



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:23 pm BST

PDB ID : 5XYA  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

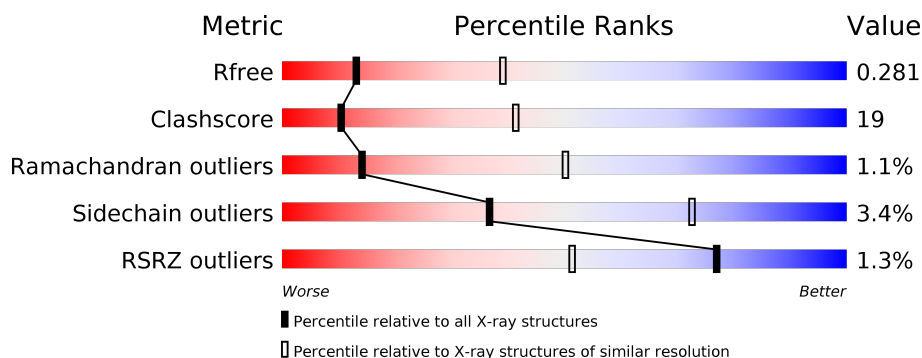
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 <div style="display: flex; justify-content: space-around; width: 100%;"> <span>%</span> <span>58%</span> <span>30%</span> <span>• 11%</span> </div>

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](#)

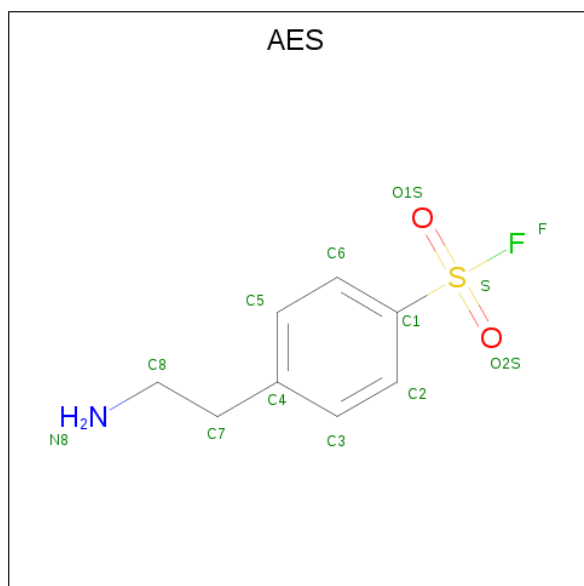
There are 4 unique types of molecules in this entry. The entry contains 10300 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: AES) (formula: C<sub>8</sub>H<sub>10</sub>FNO<sub>2</sub>S).



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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

