



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2017 – 03:19 PM EST

PDB ID : 5VYJ  
Title : Crystal structure of the photosynthetic phosphoenolpyruvate carboxylase isoenzyme from maize in complex with Gly  
Authors : Gonzalez-Segura, L.; Guemez-Toro, R.; Munoz-Clares, R.A.  
Deposited on : unknown  
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

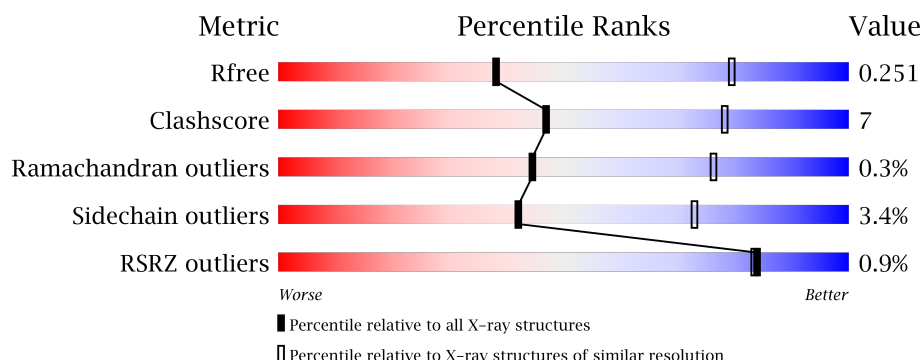
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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. 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	970	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;">73% 20% • 5%</div> </div> </div>
1	B	970	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;">74% 20% • 5%</div> </div> </div>
1	C	970	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;">75% 19% • 5%</div> </div> </div>
1	D	970	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;">76% 18% • 5%</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	1003	-	-	-	X
3	ACT	C	1002	-	-	-	X
3	ACT	C	1004	-	-	-	X
3	ACT	C	1005	-	-	-	X
3	ACT	D	1003	-	-	-	X
3	ACT	D	1004	-	-	-	X

## 2 Entry composition [i](#)

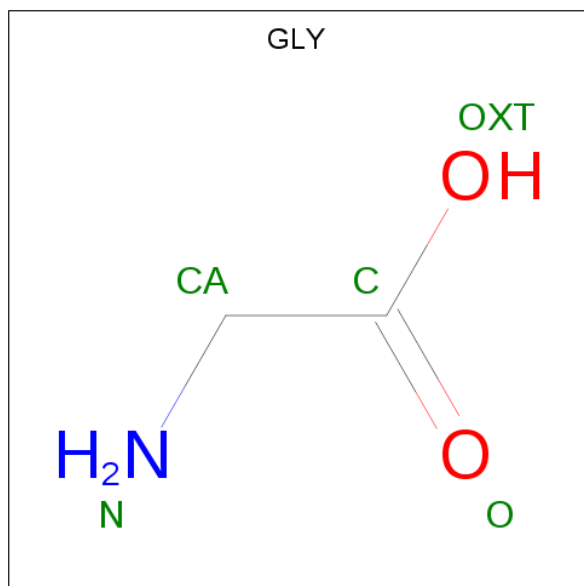
There are 3 unique types of molecules in this entry. The entry contains 29339 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphoenolpyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	918	Total	C	N	O	S	0	0	0
			7318	4646	1275	1367	30			
1	B	917	Total	C	N	O	S	0	0	0
			7309	4640	1274	1365	30			
1	C	918	Total	C	N	O	S	0	0	0
			7318	4645	1275	1368	30			
1	D	918	Total	C	N	O	S	0	0	0
			7317	4646	1275	1366	30			

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	B	1	Total	C	N	O	0	0
			5	2	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			5	2	1	2		
2	C	1	Total	C	N	O	0	0
			5	2	1	2		
2	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0

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 ( $\text{RSRZ} > 2$ ). 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.

Chain A: %

73% 20% 5%

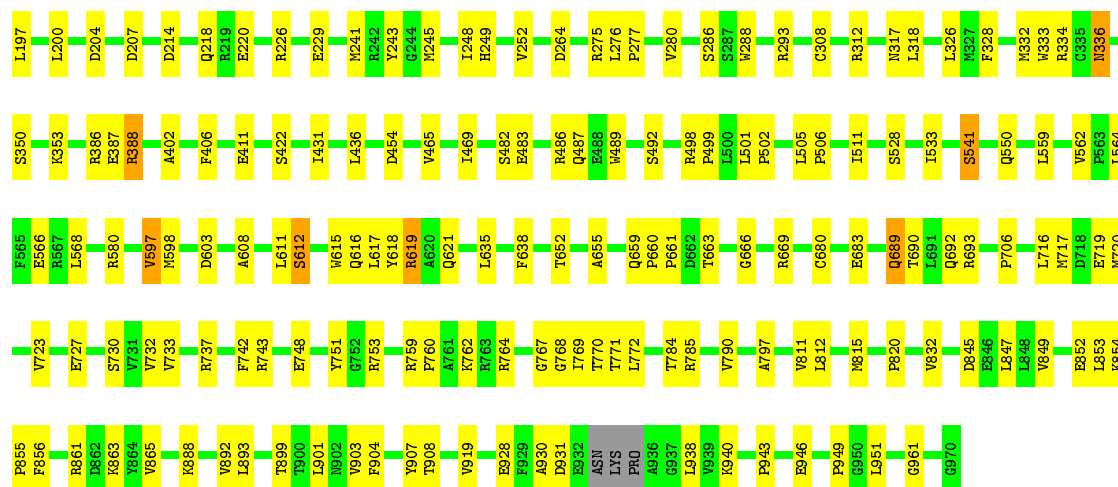
L938	F809	I515	K353	L87	MET
V939	I664	P625	T354	T88	ALA
K940	N865	P625	T355	G89	SER
P943	G666	S528	T357	L90	THR
P948	R669	P631	T358	L97	LYS
L951	E683	I533	F361	I102	ALA
L955	Q692	S541	I365	L103	PRO
G961	R693	Q650	P366	L106	GLY
G970	T698	L699	E369	A109	GLU
	E832	E700	V373	R121	LYS
	K853	M703	R379	R122	HIS
	P855	P706	R388	K125	SER
	K863	M720	L393	L252	ILE
	L871	E727	S401	L253	ASP
	L872	S730	A402	K254	ALA
	R878	D879	F406	R257	GLN
	I880	V732	K594	L267	LEU
	L881	V733	Q595	R268	GLY
	E882	K734	Q596	N269	ARG
	P885	F742	V597	L272	GLY
	F886	R743	L413	L276	GLN
	L887	P747	E414	P277	LEU
	K888	E748	P415	V280	GLY
	Q889	T750	L416	L283	PHE
		G757	Q419	E144	ALA
		L901	S612	E145	PRO
		N902	K762	R149	GLY
		P903	R763	K156	LYS
		F904	R764	L52	VAL
		L909	G766	L57	SER
		V919	G767	F60	GLU
		Q922	G768	D171	ASP
		P923	I769	E66	GLY
		P924	T770	D70	LYS
		L925	T771	T177	LEU
			T777	T179	ALA
			W781	R184	GLY
			T784	Q188	SER
			A797	G81	GLU
				E82	THR
				K189	ASP
				R192	GLY
				P193	LEU
				R194	GLY
				P195	ALA
				R196	PRO
				P197	GLY
				R198	LEU
				P199	GLY
				R200	ALA
				P201	PRO
				R202	GLY
				P203	LEU
				R204	GLY
				P205	ALA
				R206	PRO
				P207	GLY
				R208	LEU
				P209	GLY
				R210	ALA
				P211	PRO
				R212	GLY
				P213	LEU
				R214	GLY
				P215	ALA
				R216	PRO
				P217	GLY
				R218	LEU
				P219	GLY
				R220	ALA
				P221	PRO
				R222	GLY
				P223	LEU
				R224	GLY
				P225	ALA
				R226	PRO
				P227	GLY
				R228	LEU
				P229	GLY
				R230	ALA
	</				

