



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:35 PM UTC

PDB ID : 5XYA / pdb_00005xya
Title : Crystal structure of a serine protease from Streptococcus species
Authors : Jobichen, C.; Sivaraman, J.
Deposited on : 2017-07-06
Resolution : 3.00 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

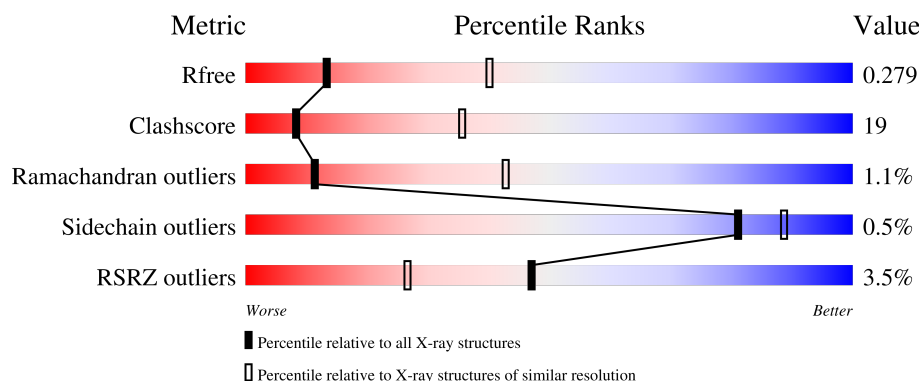
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1530	

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
3	SO4	A	1704	-	-	X	-

2 Entry composition [i](#)

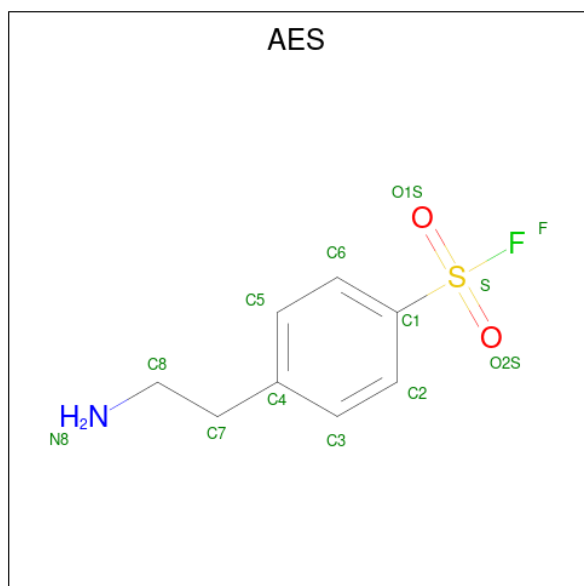
There are 4 unique types of molecules in this entry. The entry contains 10300 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chemokine protease C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1358	Total	C	N	O	Se	0	0	0
			10269	6462	1764	2019	24			

- Molecule 2 is 4-(2-AMINOETHYL)BENZENESULFONYL FLUORIDE (CCD ID: AES) (formula: C₈H₁₀FNO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	8	1	2	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Ca	0	0
			4	4		

PHE	SER	K1449	V1344	T1032		
	SER	K1450	A1236		L1124	
ARG	SER	Y1450	M1347	G1237	P1125	R1033
	LYS	T1451	K1348			R1034
LYS	THR	V1452	Y1349	I1241	T1127	P1037
	ASP		Y1350	E1242	L1128	E1038
THR	HIS	L1455	I1351		G1129	P1039
	LYS	P1352	P1352	W1246	K1130	L1040
LYS	VAL	L1464	K1353	Y1247	T1131	K1041
	ASP			G1248		D1042
PHE	SER	F1480	D1356		Y1142	
	LYS		G1357			
LYS	ASN	V1483	S1358	R1252		L1045
	ASN		Y1359	V1256	L1152	A1046
SER	SER	K1486	T1360	M1257	E1153	G1047
	GLN	M1487	I1361		M1154	V1048
ALA	ALA	T1496	S1362	Y1261		D1051
	LEU		K1363		D1158	
THR	THR		R1364	V1285	V1162	F1054
	ALA	F1499	D1365	T1266		Y1055
SER	SER	D1500	G1366	Y1267	A1166	L1056
	ALA	H1501	V1367	K1277	V1171	P1063
THR	THR	L1502	T1368	Q1278	H1172	P1064
	PRO	L1503	L1369	S1279		T1065
THR	THR		S1370	T1280	S1178	P1066
	LYS	L1521	D1371	I1281	Q1179	T1067
THR	THR	E1522	Y1372	S1282	L1180	L1068
	THR	Q1523	Y1373		T1181	
PRO	PRO	Y1526	Y1374	G1283	K1182	V1075
	ALA		E1377	R1294		S1076
THR	THR	Y1531			F1187	V1077
	ALA	G1532	A1380	T1297	F1188	
LYS	LYS	K1533		I1298	I1189	N1080
	ALA		V1383	N1299	S1190	K1081
LEU	LEU	Q1536		G1300	P1191	
	PRO		L1388	V1301	N1192	R1086
SER	SER	Y1540		D1302	E1193	
	SER		K1396	H1303	D1194	F1092
GLY	GLY	V1544	D1397		K1197	D1097
	GLY	S1545		D1307		
LYS	LYS	L1546	V1400			
	NSE	P1547		S1314	V1200	G1102
GLY	GLY	K1548	F1403			
	LEU	G1549		E1320	K1203	Y1105
LYS	LYS	Y1550	D1406	F1323	G1204	Y1106
	LEU	R1551		Y1324	L1205	M1107
ARG	ARG	L1552	P1410	L1325		T1108
	ILE	E1553			Y1210	E1109
VAL	VAL		T1415			
	GLY	E1564	Y1416	R1331	L1213	D1110
LEU	LEU	V1565	N1417	K1332	T1214	F1111
	VAL					A1112
LEU	LEU	R1571	R1423	E1337	Y1218	N1114
	LEU		D1424	G1338		V1115
GLY	GLY	K1574	A1425	K1339	H1223	A1116
	LEU	VAL		D1340	Q1224	T1117
THR	THR	GLY	Y1435	G1341	K1225	A1118
	CYS	ASP		I1342		K1119
VAL	VAL	ALA	G1440	T1243		L1120

