



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 07:58 PM JST

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

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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

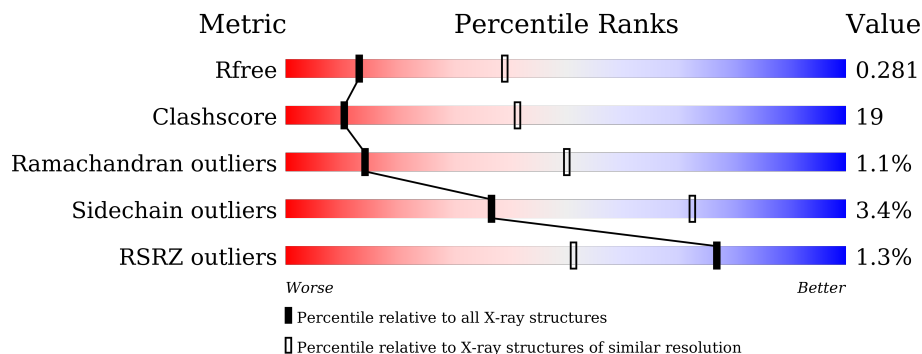
1 Overall quality at a glance

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 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](#)

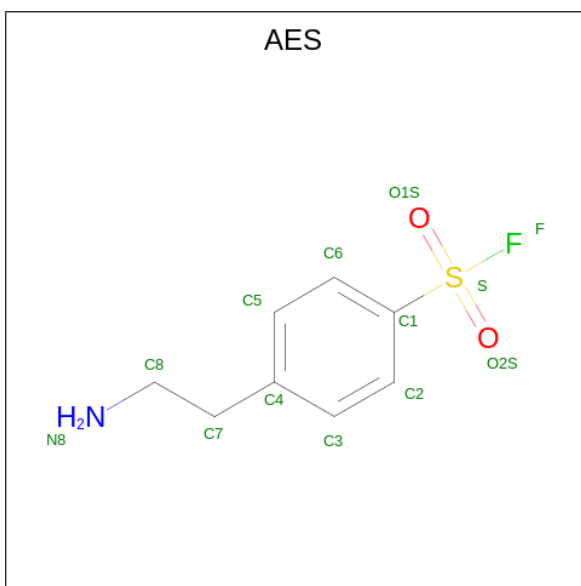
There are 4 unique types of molecules in this entry. The entry contains 10300 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	Se			
1	A	1358	10269	6462	1764	2019	24	0	0	0

- Molecule 2 is 4-(2-AMINOETHYL)BENZENESULFONYL FLUORIDE (three-letter code: AES) (formula: C₈H₁₀FNO₂S).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

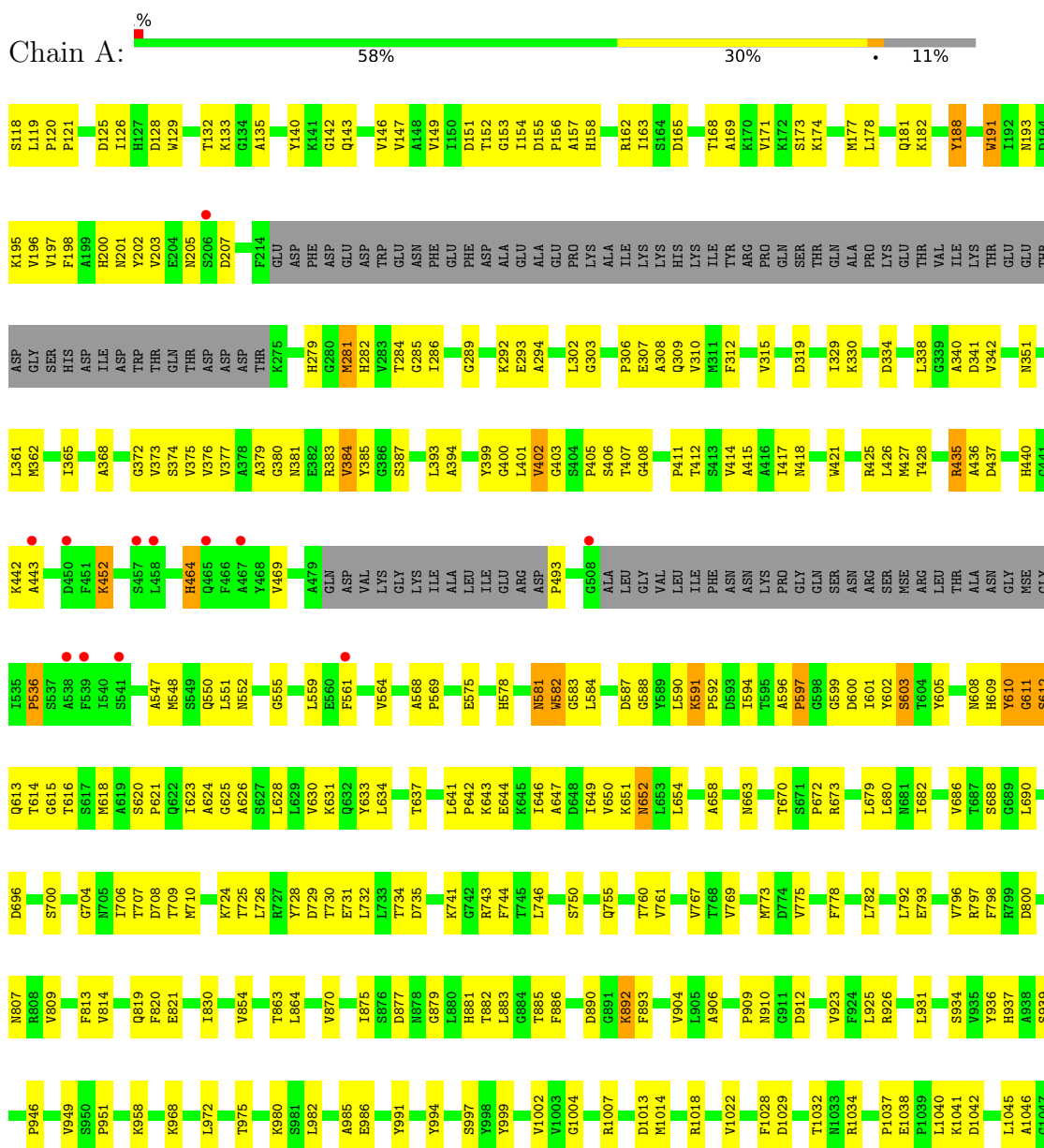
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