Chain B:

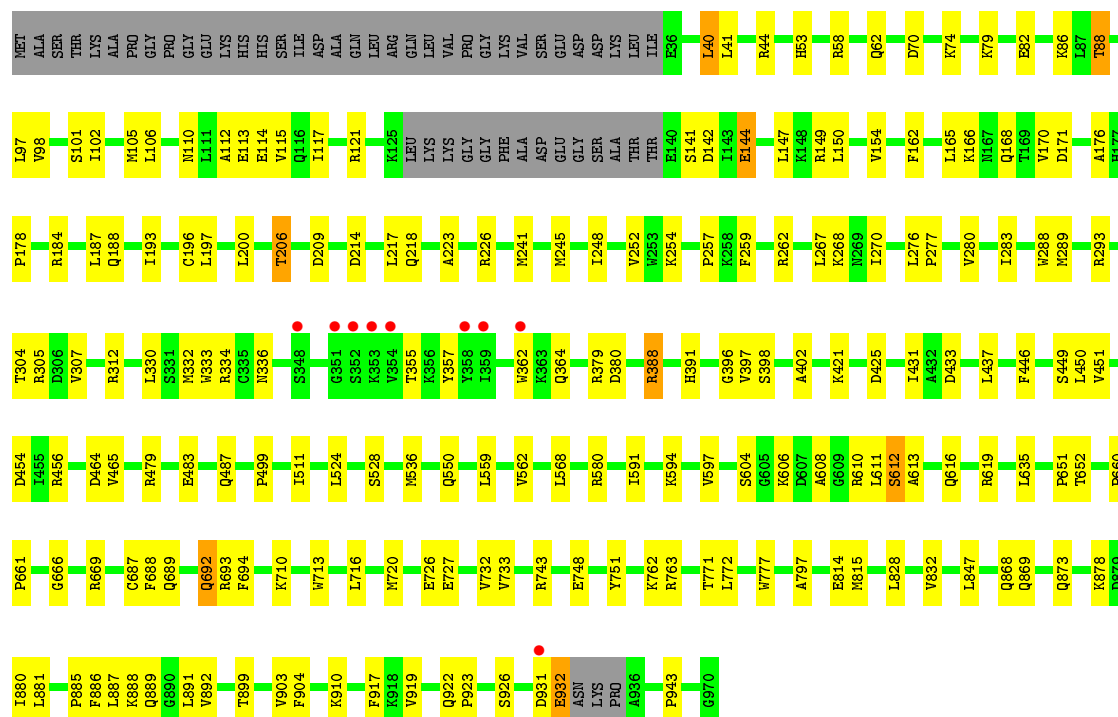
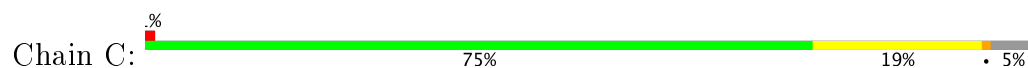
74% 20% 5%

Met Ala Thr Lys Pro Gly Glu Lys His Ser Ile Asp Asn Gln Leu Arg Gln Val Pro Gly Lys Val Ser Glu Asp Asn Lys Lys Leu Ile P36 Y37 D38 A39 L40 L41 V42 D43 R44 F45 L46 L52 P55 S56 L57 R58 D76 K79 L83

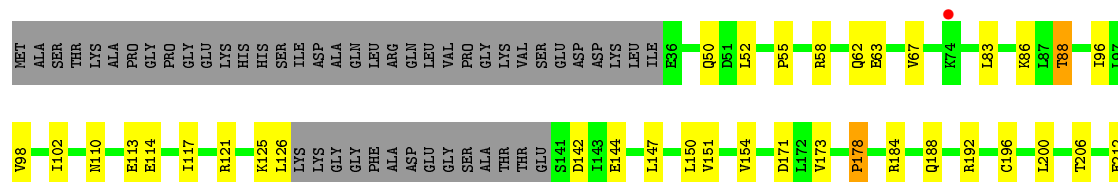
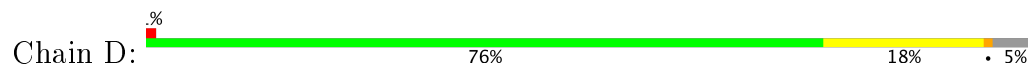
T88 L97 V98 S101 I102 L103 M104 H105 L106 H107 L108 A112 E113 I117 R121 K125 L126 LYS LYS LYS GLY GLY PHE ALA ASP GLU GLY SER SER ALA THR THR THR GLU S141 L147 V161 Q168 Q168 D171 L172 V173 P178 R184 S185 L186 L187 Q188 R192 L196



