



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 07:26 AM EDT

PDB ID : 6QWS
Title : Crystal structure of the Ski2 RNA-helicase Brr2 from *Chaetomium thermophilum* in the apo state
Authors : Absmeier, E.; Santos, K.F.; Wahl, M.C.
Deposited on : 2019-03-06
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

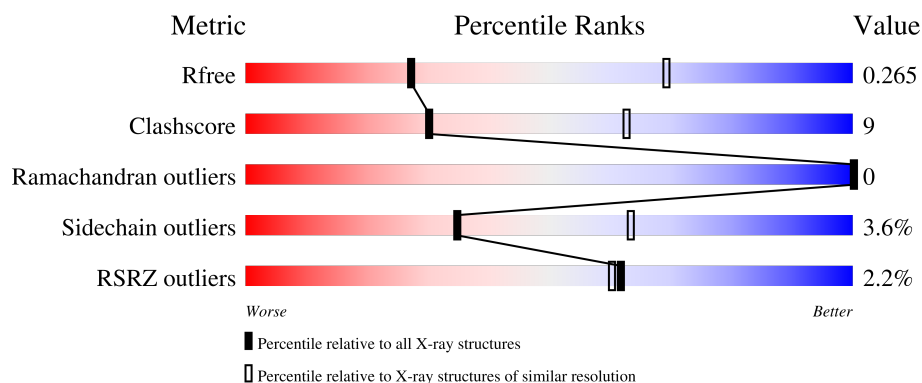
1 Overall quality at a glance

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1725	

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	2203	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	2204	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13495 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.

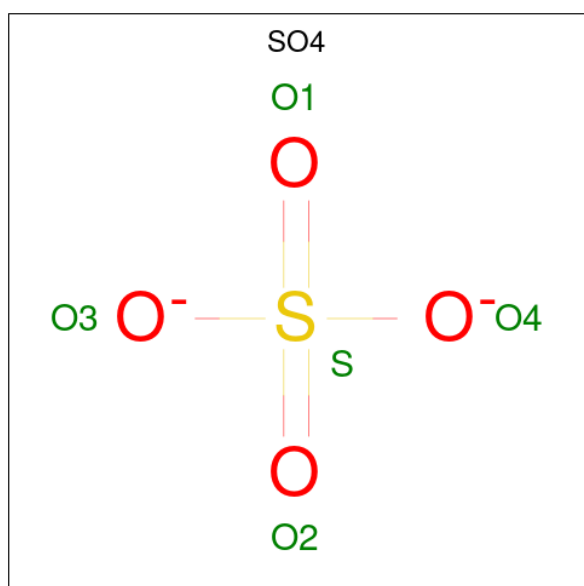
- Molecule 1 is a protein called Pre-mRNA splicing helicase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1680	13463	8607	2290	2502	64	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	GLY	-	expression tag	UNP G0S0B9
A	470	ALA	-	expression tag	UNP G0S0B9
A	471	GLU	-	expression tag	UNP G0S0B9
A	472	PHE	-	expression tag	UNP G0S0B9