4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	190.53Å 190.53Å 248.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 3.00 19.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.90-3.00) 98.7 (19.90-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.72 (at 2.86Å)	Xtriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, R_{free}	0.223 , 0.278 0.227 , 0.279	Depositor DCC
R_{free} test set	1990 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 17.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10300	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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

5.1 Standard geometry

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

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	0.61	2/10444 (0.0%)	0.88	15/14117 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1300	GLY	C-O	-5.48	1.20	1.24
1	A	580	SER	C-O	-5.36	1.17	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	VAL	CA-C-N	-7.42	115.39	122.66
1	A	402	VAL	C-N-CA	-7.42	115.39	122.66
1	A	536	PRO	N-CA-CB	7.24	110.85	103.25
1	A	1487	MSE	N-CA-C	7.21	120.38	109.41
1	A	493	PRO	N-CA-CB	6.94	110.63	103.00
1	A	1299	ASN	CB-CA-C	5.79	123.35	116.63
1	A	612	SER	CA-C-N	-5.74	110.57	121.54
1	A	612	SER	C-N-CA	-5.74	110.57	121.54
1	A	1297	THR	CB-CA-C	5.70	120.08	110.79
1	A	610	TYR	CB-CA-C	5.69	121.45	109.79
1	A	1550	TYR	N-CA-C	5.30	120.23	113.18
1	A	908	SER	CA-C-N	5.04	126.15	119.84
1	A	908	SER	C-N-CA	5.04	126.15	119.84
1	A	1051	ASP	CA-C-N	-5.04	112.93	121.85
1	A	1051	ASP	C-N-CA	-5.04	112.93	121.85

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	10269	0	9868	387	0
2	A	12	0	10	2	0
3	A	15	0	0	2	0
4	A	4	0	0	0	0
All	All	10300	0	9878	387	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 19.