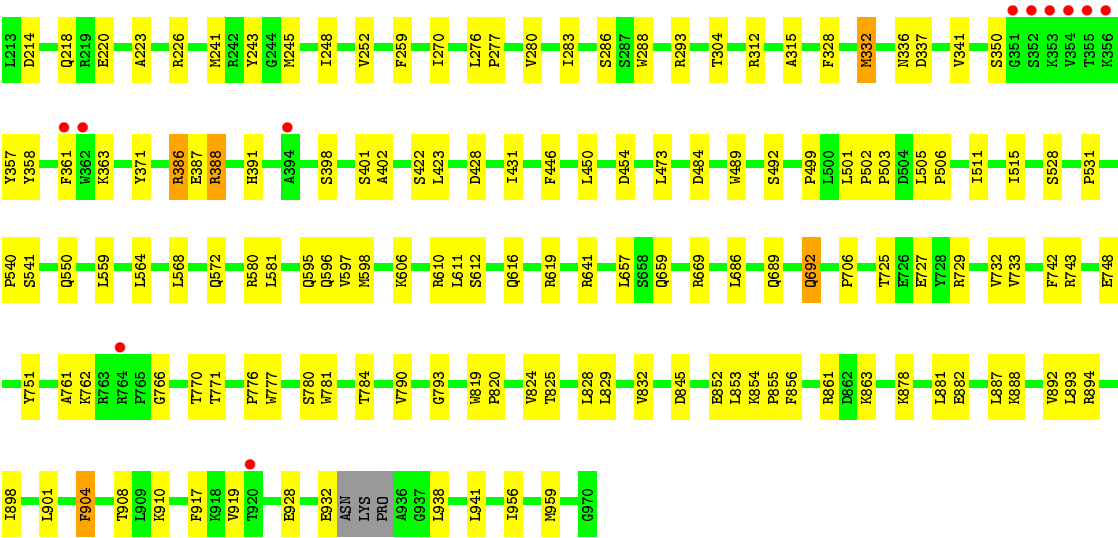
• Molecule 1: Phosphoenolpyruvate carboxylase



• Molecule 1: Phosphoenolpyruvate carboxylase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.95Å 167.24Å 242.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.08 – 3.30 57.08 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.2 (57.08-3.30) 93.3 (57.08-3.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.210 , 0.253 0.207 , 0.251	Depositor DCC
$R_{free}$ test set	4508 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	29339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.4006e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ACT

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	0.34	0/7473	0.51	0/10119
1	B	0.35	0/7464	0.53	0/10108
1	C	0.33	0/7473	0.50	0/10120
1	D	0.33	0/7472	0.50	0/10119
All	All	0.34	0/29882	0.51	0/40466

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7318	0	7314	114	0
1	B	7309	0	7303	114	0
1	C	7318	0	7309	100	0
1	D	7317	0	7314	98	0
2	A	5	0	2	1	0
2	B	10	0	4	1	0
2	C	5	0	2	1	0
2	D	5	0	2	0	0
3	A	12	0	9	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	9	0	0
3	C	16	0	12	0	0
3	D	12	0	9	1	0
All	All	29339	0	29289	414	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 7.

