



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:50 pm BST

PDB ID : 5XYR  
Title : Crystal structure of a serine protease from Streptococcus species  
Authors : Jobichen, C.; Sivaraman, J.  
Deposited on : 2017-07-10  
Resolution : 2.80 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

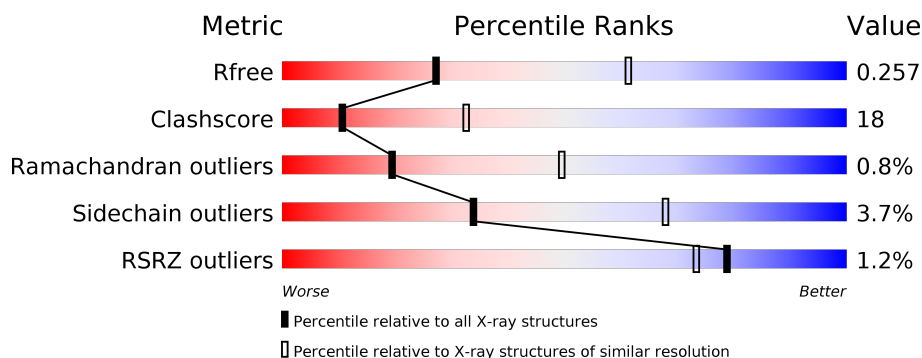
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	1647	<div> <div></div> <div>57%</div> <div>25%</div> <div>•</div> <div>16%</div> </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
2	CL	A	1701	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10518 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	1380	Total	C	N	O	Se	0	0	0
			10481	6584	1799	2074	24			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

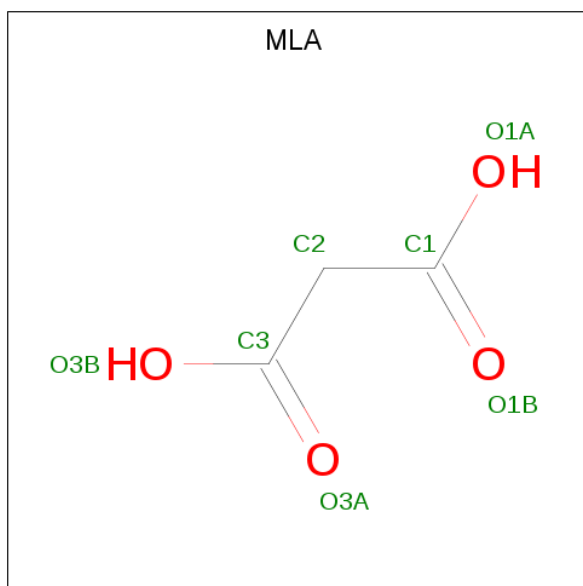
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		

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



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

- Molecule 5 is MALONIC ACID (three-letter code: MLA) (formula:  $C_3H_4O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		

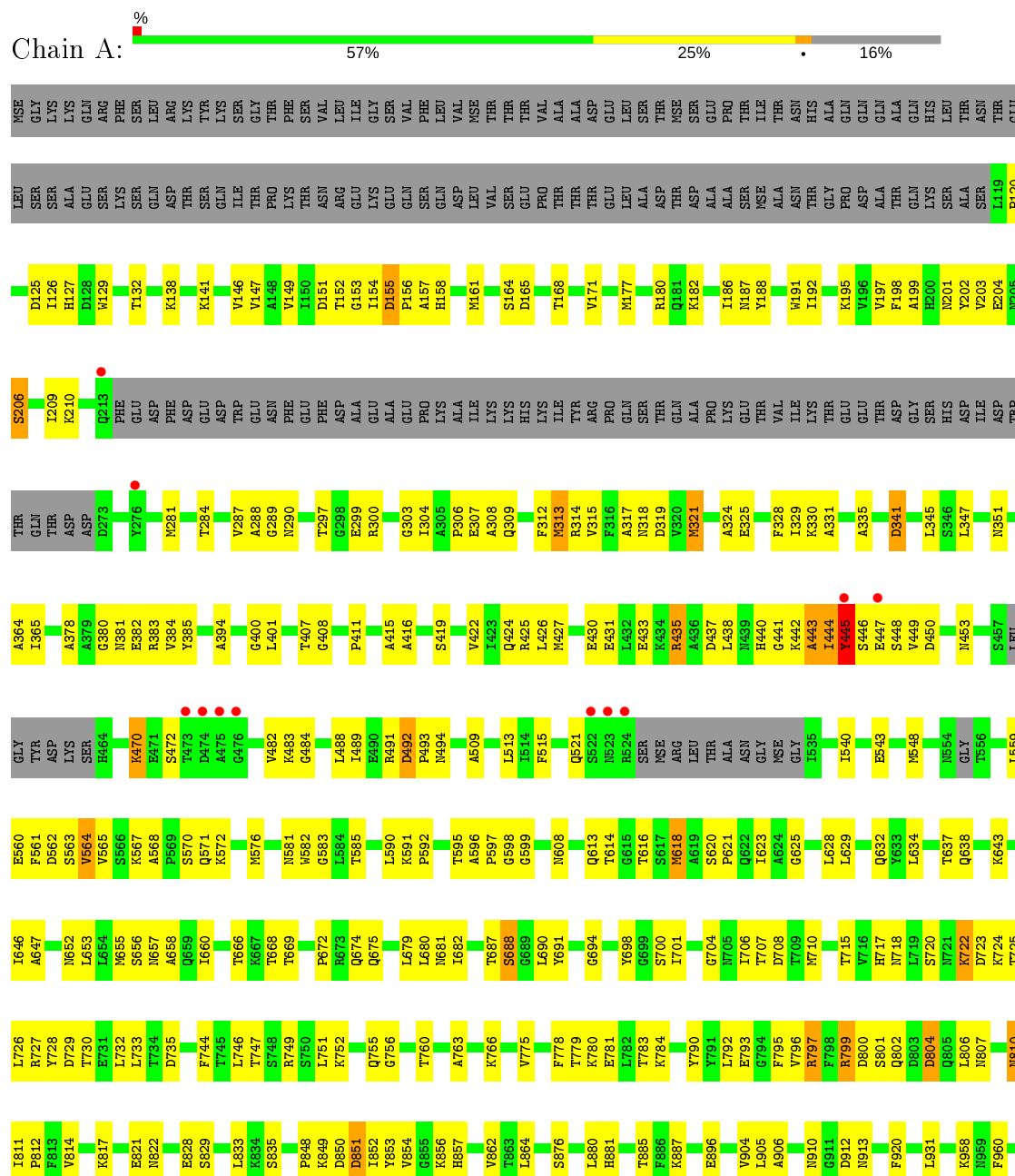
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	21	Total	O	0	0
			21	21		