- 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

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

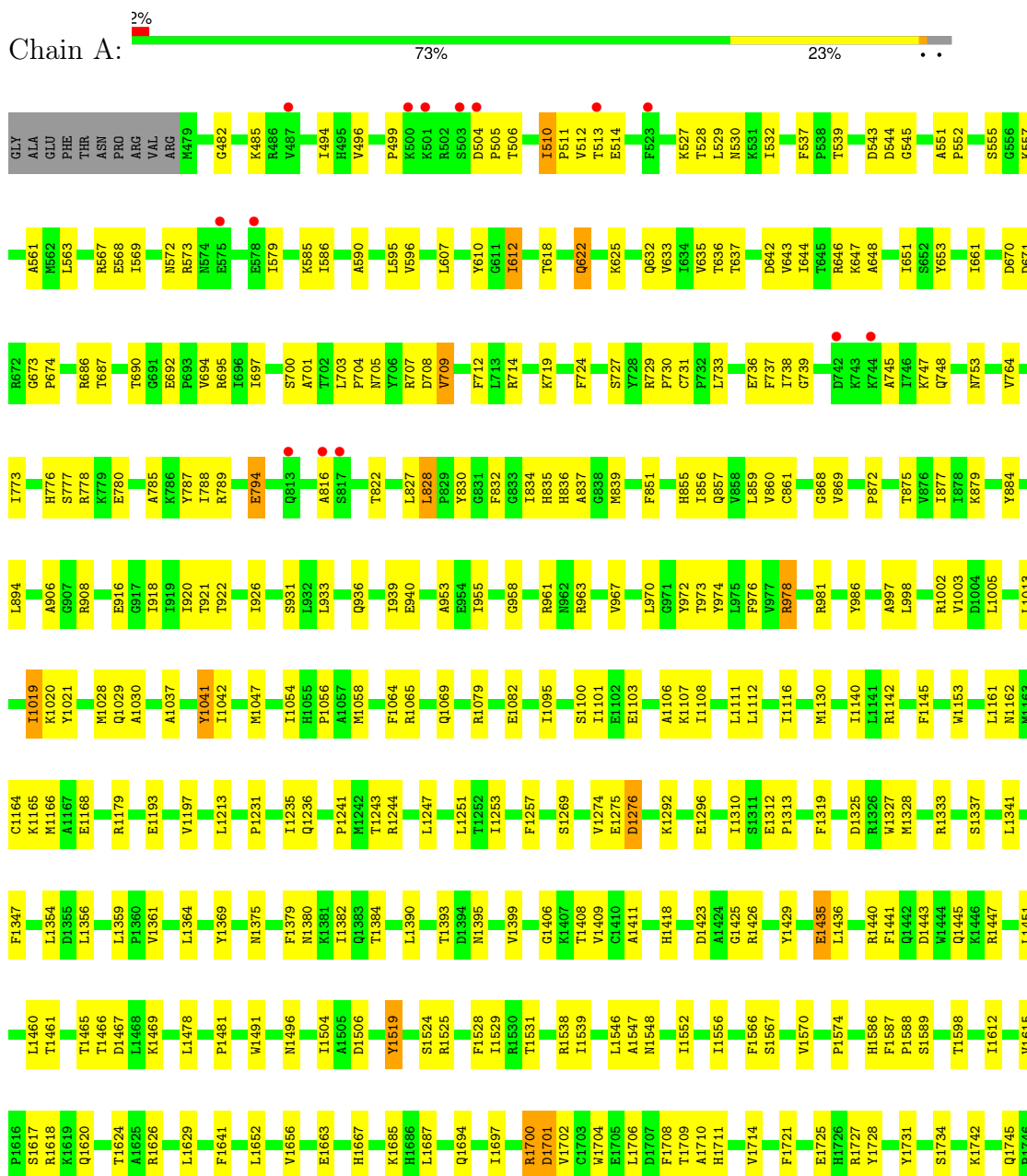
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		

3 Residue-property plots

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

- Molecule 1: Pre-mRNA splicing helicase-like protein



K2073	L2141	S1747	R1914
Y2074	A2142	G1750	R1915
P2075	I2143	H1916	E1917
D2076	K2144	V1755	L1758
I2077	R2145	N1771	E1777
T2078	V2148	P1785	M1953
L2079	G2149	V1789	R1954
E2080	K2150	I1792	M1955
F2081	E2151	I1797	D1960
E2082	L2152	E1798	D1964
VAL	L2156	S1799	Q1965
ASP	E2157	D1802	E1966
ASP	PHE	N1805	Q1970
PRO	VAL	V1806	L1975
ASN	VAL	I1807	A1978
ASN	VAL	A1810	I1979
ILE	PRO	T1811	V1980
ARG	SER	F1812	D1981
ALA	PRO	Y1813	I2101
GLY	PRO	R1815	E2102
GLU	G2164	K1846	T1982
P2084	L2168	I1853	G1987
L2097	L2172	I1854	N1990
K2098	V2173	E1855	Q1999
I2099	S2174	M1856	A2004
H2100	V2178	D1857	F2018
I2101	S2185	T1862	T2019
E2102	PHE	V1863	V2022
R2103	SER	A1864	V2025
E2104	VAL	A1869	T2031
LEU	ASN	M1884	D2036
GLU	ASN	F1885	F2037
GLU	VAL	K1892	M2038
ASP	ALA	S1893	N2041
GLU	GLU	E1900	N2046
GLU	GLY	F1901	L2056
PHE		V1902	T2070
D2112		T1903	N2071
P2113		A1904	N2072
T2114			
V2115			
P2121			
G2122			
K2123			
K2124			
S2125			
V2128			
W2129			
G2133			
E2134			
E2135			
S2136			
T2137			
LYS			
THR			
LEU			

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	124.52Å 124.52Å 128.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.63 – 3.30 44.63 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.63-3.30) 99.9 (44.63-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.206 , 0.262 0.210 , 0.265	Depositor DCC
R_{free} test set	1977 reflections (5.93%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.055 for h,-h-k,-l 0.039 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13495	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.25	0/13759	0.43	0/18658

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13463	0	13535	251	0
2	A	30	0	0	3	0
3	A	2	0	0	0	0
All	All	13495	0	13535	251	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 9.