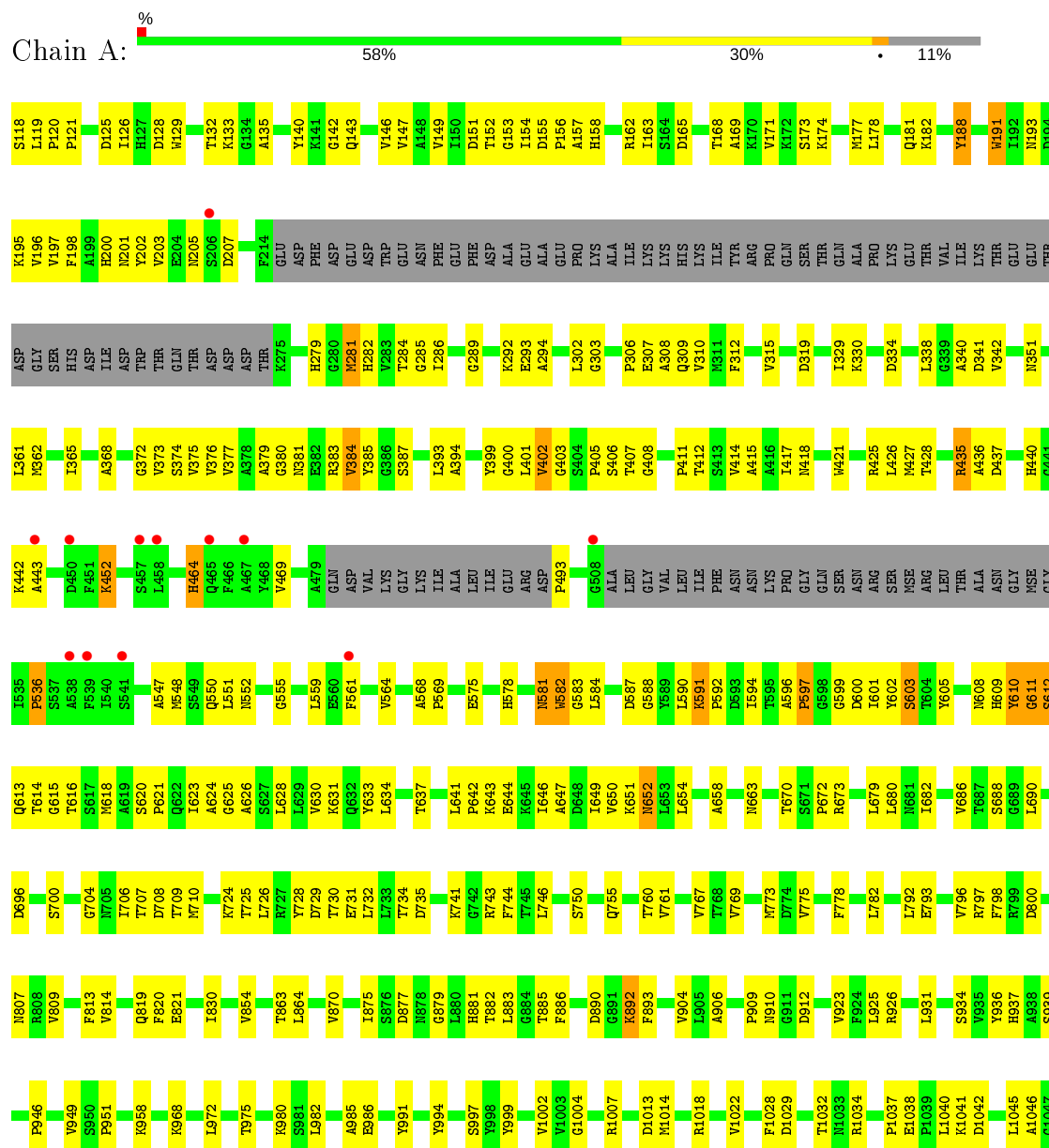
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

### 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 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: Chemokine protease C