### 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



ARG	S969	L1094	M1257	K1392	T1560
ILE	Y994	F1095	M1287	A1393	L1561
VAL	Y995	L1096	R1268	V1394	P1562
GLY	Y996	M1107	D1269	L1407	L1570
LEU	Y999	V1108	K1273	P1408	R1571
VAL		E1109	E1274	V1409	L1572
LEU		D1110		P1410	V1573
LEU		F1111	I1281	E1411	K1574
GLY	G1004	A1112	D1285	D1412	VAL
LEU	R1007	V1115	R1286	I1415	GLY
THR		A1116	K1287	E1453	THR
CYS	M1010	I1117	P1288	L1454	ASP
ALA	T1011	A1118	M1289	T1456	ASP
VAL	F1012	L1124	T1291	Y1457	HIS
SER	D1013	P1125	Q1292	A1461	LYS
ARG	M1014	G1129	R1293	A1462	LYS
LYS	D1017	I1133	G1294	L1463	VAL
SER	R1018	K1134	D1302	L1464	MSE
THR	Q1019	L1135	H1303	I1469	SER
ASP	V1022	K1136	D1307	D1477	LYS
THR	L1023	L1152	K1310	M1487	ASN
LYS	S1024	Q1156	S1314	T1488	ASN
ASP	Q1025	T1159	I1317	M1489	GLN
THR	F1028	G1160	V1318	S1493	ALA
LEU	N1033	L1161	R1319	Q1494	ALA
THR	E1038	L1180	E1321	D1500	ALA
ALA	K1041	M1183	Y1324	L1503	THR
SER	D1042	D1186	K1339	A1514	THR
THR	R1043	F1187	K1353	Q1515	LYS
THR	A1046	F1188	K1359	Q1516	THR
LYS	R1049	K1197	T1360	Q1517	PRO
THR	D1051	V1200	D1365	Y1526	ALA
ALA	F1054	Y1210	D1370	V1527	THR
THR	R1058	D1212	D1371	K1533	ALA
LYS	D1060	M1216	V1376	G1538	ALA
LEU	Y1074	S1231	E1377	V1544	THR
THR	V1077	Q1233	D1378	L1546	GLY
LYS	E1078	A1234	R1379	Y1550	GLU
GLY	D1079	G1235	V1383	R1551	LYS
THR	N1080	A1236	I1389	I1552	MSE
LYS	K1081	G1237		E1553	GLY
LYS	E1085	A1238			LEU
LEU	R1086				LYS
					LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.62Å 191.62Å 250.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.80 19.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.99-2.80) 99.3 (19.99-2.80)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.79Å)	Xtriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, $R_{free}$	0.209 , 0.257 0.211 , 0.257	Depositor DCC
$R_{free}$ test set	1956 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 20.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.57	0/10657	0.72	2/14404 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	445	TYR	CB-CA-C	-5.47	99.45	110.40
1	A	155	ASP	N-CA-C	-5.03	97.43	111.00

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	10481	0	10083	378	0
2	A	1	0	0	9	0
3	A	3	0	0	0	0
4	A	5	0	0	0	0
5	A	7	0	2	0	0
6	A	21	0	0	3	0
All	All	10518	0	10085	378	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 18.