All (387) 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:188:TYR:OH	1:A:330:LYS:HE3	1.32	1.25
1:A:401:LEU:O	1:A:581:ASN:ND2	1.82	1.12
1:A:412:THR:HG22	1:A:651:LYS:HD3	1.40	1.04
1:A:910:ASN:ND2	1:A:912:ASP:OD1	1.94	1.00
1:A:188:TYR:OH	1:A:330:LYS:CE	2.13	0.95
1:A:402:VAL:HA	1:A:581:ASN:HD22	1.34	0.90
1:A:362:MSE:HE1	1:A:405:PRO:HB3	1.51	0.90
1:A:1190:SER:O	1:A:1192:ASN:OD1	1.89	0.90
1:A:1102:GLY:HA2	1:A:1120:LEU:HB2	1.55	0.88
1:A:142:GLY:H	1:A:306:PRO:HD2	1.40	0.87
1:A:302:LEU:HD21	1:A:306:PRO:HB3	1.60	0.83
1:A:603:SER:H	1:A:611:GLY:HA3	1.44	0.83
1:A:710:MSE:HE3	1:A:775:VAL:HG11	1.60	0.81
1:A:383:ARG:HG2	1:A:384:VAL:HG22	1.62	0.81
1:A:1127:THR:HG23	1:A:1130:LYS:HE2	1.65	0.78
1:A:149:VAL:HG13	1:A:312:PHE:HD2	1.49	0.77
1:A:158:HIS:CD2	1:A:608:ASN:H	2.02	0.77
1:A:582:TRP:HD1	1:A:583:GLY:H	1.32	0.76
1:A:679:LEU:HD23	1:A:680:LEU:N	2.01	0.76
1:A:282:HIS:CE1	1:A:612:SER:O	2.39	0.76
1:A:1294:ARG:HD2	1:A:1396:LYS:HE3	1.66	0.75
1:A:154:ILE:HG22	1:A:155:ASP:H	1.52	0.75
1:A:146:VAL:HG23	1:A:340:ALA:HA	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:HIS:HD2	1:A:608:ASN:H	1.36	0.73
1:A:885:THR:HG21	1:A:893:PHE:HB3	1.71	0.73
1:A:132:THR:HA	1:A:682:ILE:HD11	1.71	0.72
1:A:582:TRP:CD1	1:A:583:GLY:H	2.06	0.71
1:A:1152:LEU:HD23	1:A:1154:MSE:HE1	1.72	0.71
1:A:147:VAL:HG23	1:A:342:VAL:HG13	1.74	0.70
1:A:174:LYS:HB3	1:A:191:TRP:NE1	2.07	0.70
1:A:1054:PHE:HE2	1:A:1107:MSE:HE3	1.57	0.70
1:A:171:VAL:HG21	1:A:197:VAL:HG11	1.75	0.69
1:A:885:THR:CG2	1:A:893:PHE:HB3	2.23	0.69
1:A:631:LYS:HE2	1:A:646:ILE:HG12	1.75	0.68
1:A:142:GLY:N	1:A:306:PRO:HD2	2.08	0.68
1:A:394:ALA:HA	1:A:744:PHE:CE2	2.29	0.68
1:A:1363:LYS:HZ1	1:A:1369:LEU:HB2	1.59	0.68
1:A:407:THR:HA	1:A:591:LYS:HD3	1.76	0.67
1:A:1499:PHE:CE2	1:A:1503:LEU:HD11	2.29	0.67
1:A:1400:VAL:HG13	1:A:1480:PHE:HD1	1.60	0.67
1:A:798:PHE:HB2	1:A:809:VAL:O	1.95	0.67
1:A:365:ILE:HG23	1:A:375:VAL:HG21	1.75	0.67
1:A:402:VAL:HA	1:A:581:ASN:ND2	2.09	0.66
1:A:1415:ILE:HG22	1:A:1417:ASN:H	1.60	0.66
1:A:630:VAL:HG12	1:A:634:LEU:HD11	1.78	0.66
1:A:643:LYS:HG3	1:A:644:GLU:OE1	1.95	0.66
1:A:937:HIS:ND1	1:A:939:SER:HB3	2.11	0.66
1:A:372:GLY:HA2	1:A:646:ILE:HG21	1.78	0.66
1:A:201:ASN:HB3	1:A:207:ASP:H	1.60	0.65
1:A:1546:LEU:HD13	1:A:1550:TYR:HB3	1.78	0.65
1:A:951:PRO:HA	1:A:1252:ARG:NH2	2.12	0.65
1:A:279:HIS:NE2	2:A:1701:AES:O1S	2.29	0.64
1:A:1110:ASP:HB3	1:A:1113:GLY:H	1.62	0.64
1:A:1546:LEU:HD11	1:A:1552:ILE:HG13	1.79	0.64
1:A:1403:PHE:HD1	1:A:1483:VAL:HG22	1.62	0.64
1:A:135:ALA:HB2	1:A:686:VAL:HG21	1.79	0.64
1:A:195:LYS:NZ	1:A:308:ALA:O	2.26	0.64
1:A:625:GLY:HA2	1:A:628:LEU:HD12	1.80	0.64
1:A:400:GLY:HA3	1:A:583:GLY:HA3	1.79	0.63
1:A:1029:ASP:OD2	1:A:1032:THR:HG22	1.98	0.63
1:A:1377:GLU:HB2	1:A:1383:VAL:HG22	1.81	0.63
1:A:708:ASP:OD1	1:A:709:THR:HG23	1.98	0.63
1:A:402:VAL:HG22	1:A:582:TRP:O	1.99	0.62
1:A:427:MSE:SE	1:A:559:LEU:HD11	2.49	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:MSE:HE2	1:A:1117:ILE:HD11	1.81	0.62
1:A:631:LYS:HG3	1:A:646:ILE:HD11	1.79	0.62
1:A:985:ALA:HA	1:A:1233:GLN:HG3	1.81	0.62
1:A:464:HIS:O	1:A:464:HIS:ND1	2.33	0.62
1:A:1192:ASN:OD1	1:A:1192:ASN:N	2.32	0.61
1:A:1192:ASN:ND2	1:A:1194:ASP:OD1	2.33	0.61
1:A:154:ILE:HD11	1:A:312:PHE:CG	2.35	0.61
1:A:1130:LYS:HB2	1:A:1131:THR:HG22	1.82	0.61
1:A:464:HIS:HB2	1:A:555:GLY:O	2.00	0.61
1:A:641:LEU:HD21	1:A:649:ILE:HD12	1.81	0.61
1:A:1205:LEU:HD12	1:A:1205:LEU:H	1.66	0.61
1:A:587:ASP:HA	1:A:1002:VAL:HG12	1.82	0.61
1:A:1496:THR:OG1	3:A:1704:SO4:O1	2.13	0.60
1:A:400:GLY:CA	1:A:583:GLY:HA3	2.31	0.60
1:A:149:VAL:HG21	1:A:284:THR:HG22	1.82	0.60
1:A:200:HIS:HB3	1:A:202:TYR:CE1	2.36	0.60
1:A:1353:LYS:HG3	1:A:1359:TYR:CZ	2.35	0.60
1:A:728:TYR:HB3	1:A:798:PHE:CE1	2.36	0.60
1:A:994:TYR:HB2	1:A:1014:MSE:HE2	1.82	0.60
1:A:673:ARG:HG3	1:A:793:GLU:OE2	2.02	0.60
1:A:403:GLY:C	1:A:407:THR:HG23	2.27	0.60
1:A:146:VAL:HG12	1:A:309:GLN:HB2	1.84	0.60
1:A:706:ILE:HD12	1:A:710:MSE:HG2	1.82	0.60
1:A:1127:THR:HA	1:A:1130:LYS:NZ	2.16	0.59
1:A:679:LEU:HD23	1:A:680:LEU:H	1.66	0.59
1:A:603:SER:O	1:A:611:GLY:N	2.35	0.59
1:A:383:ARG:O	1:A:384:VAL:HG13	2.03	0.59
1:A:402:VAL:CA	1:A:581:ASN:HD22	2.14	0.59
1:A:149:VAL:HG11	1:A:284:THR:HG22	1.85	0.58
1:A:741:LYS:HD2	1:A:743:ARG:HD2	1.86	0.58
1:A:761:VAL:HG23	1:A:767:VAL:HG12	1.85	0.58
1:A:380:GLY:H	1:A:616:THR:HG21	1.69	0.58