LEU	THR	■	D1365	M1257	E1153	V1048
	ALA	K1486	G1366	■	M1154	R1049
	SER	M1487	V1265	V1266	V1162	F1054
	THR	T1496	T1368	T1267	■	F1055
	ALA	■	L1369	■	A1166	L1056
	PRO	F1499	S1370	■	■	D1060
	THR	D1500	D1371	Q1276	V1171	■
	LYS	H1501	Y1372	K1277	H1172	P1063
	THR	L1502	Y1373	Q1278	■	Y1064
	THR	L1503	Y1374	Y1279	S1178	T1065
THR	THR	■	E1377	T1280	Q1179	V1066
	PRO	L1521	A1380	I1281	L1180	■
	ALA	E1522	■	S1282	F1187	T1067
	THR	Q1523	■	■	F1188	I1068
	ALA	Y1526	V1383	G1293	T1189	V1075
	LYS	■	L1388	R1294	S1190	S1076
	ALA	Y1531	■	■	P1191	V1077
	LEU	G1532	K1396	M1299	N1192	■
	PRO	K1533	D1397	G1300	E1193	N1080
	SER	■	■	V1301	D1194	K1081
THR	THR	■	■	D1302	■	■
	GLY	V1544	V1400	H1303	■	K1086
	GLU	S1545	■	■	K1197	■
	LYS	L1546	F1403	D1307	V1200	F1092
	MSE	P1547	■	■	■	■
	GLY	K1548	D1406	S1314	K1203	D1097
	LEU	G1549	■	■	G1204	■
	LYS	Y1550	P1410	E1320	L1205	G1102
	LEU	R1551	T1415	F1323	N1208	Y1105
	ARG	I1552	V1416	Y1324	V1209	M1106
ILE	VAL	E1553	N1417	L1325	Y1210	M1107
	GLY	■	■	■	■	V1108
	LEU	E1564	R1423	R1331	L1213	E1109
	VAL	V1565	D1424	K1332	T1214	D1110
	LEU	■	A1425	■	■	F1111
	LEU	R1571	■	E1337	Y1218	A1112
	GLY	■	Y1435	■	■	G1113
	GLY	K1574	■	I1342	H1223	N1114
	THR	GLY	G1440	T1343	Q1224	V1115
	CYS	ASP	ALA	V1344	K1225	A1116
PHE	ALA	■	K1449	■	■	I1117
	SER	■	Y1450	M1347	Q1233	K1119
	ASP	ASP	T1451	V1349	A1118	■
	ARG	SER	V1452	■	■	L1120
	LYS	THR	■	Y1350	A1236	■
	LYS	GLY	L1455	L1351	■	■
	SER	ASP	■	P1352	S1239	L1124
	SER	THR	H15	K1353	A1240	P1125
	LYS	LYS	E1465	■	I1241	K1126
	ASP	VAL	S1466	D1356	E1242	T1127
GLY	MSE	■	■	G1357	■	L1128
	SER	SER	■	■	■	■
	LYS	LYS	S1475	S1358	V1246	G1129
	LYS	ASN	A1476	T1359	Y1247	K1130
	ASN	ASN	D1477	T1360	G1248	T1131
	SER	SER	■	I1361	■	■
	SER	SER	F1480	S1362	R1252	Y1142
	ALA	GLN	■	K1363	■	■
	ALA	■	V1483	K1364	V1066	V1150
	ALA	■	■	■	■	■

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.53Å 190.53Å 248.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 3.00 49.84 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.90-3.00) 88.1 (49.84-2.85)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.72 (at 2.86Å)	Xtriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, $R_{free}$	0.223 , 0.278 0.227 , 0.281	Depositor DCC
$R_{free}$ test set	1990 reflections (3.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 30.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	10300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical 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: AES, CA, 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	0.62	0/10444	0.78	4/14117 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1299	ASN	CB-CA-C	6.47	123.35	110.40
1	A	536	PRO	N-CA-CB	6.29	110.85	103.30
1	A	493	PRO	N-CA-CB	6.11	110.63	103.30
1	A	610	TYR	CB-CA-C	5.53	121.45	110.40