All (378) 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:383:ARG:NH2	1:A:746:LEU:CD1	1.77	1.45
1:A:383:ARG:NH2	1:A:746:LEU:HD12	1.06	1.36
1:A:447:GLU:OE2	1:A:453:ASN:CB	1.74	1.34
1:A:445:TYR:HE1	1:A:561:PHE:CE1	1.44	1.34
1:A:383:ARG:CZ	1:A:746:LEU:CD1	2.20	1.19
1:A:445:TYR:CE1	1:A:561:PHE:CE1	2.35	1.15
1:A:383:ARG:CZ	1:A:746:LEU:HD13	1.79	1.12
1:A:445:TYR:CE1	1:A:561:PHE:HE1	1.68	1.10
1:A:563:SER:O	1:A:564:VAL:O	1.73	1.06
1:A:1319:ARG:NH1	6:A:1801:HOH:O	1.86	1.04
1:A:441:GLY:HA2	1:A:548:MSE:HE1	1.40	1.04
1:A:1552:ILE:HD12	1:A:1553:GLU:H	1.25	0.99
1:A:380:GLY:H	1:A:616:THR:HG21	1.30	0.96
1:A:1268:ARG:HG3	1:A:1274:GLU:OE1	1.67	0.94
1:A:154:ILE:HD11	1:A:312:PHE:CD2	2.03	0.93
1:A:154:ILE:CD1	1:A:312:PHE:CG	2.53	0.91
1:A:154:ILE:HD11	1:A:312:PHE:CG	2.07	0.90
1:A:1159:THR:HG23	1:A:1161:LEU:H	1.36	0.89
1:A:1285:ASP:HB3	1:A:1411:GLU:HG3	1.56	0.88
1:A:484:GLY:HA2	1:A:509:ALA:H	1.38	0.87
1:A:445:TYR:HH	1:A:561:PHE:HD1	0.89	0.86
1:A:154:ILE:HD11	1:A:312:PHE:CB	2.06	0.85
1:A:383:ARG:HH21	1:A:746:LEU:CD1	1.64	0.84
1:A:154:ILE:CD1	1:A:312:PHE:CB	2.56	0.83
1:A:599:GLY:HA2	1:A:614:THR:HG23	1.60	0.83
1:A:613:GLN:HB3	1:A:618:MSE:HE2	1.61	0.82
1:A:154:ILE:HD11	1:A:312:PHE:HB2	1.62	0.81
1:A:445:TYR:HE1	1:A:561:PHE:CD1	1.99	0.80
1:A:289:GLY:HA2	1:A:303:GLY:H	1.47	0.79
1:A:445:TYR:CE1	1:A:561:PHE:CD1	2.70	0.79
1:A:378:ALA:HB1	1:A:616:THR:HG23	1.65	0.78
1:A:154:ILE:HG22	1:A:155:ASP:N	1.98	0.77
1:A:896:GLU:OE1	1:A:1049:ARG:NH1	2.16	0.77
1:A:153:GLY:N	1:A:312:PHE:HZ	1.82	0.77
1:A:318:ASN:H	1:A:321:MSE:HE2	1.49	0.76
1:A:445:TYR:HE1	1:A:561:PHE:HE1	0.82	0.76
1:A:1552:ILE:HD12	1:A:1553:GLU:N	2.01	0.75
1:A:1457:TYR:CE1	1:A:1487:MSE:HE1	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:NZ	1:A:308:ALA:O	2.20	0.74
1:A:445:TYR:OH	1:A:561:PHE:HD1	1.67	0.74
1:A:383:ARG:HG2	1:A:384:VAL:HG22	1.69	0.74
1:A:153:GLY:H	1:A:312:PHE:HZ	1.31	0.74
1:A:154:ILE:CD1	1:A:312:PHE:CD2	2.70	0.74
1:A:1303:HIS:CE1	1:A:1360:THR:HG22	2.23	0.74
1:A:425:ARG:O	1:A:445:TYR:CE2	2.41	0.73
1:A:132:THR:HB	1:A:682:ILE:HD12	1.71	0.73
1:A:161:MSE:HE3	1:A:281:MSE:CE	2.20	0.72
1:A:177:MSE:HE3	1:A:198:PHE:HB2	1.71	0.72
1:A:394:ALA:HA	1:A:744:PHE:CE2	2.24	0.72
1:A:161:MSE:HE3	1:A:281:MSE:HE1	1.72	0.71
1:A:426:LEU:HD11	1:A:568:ALA:HB2	1.72	0.71
1:A:728:TYR:CE1	1:A:756:GLY:HA3	2.26	0.70
1:A:707:THR:HG23	1:A:708:ASP:H	1.56	0.70
1:A:383:ARG:CZ	1:A:746:LEU:HD12	1.96	0.70
1:A:1019:GLN:O	2:A:1701:CL:CL	2.49	0.68
1:A:154:ILE:CG2	1:A:155:ASP:N	2.56	0.68
1:A:383:ARG:NE	1:A:746:LEU:CD1	2.56	0.68
1:A:994:TYR:HB2	1:A:1014:MSE:HE2	1.74	0.68
1:A:1133:ILE:O	1:A:1133:ILE:HD12	1.94	0.68
1:A:177:MSE:CE	1:A:197:VAL:HG12	2.24	0.67
1:A:999:TYR:CE1	1:A:1007:ARG:HG3	2.29	0.67
1:A:489:ILE:HG22	1:A:515:PHE:HE2	1.58	0.66
1:A:489:ILE:HG22	1:A:515:PHE:CE2	2.30	0.66
1:A:383:ARG:NH2	1:A:746:LEU:HD13	1.85	0.66
1:A:177:MSE:HE2	1:A:197:VAL:CG1	2.26	0.66
1:A:1365:ASP:O	6:A:1802:HOH:O	2.14	0.65
1:A:1544:VAL:HG21	1:A:1552:ILE:HG21	1.78	0.65
1:A:154:ILE:HD12	1:A:312:PHE:CG	2.31	0.65
1:A:156:PRO:HG2	1:A:192:ILE:HD13	1.78	0.65
1:A:154:ILE:HD12	1:A:312:PHE:CB	2.26	0.65
1:A:141:LYS:O	1:A:632:GLN:NE2	2.29	0.65
1:A:563:SER:C	1:A:564:VAL:O	2.36	0.64
1:A:1493:SER:OG	1:A:1560:THR:HG23	1.97	0.64
1:A:1291:THR:HG22	1:A:1292:GLN:H	1.63	0.64
1:A:829:SER:HB3	1:A:1010:MSE:HE3	1.79	0.64
1:A:127:HIS:ND1	1:A:132:THR:HG21	2.13	0.64