All (414) 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:B:388:ARG:HH12	1:B:402:ALA:HA	1.39	0.88
1:D:743:ARG:HH22	1:D:762:LYS:HE3	1.43	0.82
1:B:386:ARG:NH1	1:B:387:GLU:OE1	2.17	0.77
1:C:362:TRP:NE1	1:C:380:ASP:OD2	2.19	0.75
1:B:568:LEU:HD22	1:B:608:ALA:HB2	1.67	0.74
1:A:465:VAL:HG22	1:A:511:ILE:HG23	1.69	0.74
1:B:276:LEU:HD12	1:B:277:PRO:HD2	1.71	0.72
1:C:720:MET:HB3	1:C:797:ALA:HB1	1.70	0.72
1:D:88:THR:HB	1:D:919:VAL:HG21	1.72	0.72
1:C:487:GLN:OE1	1:C:580:ARG:NH1	2.24	0.71
1:B:465:VAL:HG22	1:B:511:ILE:HG23	1.72	0.70
1:C:568:LEU:HD22	1:C:608:ALA:HB2	1.73	0.69
1:B:812:LEU:HA	1:B:815:MET:HE3	1.76	0.68
1:C:88:THR:HB	1:C:919:VAL:HG11	1.75	0.66
1:A:293:ARG:NH2	1:A:304:THR:OG1	2.27	0.66
1:D:312:ARG:HH21	1:D:528:SER:HB3	1.60	0.66
1:C:41:LEU:HD12	1:C:112:ALA:HB2	1.79	0.65
1:A:192:ARG:NH1	1:A:220:GLU:OE1	2.30	0.65
1:A:103:LEU:HD13	1:A:961:GLY:HA2	1.78	0.65
1:D:259:PHE:HE1	1:D:692:GLN:HE21	1.45	0.64
1:A:937:GLY:HA2	1:A:940:LYS:HD2	1.79	0.64
1:C:40:LEU:HG	1:C:44:ARG:HH21	1.62	0.63
1:D:171:ASP:HB3	1:D:669:ARG:HG2	1.80	0.63
1:A:720:MET:HB3	1:A:797:ALA:HB1	1.81	0.63
1:D:288:TRP:CD1	1:D:454:ASP:HB2	2.35	0.62
1:D:564:LEU:HD13	1:D:598:MET:HG2	1.80	0.62
1:D:659:GLN:HA	3:D:1004:ACT:H1	1.81	0.62
1:C:293:ARG:NH2	1:C:304:THR:OG1	2.32	0.61
1:C:178:PRO:O	1:C:751:TYR:OH	2.17	0.61
1:A:606:LYS:HG3	1:A:777:TRP:CD1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:THR:HB	1:C:209:ASP:H	1.67	0.60
1:B:505:LEU:HD12	1:B:506:PRO:HD2	1.83	0.60
1:D:336:ASN:HD22	1:D:422:SER:HA	1.66	0.60
1:A:361:PHE:HD2	1:A:379:ARG:HH12	1.49	0.60
1:B:501:LEU:HD12	1:B:502:PRO:HD2	1.84	0.60
1:A:706:PRO:HB3	1:A:820:PRO:HG2	1.84	0.59
1:C:276:LEU:HD12	1:C:277:PRO:HD2	1.84	0.59
1:A:499:PRO:HB2	1:C:499:PRO:HB2	1.84	0.59
1:C:743:ARG:NH1	1:C:748:GLU:OE2	2.35	0.59
1:D:428:ASP:HB3	1:D:431:ILE:HD12	1.82	0.59
1:A:241:MET:HG3	1:A:307:VAL:HG13	1.84	0.59
1:A:764:ARG:HG3	1:A:765:PRO:HD2	1.84	0.59
1:A:657:LEU:HG	1:A:820:PRO:HB3	1.86	0.58
1:A:428:ASP:HB3	1:A:431:ILE:HD12	1.84	0.58
1:B:173:VAL:HG22	1:B:286:SER:HB2	1.84	0.58
1:D:790:VAL:HG11	1:D:832:VAL:HG21	1.85	0.58
1:B:487:GLN:OE1	1:B:580:ARG:NH1	2.36	0.58
1:B:103:LEU:HD13	1:B:961:GLY:HA2	1.86	0.58
1:A:171:ASP:HB3	1:A:669:ARG:HG2	1.85	0.57
1:C:421:LYS:NZ	1:C:425:ASP:OD2	2.35	0.57
1:C:597:VAL:HG12	1:C:635:LEU:HD11	1.87	0.57
1:C:355:THR:HG22	1:C:357:TYR:HB3	1.86	0.57
1:D:568:LEU:HD12	1:D:616:GLN:HG2	1.86	0.57
1:B:248:ILE:HA	1:B:252:VAL:HB	1.87	0.57
1:C:115:VAL:HG21	1:C:197:LEU:HD23	1.86	0.57
1:D:63:GLU:OE1	1:D:86:LYS:NZ	2.34	0.57
1:D:147:LEU:HB3	1:D:270:ILE:HD13	1.87	0.57
1:B:88:THR:HB	1:B:919:VAL:HG21	1.85	0.57
1:C:604:SER:HB3	1:C:613:ALA:HB1	1.87	0.57
1:A:49:LEU:HD11	1:A:57:LEU:HD22	1.87	0.57
1:B:770:THR:HG23	1:B:771:THR:HG23	1.87	0.56
1:B:727:GLU:OE2	1:B:863:LYS:NZ	2.38	0.56
1:C:550:GLN:OE1	1:C:559:LEU:N	2.38	0.56
1:C:248:ILE:HA	1:C:252:VAL:HB	1.88	0.56
1:C:312:ARG:HH21	1:C:528:SER:HB3	1.70	0.56
1:A:767:GLY:O	1:A:770:THR:HG22	2.05	0.56
1:B:184:ARG:O	1:B:188:GLN:HG3	2.06	0.56
1:C:110:ASN:O	1:C:114:GLU:HG3	2.06	0.56
1:D:725:THR:HG22	1:D:729:ARG:HD2	1.86	0.55
1:D:96:ILE:HG21	1:D:938:LEU:HD21	1.87	0.55
1:A:288:TRP:CD1	1:A:454:ASP:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:NH1	1:B:928:GLU:OE2	2.38	0.55
1:D:388:ARG:HH12	1:D:402:ALA:HA	1.71	0.55
1:A:52:LEU:HD13	1:A:226:ARG:NH1	2.21	0.55
1:C:101:SER:O	1:C:105:MET:HG3	2.06	0.55
1:A:88:THR:HB	1:A:919:VAL:HG21	1.89	0.55
1:B:930:ALA:HB3	1:B:931:ASP:HA	1.88	0.55
1:A:178:PRO:O	1:A:751:TYR:OH	2.24	0.55
1:C:241:MET:O	1:C:245:MET:HG2	2.06	0.55
1:D:67:VAL:HG11	1:D:83:LEU:HB2	1.89	0.55
1:D:121:ARG:NH1	1:D:689:GLN:OE1	2.41	0.54
1:B:550:GLN:OE1	1:B:559:LEU:N	2.40	0.54
1:A:652:THR:HB	1:A:693:ARG:HD3	1.90	0.54
1:B:288:TRP:CD1	1:B:454:ASP:HB2	2.42	0.54
1:A:730:SER:HA	1:A:734:LYS:HE3	1.88	0.54
1:B:499:PRO:HB2	1:D:499:PRO:HB2	1.88	0.54
1:A:727:GLU:OE2	1:A:863:LYS:NZ	2.40	0.54
1:D:501:LEU:HD12	1:D:502:PRO:HD2	1.90	0.54
1:C:196:CYS:O	1:C:200:LEU:HB2	2.08	0.53
1:A:602:SER:HB2	3:A:1002:ACT:H1	1.90	0.53
1:A:189:LYS:HG2	1:A:192:ARG:HH12	1.73	0.53
1:A:743:ARG:NH1	1:A:748:GLU:OE2	2.41	0.53
1:C:165:LEU:HD12	1:C:267:LEU:HD21	1.91	0.53
1:A:568:LEU:HD12	1:A:616:GLN:HG2	1.91	0.53
1:B:171:ASP:HB3	1:B:669:ARG:HG2	1.90	0.53
1:C:184:ARG:O	1:C:188:GLN:HG3	2.09	0.52
1:A:621:GLN:HG2	1:A:637:LEU:HD13	1.92	0.52
1:C:70:ASP:HB3	1:C:79:LYS:HE3	1.91	0.52
1:A:149:ARG:NH1	1:A:700:GLU:OE1	2.42	0.52
1:A:742:PHE:CZ	1:A:748:GLU:HG3	2.43	0.52
1:A:872:LEU:HD21	1:A:880:ILE:HD12	1.91	0.52
1:B:312:ARG:HH21	1:B:528:SER:HB3	1.74	0.52
1:B:716:LEU:HD23	1:B:815:MET:HE2	1.92	0.52
1:C:141:SER:OG	1:C:149:ARG:NH2	2.41	0.52