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	375	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	375	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 (375) 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:1190:SER:O	1:A:1192:ASN:OD1	1.89	0.90
1:A:362:MSE:HE1	1:A:405:PRO:HB3	1.51	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
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: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:1054:PHE:HE2	1:A:1107:MSE:HE3	1.57	0.70
1:A:174:LYS:HB3	1:A:191:TRP:NE1	2.07	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1546:LEU:HD13	1:A:1550:TYR:HB3	1.78	0.65
1:A:201:ASN:HB3	1:A:207:ASP:H	1.60	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:1029:ASP:OD2	1:A:1032:THR:HG22	1.98	0.63
1:A:400:GLY:HA3	1:A:583:GLY:HA3	1.79	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:1107:MSE:HE2	1:A:1117:ILE:HD11	1.81	0.62
1:A:427:MSE:SE	1:A:559:LEU:HD11	2.49	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:1353:LYS:HG3	1:A:1359:TYR:CZ	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1056:LEU:HD13	1:A:1063:PRO:HB2	1.85	0.58
1:A:376:VAL:HG12	1:A:620:SER:OG	2.03	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
1:A:1325:LEU:HA	1:A:1347:ASN:O	2.05	0.57
1:A:384:VAL:HG12	1:A:399:TYR:HD1	1.69	0.57
1:A:1127:THR:HA	1:A:1130:LYS:HZ3	1.69	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:1397:ASP:N	1:A:1397:ASP:OD1	2.26	0.56
1:A:602:TYR:CE2	1:A:610:TYR:HB3	2.41	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: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:1200:VAL:HG21	1:A:1281:ILE:HG13	1.87	0.56
1:A:143:GLN:HA	1:A:307:GLU:O	2.06	0.56
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:403:GLY:C	1:A:407:THR:HG23	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:633:TYR:O	1:A:637:THR:HG23	2.06	0.54
1:A:630:VAL:HB	1:A:650:VAL:HG23	1.89	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:910:ASN:N	1:A:910:ASN:OD1	2.39	0.53
1:A:1188:PHE:O	1:A:1197:LYS:HE3	2.09	0.53
1:A:704:GLY:HA2	1:A:1526:TYR:CE2	2.44	0.53
1:A:1110:ASP:HB2	1:A:1114:ASN:O	2.08	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
1:A:428:THR:HG22	1:A:442:LYS:HG2	1.91	0.52
1:A:1423:ARG:HB2	1:A:1451:THR:HG23	1.92	0.52
1:A:731:GLU:OE2	1:A:750:SER:OG	2.27	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:1571:ARG:HH11	1:A:1571:ARG:HB3	1.75	0.52
1:A:435:ARG:C	1:A:437:ASP:H	2.13	0.51
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: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:282:HIS:HE1	1:A:612:SER:H	1.59	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:730:THR:OG1	1:A:796:VAL:HG22	2.11	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:152:THR:O	1:A:152:THR:OG1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:VAL:HG12	1:A:1142:TYR:CG	2.46	0.51
1:A:165:ASP:O	1:A:168:THR:HG22	2.11	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: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:177:MSE:HE3	1:A:177:MSE:HA	1.92	0.50
1:A:156:PRO:O	1:A:193:ASN:ND2	2.45	0.50
1:A:1323:PHE:CE2	1:A:1348:LYS:HE3	2.46	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:731:GLU:OE1	1:A:797:ARG:NH2	2.33	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
1:A:1166:ALA:HB2	1:A:1178:SER:CB	2.42	0.49
1:A:1363:LYS:HZ3	1:A:1369:LEU:H	1.60	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:672:PRO:HD2	1:A:793:GLU:CD	2.33	0.49
1:A:1188:PHE:CD2	1:A:1314:SER:HB2	2.47	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:428:THR:HG22	1:A:442:LYS:CG	2.43	0.48
1:A:910:ASN:CG	1:A:912:ASP:OD1	2.48	0.48
1:A:1004:GLY:N	3:A:1704:SO4:O4	2.46	0.48
1:A:1075:VAL:HB	1:A:1344:VAL:HG21	1.94	0.48
1:A:414:VAL:HG21	1:A:620:SER:HA	1.96	0.48
1:A:282:HIS:HE1	1:A:612:SER:O	1.95	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:1277:LYS:HB3	1:A:1279:TYR:CE1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:TYR:HB3	1:A:798:PHE:CD1	2.48	0.48
1:A:417:ILE:HG13	1:A:575:GLU:O	2.13	0.48
1:A:904:VAL:HG11	1:A:1111:PHE:CD2	2.49	0.48
1:A:302:LEU:HD23	1:A:303:GLY:H	1.79	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:704:GLY:HA2	1:A:1526:TYR:CZ	2.50	0.47
1:A:1068:ILE:HG21	1:A:1331:ARG:HD3	1.97	0.46
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: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:1521:LEU:HA	1:A:1521:LEU:HD23	1.58	0.46
1:A:153:GLY:H	1:A:312:PHE:HZ	1.63	0.46
1:A:1361:ILE:HG12	1:A:1388:LEU:CD1	2.45	0.46
1:A:1188:PHE:HB2	1:A:1380:ALA:HA	1.97	0.46