1:A:1453:GLU:HG3	1:A:1469:ILE:HG12	1.80	0.64
1:A:201:ASN:HA	1:A:314:ARG:HB3	1.78	0.64
1:A:706:ILE:HD11	1:A:792:LEU:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ARG:HH21	1:A:746:LEU:HD12	0.70	0.63
1:A:783:THR:HG22	1:A:790:TYR:HE1	1.63	0.63
1:A:351:ASN:ND2	1:A:958:LYS:HE3	2.13	0.62
1:A:445:TYR:OH	1:A:561:PHE:CD1	2.47	0.61
1:A:706:ILE:CD1	1:A:792:LEU:HD12	2.30	0.61
1:A:853:TYR:O	1:A:856:LYS:HB2	1.99	0.61
1:A:1042:ASP:OD2	2:A:1701:CL:CL	2.55	0.61
1:A:1493:SER:CB	1:A:1560:THR:HG23	2.31	0.61
1:A:443:ALA:HB2	1:A:548:MSE:SE	2.51	0.61
1:A:710:MSE:HE1	1:A:792:LEU:HB3	1.82	0.61
1:A:153:GLY:N	1:A:312:PHE:CZ	2.67	0.60
1:A:154:ILE:HG22	1:A:156:PRO:N	2.17	0.60
1:A:1292:GLN:HG2	1:A:1394:VAL:HG11	1.82	0.60
1:A:862:VAL:HG11	1:A:880:LEU:HD13	1.84	0.60
1:A:1017:ASP:OD2	2:A:1701:CL:CL	2.56	0.60
1:A:328:PHE:CZ	1:A:347:LEU:HD13	2.37	0.60
1:A:424:GLN:O	1:A:565:VAL:HA	2.02	0.59
1:A:1464:LEU:CA	1:A:1487:MSE:HE3	2.32	0.59
1:A:321:MSE:HB3	1:A:1456:THR:OG1	2.02	0.59
1:A:1377:GLU:HG3	1:A:1383:VAL:HG22	1.84	0.59
1:A:1159:THR:HG21	1:A:1183:MSE:O	2.03	0.59
1:A:154:ILE:HD12	1:A:312:PHE:HB3	1.85	0.59
1:A:729:ASP:HB3	1:A:755:GLN:HG3	1.83	0.58
1:A:441:GLY:CA	1:A:548:MSE:HE1	2.24	0.58
1:A:669:THR:HB	1:A:733:LEU:HD21	1.84	0.58
1:A:380:GLY:N	1:A:616:THR:HG21	2.10	0.58
1:A:1415:ILE:HD13	1:A:1489:MSE:HE1	1.84	0.58
1:A:910:ASN:ND2	1:A:912:ASP:OD2	2.36	0.58
1:A:1212:ASP:OD2	1:A:1268:ARG:NH2	2.33	0.58
1:A:727:ARG:HE	1:A:801:SER:HA	1.69	0.58
1:A:1004:GLY:HA3	1:A:1527:VAL:HB	1.86	0.58
1:A:202:TYR:HB2	1:A:315:VAL:HG22	1.85	0.58
1:A:1033:ASN:OD1	1:A:1096:LEU:HD12	2.04	0.57
1:A:1042:ASP:OD2	1:A:1046:ALA:O	2.21	0.57
1:A:1353:LYS:HG3	1:A:1359:TYR:CZ	2.39	0.57
1:A:313:MSE:HE2	1:A:335:ALA:HB2	1.87	0.57
1:A:154:ILE:O	1:A:210:LYS:HA	2.04	0.57
1:A:1464:LEU:N	1:A:1487:MSE:HE3	2.20	0.57
1:A:430:GLU:HG2	1:A:431:GLU:OE1	2.05	0.57
1:A:447:GLU:CD	1:A:453:ASN:CB	2.67	0.56
1:A:435:ARG:NH1	1:A:437:ASP:OD2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:PHE:O	1:A:1197:LYS:HE2	2.04	0.56
1:A:1551:ARG:HD3	1:A:1553:GLU:HG3	1.87	0.56
1:A:154:ILE:CD1	1:A:312:PHE:HB2	2.30	0.56
1:A:177:MSE:HE2	1:A:197:VAL:HG13	1.88	0.56
1:A:400:GLY:O	1:A:401:LEU:HD23	2.06	0.56
1:A:694:GLY:HA3	1:A:701:ILE:HD11	1.88	0.56
1:A:857:HIS:HA	1:A:969:SER:HB3	1.87	0.56
1:A:186:ILE:HG13	1:A:188:TYR:CE1	2.41	0.56
1:A:177:MSE:HE2	1:A:197:VAL:HG12	1.87	0.55
1:A:177:MSE:CE	1:A:197:VAL:O	2.55	0.55
1:A:920:PHE:CD1	1:A:996:VAL:HG21	2.42	0.55
1:A:177:MSE:CE	1:A:198:PHE:HB2	2.36	0.55
1:A:287:VAL:HG23	1:A:625:GLY:N	2.22	0.55
1:A:491:ARG:HG3	1:A:492:ASP:N	2.21	0.55
1:A:182:LYS:HE3	1:A:187:ASN:HB3	1.89	0.55
1:A:126:ILE:HG23	1:A:597:PRO:HG2	1.88	0.55
1:A:177:MSE:HG2	1:A:191:TRP:HB2	1.88	0.55
1:A:1291:THR:HG22	1:A:1292:GLN:N	2.22	0.54
1:A:1028:PHE:H	1:A:1133:ILE:CD1	2.20	0.54
1:A:484:GLY:CA	1:A:509:ALA:H	2.14	0.54
1:A:1303:HIS:NE2	1:A:1360:THR:HG22	2.21	0.54
1:A:304:ILE:O	1:A:629:LEU:HD11	2.06	0.54
1:A:582:TRP:HD1	1:A:583:GLY:H	1.55	0.54
1:A:829:SER:HB3	1:A:1010:MSE:CE	2.37	0.54
1:A:120:PRO:HG2	1:A:300:ARG:HG3	1.89	0.54
1:A:1544:VAL:HG21	1:A:1552:ILE:CG2	2.37	0.54
1:A:154:ILE:HG13	1:A:312:PHE:CD2	2.43	0.54
1:A:431:GLU:OE1	1:A:431:GLU:N	2.38	0.54
1:A:724:LYS:HG2	1:A:807:ASN:OD1	2.07	0.54
1:A:1049:ARG:HB2	1:A:1111:PHE:CD1	2.43	0.54
1:A:154:ILE:HG13	1:A:312:PHE:CE2	2.43	0.54
1:A:582:TRP:CH2	1:A:746:LEU:HB3	2.43	0.54