1:B:214:ASP:O	1:B:218:GLN:HG2	2.09	0.52
1:C:142:ASP:HB2	1:C:692:GLN:OE1	2.09	0.52
1:A:550:GLN:OE1	1:A:559:LEU:N	2.42	0.52
1:B:336:ASN:HD22	1:B:422:SER:HB2	1.75	0.52
1:B:249:HIS:CD2	1:B:318:LEU:HD21	2.44	0.52
1:D:904:PHE:O	1:D:908:THR:OG1	2.18	0.51
1:C:241:MET:HG3	1:C:307:VAL:HG13	1.92	0.51
1:C:465:VAL:HG22	1:C:511:ILE:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:TRP:CZ2	1:B:619:ARG:HD2	2.46	0.51
1:D:113:GLU:O	1:D:117:ILE:HG12	2.11	0.51
1:B:498:ARG:HD2	1:D:473:LEU:HD13	1.92	0.51
1:A:568:LEU:HD22	1:A:608:ALA:HB2	1.93	0.51
1:D:388:ARG:NH1	1:D:401:SER:O	2.43	0.51
1:A:276:LEU:HD12	1:A:277:PRO:HD2	1.92	0.51
1:B:652:THR:HB	1:B:693:ARG:HD3	1.93	0.51
1:C:433:ASP:HA	1:C:437:LEU:HB2	1.92	0.51
1:B:333:TRP:CZ3	1:B:334:ARG:HG2	2.45	0.51
1:B:52:LEU:HD13	1:B:226:ARG:HH11	1.76	0.50
1:B:566:GLU:HG2	1:B:603:ASP:HB2	1.92	0.50
1:B:732:VAL:HG23	1:B:733:VAL:HG23	1.92	0.50
1:A:595:GLN:NE2	1:A:596:GLN:O	2.43	0.50
1:D:489:TRP:O	1:D:492:SER:OG	2.25	0.50
1:C:226:ARG:NE	1:D:428:ASP:OD1	2.43	0.50
1:A:237:PRO:HB2	1:A:303:VAL:HG11	1.94	0.50
1:B:102:ILE:HG21	1:B:901:LEU:HG	1.94	0.50
1:D:184:ARG:O	1:D:188:GLN:HG3	2.12	0.50
1:D:241:MET:O	1:D:245:MET:HG2	2.11	0.50
1:D:248:ILE:HA	1:D:252:VAL:HB	1.93	0.50
1:C:606:LYS:HG3	1:C:777:TRP:CD1	2.47	0.50
1:C:168:GLN:HG3	1:C:666:GLY:HA2	1.93	0.50
1:D:910:LYS:HE2	1:D:917:PHE:CD1	2.46	0.50
1:A:467:ASP:OD1	1:A:477:SER:OG	2.26	0.50
1:C:710:LYS:NZ	1:C:814:GLU:OE1	2.45	0.50
1:A:52:LEU:HD13	1:A:226:ARG:HH11	1.77	0.49
1:A:812:LEU:HA	1:A:815:MET:HE2	1.94	0.49
1:B:196:CYS:O	1:B:200:LEU:HB2	2.12	0.49
1:C:446:PHE:HB3	1:C:450:LEU:HD12	1.94	0.49
1:D:761:ALA:HB1	1:D:776:PRO:HG3	1.93	0.49
1:A:168:GLN:HG3	1:A:666:GLY:HA2	1.94	0.49
1:A:747:PRO:HB3	1:A:909:LEU:HD11	1.94	0.49
1:A:102:ILE:HG21	1:A:901:LEU:HG	1.94	0.49
1:B:326:LEU:HD21	1:B:436:LEU:HD13	1.94	0.49
1:D:276:LEU:HD12	1:D:277:PRO:HD2	1.93	0.49
1:C:171:ASP:HB3	1:C:669:ARG:HG2	1.95	0.49
1:A:241:MET:O	1:A:245:MET:HG2	2.13	0.49
1:B:680:CYS:HB3	1:B:690:THR:HG21	1.94	0.49
1:C:591:ILE:HB	1:C:594:LYS:O	2.13	0.49
1:D:277:PRO:HG2	1:D:280:VAL:HG23	1.94	0.49
1:D:337:ASP:O	1:D:341:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:O	1:A:188:GLN:HG3	2.13	0.49
1:D:386:ARG:NH1	1:D:387:GLU:OE2	2.46	0.49
1:A:388:ARG:NH1	1:A:401:SER:O	2.45	0.49
1:C:568:LEU:HD12	1:C:616:GLN:HG2	1.95	0.49
1:A:357:TYR:HD2	1:A:358:TYR:N	2.11	0.48
1:B:483:GLU:OE1	1:B:541:SER:HB3	2.13	0.48
1:A:248:ILE:HA	1:A:252:VAL:HB	1.95	0.48
1:A:948:PRO:HB2	1:A:951:LEU:HD12	1.96	0.48
1:B:564:LEU:HD13	1:B:598:MET:HG2	1.96	0.48
1:B:706:PRO:HB3	1:B:820:PRO:HG2	1.94	0.48
1:C:922:GLN:HB3	1:C:923:PRO:HD2	1.95	0.48
1:D:178:PRO:O	1:D:751:TYR:OH	2.31	0.48
1:A:854:LYS:N	1:A:855:PRO:HD2	2.28	0.48
1:B:113:GLU:O	1:B:117:ILE:HG12	2.14	0.48
1:D:110:ASN:O	1:D:114:GLU:HG3	2.14	0.48
1:D:894:ARG:HG2	1:D:898:ILE:HD11	1.94	0.48
1:B:742:PHE:CZ	1:B:748:GLU:HG3	2.48	0.48
1:A:122:ARG:NH1	1:B:204:ASP:OD2	2.45	0.47
1:C:652:THR:HB	1:C:693:ARG:HD3	1.96	0.47
1:D:595:GLN:NE2	1:D:596:GLN:O	2.47	0.47
1:C:888:LYS:O	1:C:892:VAL:HG23	2.13	0.47
1:D:641:ARG:HH12	1:D:659:GLN:NE2	2.12	0.47
1:B:719:GLU:O	1:B:723:VAL:HG23	2.15	0.47
1:B:767:GLY:O	1:B:770:THR:HG22	2.13	0.47
1:B:743:ARG:NH1	1:B:748:GLU:OE2	2.47	0.47
1:D:173:VAL:HG22	1:D:286:SER:HB2	1.96	0.47
1:B:502:PRO:HG2	1:B:505:LEU:HB2	1.97	0.47
1:B:83:LEU:HD23	1:B:903:VAL:HG21	1.97	0.47
1:C:868:GLN:NE2	1:C:880:ILE:HD12	2.29	0.47
1:C:162:PHE:CE2	1:C:166:LYS:HD2	2.50	0.47
1:D:770:THR:HG23	1:D:771:THR:HG23	1.96	0.47
1:A:525:PRO:O	1:A:528:SER:OG	2.33	0.47
1:C:288:TRP:CD1	1:C:454:ASP:HB2	2.50	0.47
1:A:144:GLU:CD	1:A:269:ASN:HD22	2.18	0.47
1:A:293:ARG:HG2	1:A:456:ARG:O	2.15	0.47
1:A:70:ASP:HB3	1:A:79:LYS:HE3	1.97	0.47
1:B:41:LEU:HD21	1:B:197:LEU:HD13	1.97	0.47
1:B:655:ALA:O	1:B:659:GLN:HG3	2.14	0.47
1:A:750:GLU:HG3	1:A:955:LEU:HD21	1.97	0.47
1:C:464:ASP:OD1	1:C:479:ARG:NH2	2.45	0.47
1:A:267:LEU:O	1:A:272:ILE:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ARG:HH12	1:A:402:ALA:HA	1.80	0.47
1:A:826:LEU:HB3	1:A:871:LEU:HD11	1.97	0.47
1:B:618:TYR:CD2	1:B:660:PRO:HD3	2.50	0.47
1:B:720:MET:HB3	1:B:797:ALA:HB1	1.96	0.47
1:A:86:LYS:O	1:A:922:GLN:NE2	2.48	0.46
1:D:606:LYS:HG3	1:D:777:TRP:CD1	2.50	0.46
1:D:142:ASP:HB2	1:D:692:GLN:OE1	2.15	0.46
1:C:388:ARG:HH12	1:C:402:ALA:HA	1.80	0.46
1:C:41:LEU:HD11	1:C:197:LEU:HD22	1.97	0.46
1:C:449:SER:O	1:C:451:VAL:N	2.44	0.46
1:C:86:LYS:O	1:C:922:GLN:NE2	2.48	0.46
1:D:196:CYS:O	1:D:200:LEU:HB2	2.15	0.46
1:B:121:ARG:NH2	1:B:693:ARG:HH22	2.14	0.46
1:A:845:ASP:HA	1:A:849:VAL:HG23	1.97	0.46
1:B:568:LEU:HD12	1:B:616:GLN:HG2	1.97	0.46