All (251) 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:572:ASN:HB3	1:A:579:ILE:HG21	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1615:VAL:HG21	1:A:1624:THR:HG21	1.67	0.76
1:A:610:TYR:HB2	1:A:612:ILE:HG22	1.69	0.75
1:A:931:SER:HB2	1:A:936:GLN:HB3	1.70	0.74
1:A:1179:ARG:NH1	1:A:1193:GLU:OE1	2.20	0.74
1:A:510:ILE:HG22	1:A:511:PRO:HD2	1.70	0.72
1:A:816:ALA:HB1	1:A:828:LEU:HD21	1.73	0.71
1:A:1902:VAL:HG13	1:A:1975:LEU:HD22	1.73	0.71
1:A:1461:THR:HG22	1:A:1467:ASP:HB3	1.74	0.69
1:A:739:GLY:HA3	1:A:926:ILE:HD11	1.76	0.67
1:A:1855:GLU:HG3	1:A:1856:MET:H	1.59	0.67
1:A:745:ALA:HB3	1:A:747:LYS:HG2	1.75	0.67
1:A:1241:PRO:HG3	1:A:1341:LEU:HD11	1.77	0.67
1:A:1460:LEU:HD22	1:A:1467:ASP:HB2	1.76	0.65
1:A:1999:GLN:HB3	1:A:2178:VAL:HG22	1.79	0.65
1:A:1915:ARG:NH1	2:A:2204:SO4:O2	2.30	0.64
1:A:1652:LEU:HD13	1:A:1687:LEU:HD11	1.79	0.63
1:A:777:SER:HB3	1:A:780:GLU:HB2	1.80	0.63
1:A:778:ARG:HG3	1:A:836:HIS:HB2	1.80	0.62
1:A:1711:HIS:NE2	1:A:1747:SER:OG	2.32	0.62
1:A:2074:TYR:HD1	1:A:2075:PRO:HD2	1.66	0.61
1:A:670:ASP:OD1	1:A:671:ASP:N	2.33	0.61
1:A:690:THR:HG23	1:A:692:GLU:H	1.66	0.61
1:A:1598:THR:HG23	1:A:1714:VAL:HG21	1.83	0.60
1:A:1893:SER:H	1:A:1990:ASN:HD22	1.48	0.60
1:A:738:ILE:HB	1:A:920:ILE:HG22	1.83	0.60
1:A:1954:ARG:NH1	1:A:2004:ALA:O	2.35	0.60
1:A:586:ILE:HB	1:A:633:VAL:HG22	1.84	0.60
1:A:1799:SER:H	1:A:1802:ASP:HB2	1.67	0.60
1:A:963:ARG:NH1	1:A:1021:TYR:OH	2.33	0.60
1:A:773:ILE:HB	1:A:860:VAL:HG12	1.83	0.60
1:A:1612:ILE:HG13	1:A:1710:ALA:HB2	1.85	0.59
1:A:1426:ARG:NH1	1:A:1496:ASN:OD1	2.35	0.59
1:A:2077:ILE:HG21	1:A:2102:GLU:HB3	1.85	0.58
1:A:2148:VAL:HA	1:A:2152:LEU:HD12	1.83	0.58
1:A:1539:ILE:HG21	1:A:1556:ILE:HD11	1.86	0.58
1:A:561:ALA:HB1	1:A:661:ILE:HD13	1.85	0.57
1:A:1243:THR:HG22	1:A:1244:ARG:H	1.70	0.57
1:A:1624:THR:HG23	1:A:1697:ILE:HD13	1.87	0.57
1:A:1042:ILE:HD12	1:A:1140:ILE:HD13	1.87	0.57
1:A:485:LYS:HG2	1:A:494:ILE:HG12	1.87	0.57
1:A:1853:ILE:HG13	1:A:1869:ALA:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:LYS:HD2	1:A:644:ILE:HD11	1.85	0.57
1:A:973:THR:HG23	1:A:976:PHE:H	1.70	0.57
1:A:884:TYR:OH	1:A:1079:ARG:NH1	2.36	0.56
1:A:1586:HIS:NE2	2:A:2204:SO4:O2	2.35	0.56
1:A:2129:TRP:CD1	1:A:2145:ARG:HG3	2.41	0.56
1:A:785:ALA:HB2	1:A:860:VAL:HG21	1.87	0.56
1:A:1054:ILE:HG22	1:A:1153:TRP:HZ3	1.70	0.55