1:A:730:THR:HB	1:A:796:VAL:HG12	1.88	0.54
1:A:290:ASN:ND2	1:A:307:GLU:OE1	2.39	0.54
1:A:655:MSE:HE1	1:A:700:SER:HB2	1.89	0.54
1:A:799:ARG:HB3	1:A:804:ASP:HB2	1.90	0.54
1:A:1317:ILE:HD12	1:A:1376:VAL:HB	1.89	0.53
1:A:1514:ALA:O	1:A:1515:GLN:HB2	2.08	0.53
1:A:177:MSE:HE1	1:A:197:VAL:HG12	1.90	0.53
1:A:203:VAL:O	1:A:204:GLU:HG2	2.07	0.53
1:A:380:GLY:HA3	1:A:581:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:CG1	1:A:312:PHE:CD2	2.91	0.53
1:A:435:ARG:NH1	1:A:438:LEU:HG	2.23	0.53
1:A:724:LYS:HB3	1:A:726:LEU:HD21	1.88	0.53
1:A:445:TYR:CZ	1:A:561:PHE:CD1	2.96	0.53
1:A:1457:TYR:CD1	1:A:1487:MSE:HE1	2.43	0.53
1:A:521:GLN:NE2	1:A:543:GLU:O	2.42	0.53
1:A:154:ILE:CG2	1:A:155:ASP:H	2.22	0.53
1:A:319:ASP:N	1:A:319:ASP:OD1	2.40	0.53
1:A:438:LEU:HD13	1:A:548:MSE:HG3	1.91	0.53
1:A:1152:LEU:HD12	1:A:1180:LEU:HD23	1.91	0.52
1:A:313:MSE:HG2	1:A:331:ALA:HB1	1.91	0.52
1:A:483:LYS:CB	1:A:509:ALA:HB2	2.39	0.52
1:A:723:ASP:OD1	1:A:763:ALA:HB2	2.09	0.52
1:A:1028:PHE:H	1:A:1133:ILE:HD11	1.74	0.52
1:A:484:GLY:H	1:A:509:ALA:HA	1.73	0.52
1:A:623:ILE:HD13	1:A:680:LEU:HD22	1.92	0.52
1:A:559:LEU:HD23	1:A:560:GLU:N	2.25	0.52
1:A:1124:LEU:HD12	1:A:1125:PRO:HD2	1.92	0.51
1:A:634:LEU:HD21	1:A:653:LEU:HD11	1.91	0.51
1:A:381:ASN:OD1	1:A:616:THR:HG22	2.10	0.51
1:A:779:THR:O	1:A:783:THR:HG23	2.10	0.51
1:A:660:ILE:HD13	1:A:795:PHE:CG	2.46	0.51
1:A:1017:ASP:OD1	2:A:1701:CL:CL	2.66	0.51
1:A:730:THR:HG22	1:A:796:VAL:HB	1.92	0.51
1:A:1107:MSE:HB2	1:A:1117:ILE:HG12	1.92	0.51
1:A:595:THR:OG1	1:A:675:GLN:O	2.29	0.51
1:A:1049:ARG:HB2	1:A:1111:PHE:CE1	2.46	0.50
1:A:590:LEU:HD22	1:A:814:VAL:HG12	1.92	0.50
1:A:576:MSE:CE	1:A:675:GLN:HA	2.42	0.50
1:A:146:VAL:HG23	1:A:309:GLN:O	2.11	0.50
1:A:1186:ASP:OD1	1:A:1379:ARG:NH1	2.43	0.50
1:A:1392:LYS:C	1:A:1394:VAL:H	2.15	0.50
1:A:591:LYS:HA	1:A:592:PRO:O	2.11	0.50
1:A:470:LYS:HA	1:A:489:ILE:HD13	1.92	0.50
1:A:896:GLU:CD	1:A:1049:ARG:NH1	2.66	0.50
1:A:1538:GLY:O	1:A:1560:THR:HB	2.12	0.50
1:A:730:THR:CG2	1:A:796:VAL:HG12	2.42	0.50
1:A:149:VAL:HG11	1:A:284:THR:HG23	1.94	0.50
1:A:321:MSE:HE1	1:A:324:ALA:HB2	1.92	0.50
1:A:147:VAL:HB	1:A:628:LEU:HD11	1.94	0.50
1:A:426:LEU:O	1:A:562:ASP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:VAL:HG23	1:A:570:SER:HB2	1.94	0.49
1:A:710:MSE:HE1	1:A:732:LEU:HD21	1.92	0.49
1:A:289:GLY:N	1:A:306:PRO:HA	2.26	0.49
1:A:1546:LEU:HD22	1:A:1550:TYR:HB2	1.94	0.49
1:A:202:TYR:CE1	1:A:313:MSE:HG3	2.47	0.49
1:A:1216:ASN:OD1	1:A:1231:SER:OG	2.27	0.49
1:A:1544:VAL:HG23	1:A:1546:LEU:HD12	1.95	0.49
1:A:1110:ASP:OD2	2:A:1701:CL:CL	2.68	0.49
1:A:1200:VAL:HG21	1:A:1281:ILE:HG13	1.95	0.49
1:A:1493:SER:OG	1:A:1560:THR:CG2	2.60	0.49
1:A:446:SER:CA	1:A:543:GLU:H	2.25	0.49
1:A:658:ALA:O	1:A:810:ASN:ND2	2.45	0.49
1:A:1043:ARG:O	2:A:1701:CL:CL	2.68	0.49
1:A:422:VAL:CG1	1:A:424:GLN:HG3	2.43	0.49
1:A:690:LEU:HD21	1:A:724:LYS:HD3	1.94	0.49
1:A:790:TYR:OH	1:A:817:LYS:HD3	2.13	0.49
1:A:177:MSE:HE3	1:A:197:VAL:O	2.13	0.49
1:A:1544:VAL:CG2	1:A:1552:ILE:HG21	2.43	0.48
1:A:780:LYS:HE3	1:A:784:LYS:HE3	1.96	0.48
1:A:1042:ASP:OD1	2:A:1701:CL:CL	2.69	0.48
1:A:489:ILE:HA	1:A:513:LEU:O	2.13	0.48
1:A:660:ILE:HD11	1:A:810:ASN:HB3	1.94	0.48
1:A:1133:ILE:HD12	1:A:1133:ILE:C	2.34	0.48
1:A:400:GLY:HA2	1:A:583:GLY:HA3	1.95	0.48
1:A:1415:ILE:HD11	1:A:1461:ALA:HB1	1.95	0.48
1:A:749:ARG:NH2	1:A:781:GLU:OE2	2.47	0.47