1:A:60:PHE:CE2	1:A:90:LEU:HD11	2.50	0.46
1:A:885:PRO:O	1:A:887:LEU:N	2.49	0.46
1:B:178:PRO:O	1:B:751:TYR:OH	2.33	0.46
1:A:102:ILE:O	1:A:106:LEU:HB2	2.16	0.46
1:A:732:VAL:HG23	1:A:733:VAL:HG23	1.98	0.46
1:C:259:PHE:HA	1:C:688:PHE:HE1	1.81	0.46
1:A:254:LYS:O	1:A:257:PRO:HD2	2.15	0.46
1:B:861:ARG:O	1:B:865:VAL:HG23	2.16	0.46
1:D:781:TRP:HA	1:D:784:THR:HG22	1.98	0.46
1:A:446:PHE:HB3	1:A:450:LEU:HA	1.98	0.45
1:D:505:LEU:HD12	1:D:506:PRO:HD2	1.98	0.45
1:B:406:PHE:HD1	1:B:411:GLU:HG2	1.81	0.45
1:B:617:LEU:O	1:B:621:GLN:HG3	2.17	0.45
1:B:241:MET:O	1:B:245:MET:HG2	2.15	0.45
1:A:121:ARG:NH2	1:A:693:ARG:HH22	2.14	0.45
1:B:811:VAL:HG12	1:B:815:MET:HE2	1.99	0.45
1:C:53:HIS:HD1	1:C:926:SER:HG	1.64	0.45
1:D:446:PHE:HB3	1:D:450:LEU:HD12	1.99	0.45
1:B:52:LEU:HD13	1:B:226:ARG:NH1	2.32	0.45
1:A:730:SER:HA	1:A:734:LYS:HB2	1.97	0.45
1:C:147:LEU:HB3	1:C:270:ILE:HD13	1.98	0.45
1:C:40:LEU:HG	1:C:44:ARG:NH2	2.31	0.45
1:D:102:ILE:HG21	1:D:901:LEU:HG	1.98	0.45
1:A:598:MET:HA	1:A:638:PHE:HB3	1.99	0.45
1:A:762:LYS:HE3	1:A:771:THR:OG1	2.17	0.45
1:B:615:TRP:HB2	1:B:717:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LYS:O	1:A:82:GLU:HG2	2.17	0.45
1:B:533:ILE:HG12	1:B:562:VAL:HG22	1.99	0.45
1:C:254:LYS:O	1:C:257:PRO:HD2	2.17	0.45
1:C:732:VAL:HG23	1:C:733:VAL:HG23	1.99	0.45
1:D:357:TYR:HD2	1:D:358:TYR:CD2	2.35	0.45
1:B:98:VAL:O	1:B:102:ILE:HG12	2.16	0.45
1:B:106:LEU:HD12	1:B:106:LEU:HA	1.80	0.45
1:B:908:THR:HG23	1:B:951:LEU:HD22	1.99	0.45
1:A:511:ILE:O	1:A:515:ILE:HG13	2.17	0.44
1:A:591:ILE:HB	1:A:594:LYS:O	2.17	0.44
1:B:147:LEU:HD22	1:B:161:VAL:HG11	1.99	0.44
1:D:150:LEU:HD23	1:D:154:VAL:HG21	1.97	0.44
1:D:568:LEU:O	1:D:572:GLN:HG3	2.17	0.44
1:A:597:VAL:CG1	1:A:635:LEU:HD11	2.47	0.44
1:B:888:LYS:O	1:B:892:VAL:HG23	2.17	0.44
1:C:305:ARG:HA	1:C:524:LEU:HD11	1.99	0.44
1:D:657:LEU:HD12	1:D:706:PRO:HG3	1.98	0.44
1:B:336:ASN:HD22	1:B:422:SER:CB	2.30	0.44
1:B:489:TRP:O	1:B:492:SER:OG	2.28	0.44
1:B:598:MET:HA	1:B:638:PHE:HB3	2.00	0.44
1:B:854:LYS:N	1:B:855:PRO:HD2	2.32	0.44
1:A:416:LEU:O	1:A:419:CYS:HB2	2.18	0.44
1:A:615:TRP:CE2	1:A:619:ARG:HD2	2.52	0.44
1:A:533:ILE:HG12	1:A:562:VAL:HG22	1.99	0.44
1:A:734:LYS:HE3	1:A:734:LYS:HB2	1.83	0.44
1:D:454:ASP:OD1	1:D:531:PRO:HD2	2.18	0.44
1:C:334:ARG:NH1	1:D:928:GLU:OE2	2.51	0.44
1:A:601:TYR:HE2	3:A:1004:ACT:H1	1.83	0.44
1:D:828:LEU:O	1:D:832:VAL:HG23	2.18	0.44
1:A:177:HIS:O	1:A:179:THR:N	2.50	0.44
1:B:277:PRO:HG2	1:B:280:VAL:CG2	2.48	0.44
1:B:168:GLN:HG3	1:B:666:GLY:HA2	2.00	0.44
1:C:391:HIS:HB2	1:C:398:SER:HB2	2.00	0.44
1:A:277:PRO:HG2	1:A:280:VAL:HG23	2.00	0.44
1:A:40:LEU:O	1:A:44:ARG:HG3	2.18	0.44
1:A:604:SER:O	1:A:607:ASP:N	2.50	0.44
1:C:536:MET:HE3	1:C:763:ARG:HH22	1.83	0.44
1:A:141:SER:HB2	1:A:145:GLU:OE1	2.18	0.43
1:A:406:PHE:CE1	1:A:412:PHE:HA	2.53	0.43
1:C:41:LEU:HD21	1:C:197:LEU:HD13	2.00	0.43
1:D:147:LEU:O	1:D:151:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:657:LEU:HG	1:D:820:PRO:HB3	2.00	0.43
1:A:888:LYS:O	1:A:892:VAL:HG23	2.17	0.43
1:A:647:ARG:NE	1:A:970:GLY:OXT	2.51	0.43
1:B:469:ILE:HD11	1:B:501:LEU:HD13	1.99	0.43
2:A:1001:GLY:N	1:B:229:GLU:OE1	2.52	0.43
1:B:406:PHE:CD1	1:B:411:GLU:HG2	2.52	0.43
1:B:40:LEU:O	1:B:44:ARG:HG3	2.18	0.43
1:B:737:ARG:HB3	1:B:853:LEU:HD21	2.00	0.43
1:C:113:GLU:O	1:C:117:ILE:HG12	2.17	0.43
1:C:305:ARG:HH22	1:C:396:GLY:HA2	1.83	0.43
1:D:540:PRO:HB3	1:D:581:LEU:HG	1.99	0.43
1:B:42:VAL:HG13	1:B:105:MET:HE2	1.99	0.43
1:B:97:LEU:HD11	1:B:938:LEU:HD13	1.99	0.43
1:C:193:ILE:HG23	1:C:217:LEU:HD11	1.99	0.43
1:A:365:ILE:HG21	1:A:373:VAL:HG22	2.00	0.43
1:A:178:PRO:HB3	1:A:757:GLY:HA3	2.01	0.43
1:B:716:LEU:HD23	1:B:815:MET:CE	2.47	0.43
1:C:885:PRO:O	1:C:887:LEU:N	2.48	0.43
1:D:727:GLU:OE2	1:D:863:LYS:NZ	2.52	0.43
1:D:742:PHE:CZ	1:D:748:GLU:HG3	2.54	0.43
1:A:886:PHE:HA	1:A:889:GLN:HB2	2.00	0.43
1:B:597:VAL:HG12	1:B:635:LEU:HD11	2.00	0.43
1:B:608:ALA:HB1	1:B:612:SER:HB2	2.00	0.43
1:C:931:ASP:OD1	1:C:931:ASP:N	2.50	0.43
1:D:610:ARG:HA	1:D:610:ARG:HD2	1.90	0.43
1:C:176:ALA:HB2	1:C:289:MET:HG2	2.01	0.43
1:C:70:ASP:O	1:C:74:LYS:HG2	2.17	0.43
1:D:766:GLY:O	1:D:771:THR:HG21	2.19	0.43
1:D:776:PRO:O	1:D:780:SER:OG	2.33	0.43
1:A:781:TRP:HA	1:A:784:THR:HG22	2.00	0.43
1:B:249:HIS:HD2	1:B:318:LEU:HD21	1.84	0.43
1:C:886:PHE:HA	1:C:889:GLN:HB2	2.00	0.43
1:D:50:GLN:HG3	1:D:55:PRO:HA	1.99	0.43
1:D:727:GLU:HG2	1:D:793:GLY:HA2	2.00	0.43
1:D:956:ILE:HA	1:D:959:MET:CE	2.49	0.43
1:A:223:ALA:HA	1:B:431:ILE:HD11	2.01	0.43
1:A:899:THR:O	1:A:903:VAL:HG23	2.19	0.43
1:A:922:GLN:HB3	1:A:923:PRO:HD2	2.01	0.43
1:C:98:VAL:O	1:C:102:ILE:HG12	2.19	0.43
1:C:608:ALA:HB1	1:C:612:SER:HB2	2.00	0.43