3 Residue-property plots i

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: Chemokine protease C



V1048	E1153	M1257	D1365	K1486	LEU
R1049	M1154	V1265	G1366	M1487	THR
F1054	V1162	T1266	V1367	T1368	ALA
Y1055	L1369	Y1267	T1368	L1369	SER
L1056	A1166	H1275	S1370	T1496	ALA
D1060	V1171	Q1276	D1371	F1499	THR
P1063	H1172	K1277	Y1372	D1500	PRO
Y1064	S1178	Q1278	Y1373	H1501	THR
T1065	Q1179	T1280	Y1374	L1502	THR
V1066	L1180	I1281	E1377	L1503	THR
T1067	F1187	S1282	A1380	L1521	THR
I1068	F1188	G1293	V1383	E1522	ALA
V1075	I1189	R1294	V1383	Q1523	THR
S1076	S1190	M1299	L1388	Y1526	ALA
V1077	P1191	G1300	L1388	Y1531	ALA
M1080	M1192	V1301	K1396	Y1531	LEU
K1081	E1193	D1302	D1397	G1532	PRO
R1086	D1194	H1303	V1400	K1533	SER
F1092	K1197	D1307	F1403	V1544	THR
D1097	V1200	S1314	D1406	S1545	GLU
G1102	K1203	E1320	P1410	L1546	GLY
Y1105	G1204	E1320	P1410	P1547	MSE
Y1106	L1205	F1323	I1415	K1548	GLY
M1107	M1208	Y1324	V1416	G1549	LEU
V1108	Y1209	L1325	M1417	Y1550	LEU
E1109	Y1210	R1331	R1423	R1551	LEU
D1110	L1213	K1332	D1424	I1552	ARG
F1111	T1214	E1337	A1425	E1553	ILE
A1112	Y1218	T1342	Y1435	E1564	VAL
G1113	H1223	T1343	G1440	V1565	GLY
M1114	Q1224	V1344	T1343	R1571	LEU
V1115	K1225	M1347	K1449	K1574	LEU
A1116	Q1233	K1348	Y1450	VAL	GLY
I1117	A1236	V1349	T1451	VAL	THR
A1118	L1120	I1351	V1452	ALA	ASP
L1124	S1239	P1352	L1455	ALA	SER
P1125	A1240	K1353	L1464	ASP	THR
Q1126	L1241	D1356	E1465	HIS	LYS
T1127	E1242	G1357	S1466	VAL	LYS
L1128	V1246	S1358	S1475	MSE	ASP
G1129	Y1247	Y1359	A1476	SER	THR
K1130	G1248	T1360	D1477	SER	SER
T1131	R1252	I1361	F1480	LYS	LYS
Y1142	V1256	K1363	V1483	ASN	ASN
L1152		S1362		SER	SER
		R1364		GLN	GLN
				ALA	ALA

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 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
$\langle I/\sigma(I) \rangle$ ¹	4.72 (at 2.86Å)	Xtrriage
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 ²)	37.2	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10300	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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 [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	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: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
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: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: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: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
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

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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: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
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: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: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: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: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: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: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
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: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:435:ARG:C	1:A:437:ASP:H	2.13	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:152:THR:O	1:A:152:THR:OG1	2.28	0.51
1:A:1188:PHE:HA	1:A:1282:SER:O	2.10	0.51

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:704:GLY:HA2	1:A:1526:TYR:CZ	2.50	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: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:1064:TYR:OH	1:A:1337:GLU:OE1	2.22	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: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: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: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

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

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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: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:119:LEU:C	1:A:121:PRO:HD3	2.39	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:729:ASP:HB3	1:A:755:GLN:CD	2.41	0.41
1:A:1363:LYS:HZ1	1:A:1369:LEU:HB2	1.84	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: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: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: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:406:SER:C	1:A:408:GLY:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:ASP:HB2	1:A:1048:VAL:CG2	2.50	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: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
1:A:1210:TYR:HD1	1:A:1267:TYR:CG	2.39	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 [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	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

Sometimes 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 [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

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	1704	-	4,4,4	0.54	0	6,6,6	0.82	0
3	SO4	A	1702	-	4,4,4	0.65	0	6,6,6	0.58	0
3	SO4	A	1703	-	4,4,4	0.41	0	6,6,6	0.56	0
2	AES	A	1701	1	8,12,13	0.69	0	13,15,18	1.67	3 (23%)

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	C2-C1-C6	-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
3	A	1704	SO4	2	0
2	A	1701	AES	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%)	-0.54	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 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
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
4	CA	A	1707	1/1	0.96	0.14	21,21,21,21	0
3	SO4	A	1703	5/5	0.96	0.17	37,42,57,73	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.