1:A:555:SER:HA	1:A:730:PRO:HD3	1.89	0.55
1:A:875:THR:HG22	1:A:916:GLU:HB2	1.87	0.55
1:A:1235:ILE:HG22	1:A:1253:ILE:HG12	1.88	0.55
1:A:1617:SER:HB3	1:A:1620:GLN:HB2	1.88	0.55
1:A:714:ARG:NH1	1:A:972:TYR:HA	2.22	0.55
1:A:1244:ARG:NH1	1:A:1312:GLU:OE2	2.40	0.54
1:A:736:GLU:HB3	1:A:918:ILE:HG13	1.88	0.54
1:A:1056:PRO:HG3	1:A:1153:TRP:CE2	2.43	0.54
1:A:1418:HIS:NE2	1:A:1425:GLY:O	2.37	0.54
1:A:1641:PHE:HB3	1:A:1694:GLN:HB3	1.89	0.54
1:A:1914:ARG:NH2	1:A:1964:ASP:OD2	2.40	0.54
1:A:545:GLY:O	1:A:695:ARG:NH1	2.40	0.54
1:A:1275:GLU:OE2	1:A:1333:ARG:NH2	2.41	0.54
1:A:1546:LEU:HD13	1:A:1552:ILE:HD12	1.90	0.54
1:A:1618:ARG:NH2	1:A:1964:ASP:OD1	2.39	0.54
1:A:622:GLN:HA	1:A:625:LYS:HZ3	1.73	0.53
1:A:2031:ILE:HG23	1:A:2037:PHE:HB2	1.89	0.53
1:A:753:ASN:HB3	1:A:787:TYR:CE1	2.43	0.53
1:A:997:ALA:O	1:A:1002:ARG:NH1	2.41	0.53
1:A:1429:TYR:CE1	1:A:1440:ARG:HG2	2.44	0.53
1:A:1525:ARG:HG2	1:A:1529:ILE:HD13	1.90	0.53
1:A:703:LEU:HG	1:A:704:PRO:HD2	1.91	0.53
1:A:1037:ALA:HB2	1:A:1047:MET:HG3	1.90	0.52
1:A:921:THR:OG1	1:A:922:THR:N	2.42	0.52
1:A:1587:PHE:HB3	1:A:1588:PRO:HD3	1.92	0.52
1:A:532:ILE:HD11	1:A:724:PHE:CG	2.44	0.52
1:A:1380:ASN:O	1:A:1384:THR:HG23	2.10	0.52
1:A:970:LEU:O	1:A:973:THR:HG22	2.10	0.52
1:A:1197:VAL:HG11	1:A:1213:LEU:HD21	1.92	0.52
1:A:512:VAL:HG13	1:A:514:GLU:H	1.75	0.52
1:A:527:LYS:HG3	1:A:528:THR:H	1.75	0.51
1:A:1966:GLU:O	1:A:1970:GLN:HG2	2.09	0.51
1:A:1701:ASP:N	1:A:1701:ASP:OD1	2.42	0.51
1:A:773:ILE:HG23	1:A:877:ILE:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ALA:HB1	1:A:595:LEU:HD23	1.92	0.51
1:A:612:ILE:HG13	1:A:632:GLN:HB3	1.91	0.51
1:A:1586:HIS:HB3	1:A:1589:SER:HB2	1.92	0.51
1:A:642:ASP:OD2	1:A:1041:TYR:OH	2.21	0.51
1:A:1247:LEU:HD11	1:A:1310:ILE:HD12	1.93	0.51
1:A:1443:ASP:OD2	1:A:1447:ARG:NH1	2.44	0.51
1:A:1142:ARG:NH2	1:A:1325:ASP:OD1	2.42	0.51
1:A:1652:LEU:O	1:A:1656:VAL:HG23	2.10	0.51
1:A:1810:THR:HG23	1:A:1813:TYR:H	1.76	0.50
1:A:510:ILE:HD12	1:A:529:LEU:HB3	1.93	0.50
1:A:700:SER:OG	1:A:701:ALA:N	2.44	0.50
1:A:1101:ILE:O	1:A:1103:GLU:N	2.45	0.50
1:A:764:VAL:HG21	1:A:857:GLN:HB3	1.93	0.50
1:A:1231:PRO:HG2	1:A:1327:TRP:CD1	2.47	0.50
1:A:607:LEU:HD13	1:A:612:ILE:HD13	1.94	0.50
1:A:1112:LEU:O	1:A:1116:ILE:HG12	2.12	0.50
1:A:1855:GLU:HB3	1:A:1864:ALA:H	1.76	0.50
1:A:1390:LEU:HA	1:A:1538:ARG:HH22	1.76	0.50
