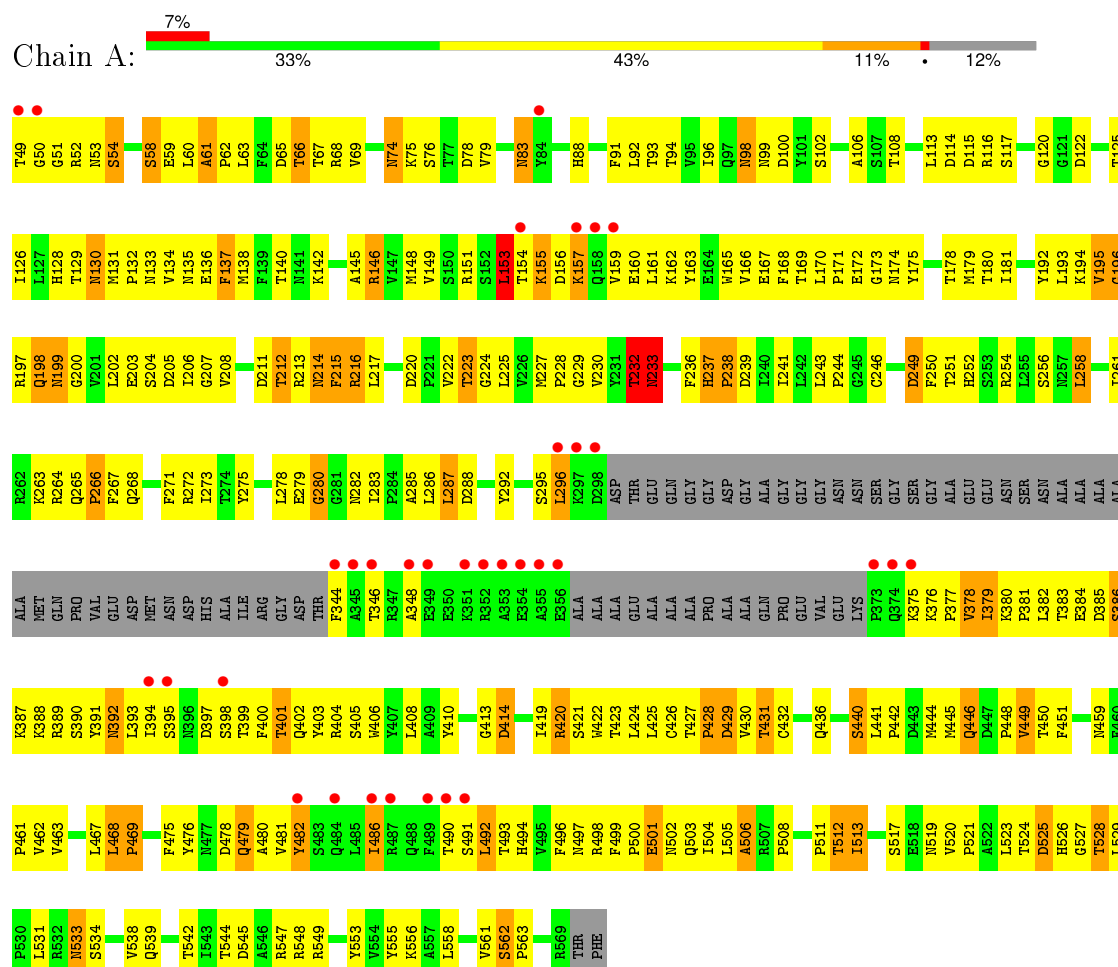


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	15	1	3	1		
3	A	1	Total	C	N	O	S	0	0
			20	15	1	3	1		

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 ($\text{RSRZ} > 2$). 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: Penton protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	80.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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

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 46.

All (337) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:MET:HB2	1:A:539:GLN:OE1	2.01	0.61
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	1 5

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	13	45

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

Mol	Chain	Res	Type
1	A	58	SER
1	A	76	SER
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
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 [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](#)

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	3.19	2 (50%)	6,6,6	2.96	4 (66%)
3	C15	A	998	-	18,19,21	2.87	1 (5%)	19,21,26	1.80	3 (15%)
3	C15	A	999	-	18,19,21	2.79	1 (5%)	19,21,26	1.64	2 (10%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	SO4	O3-S	-4.23	1.32	1.47
2	A	700	SO4	O1-S	4.74	1.63	1.47
3	A	999	C15	O3S-S1	11.60	1.76	1.46
3	A	998	C15	O3S-S1	12.03	1.77	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	SO4	O4-S-O3	-4.49	90.73	108.98
2	A	700	SO4	O4-S-O1	-3.49	77.68	110.19
2	A	700	SO4	O4-S-O2	-2.87	83.46	110.19
3	A	998	C15	O3S-S1-O1S	-2.51	105.76	111.61
3	A	999	C15	O3S-S1-O1S	-2.40	106.02	111.61
3	A	998	C15	C9-C8-C7	-2.08	103.80	114.53
2	A	700	SO4	O2-S-O1	3.24	119.76	109.50
3	A	999	C15	O2S-S1-C1	5.38	111.49	106.91
3	A	998	C15	O2S-S1-C1	6.19	112.19	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	998	C15	2	0
3	A	999	C15	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	460/523 (87%)	0.14	34 (7%) 17 14	30, 54, 150, 186	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	ALA	12.1
1	A	352	ARG	11.7
1	A	356	GLU	10.1
1	A	355	ALA	6.3
1	A	297	LYS	5.2
1	A	345	ALA	5.1
1	A	344	PHE	5.0
1	A	158	GLN	4.8
1	A	351	LYS	4.4
1	A	373	PRO	4.2
1	A	490	THR	3.6
1	A	486	ILE	3.5
1	A	159	VAL	3.5
1	A	154	THR	3.2
1	A	50	GLY	3.2
1	A	484	GLN	3.2
1	A	374	GLN	3.0
1	A	49	THR	2.9
1	A	491	SER	2.9
1	A	298	ASP	2.9
1	A	489	PHE	2.9
1	A	348	ALA	2.9
1	A	482	TYR	2.9
1	A	346	THR	2.8
1	A	296	LEU	2.7
1	A	354	GLU	2.7
1	A	157	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	394	ILE	2.7
1	A	375	LYS	2.6
1	A	487	ARG	2.5
1	A	349	GLU	2.5
1	A	398	SER	2.4
1	A	395	SER	2.2
1	A	84	TYR	2.2

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

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

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	C15	A	999	20/22	0.78	0.36	3.02	70,83,94,94	0
2	SO4	A	700	5/5	0.72	0.38	-	166,166,166,166	0
3	C15	A	998	20/22	0.63	0.47	-	91,95,113,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.