1:A:1500:ASP:HB3	1:A:1501:HIS:ND1	2.31	0.46
1:A:663:ASN:HB2	1:A:670:THR:HG23	1.96	0.46
1:A:1064:TYR:OH	1:A:1337:GLU:OE1	2.22	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:1152:LEU:HB3	1:A:1154:MSE:HE2	1.96	0.46
1:A:289:GLY:O	1:A:302:LEU:HA	2.16	0.46
1:A:649:ILE:O	1:A:652:ASN:N	2.48	0.46
1:A:385:TYR:CE1	1:A:925:LEU:HA	2.51	0.46
1:A:408:GLY:C	1:A:411:PRO:HD2	2.36	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:1046:ALA:HB3	1:A:1110:ASP:OD1	2.16	0.46
1:A:188:TYR:CG	1:A:200:HIS:CE1	3.04	0.46
1:A:972:LEU:O	1:A:975:THR:OG1	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1551:ARG:NH2	1:A:1553:GLU:OE2	2.50	0.45
1:A:782:LEU:HD23	1:A:782:LEU:HA	1.72	0.45
1:A:724:LYS:HD2	1:A:807:ASN:OD1	2.16	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: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:383:ARG:HD3	1:A:387:SER:HB2	1.99	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:568:ALA:HB1	1:A:569:PRO:HD2	1.99	0.45
1:A:1455:LEU:HA	1:A:1455:LEU:HD23	1.57	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:1303:HIS:NE2	1:A:1360:THR:HG23	2.32	0.45
1:A:154:ILE:HD11	1:A:312:PHE:CB	2.47	0.45
1:A:1066:VAL:HG22	1:A:1077:VAL:HG23	1.98	0.45
1:A:870:VAL:HG12	1:A:1142:TYR:CD1	2.52	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:1544:VAL:HG11	1:A:1552:ILE:HD12	2.00	0.44
1:A:596:ALA:HB2	1:A:623:ILE:HD11	1.99	0.44
1:A:135:ALA:CB	1:A:686:VAL:HG21	2.48	0.44
1:A:991:TYR:HE1	1:A:1013:ASP:HB3	1.82	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:293:GLU:HG3	1:A:294:ALA:N	2.33	0.44
1:A:142:GLY:HA3	1:A:307:GLU:H	1.82	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:1564:GLU:HG3	1:A:1565:VAL:N	2.33	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1166:ALA:HB2	1:A:1178:SER:HB3	2.00	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:1320:GLU:HG2	1:A:1374:TYR:HE1	1.83	0.43
1:A:351:ASN:OD1	1:A:958:LYS:HE3	2.17	0.43
1:A:119:LEU:C	1:A:121:PRO:HD3	2.39	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:1363:LYS:HZ3	1:A:1369:LEU:N	2.16	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
1:A:877:ASP:N	1:A:877:ASP:OD1	2.51	0.43
1:A:1364:ARG:HB2	1:A:1367:VAL:CG1	2.49	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:680:LEU:HD11	1:A:682:ILE:HG22	2.00	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: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: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: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:821:GLU:HA	1:A:1002:VAL:CG2	2.49	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:949:VAL:O	1:A:1252:ARG:NH2	2.50	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: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:875:ILE:HD11	1:A:1342:ILE:O	2.18	0.42
1:A:426:LEU:HD22	1:A:442:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:GLY:HA3	2:A:1701:AES:H6	2.01	0.42
1:A:892:LYS:HD2	1:A:892:LYS:N	2.34	0.42
1:A:1350:TYR:O	1:A:1351:ILE:HD13	2.18	0.42
1:A:875:ILE:HA	1:A:875:ILE:HD13	1.86	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: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: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
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:118:SER:C	1:A:120:PRO:HD3	2.40	0.42
1:A:931:LEU:C	1:A:931:LEU:HD23	2.40	0.42
1:A:1363:LYS:HZ1	1:A:1369:LEU:HB2	1.84	0.41
1:A:729:ASP:HB3	1:A:755:GLN:CD	2.41	0.41
1:A:1406:ASP:HB3	1:A:1486:LYS:HA	2.01	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:982:LEU:HA	1:A:982:LEU:HD23	1.89	0.41
1:A:601:ILE:HG22	1:A:602:TYR:N	2.35	0.41
1:A:1241:ILE:HG13	1:A:1242:GLU: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: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:174:LYS:HB3	1:A:191:TRP:CE2	2.55	0.41
1:A:885:THR:C	1:A:886:PHE:CD1	2.94	0.41
1:A:1110:ASP:HB3	1:A:1113:GLY:N	2.32	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:1040:LEU:HA	1:A:1040:LEU:HD23	1.77	0.41
1:A:135:ALA:O	1:A:140:TYR:HB2	2.21	0.41
1:A:1042:ASP:HB2	1:A:1048:VAL:CG2	2.50	0.40
1:A:173:SER:HA	1:A:191:TRP:CZ3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:SER:C	1:A:408:GLY:H	2.25	0.40
1:A:1521:LEU:CD2	1:A:1533:LYS:HB2	2.51	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: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:1210:TYR:HD1	1:A:1267:TYR:CG	2.39	0.40
1:A:584:LEU:HD13	1:A:588:GLY:C	2.41	0.40
1:A:830:ILE:HD12	1:A:830:ILE:HA	1.83	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	1350/1530 (88%)	1159 (86%)	176 (13%)	15 (1%)	14	50