1:A:596:VAL:HB	1:A:635:VAL:HG23	1.93	0.49
1:A:1915:ARG:NH1	2:A:2204:SO4:S	2.86	0.49
1:A:709:VAL:HA	1:A:712:PHE:HB3	1.95	0.49
1:A:1904:ALA:HB2	1:A:1941:HIS:CE1	2.48	0.49
1:A:1364:LEU:HD22	1:A:1369:TYR:HB3	1.94	0.48
1:A:1162:ASN:O	1:A:1166:MET:HG3	2.12	0.48
1:A:646:ARG:HD2	1:A:953:ALA:HB1	1.96	0.48
1:A:729:ARG:NE	1:A:731:CYS:O	2.36	0.48
1:A:822:THR:HG21	1:A:839:MET:HG2	1.95	0.48
1:A:686:ARG:O	1:A:690:THR:HG22	2.14	0.48
1:A:648:ALA:HB1	1:A:651:ILE:HD11	1.96	0.48
1:A:1528:PHE:HA	1:A:1531:THR:HG22	1.95	0.48
1:A:1706:LEU:HB3	1:A:1742:LYS:HE2	1.95	0.48
1:A:544:ASP:CG	1:A:567:ARG:HH21	2.17	0.48
1:A:539:THR:HG23	1:A:719:LYS:HG3	1.96	0.48
1:A:1885:PHE:HZ	1:A:1975:LEU:HD21	1.77	0.48
1:A:482:GLY:HA3	1:A:496:VAL:HG22	1.95	0.47
1:A:789:ARG:HH22	1:A:827:LEU:HD23	1.79	0.47
1:A:851:PHE:HB2	1:A:856:ILE:HD11	1.96	0.47
1:A:877:ILE:HD13	1:A:918:ILE:HB	1.96	0.47
1:A:709:VAL:HG12	1:A:974:TYR:CE1	2.49	0.47
1:A:1574:PRO:HD2	1:A:1750:GLY:O	2.15	0.47
1:A:733:LEU:HD21	1:A:906:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:ILE:HB	1:A:832:PHE:HE2	1.79	0.47
1:A:1406:GLY:O	1:A:1409:VAL:HG22	2.14	0.47
1:A:1436:LEU:HD21	1:A:1704:TRP:HB3	1.96	0.47
1:A:1725:GLU:HB3	1:A:1727:ARG:HG2	1.97	0.47
1:A:1100:SER:HB2	1:A:1106:ALA:HB2	1.96	0.47
1:A:551:ALA:HB3	1:A:557:LYS:HE2	1.96	0.47
1:A:1892:LYS:HA	1:A:1990:ASN:HB3	1.96	0.47
1:A:1292:LYS:O	1:A:1296:GLU:HG2	2.14	0.46
1:A:955:ILE:HG22	1:A:1030:ALA:HB2	1.97	0.46
1:A:1065:ARG:O	1:A:1069:GLN:HG2	2.15	0.46
1:A:552:PRO:O	1:A:557:LYS:HE3	2.15	0.46
1:A:998:LEU:O	1:A:1002:ARG:HG3	2.15	0.46
1:A:778:ARG:HH21	1:A:837:ALA:HB2	1.80	0.46
1:A:1466:THR:HA	1:A:1469:LYS:HE2	1.97	0.46
1:A:1792:ILE:HG12	1:A:1797:ILE:HG23	1.98	0.46
1:A:2121:PRO:O	1:A:2123:LYS:NZ	2.46	0.46
1:A:2135:GLU:N	1:A:2135:GLU:OE1	2.48	0.46
1:A:1347:PHE:CE2	1:A:1547:ALA:HB1	2.51	0.46
1:A:1435:GLU:OE1	1:A:1704:TRP:HB2	2.16	0.46
1:A:1082:GLU:OE2	1:A:1107:LYS:NZ	2.36	0.46
1:A:709:VAL:HG12	1:A:974:TYR:CZ	2.50	0.45
1:A:2097:LEU:N	1:A:2156:LEU:O	2.46	0.45
1:A:512:VAL:HA	1:A:528:THR:HG22	1.97	0.45
1:A:1914:ARG:NH1	1:A:1960:ASP:HB3	2.31	0.45
1:A:568:GLU:OE2	1:A:572:ASN:ND2	2.50	0.45
1:A:705:ASN:HD21	1:A:939:ILE:HB	1.80	0.45
1:A:1810:THR:HG21	1:A:1812:PHE:HD2	1.80	0.45
1:A:1145:PHE:CE1	1:A:1161:LEU:HB2	2.52	0.45
1:A:1465:THR:HG23	1:A:1466:THR:HG23	1.99	0.45