1:B:753:ARG:NH2	1:B:946:GLU:OE1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ARG:HG2	1:C:456:ARG:O	2.19	0.43
1:D:391:HIS:HB2	1:D:398:SER:HB2	2.00	0.43
1:A:762:LYS:NZ	1:A:768:GLY:O	2.41	0.42
1:B:845:ASP:HA	1:B:849:VAL:HG23	2.00	0.42
1:D:214:ASP:O	1:D:218:GLN:HG2	2.19	0.42
1:D:580:ARG:HA	1:D:580:ARG:HD3	1.89	0.42
1:B:264:ASP:CG	1:B:275:ARG:HB3	2.40	0.42
1:B:76:ASP:HB3	1:B:79:LYS:H	1.84	0.42
1:C:214:ASP:O	1:C:218:GLN:HG2	2.19	0.42
1:C:121:ARG:NH1	1:C:689:GLN:OE1	2.52	0.42
1:C:716:LEU:HD23	1:C:815:MET:HE1	2.00	0.42
1:D:192:ARG:HD2	1:D:220:GLU:OE2	2.20	0.42
1:A:163:GLU:HA	1:A:166:LYS:HD3	2.00	0.42
1:A:412:PHE:O	1:A:415:PRO:HD2	2.19	0.42
1:B:41:LEU:HD13	1:B:108:LEU:HD22	2.02	0.42
1:C:223:ALA:HA	1:D:332:MET:HE1	2.01	0.42
1:D:732:VAL:HG23	1:D:733:VAL:HG23	2.00	0.42
1:A:366:PRO:HD2	1:A:369:GLU:OE2	2.20	0.42
1:C:334:ARG:NH2	2:C:1001:GLY:O	2.52	0.42
1:D:502:PRO:HG2	1:D:505:LEU:HB2	2.00	0.42
1:D:819:TRP:HD1	1:D:820:PRO:HD2	1.84	0.42
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.75	0.42
1:C:262:ARG:NH2	1:D:212:GLU:OE2	2.53	0.42
1:D:820:PRO:O	1:D:824:VAL:HG23	2.20	0.42
1:B:853:LEU:O	1:B:856:PHE:HB3	2.20	0.42
1:D:371:TYR:CE1	1:D:423:LEU:HG	2.55	0.42
1:A:357:TYR:CD2	1:A:358:TYR:N	2.88	0.42
1:A:878:LYS:HE2	1:A:882:GLU:HG3	2.01	0.42
1:A:664:ILE:HG21	1:A:698:THR:HG23	2.02	0.42
1:B:759:ARG:HG2	1:B:760:PRO:O	2.20	0.42
1:D:845:ASP:CG	1:D:861:ARG:HH12	2.23	0.42
1:C:150:LEU:HD23	1:C:154:VAL:HG21	2.01	0.41
1:D:502:PRO:HA	1:D:503:PRO:HD3	1.81	0.41
1:C:106:LEU:HA	1:C:106:LEU:HD12	1.75	0.41
1:D:336:ASN:ND2	1:D:422:SER:HA	2.32	0.41
1:A:106:LEU:O	1:A:109:ALA:HB3	2.19	0.41
1:B:187:LEU:HA	1:B:187:LEU:HD23	1.79	0.41
1:C:881:LEU:HA	1:C:881:LEU:HD23	1.83	0.41
1:C:431:ILE:HD11	1:D:223:ALA:HA	2.01	0.41
1:A:156:LYS:HE3	1:A:703:MET:HB3	2.02	0.41
1:A:580:ARG:O	1:A:584:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:GLN:OE1	1:B:693:ARG:NH1	2.54	0.41
1:B:785:ARG:NH2	1:B:899:THR:OG1	2.52	0.41
1:B:101:SER:O	1:B:105:MET:HG3	2.21	0.41
1:C:762:LYS:HD2	1:C:772:LEU:HA	2.02	0.41
1:D:52:LEU:HD13	1:D:226:ARG:HD2	2.02	0.41
1:D:259:PHE:HE1	1:D:692:GLN:NE2	2.16	0.41
1:D:293:ARG:NH2	1:D:304:THR:OG1	2.52	0.41
1:D:881:LEU:HD11	1:D:887:LEU:HD23	2.02	0.41
1:A:409:ILE:HG22	1:A:413:LEU:HD12	2.02	0.41
1:B:790:VAL:HG11	1:B:832:VAL:HG21	2.03	0.41
1:C:170:VAL:HG11	1:C:694:PHE:HB3	2.01	0.41
1:A:450:LEU:HD12	1:A:450:LEU:HA	1.90	0.41
1:B:308:CYS:O	1:B:312:ARG:HG3	2.21	0.41
1:C:268:LYS:HE2	1:C:268:LYS:HB3	1.80	0.41
1:C:660:PRO:HA	1:C:661:PRO:HD3	1.92	0.41
1:D:315:ALA:HB2	1:D:450:LEU:HB2	2.02	0.41
1:D:854:LYS:N	1:D:855:PRO:HD2	2.36	0.41
1:D:888:LYS:O	1:D:892:VAL:HG23	2.21	0.41
1:B:334:ARG:NH2	2:B:1002:GLY:OXT	2.54	0.41
1:B:55:PRO:O	1:B:56:SER:OG	2.23	0.41
1:C:483:GLU:O	1:C:487:GLN:HG3	2.21	0.41
1:C:828:LEU:O	1:C:832:VAL:HG23	2.21	0.41
1:C:910:LYS:HG2	1:C:917:PHE:CD2	2.56	0.41
1:A:365:ILE:HA	1:A:366:PRO:HD3	1.94	0.41
1:A:938:LEU:O	1:A:938:LEU:HD23	2.21	0.41
1:B:46:LEU:HA	1:B:46:LEU:HD23	1.81	0.41
1:C:102:ILE:O	1:C:106:LEU:HB2	2.21	0.41
1:C:277:PRO:HG2	1:C:280:VAL:HG23	2.03	0.41
1:C:710:LYS:HD2	1:C:713:TRP:CE2	2.56	0.41
1:D:98:VAL:O	1:D:102:ILE:HG12	2.21	0.41
1:D:550:GLN:OE1	1:D:559:LEU:N	2.51	0.41
1:B:277:PRO:HG2	1:B:280:VAL:HG23	2.02	0.40
1:B:661:PRO:O	1:B:663:THR:HG23	2.21	0.40
1:B:762:LYS:HE2	1:B:772:LEU:HD13	2.04	0.40
1:C:144:GLU:OE2	1:C:262:ARG:HD2	2.21	0.40
1:C:899:THR:O	1:C:903:VAL:HG23	2.21	0.40
1:B:192:ARG:HD2	1:B:220:GLU:OE1	2.20	0.40
1:B:638:PHE:CD1	1:B:669:ARG:HB2	2.56	0.40
1:C:932:GLU:H	1:C:932:GLU:HG3	1.52	0.40
1:A:770:THR:HG23	1:A:771:THR:HG23	2.03	0.40
1:C:333:TRP:CD2	1:D:941:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:MET:HE3	1:A:313:MET:HB2	1.97	0.40
1:A:325:GLU:O	1:A:329:GLU:HG3	2.21	0.40
1:B:37:TYR:HB3	1:B:112:ALA:HB1	2.04	0.40
1:B:727:GLU:O	1:B:730:SER:OG	2.29	0.40
1:B:847:LEU:HD21	1:B:907:TYR:CZ	2.57	0.40
1:B:930:ALA:N	1:B:931:ASP:HB2	2.37	0.40
1:D:125:LYS:O	1:D:126:LEU:HG	2.22	0.40
1:D:686:LEU:HA	1:D:686:LEU:HD23	1.89	0.40
1:D:853:LEU:O	1:D:856:PHE:HB3	2.21	0.40
1:A:57:LEU:HA	1:A:925:LEU:HD23	2.03	0.40
1:B:482:SER:O	1:B:486:ARG:HG3	2.22	0.40
1:B:660:PRO:HA	1:B:661:PRO:HD3	2.00	0.40
1:C:869:GLN:O	1:C:873:GLN:HG3	2.22	0.40
1:D:511:ILE:O	1:D:515:ILE:HG13	2.21	0.40
1:D:829:LEU:HA	1:D:829:LEU:HD23	1.89	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	912/970 (94%)	855 (94%)	53 (6%)	4 (0%)	38	71
1	B	911/970 (94%)	863 (95%)	44 (5%)	4 (0%)	38	71
1	C	912/970 (94%)	867 (95%)	42 (5%)	3 (0%)	44	76
1	D	912/970 (94%)	857 (94%)	54 (6%)	1 (0%)	55	85
All	All	3647/3880 (94%)	3442 (94%)	193 (5%)	12 (0%)	44	76