1:A:631:LYS:HA	1:A:634:LEU:HD12	1.85	0.58
1:A:931:LEU:HA	1:A:997:SER:O	2.03	0.58
1:A:143:GLN:N	1:A:307:GLU:HB3	2.19	0.58
1:A:376:VAL:HG12	1:A:620:SER:OG	2.03	0.58
1:A:1056:LEU:HD13	1:A:1063:PRO:HB2	1.85	0.58
1:A:146:VAL:CG2	1:A:340:ALA:HA	2.34	0.57
1:A:647:ALA:HA	1:A:650:VAL:HG12	1.86	0.57
1:A:999:TYR:CZ	1:A:1007:ARG:HB2	2.39	0.57
1:A:418:ASN:HA	1:A:599:GLY:HA3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ASN:CG	1:A:912:ASP:OD1	2.48	0.57
1:A:384:VAL:HG12	1:A:399:TYR:HD1	1.69	0.57
1:A:1325:LEU:HA	1:A:1347:ASN:O	2.05	0.57
1:A:1109:GLU:HG2	1:A:1115:VAL:HG22	1.87	0.57
1:A:1464:LEU:HA	1:A:1487:MSE:HG2	1.87	0.57
1:A:690:LEU:HD21	1:A:726:LEU:HD11	1.85	0.57
1:A:602:TYR:CE2	1:A:610:TYR:HB3	2.41	0.56
1:A:1397:ASP:OD1	1:A:1397:ASP:N	2.26	0.56
1:A:128:ASP:OD2	1:A:133:LYS:NZ	2.38	0.56
1:A:854:VAL:HB	1:A:881:HIS:HA	1.87	0.56
1:A:1158:ASP:OD2	1:A:1182:LYS:NZ	2.38	0.56
1:A:188:TYR:HH	1:A:330:LYS:HE3	1.65	0.56
1:A:202:TYR:OH	1:A:334:ASP:OD2	2.22	0.56
1:A:548:MSE:O	1:A:551:LEU:N	2.38	0.56
1:A:594:ILE:HD13	1:A:623:ILE:HD12	1.87	0.56
1:A:143:GLN:HA	1:A:307:GLU:O	2.06	0.56
1:A:1200:VAL:HG21	1:A:1281:ILE:HG13	1.87	0.56
1:A:435:ARG:C	1:A:437:ASP:H	2.13	0.55
1:A:341:ASP:O	1:A:373:VAL:HA	2.05	0.55
1:A:904:VAL:HG11	1:A:1111:PHE:CG	2.42	0.55
1:A:1064:TYR:OH	1:A:1337:GLU:OE1	2.22	0.55
1:A:658:ALA:HB1	1:A:679:LEU:O	2.06	0.55
1:A:1154:MSE:HE3	1:A:1203:LYS:HD3	1.87	0.55
1:A:156:PRO:HB2	1:A:196:VAL:HG21	1.89	0.55
1:A:435:ARG:NH1	1:A:437:ASP:OD1	2.39	0.55
1:A:630:VAL:HB	1:A:650:VAL:HG23	1.89	0.54
1:A:633:TYR:O	1:A:637:THR:HG23	2.06	0.54
1:A:126:ILE:HD11	1:A:597:PRO:HG2	1.88	0.54
1:A:154:ILE:HG22	1:A:155:ASP:N	2.20	0.54
1:A:1400:VAL:HG13	1:A:1480:PHE:CD1	2.41	0.54
1:A:625:GLY:O	1:A:628:LEU:HB2	2.07	0.54
1:A:329:ILE:HG12	1:A:361:LEU:HD13	1.90	0.54
1:A:452:LYS:H	1:A:452:LYS:HD2	1.73	0.53
1:A:162:ARG:HG2	1:A:292:LYS:NZ	2.23	0.53
1:A:672:PRO:HD2	1:A:793:GLU:CD	2.33	0.53
1:A:910:ASN:OD1	1:A:910:ASN:N	2.39	0.53
1:A:704:GLY:HA2	1:A:1526:TYR:CE2	2.44	0.53
1:A:1188:PHE:O	1:A:1197:LYS:HE3	2.09	0.53
1:A:591:LYS:HA	1:A:592:PRO:O	2.09	0.53
1:A:688:SER:OG	1:A:690:LEU:HB2	2.07	0.53
1:A:882:THR:O	1:A:885:THR:HB	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:ASP:HB2	1:A:1114:ASN:O	2.08	0.53
1:A:428:THR:HG22	1:A:442:LYS:HG2	1.91	0.52
1:A:731:GLU:OE2	1:A:750:SER:OG	2.27	0.52
1:A:1423:ARG:HB2	1:A:1451:THR:HG23	1.92	0.52
1:A:169:ALA:HB1	1:A:309:GLN:NE2	2.24	0.52
1:A:630:VAL:O	1:A:633:TYR:HB3	2.09	0.52
1:A:149:VAL:HG13	1:A:312:PHE:CD2	2.38	0.52
1:A:1127:THR:HA	1:A:1130:LYS:HZ3	1.75	0.52
1:A:1571:ARG:HH11	1:A:1571:ARG:HB3	1.75	0.52
1:A:286:ILE:HD11	1:A:601:ILE:HG21	1.91	0.51
1:A:1403:PHE:HD1	1:A:1483:VAL:CG2	2.23	0.51
1:A:1265:VAL:HB	1:A:1277:LYS:HB2	1.90	0.51
1:A:282:HIS:HE1	1:A:612:SER:H	1.59	0.51
1:A:1028:PHE:HA	1:A:1034:ARG:O	2.10	0.51
1:A:1403:PHE:CD1	1:A:1483:VAL:HG22	2.45	0.51
1:A:730:THR:OG1	1:A:796:VAL:HG22	2.11	0.51
1:A:1042:ASP:HB2	1:A:1048:VAL:HG23	1.91	0.51
1:A:1246:TRP:CZ2	1:A:1248:GLY:HA2	2.45	0.51
1:A:177:MSE:HE1	1:A:338:LEU:HG	1.91	0.51
1:A:643:LYS:O	1:A:646:ILE:HG22	2.10	0.51
1:A:1188:PHE:HA	1:A:1282:SER:O	2.10	0.51
1:A:165:ASP:O	1:A:168:THR:HG22	2.11	0.51
1:A:870:VAL:HG12	1:A:1142:TYR:CG	2.46	0.51
1:A:384:VAL:HG21	1:A:746:LEU:HD11	1.92	0.51
1:A:773:MSE:HE1	1:A:813:PHE:CZ	2.46	0.51
1:A:408:GLY:C	1:A:411:PRO:HD2	2.36	0.50
1:A:550:GLN:O	1:A:552:ASN:N	2.44	0.50
1:A:1213:LEU:HB3	1:A:1236:ALA:O	2.11	0.50
1:A:1435:TYR:CD1	1:A:1440:GLY:HA2	2.46	0.50
1:A:156:PRO:O	1:A:193:ASN:ND2	2.45	0.50
1:A:177:MSE:HE3	1:A:177:MSE:HA	1.92	0.50
1:A:1323:PHE:CE2	1:A:1348:LYS:HE3	2.46	0.50
1:A:731:GLU:OE1	1:A:797:ARG:NH2	2.33	0.50
1:A:1107:MSE:HE2	1:A:1117:ILE:CD1	2.42	0.50
1:A:1246:TRP:CE2	1:A:1248:GLY:HA2	2.47	0.50
1:A:1521:LEU:HD21	1:A:1533:LYS:HB2	1.94	0.50
1:A:1571:ARG:HB3	1:A:1571:ARG:NH1	2.26	0.50
1:A:125:ASP:HB3	1:A:421:TRP:HB2	1.93	0.50
1:A:1068:ILE:HG12	1:A:1075:VAL:HG22	1.93	0.50
1:A:1452:VAL:HG11	1:A:1483:VAL:HG21	1.93	0.50
1:A:1124:LEU:HD23	1:A:1124:LEU:H	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1166:ALA:HB2	1:A:1178:SER:CB	2.42	0.49
1:A:725:THR:OG1	1:A:760:THR:HG22	2.12	0.49
1:A:178:LEU:O	1:A:182:LYS:HG2	2.12	0.49
1:A:443:ALA:HB1	1:A:547:ALA:HB1	1.95	0.49
1:A:399:TYR:OH	1:A:673:ARG:NH2	2.46	0.49
1:A:1188:PHE:CD2	1:A:1314:SER:HB2	2.47	0.48