1:A:776:HIS:NE2	1:A:894:LEU:HD11	2.31	0.45
1:A:1359:LEU:H	1:A:1384:THR:CG2	2.30	0.45
1:A:1893:SER:N	1:A:1990:ASN:HB3	2.31	0.45
1:A:543:ASP:OD1	1:A:544:ASP:N	2.50	0.45
1:A:794:GLU:H	1:A:794:GLU:HG3	1.63	0.45
1:A:872:PRO:HG2	1:A:908:ARG:HG2	1.98	0.45
1:A:1243:THR:HG23	1:A:1347:PHE:CZ	2.52	0.45
1:A:868:GLY:O	1:A:869:VAL:HG23	2.16	0.44
1:A:1020:LYS:HE2	1:A:1029:GLN:HB3	1.99	0.44
1:A:2128:TRP:HB3	1:A:2172:LEU:HD21	1.99	0.44
1:A:737:PHE:CZ	1:A:933:LEU:HD12	2.52	0.44
1:A:1274:VAL:HA	1:A:1319:PHE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:PHE:CZ	1:A:1445:GLN:HG3	2.52	0.44
1:A:1914:ARG:NH2	1:A:1917:GLU:OE1	2.51	0.44
1:A:673:GLY:N	1:A:674:PRO:HD2	2.33	0.44
1:A:1411:ALA:HB1	1:A:1504:ILE:HD13	1.99	0.44
1:A:2077:ILE:HG12	1:A:2104:GLU:HG2	1.99	0.44
1:A:2097:LEU:HB2	1:A:2156:LEU:HD23	1.98	0.44
1:A:1165:LYS:HD3	1:A:1328:MET:HA	1.99	0.44
1:A:1429:TYR:HB3	1:A:1478:LEU:HD22	1.99	0.44
1:A:2019:THR:HB	1:A:2022:VAL:HG23	1.99	0.44
1:A:879:LYS:HG2	1:A:920:ILE:HD11	2.00	0.44
1:A:1709:THR:HG22	1:A:1745:GLN:HG3	2.00	0.44
1:A:1799:SER:HB3	1:A:1862:THR:HA	1.98	0.44
1:A:494:ILE:HB	1:A:737:PHE:HB2	1.99	0.44
1:A:958:GLY:HA2	1:A:961:ARG:HD3	1.98	0.44
1:A:2128:TRP:CH2	1:A:2174:SER:HB3	2.53	0.44
1:A:1005:LEU:HD12	1:A:1005:LEU:HA	1.85	0.44
1:A:1700:ARG:HD3	1:A:1731:TYR:CE1	2.52	0.44
1:A:1777:GLU:OE2	1:A:1815:ARG:NH1	2.51	0.44
1:A:2038:MET:SD	1:A:2070:THR:HG21	2.58	0.44
1:A:1056:PRO:HG3	1:A:1153:TRP:CD2	2.53	0.43
1:A:2123:LYS:H	1:A:2123:LYS:HD2	1.83	0.43
1:A:1064:PHE:HE2	1:A:1095:ILE:HG13	1.82	0.43
1:A:708:ASP:OD2	1:A:981:ARG:NH2	2.51	0.43
1:A:661:ILE:HG12	1:A:697:ILE:HB	1.99	0.43
1:A:1364:LEU:HD12	1:A:1364:LEU:H	1.82	0.43
1:A:1361:VAL:HA	1:A:1379:PHE:HE2	1.82	0.43
1:A:1013:LEU:HB3	1:A:1019:ILE:HB	2.01	0.43
1:A:1721:PHE:HB2	1:A:1728:TYR:CE1	2.53	0.43
1:A:1276:ASP:OD1	1:A:1276:ASP:N	2.52	0.43
1:A:512:VAL:HG22	1:A:513:THR:H	1.84	0.43
1:A:537:PHE:HD1	1:A:563:LEU:HD13	1.82	0.43
1:A:643:VAL:O	1:A:647:LYS:HG2	2.18	0.43
1:A:1807:ALA:O	1:A:1810:THR:HG22	2.19	0.43
1:A:1382:ILE:HG23	1:A:1566:PHE:CE2	2.53	0.43
1:A:687:THR:HG21	1:A:694:VAL:HB	2.01	0.43
1:A:1021:TYR:HD1	1:A:1028:MET:HB3	1.83	0.43
1:A:1054:ILE:HG22	1:A:1153:TRP:CZ3	2.52	0.43
1:A:2101:ILE:O	1:A:2151:GLU:HA	2.19	0.43
1:A:1435:GLU:H	1:A:1435:GLU:HG3	1.48	0.42