1:A:1210:TYR:CD1	1:A:1238:ALA:HB2	2.49	0.47
1:A:1552:ILE:CD1	1:A:1553:GLU:N	2.75	0.47
1:A:165:ASP:OD2	1:A:168:THR:HG23	2.14	0.47
1:A:717:HIS:ND1	1:A:766:LYS:HD2	2.29	0.47
1:A:725:THR:HA	1:A:760:THR:HA	1.97	0.47
1:A:400:GLY:CA	1:A:583:GLY:HA3	2.45	0.47
1:A:1561:LEU:HB3	1:A:1562:PRO:HD2	1.97	0.47
1:A:666:THR:O	1:A:668:THR:HG23	2.13	0.47
1:A:849:LYS:HE3	1:A:850:ASP:OD2	2.15	0.47
1:A:1077:VAL:C	1:A:1078:GLU:HG2	2.34	0.47
1:A:1135:LEU:HD12	1:A:1136:LYS:N	2.30	0.47
1:A:385:TYR:HD2	1:A:958:LYS:HD3	1.79	0.47
1:A:1109:GLU:HB3	1:A:1115:VAL:HG12	1.95	0.47
1:A:401:LEU:HD11	1:A:960:PHE:HB2	1.97	0.47
1:A:1051:ASP:HB3	1:A:1108:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:LEU:HD12	1:A:1136:LYS:H	1.80	0.47
1:A:313:MSE:N	1:A:313:MSE:SE	2.98	0.47
1:A:1156:GLN:NE2	1:A:1156:GLN:O	2.46	0.46
1:A:1500:ASP:HB2	1:A:1571:ARG:HA	1.96	0.46
1:A:146:VAL:HA	1:A:309:GLN:O	2.15	0.46
1:A:1107:MSE:HG3	1:A:1117:ILE:HG12	1.97	0.46
1:A:1010:MSE:HE2	1:A:1012:PHE:CZ	2.50	0.46
1:A:195:LYS:HZ1	1:A:288:ALA:HB1	1.81	0.46
1:A:582:TRP:CE2	1:A:674:GLN:HB2	2.50	0.46
1:A:1455:LEU:HA	1:A:1455:LEU:HD23	1.74	0.46
1:A:1551:ARG:HG3	1:A:1573:VAL:HG23	1.98	0.46
1:A:488:LEU:O	1:A:513:LEU:N	2.49	0.46
1:A:1494:GLN:HE22	1:A:1533:LYS:C	2.20	0.46
1:A:297:THR:HG23	1:A:299:GLU:H	1.81	0.46
1:A:1392:LYS:O	1:A:1393:ALA:HB3	2.16	0.46
1:A:177:MSE:HE2	1:A:197:VAL:O	2.16	0.46
1:A:729:ASP:OD2	1:A:797:ARG:NH2	2.49	0.45
1:A:797:ARG:HD3	1:A:797:ARG:N	2.31	0.45
1:A:151:ASP:O	1:A:314:ARG:HA	2.16	0.45
1:A:1022:VAL:HG22	1:A:1041:LYS:O	2.16	0.45
1:A:1370:SER:OG	1:A:1389:ARG:HD2	2.16	0.45
1:A:854:VAL:HB	1:A:881:HIS:HA	1.98	0.45
1:A:1054:PHE:HE2	1:A:1107:MSE:HE3	1.82	0.45
1:A:1409:VAL:HB	1:A:1410:PRO:HD2	1.98	0.45
1:A:158:HIS:CD2	1:A:608:ASN:HA	2.51	0.45
1:A:656:SER:HA	1:A:810:ASN:O	2.17	0.45
1:A:646:ILE:HG23	1:A:647:ALA:N	2.32	0.45
1:A:129:TRP:HZ3	1:A:419:SER:HA	1.81	0.45
1:A:155:ASP:O	1:A:157:ALA:N	2.50	0.45
1:A:660:ILE:HD11	1:A:810:ASN:CB	2.47	0.45
1:A:1464:LEU:HA	1:A:1487:MSE:HE3	1.98	0.45
1:A:444:ILE:N	1:A:444:ILE:HD13	2.32	0.45
1:A:905:LEU:HB2	1:A:1013:ASP:O	2.17	0.44
1:A:1503:LEU:HD23	1:A:1572:LEU:HD13	1.98	0.44
1:A:995:VAL:HG22	1:A:1011:THR:HG23	1.99	0.44
1:A:1085:GLU:HG2	1:A:1086:ARG:N	2.32	0.44
1:A:1269:ASP:HB2	1:A:1273:LYS:O	2.17	0.44
1:A:155:ASP:H	1:A:281:MSE:SE	2.50	0.44
1:A:521:GLN:CD	1:A:571:GLN:HE22	2.20	0.44
1:A:177:MSE:O	1:A:180:ARG:N	2.46	0.44
1:A:1233:GLN:HA	1:A:1233:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1544:VAL:HG21	1:A:1546:LEU:HD11	1.98	0.44
1:A:427:MSE:SE	1:A:561:PHE:CE1	3.21	0.44
1:A:442:LYS:C	1:A:444:ILE:H	2.18	0.44
1:A:751:LEU:O	1:A:752:LYS:HG2	2.18	0.44
1:A:1025:GLN:O	1:A:1038:GLU:HG2	2.16	0.44
1:A:138:LYS:HE3	1:A:687:THR:HG22	1.99	0.44
1:A:848:PRO:HG2	1:A:851:ASP:HB2	2.00	0.44
1:A:643:LYS:O	1:A:646:ILE:HG22	2.18	0.44
1:A:317:ALA:HA	1:A:321:MSE:HE1	2.00	0.44
1:A:445:TYR:CZ	1:A:561:PHE:HD1	2.32	0.44
1:A:1183:MSE:HE3	1:A:1187:PHE:CD1	2.53	0.44
1:A:1291:THR:CG2	1:A:1307:ASP:OD2	2.66	0.44
1:A:657:ASN:O	1:A:681:ASN:HB3	2.17	0.44
1:A:710:MSE:HE2	1:A:792:LEU:HD13	2.00	0.43
1:A:852:ILE:HB	1:A:885:THR:HG21	2.00	0.43
1:A:146:VAL:O	1:A:341:ASP:HB2	2.18	0.43
1:A:1324:TYR:HA	1:A:1371:ASP:O	2.18	0.43
1:A:289:GLY:H	1:A:306:PRO:HA	1.84	0.43
1:A:1023:LEU:HD13	1:A:1118:ALA:HB2	1.98	0.43
1:A:1054:PHE:CE2	1:A:1107:MSE:HE3	2.52	0.43