1:A:428:THR:HG22	1:A:442:LYS:CG	2.43	0.48
1:A:1257:MSE:SE	1:A:1410:PRO:HD3	2.63	0.48
1:A:1423:ARG:HB2	1:A:1451:THR:CG2	2.42	0.48
1:A:1502:LEU:HD12	1:A:1502:LEU:H	1.78	0.48
1:A:1004:GLY:N	3:A:1704:SO4:O4	2.46	0.48
1:A:282:HIS:HE1	1:A:612:SER:O	1.95	0.48
1:A:414:VAL:HG21	1:A:620:SER:HA	1.96	0.48
1:A:1075:VAL:HB	1:A:1344:VAL:HG21	1.94	0.48
1:A:1045:LEU:HD12	1:A:1045:LEU:H	1.78	0.48
1:A:1425:ALA:HB2	1:A:1449:LYS:HB3	1.94	0.48
1:A:119:LEU:C	1:A:121:PRO:HD3	2.39	0.48
1:A:707:THR:HG23	1:A:709:THR:H	1.79	0.48
1:A:710:MSE:HE2	1:A:792:LEU:HD13	1.95	0.48
1:A:728:TYR:HB3	1:A:798:PHE:CD1	2.48	0.48
1:A:1277:LYS:HB3	1:A:1279:TYR:CE1	2.49	0.48
1:A:417:ILE:HG13	1:A:575:GLU:O	2.13	0.48
1:A:302:LEU:HD23	1:A:303:GLY:H	1.79	0.48
1:A:904:VAL:HG11	1:A:1111:PHE:CD2	2.49	0.48
1:A:368:ALA:HB1	1:A:373:VAL:HB	1.95	0.47
1:A:155:ASP:O	1:A:157:ALA:N	2.47	0.47
1:A:590:LEU:O	1:A:591:LYS:HG2	2.14	0.47
1:A:1022:VAL:HG22	1:A:1041:LYS:O	2.15	0.47
1:A:118:SER:C	1:A:120:PRO:HD3	2.40	0.47
1:A:704:GLY:HA2	1:A:1526:TYR:CZ	2.50	0.47
1:A:931:LEU:C	1:A:931:LEU:HD23	2.40	0.47
1:A:403:GLY:O	1:A:406:SER:OG	2.29	0.46
1:A:415:ALA:HB2	1:A:592:PRO:HG3	1.96	0.46
1:A:1068:ILE:HG21	1:A:1331:ARG:HD3	1.97	0.46
1:A:302:LEU:HD23	1:A:303:GLY:N	2.29	0.46
1:A:626:ALA:HB1	1:A:654:LEU:HD21	1.96	0.46
1:A:710:MSE:HE1	1:A:732:LEU:HD11	1.97	0.46
1:A:153:GLY:H	1:A:312:PHE:HZ	1.63	0.46
1:A:1521:LEU:HD23	1:A:1521:LEU:HA	1.58	0.46
1:A:663:ASN:HB2	1:A:670:THR:HG23	1.96	0.46
1:A:729:ASP:HB3	1:A:755:GLN:CD	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:PHE:HB2	1:A:1380:ALA:HA	1.97	0.46
1:A:1361:ILE:HG12	1:A:1388:LEU:CD1	2.45	0.46
1:A:1500:ASP:HB3	1:A:1501:HIS:ND1	2.31	0.46
1:A:201:ASN:OD1	1:A:203:VAL:HG12	2.14	0.46
1:A:293:GLU:HG3	1:A:294:ALA:H	1.81	0.46
1:A:289:GLY:O	1:A:302:LEU:HA	2.16	0.46
1:A:1152:LEU:HB3	1:A:1154:MSE:HE2	1.96	0.46
1:A:385:TYR:CE1	1:A:925:LEU:HA	2.51	0.46
1:A:649:ILE:O	1:A:652:ASN:N	2.48	0.46
1:A:435:ARG:O	1:A:437:ASP:N	2.49	0.46
1:A:641:LEU:HD12	1:A:642:PRO:HD2	1.97	0.46
1:A:934:SER:HB2	1:A:936:TYR:CE1	2.51	0.46
1:A:936:TYR:N	1:A:936:TYR:CD1	2.84	0.46
1:A:188:TYR:CG	1:A:200:HIS:CE1	3.04	0.46
1:A:885:THR:C	1:A:886:PHE:CD1	2.94	0.46
1:A:972:LEU:O	1:A:975:THR:OG1	2.30	0.46
1:A:1046:ALA:HB3	1:A:1110:ASP:OD1	2.16	0.46
1:A:132:THR:HA	1:A:682:ILE:CD1	2.44	0.45
1:A:202:TYR:HB2	1:A:315:VAL:HG22	1.98	0.45
1:A:620:SER:N	1:A:621:PRO:HD2	2.31	0.45
1:A:724:LYS:HD2	1:A:807:ASN:OD1	2.16	0.45
1:A:782:LEU:HD23	1:A:782:LEU:HA	1.72	0.45
1:A:1045:LEU:HD12	1:A:1045:LEU:N	2.31	0.45
1:A:1323:PHE:CZ	1:A:1348:LYS:HE3	2.51	0.45
1:A:1551:ARG:NH2	1:A:1553:GLU:OE2	2.50	0.45
1:A:820:PHE:HB3	1:A:1526:TYR:CD2	2.51	0.45
1:A:1499:PHE:CE1	1:A:1552:ILE:HD13	2.51	0.45
1:A:383:ARG:HD3	1:A:387:SER:HB2	1.99	0.45
1:A:406:SER:C	1:A:408:GLY:H	2.25	0.45
1:A:642:PRO:HB2	1:A:644:GLU:HG2	1.99	0.45
1:A:734:THR:OG1	1:A:735:ASP:N	2.49	0.45
1:A:1332:LYS:HE2	1:A:1371:ASP:OD1	2.16	0.45
1:A:1356:ASP:HB3	1:A:1358:SER:H	1.81	0.45
1:A:568:ALA:HB1	1:A:569:PRO:HD2	1.99	0.45
1:A:149:VAL:HG11	1:A:284:THR:CG2	2.46	0.45
1:A:936:TYR:CE2	1:A:946:PRO:HG3	2.52	0.45
1:A:1455:LEU:HA	1:A:1455:LEU:HD23	1.57	0.45
1:A:154:ILE:HD11	1:A:312:PHE:CB	2.47	0.45
1:A:584:LEU:HD13	1:A:588:GLY:C	2.41	0.45
1:A:1303:HIS:NE2	1:A:1360:THR:HG23	2.32	0.45
1:A:870:VAL:HG12	1:A:1142:TYR:CD1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1066:VAL:HG22	1:A:1077:VAL:HG23	1.98	0.45
1:A:726:LEU:HD23	1:A:800:ASP:HA	1.98	0.45
1:A:149:VAL:HG21	1:A:284:THR:CG2	2.46	0.44
1:A:177:MSE:O	1:A:181:GLN:HG3	2.17	0.44
1:A:621:PRO:O	1:A:624:ALA:HB3	2.17	0.44
1:A:135:ALA:CB	1:A:686:VAL:HG21	2.48	0.44
1:A:323:SER:C	1:A:325:GLU:H	2.25	0.44
1:A:596:ALA:HB2	1:A:623:ILE:HD11	1.99	0.44
1:A:991:TYR:HE1	1:A:1013:ASP:HB3	1.82	0.44
1:A:1536:GLN:O	1:A:1540:TYR:OH	2.32	0.44
1:A:1544:VAL:HG11	1:A:1552:ILE:HD12	2.00	0.44
1:A:142:GLY:HA3	1:A:307:GLU:H	1.82	0.44
1:A:293:GLU:HG3	1:A:294:ALA:N	2.33	0.44
1:A:654:LEU:HD23	1:A:654:LEU:HA	1.85	0.44
1:A:728:TYR:CE2	1:A:769:VAL:HG21	2.52	0.44
1:A:1365:ASP:OD1	1:A:1365:ASP:N	2.45	0.44
1:A:1368:THR:HG23	1:A:1370:SER:H	1.83	0.44
1:A:169:ALA:HB1	1:A:309:GLN:CD	2.43	0.44
1:A:281:MSE:O	1:A:285:GLY:N	2.42	0.44
1:A:994:TYR:HB2	1:A:1014:MSE:CE	2.47	0.44
1:A:1564:GLU:HG3	1:A:1565:VAL:N	2.33	0.44
1:A:163:ILE:HG13	1:A:307:GLU:HG3	2.00	0.44
1:A:377:VAL:HB	1:A:406:SER:HB3	1.99	0.44