1:A:1567:SER:HB3	1:A:1570:VAL:HG23	2.01	0.42
1:A:499:PRO:HB2	1:A:727:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:ARG:HH12	1:A:827:LEU:HD23	1.83	0.42
1:A:2075:PRO:HG3	1:A:2128:TRP:CZ2	2.54	0.42
1:A:504:ASP:N	1:A:505:PRO:HD3	2.35	0.42
1:A:828:LEU:O	1:A:830:TYR:N	2.53	0.42
1:A:1111:LEU:HD22	1:A:1130:MET:HB2	2.00	0.42
1:A:1164:CYS:O	1:A:1168:GLU:HG2	2.20	0.42
1:A:1429:TYR:OH	1:A:1506:ASP:OD2	2.31	0.42
1:A:1481:PRO:HB3	1:A:1519:TYR:HA	2.02	0.42
1:A:1491:TRP:CG	1:A:1529:ILE:HD11	2.55	0.42
1:A:2128:TRP:CZ3	1:A:2174:SER:HB3	2.54	0.42
1:A:835:HIS:O	1:A:861:CYS:HA	2.20	0.42
1:A:1990:ASN:N	1:A:1990:ASN:OD1	2.52	0.42
1:A:967:VAL:HG11	1:A:1003:VAL:HG22	2.03	0.41
1:A:1161:LEU:HG	1:A:1165:LYS:HE3	2.02	0.41
1:A:1393:THR:HG22	1:A:1395:ASN:H	1.85	0.41
1:A:785:ALA:HB2	1:A:860:VAL:CG2	2.50	0.41
1:A:955:ILE:HD13	1:A:1019:ILE:HD11	2.03	0.41
1:A:1702:VAL:O	1:A:1706:LEU:HB2	2.21	0.41
1:A:2025:VAL:HG13	1:A:2056:LEU:HD23	2.03	0.41
1:A:1312:GLU:HB3	1:A:1313:PRO:HD3	2.02	0.41
1:A:1777:GLU:OE1	1:A:1815:ARG:HG2	2.20	0.41
1:A:1914:ARG:HH11	1:A:1960:ASP:HB3	1.84	0.41
1:A:1953:SER:HB2	1:A:1955:MET:HG3	2.02	0.41
1:A:1978:ALA:O	1:A:1982:ILE:HG13	2.20	0.41
1:A:585:LYS:HZ2	1:A:653:TYR:HD1	1.68	0.41
1:A:590:ALA:HB3	1:A:596:VAL:CG1	2.51	0.41
1:A:636:THR:OG1	1:A:637:THR:N	2.53	0.41
1:A:940:GLU:OE1	1:A:978:ARG:NH1	2.53	0.41
1:A:1629:LEU:HD21	1:A:1667:HIS:HB2	2.01	0.41
1:A:1785:PRO:O	1:A:1789:VAL:HG23	2.21	0.41
1:A:1236:GLN:O	1:A:1251:LEU:HD12	2.20	0.41
1:A:1354:LEU:HD23	1:A:1356:LEU:HD21	2.03	0.41
1:A:1524:SER:OG	1:A:1810:THR:HA	2.20	0.41
1:A:1685:LYS:HA	1:A:1708:PHE:CE2	2.56	0.41
1:A:2115:VAL:HG23	1:A:2125:SER:HA	2.02	0.41
1:A:978:ARG:HD3	1:A:978:ARG:HA	1.93	0.41
1:A:2079:LEU:HD11	1:A:2172:LEU:HD12	2.03	0.41
1:A:510:ILE:HD12	1:A:529:LEU:CB	2.50	0.40
1:A:2081:PHE:HE1	1:A:2099:ILE:HG23	1.86	0.40
1:A:569:ILE:O	1:A:573:ARG:HB2	2.21	0.40
1:A:978:ARG:HB3	1:A:986:TYR:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1626:ARG:NH2	1:A:1663:GLU:HG2	2.37	0.40
1:A:856:ILE:HD12	1:A:859:LEU:HD13	2.03	0.40
1:A:1451:LEU:HD12	1:A:1451:LEU:HA	1.95	0.40
1:A:1980:VAL:HG11	1:A:2129:TRP:CZ3	2.56	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	1670/1725 (97%)	1601 (96%)	69 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1484/1523 (97%)	1431 (96%)	53 (4%)	35	63