1:A:448:SER:O	1:A:450:ASP:N	2.51	0.43
1:A:704:GLY:HA2	1:A:1526:TYR:CE2	2.54	0.43
1:A:1017:ASP:CG	2:A:1701:CL:CL	2.94	0.43
1:A:199:ALA:HB1	1:A:209:ILE:HG13	2.01	0.43
1:A:931:LEU:C	1:A:931:LEU:HD23	2.39	0.43
1:A:1292:GLN:HE21	1:A:1394:VAL:HG11	1.84	0.43
1:A:161:MSE:HE3	1:A:281:MSE:HE2	1.98	0.43
1:A:1257:MSE:SE	1:A:1410:PRO:HD3	2.69	0.43
1:A:204:GLU:HG3	1:A:206:SER:HB3	2.00	0.43
1:A:401:LEU:O	1:A:581:ASN:ND2	2.52	0.43
1:A:1377:GLU:HG3	1:A:1383:VAL:CG2	2.47	0.43
1:A:415:ALA:HB2	1:A:592:PRO:HG2	2.01	0.43
1:A:407:THR:HG22	1:A:585:THR:HG22	2.01	0.43
1:A:828:GLU:HB3	1:A:833:LEU:HD21	2.00	0.43
1:A:906:ALA:HB1	1:A:1112:ALA:HB2	1.99	0.43
1:A:195:LYS:NZ	1:A:288:ALA:HB1	2.34	0.43
1:A:365:ILE:HG21	1:A:411:PRO:HG3	2.01	0.42
1:A:710:MSE:CE	1:A:775:VAL:HG11	2.49	0.42
1:A:796:VAL:HG22	1:A:811:ILE:HG22	2.00	0.42
1:A:795:PHE:CE2	1:A:812:PRO:HB3	2.53	0.42
1:A:492:ASP:O	1:A:494:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:THR:HG22	1:A:638:GLN:CD	2.40	0.42
1:A:730:THR:CB	1:A:796:VAL:HG12	2.49	0.42
1:A:790:TYR:CZ	1:A:817:LYS:HD3	2.54	0.42
1:A:151:ASP:OD1	1:A:152:THR:HG23	2.20	0.42
1:A:281:MSE:HE3	1:A:284:THR:OG1	2.18	0.42
1:A:679:LEU:HG	1:A:680:LEU:N	2.33	0.42
1:A:330:LYS:HD2	1:A:330:LYS:HA	1.83	0.42
1:A:595:THR:HG22	1:A:596:ALA:N	2.34	0.42
1:A:688:SER:O	1:A:690:LEU:HD23	2.20	0.42
1:A:864:LEU:HD12	1:A:880:LEU:HD23	2.01	0.42
1:A:1319:ARG:NH1	1:A:1321:GLU:OE2	2.44	0.42
1:A:620:SER:N	1:A:621:PRO:HD2	2.35	0.42
1:A:1024:SER:OG	1:A:1038:GLU:HG3	2.19	0.42
1:A:325:GLU:O	1:A:329:ILE:HG13	2.20	0.42
1:A:904:VAL:HB	1:A:1111:PHE:CD2	2.55	0.42
1:A:1494:GLN:NE2	1:A:1533:LYS:C	2.73	0.41
1:A:1079:ASP:HB2	1:A:1081:LYS:HE3	2.02	0.41
1:A:1042:ASP:CG	2:A:1701:CL:CL	2.95	0.41
1:A:1407:LEU:CD2	1:A:1487:MSE:HB2	2.50	0.41
1:A:382:GLU:HB3	1:A:401:LEU:CD1	2.50	0.41
1:A:408:GLY:O	1:A:411:PRO:HD2	2.20	0.41
1:A:1133:ILE:CD1	1:A:1133:ILE:C	2.89	0.41
1:A:1570:LEU:HD23	1:A:1570:LEU:HA	1.79	0.41
1:A:433:GLU:HA	1:A:440:HIS:HB3	2.00	0.41
1:A:628:LEU:HD23	1:A:628:LEU:HA	1.90	0.41
1:A:416:ALA:HB1	1:A:598:GLY:HA3	2.03	0.41
1:A:720:SER:HB2	1:A:722:LYS:HD2	2.03	0.41
1:A:1028:PHE:HB3	1:A:1133:ILE:HD11	2.02	0.41
1:A:715:THR:HG22	1:A:717:HIS:CD2	2.55	0.41
1:A:1159:THR:CG2	1:A:1161:LEU:H	2.21	0.41
1:A:698:TYR:C	1:A:700:SER:H	2.24	0.41
1:A:1409:VAL:HB	1:A:1410:PRO:CD	2.50	0.41
1:A:1493:SER:CB	1:A:1560:THR:CG2	2.98	0.41
1:A:715:THR:HG22	1:A:717:HIS:NE2	2.36	0.41
1:A:672:PRO:HD2	1:A:793:GLU:HG3	2.02	0.41
1:A:1289:MSE:HE3	6:A:1808:HOH:O	2.19	0.41
1:A:171:VAL:HG11	1:A:197:VAL:HG13	2.03	0.41
1:A:800:ASP:HB2	1:A:806:LEU:O	2.21	0.41
1:A:1094:LEU:O	1:A:1096:LEU:N	2.54	0.41
1:A:284:THR:HA	1:A:287:VAL:HG12	2.03	0.41
1:A:345:LEU:HA	1:A:345:LEU:HD23	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:LEU:C	1:A:733:LEU:HD12	2.41	0.41
1:A:164:SER:HB2	1:A:307:GLU:OE2	2.21	0.40
1:A:821:GLU:HG2	1:A:822:ASN:ND2	2.36	0.40
1:A:329:ILE:HG23	1:A:364:ALA:HB2	2.02	0.40
1:A:1269:ASP:OD2	1:A:1273:LYS:HB3	2.20	0.40
1:A:125:ASP:OD2	1:A:567:LYS:HD3	2.21	0.40
1:A:590:LEU:O	1:A:591:LYS:HG2	2.21	0.40
1:A:653:LEU:HD23	1:A:691:TYR:HB3	2.04	0.40
1:A:733:LEU:N	1:A:733:LEU:HD12	2.36	0.40
1:A:912:ASP:O	1:A:913:ASN:HB2	2.20	0.40
1:A:1415:ILE:CD1	1:A:1489:MSE:HE1	2.50	0.40
1:A:876:SER:HB2	1:A:1074:TYR:OH	2.21	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	1370/1647 (83%)	1206 (88%)	153 (11%)	11 (1%)	19 49