1:A:690:LEU:CD1	1:A:724:LYS:HE2	2.47	0.44
1:A:710:MSE:HE1	1:A:792:LEU:HB3	2.00	0.44
1:A:1126:GLN:O	1:A:1128:LEU:N	2.50	0.44
1:A:1162:VAL:CG2	1:A:1180:LEU:HD11	2.48	0.44
1:A:1032:THR:HG23	1:A:1034:ARG:HB2	1.99	0.44
1:A:1277:LYS:HG3	1:A:1279:TYR:OH	2.18	0.44
1:A:1301:VAL:CG1	1:A:1362:SER:HA	2.48	0.44
1:A:1339:LYS:C	1:A:1341:GLY:H	2.24	0.44
1:A:436:ALA:HB2	1:A:440:HIS:NE2	2.33	0.44
1:A:863:THR:HG21	1:A:883:LEU:HD13	2.00	0.44
1:A:906:ALA:HB1	1:A:1112:ALA:HB2	2.00	0.44
1:A:1166:ALA:HB2	1:A:1178:SER:HB3	2.00	0.44
1:A:351:ASN:OD1	1:A:958:LYS:HE3	2.17	0.43
1:A:1320:GLU:HG2	1:A:1374:TYR:HE1	1.83	0.43
1:A:282:HIS:HD1	1:A:605:TYR:HE2	1.64	0.43
1:A:630:VAL:O	1:A:634:LEU:HD12	2.18	0.43
1:A:710:MSE:CE	1:A:775:VAL:HG11	2.39	0.43
1:A:821:GLU:HA	1:A:1002:VAL:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:ASP:N	1:A:877:ASP:OD1	2.51	0.43
1:A:1293:GLY:HA2	1:A:1307:ASP:OD1	2.19	0.43
1:A:1361:ILE:HG12	1:A:1388:LEU:HD12	2.00	0.43
1:A:1364:ARG:HB2	1:A:1367:VAL:CG1	2.49	0.43
1:A:680:LEU:HD11	1:A:682:ILE:HG22	2.00	0.43
1:A:1105:TYR:CE2	1:A:1119:LYS:HB2	2.53	0.43
1:A:1324:TYR:HB3	1:A:1372:TYR:CD2	2.54	0.43
1:A:195:LYS:HG3	1:A:310:VAL:HG12	1.99	0.43
1:A:746:LEU:HD23	1:A:746:LEU:HA	1.70	0.43
1:A:147:VAL:HB	1:A:628:LEU:HD11	2.00	0.43
1:A:923:VAL:HG22	1:A:968:LYS:O	2.19	0.43
1:A:1086:ARG:HG3	1:A:1092:PHE:CZ	2.53	0.43
1:A:1162:VAL:HG23	1:A:1180:LEU:HD11	2.00	0.43
1:A:1187:PHE:N	1:A:1187:PHE:CD1	2.86	0.43
1:A:581:ASN:O	1:A:582:TRP:HB2	2.19	0.43
1:A:590:LEU:HD23	1:A:700:SER:HB2	2.01	0.43
1:A:140:TYR:CZ	1:A:633:TYR:HA	2.54	0.43
1:A:379:ALA:O	1:A:581:ASN:ND2	2.52	0.43
1:A:821:GLU:HA	1:A:1002:VAL:CG2	2.49	0.43
1:A:949:VAL:O	1:A:1252:ARG:NH2	2.50	0.43
1:A:198:PHE:CD2	1:A:338:LEU:HD21	2.54	0.43
1:A:980:LYS:HD3	1:A:986:GLU:HG2	1.99	0.43
1:A:1218:TYR:CZ	1:A:1225:LYS:HB3	2.53	0.43
1:A:1248:GLY:O	1:A:1256:VAL:HG22	2.19	0.43
1:A:426:LEU:HD22	1:A:442:LYS:HB3	2.01	0.42
1:A:615:GLY:HA3	2:A:1701:AES:H6	2.01	0.42
1:A:875:ILE:HD11	1:A:1342:ILE:O	2.18	0.42
1:A:892:LYS:N	1:A:892:LYS:HD2	2.34	0.42
1:A:875:ILE:HD13	1:A:875:ILE:HA	1.86	0.42
1:A:1350:TYR:O	1:A:1351:ILE:HD13	2.18	0.42
1:A:342:VAL:HA	1:A:374:SER:O	2.18	0.42
1:A:393:LEU:HD23	1:A:743:ARG:HG2	2.01	0.42
1:A:864:LEU:HD12	1:A:879:GLY:O	2.20	0.42
1:A:162:ARG:HG2	1:A:292:LYS:HZ1	1.83	0.42
1:A:372:GLY:O	1:A:631:LYS:HE3	2.18	0.42
1:A:819:GLN:HB3	1:A:821:GLU:HG3	2.01	0.42
1:A:463:SER:C	1:A:465:GLN:H	2.27	0.42
1:A:1110:ASP:OD2	1:A:1114:ASN:HB2	2.19	0.42
1:A:1124:LEU:HD11	1:A:1127:THR:HG21	2.00	0.42
1:A:1223:HIS:HB2	1:A:1224:GLN:OE1	2.18	0.42
1:A:154:ILE:HG23	1:A:281:MSE:HG3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:ILE:HG23	1:A:654:LEU:HD13	2.01	0.42
1:A:820:PHE:HB3	1:A:1526:TYR:CE2	2.55	0.42
1:A:793:GLU:HB3	1:A:814:VAL:HG23	2.01	0.42
1:A:579:PHE:O	1:A:580:SER:C	2.63	0.41
1:A:738:ASP:OD2	1:A:738:ASP:C	2.63	0.41
1:A:406:SER:C	1:A:408:GLY:N	2.78	0.41
1:A:1406:ASP:HB3	1:A:1486:LYS:HA	2.01	0.41
1:A:982:LEU:HD23	1:A:982:LEU:HA	1.89	0.41
1:A:1097:ASP:OD2	1:A:1097:ASP:N	2.49	0.41
1:A:1214:THR:HG23	1:A:1266:THR:OG1	2.21	0.41
1:A:577:ASN:O	1:A:578:HIS:C	2.63	0.41
1:A:601:ILE:HG22	1:A:602:TYR:N	2.35	0.41
1:A:1544:VAL:HG21	1:A:1552:ILE:HD12	2.02	0.41
1:A:1065:THR:HG23	1:A:1080:ASN:HD21	1.86	0.41
1:A:1081:LYS:HE2	1:A:1107:MSE:HE1	2.02	0.41
1:A:1257:MSE:O	1:A:1261:TYR:OH	2.30	0.41
1:A:174:LYS:HB3	1:A:191:TRP:CE2	2.55	0.41
1:A:909:PRO:HB2	1:A:1018:ARG:HE	1.85	0.41
1:A:1171:VAL:HG23	1:A:1172:HIS:H	1.86	0.41
1:A:1544:VAL:HG21	1:A:1552:ILE:CD1	2.51	0.41
1:A:381:ASN:OD1	1:A:616:THR:HG22	2.21	0.41
1:A:883:LEU:HD12	1:A:883:LEU:HA	1.84	0.41
1:A:1110:ASP:HB3	1:A:1113:GLY:N	2.32	0.41
1:A:135:ALA:O	1:A:140:TYR:HB2	2.21	0.41
1:A:1040:LEU:HD23	1:A:1040:LEU:HA	1.77	0.41
1:A:173:SER:HA	1:A:191:TRP:CZ3	2.56	0.40
1:A:590:LEU:C	1:A:591:LYS:HG2	2.46	0.40
1:A:1042:ASP:HB2	1:A:1048:VAL:CG2	2.50	0.40
1:A:1241:ILE:HG13	1:A:1242:GLU:N	2.35	0.40
1:A:154:ILE:HD11	1:A:312:PHE:HB2	2.03	0.40
1:A:286:ILE:CG2	1:A:621:PRO:HB2	2.51	0.40
1:A:1521:LEU:CD2	1:A:1533:LYS:HB2	2.51	0.40
1:A:1500:ASP:HB2	1:A:1571:ARG:HA	2.03	0.40
1:A:1523:GLN:HA	1:A:1531:TYR:CD2	2.56	0.40
1:A:830:ILE:HD12	1:A:830:ILE:HA	1.83	0.40
1:A:1210:TYR:HD1	1:A:1267:TYR:CG	2.39	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	1350/1530 (88%)	1159 (86%)	176 (13%)	15 (1%)	11	43