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	506	THR
1	A	510	ILE

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Mol	Chain	Res	Type
1	A	530	ASN
1	A	612	ILE
1	A	618	THR
1	A	622	GLN
1	A	707	ARG
1	A	709	VAL
1	A	748	GLN
1	A	794	GLU
1	A	828	LEU
1	A	834	ILE
1	A	855	HIS
1	A	978	ARG
1	A	1019	ILE
1	A	1041	TYR
1	A	1058	MET
1	A	1108	ILE
1	A	1257	PHE
1	A	1269	SER
1	A	1276	ASP
1	A	1337	SER
1	A	1375	ASN
1	A	1399	VAL
1	A	1408	THR
1	A	1423	ASP
1	A	1435	GLU
1	A	1519	TYR
1	A	1548	ASN
1	A	1700	ARG
1	A	1701	ASP
1	A	1734	SER
1	A	1755	VAL
1	A	1758	LEU
1	A	1771	ASN
1	A	1802	ASP
1	A	1805	ASN
1	A	1812	PHE
1	A	1815	ARG
1	A	1846	LYS
1	A	1857	ASP
1	A	1884	MET
1	A	1900	GLU
1	A	1990	ASN

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Mol	Chain	Res	Type
1	A	2018	PHE
1	A	2046	ASN
1	A	2074	TYR
1	A	2112	ASP
1	A	2114	THR
1	A	2123	LYS
1	A	2150	LYS
1	A	2156	LEU
1	A	2172	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	2202	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	A	2205	-	4,4,4	0.23	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	2206	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	A	2204	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	A	2201	-	4,4,4	0.24	0	6,6,6	0.16	0
2	SO4	A	2203	-	4,4,4	0.23	0	6,6,6	0.12	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2204	SO4	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	1680/1725 (97%)	-0.02	37 (2%) 62 60	39, 79, 163, 244	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2081	PHE	5.2
1	A	2168	LEU	4.8
1	A	2079	LEU	4.6
1	A	2143	ILE	3.8
1	A	742	ASP	3.5
1	A	504	ASP	3.5
1	A	2133	GLY	3.4
1	A	2156	LEU	3.2
1	A	2141	LEU	3.2
1	A	2036	ASP	3.1
1	A	1987	GLY	3.1
1	A	513	THR	3.0
1	A	575	GLU	3.0
1	A	578	GLU	2.9
1	A	2072	ASN	2.8
1	A	817	SER	2.8
1	A	816	ALA	2.6
1	A	487	VAL	2.6
1	A	2157	GLU	2.5
1	A	503	SER	2.5
1	A	1926	ASP	2.4
1	A	500	LYS	2.4
1	A	523	PHE	2.3
1	A	2142	ALA	2.3
1	A	2073	LYS	2.3
1	A	2101	ILE	2.3
1	A	813	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	744	LYS	2.2
1	A	2149	GLY	2.2
1	A	2041	MET	2.2
1	A	2103	ARG	2.2
1	A	2104	GLU	2.2
1	A	2075	PRO	2.1
1	A	501	LYS	2.1
1	A	2038	MET	2.0
1	A	2148	VAL	2.0
1	A	2094	PRO	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	2203	5/5	0.69	0.52	125,128,134,142	0
2	SO4	A	2204	5/5	0.78	0.29	175,176,181,182	0
2	SO4	A	2202	5/5	0.87	0.25	101,102,112,122	0
2	SO4	A	2205	5/5	0.91	0.24	130,131,135,142	0
2	SO4	A	2206	5/5	0.93	0.22	112,113,118,124	0
2	SO4	A	2201	5/5	0.98	0.29	55,59,73,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.