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	482	VAL
1	A	540	ILE
1	A	564	VAL
1	A	1412	ASP
1	A	449	VAL
1	A	804	ASP
1	A	341	ASP
1	A	444	ILE
1	A	493	PRO

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Mol	Chain	Res	Type
1	A	443	ALA
1	A	492	ASP

### 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	1104/1369 (81%)	1063 (96%)	41 (4%)	34 68

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	SER
1	A	313	MSE
1	A	321	MSE
1	A	435	ARG
1	A	445	TYR
1	A	470	LYS
1	A	472	SER
1	A	572	LYS
1	A	618	MSE
1	A	652	ASN
1	A	688	SER
1	A	718	ASN
1	A	722	LYS
1	A	735	ASP
1	A	747	THR
1	A	778	PHE
1	A	797	ARG
1	A	799	ARG
1	A	802	GLN
1	A	810	ASN
1	A	835	SER
1	A	851	ASP
1	A	887	LYS
1	A	1049	ARG

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Mol	Chain	Res	Type
1	A	1058	ARG
1	A	1060	ASP
1	A	1268	ARG
1	A	1285	ASP
1	A	1287	LYS
1	A	1292	GLN
1	A	1294	ARG
1	A	1302	ASP
1	A	1310	LYS
1	A	1314	SER
1	A	1339	LYS
1	A	1411	GLU
1	A	1463	LYS
1	A	1477	ASP
1	A	1500	ASP
1	A	1517	GLN
1	A	1551	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	ASN
1	A	571	GLN
1	A	929	GLN
1	A	1494	GLN

### 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 [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z  > 2$
4	SO4	A	1705	-	4,4,4	0.47	0	6,6,6	0.94	0
5	MLA	A	1706	-	0,6,6	0.00	-	0,7,7	0.00	-

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
5	MLA	A	1706	-	-	0/0/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	1355/1647 (82%)	-0.36	16 (1%) 79 73	35, 65, 118, 148	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1237	GLY	4.6
1	A	473	THR	4.6
1	A	447	GLU	4.0
1	A	522	SER	3.9
1	A	474	ASP	3.7
1	A	475	ALA	3.1
1	A	1129	GLY	3.0
1	A	523	ASN	2.6
1	A	476	GLY	2.3
1	A	524	ARG	2.3
1	A	213	GLN	2.3
1	A	1236	ALA	2.2
1	A	276	TYR	2.2
1	A	445	TYR	2.2
1	A	1235	GLY	2.2
1	A	1551	ARG	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
3	CA	A	1703	1/1	0.79	0.24	91,91,91,91	0
5	MLA	A	1706	7/7	0.89	0.27	57,64,69,71	0
4	SO4	A	1705	5/5	0.90	0.25	66,71,88,105	0
3	CA	A	1704	1/1	0.94	0.11	51,51,51,51	0
3	CA	A	1702	1/1	0.99	0.07	44,44,44,44	0
2	CL	A	1701	1/1	1.00	0.20	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.