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	536	PRO
1	A	581	ASN
1	A	613	GLN
1	A	582	TRP
1	A	564	VAL
1	A	578	HIS
1	A	611	GLY
1	A	1037	PRO
1	A	1127	THR
1	A	205	ASN
1	A	597	PRO
1	A	1548	LYS
1	A	469	VAL
1	A	384	VAL
1	A	1038	GLU

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	1073/1271 (84%)	1068 (100%)	5 (0%)	81	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	VAL
1	A	612	SER
1	A	614	THR
1	A	923	VAL
1	A	1301	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	HIS
1	A	200	HIS
1	A	309	GLN
1	A	344	ASN
1	A	418	ASN
1	A	581	ASN
1	A	718	ASN
1	A	785	GLN
1	A	810	ASN
1	A	915	GLN
1	A	1019	GLN
1	A	1211	ASN
1	A	1402	ASN
1	A	1478	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	1702	-	4,4,4	0.72	0	6,6,6	0.52	0
2	AES	A	1701	1	10,12,13	1.05	1 (10%)	14,15,18	1.66	3 (21%)
3	SO4	A	1703	-	4,4,4	0.51	0	6,6,6	0.54	0
3	SO4	A	1704	-	4,4,4	0.62	0	6,6,6	0.81	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AES	A	1701	1	-	3/7/7/9	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1701	AES	C1-S	2.59	1.84	1.80