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

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Mol	Chain	Res	Type
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%)	1036 (97%)	37 (3%)	37 72

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	TRP
1	A	151	ASP
1	A	188	TYR
1	A	191	TRP
1	A	281	MSE
1	A	319	ASP
1	A	402	VAL
1	A	425	ARG
1	A	435	ARG
1	A	452	LYS
1	A	464	HIS
1	A	561	PHE
1	A	591	LYS
1	A	600	ASP
1	A	603	SER
1	A	609	HIS
1	A	612	SER
1	A	614	THR
1	A	618	MSE
1	A	652	ASN
1	A	696	ASP
1	A	778	PHE
1	A	890	ASP

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Mol	Chain	Res	Type
1	A	892	LYS
1	A	926	ARG
1	A	1049	ARG
1	A	1060	ASP
1	A	1110	ASP
1	A	1208	ASN
1	A	1239	SER
1	A	1275	HIS
1	A	1302	ASP
1	A	1314	SER
1	A	1466	SER
1	A	1475	SER
1	A	1477	ASP
1	A	1533	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	HIS
1	A	200	HIS
1	A	309	GLN
1	A	418	ASN
1	A	581	ASN
1	A	810	ASN
1	A	881	HIS

### 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 carbohydrates 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	0.65	0	6,6,6	0.58	0
2	AES	A	1701	1	8,12,13	0.69	0	13,15,18	1.67	3 (23%)
3	SO4	A	1703	-	4,4,4	0.41	0	6,6,6	0.56	0
3	SO4	A	1704	-	4,4,4	0.54	0	6,6,6	0.82	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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1701	AES	C5-C6-C1	3.47	122.49	119.40
2	A	1701	AES	C6-C1-C2	-3.46	117.72	121.59
2	A	1701	AES	O2S-S-C1	2.18	109.55	104.58

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
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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1333/1530 (87%)	-0.54	17 (1%)	77 51	6, 39, 88, 117	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1126	GLN	3.3
1	A	1129	GLY	3.1
1	A	465	GLN	3.0
1	A	538	ALA	3.0
1	A	1125	PRO	2.9
1	A	443	ALA	2.9
1	A	541	SER	2.6
1	A	467	ALA	2.6
1	A	458	LEU	2.6
1	A	450	ASP	2.5
1	A	1128	LEU	2.4
1	A	561	PHE	2.4
1	A	508	GLY	2.2
1	A	457	SER	2.1
1	A	1124	LEU	2.1
1	A	539	PHE	2.1
1	A	206	SER	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 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	A	1708	1/1	0.80	0.34	57,57,57,57	0
2	AES	A	1701	12/13	0.91	0.24	59,81,87,87	0
3	SO4	A	1702	5/5	0.92	0.26	28,29,60,83	0
3	SO4	A	1704	5/5	0.94	0.34	35,36,48,81	0
3	SO4	A	1703	5/5	0.96	0.17	37,42,57,73	0
4	CA	A	1707	1/1	0.96	0.14	21,21,21,21	0
4	CA	A	1705	1/1	0.98	0.10	18,18,18,18	0
4	CA	A	1706	1/1	0.98	0.10	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.