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1701	AES	C5-C6-C1	3.55	122.49	119.39
2	A	1701	AES	C2-C1-C6	-3.46	117.72	121.59
2	A	1701	AES	O2S-S-C1	2.22	109.55	104.55

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1701	AES	C2-C1-S-O2S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1701	AES	C6-C1-S-O2S
2	A	1701	AES	C4-C7-C8-N8

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1701	AES	2	0
3	A	1704	SO4	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1333/1530 (87%)	-0.13	47 (3%) 47 27	6, 39, 88, 117	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	606	ASN	5.4
1	A	206	SER	4.8
1	A	1128	LEU	4.2
1	A	467	ALA	3.9
1	A	175	GLU	3.6
1	A	607	ASP	3.6
1	A	194	ASP	3.5
1	A	547	ALA	3.5
1	A	458	LEU	3.4
1	A	536	PRO	3.4
1	A	451	PHE	3.3
1	A	450	ASP	3.3
1	A	554	ASN	3.2
1	A	539	PHE	3.1
1	A	443	ALA	3.1
1	A	537	SER	2.9
1	A	1415	ILE	2.9
1	A	535	ILE	2.9
1	A	538	ALA	2.8
1	A	296	ALA	2.8
1	A	507	HIS	2.5
1	A	454	ILE	2.5
1	A	1124	LEU	2.5
1	A	605	TYR	2.5
1	A	540	ILE	2.4
1	A	478	ASN	2.4
1	A	555	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	502	ALA	2.4
1	A	191	TRP	2.4
1	A	612	SER	2.4
1	A	213	GLN	2.3
1	A	1125	PRO	2.3
1	A	276	TYR	2.3
1	A	1237	GLY	2.3
1	A	118	SER	2.3
1	A	541	SER	2.3
1	A	277	GLU	2.2
1	A	505	LYS	2.2
1	A	278	SER	2.2
1	A	187	ASN	2.2
1	A	449	VAL	2.2
1	A	497	TYR	2.2
1	A	504	ALA	2.1
1	A	428	THR	2.1
1	A	468	TYR	2.0
1	A	441	GLY	2.0
1	A	470	LYS	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	CA	A	1708	1/1	0.73	0.34	57,57,57,57	0
2	AES	A	1701	12/13	0.81	0.21	59,81,87,87	0
3	SO4	A	1702	5/5	0.82	0.29	28,29,60,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1704	5/5	0.91	0.29	35,36,48,81	0
3	SO4	A	1703	5/5	0.93	0.19	37,42,57,73	0
4	CA	A	1706	1/1	0.99	0.05	24,24,24,24	0
4	CA	A	1707	1/1	0.99	0.02	21,21,21,21	0
4	CA	A	1705	1/1	0.99	0.03	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.