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	943	PRO
1	B	943	PRO
1	C	330	LEU
1	A	764	ARG
1	A	943	PRO
1	C	651	PRO
1	A	531	PRO
1	B	764	ARG
1	B	768	GLY
1	B	949	PRO
1	D	178	PRO
1	A	178	PRO

### 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	791/832 (95%)	768 (97%)	23 (3%)	48	75
1	B	790/832 (95%)	762 (96%)	28 (4%)	41	72
1	C	791/832 (95%)	761 (96%)	30 (4%)	38	70
1	D	791/832 (95%)	763 (96%)	28 (4%)	41	72
All	All	3163/3328 (95%)	3054 (97%)	109 (3%)	42	73

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	A	97	LEU
1	A	243	TYR
1	A	283	ILE
1	A	332	MET
1	A	336	ASN
1	A	388	ARG
1	A	393	LEU
1	A	541	SER
1	A	562	VAL

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Mol	Chain	Res	Type
1	A	597	VAL
1	A	612	SER
1	A	619	ARG
1	A	683	GLU
1	A	692	GLN
1	A	764	ARG
1	A	809	PHE
1	A	852	GLU
1	A	878	LYS
1	A	882	GLU
1	A	902	ASN
1	A	904	PHE
1	A	932	GLU
1	B	36	GLU
1	B	40	LEU
1	B	58	ARG
1	B	186	LEU
1	B	207	ASP
1	B	243	TYR
1	B	293	ARG
1	B	317	ASN
1	B	328	PHE
1	B	332	MET
1	B	336	ASN
1	B	350	SER
1	B	353	LYS
1	B	388	ARG
1	B	541	SER
1	B	597	VAL
1	B	611	LEU
1	B	612	SER
1	B	619	ARG
1	B	683	GLU
1	B	689	GLN
1	B	692	GLN
1	B	769	ILE
1	B	784	THR
1	B	852	GLU
1	B	893	LEU
1	B	904	PHE
1	B	940	LYS
1	C	40	LEU

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Mol	Chain	Res	Type
1	C	58	ARG
1	C	62	GLN
1	C	82	GLU
1	C	88	THR
1	C	97	LEU
1	C	144	GLU
1	C	206	THR
1	C	283	ILE
1	C	332	MET
1	C	336	ASN
1	C	364	GLN
1	C	379	ARG
1	C	388	ARG
1	C	397	VAL
1	C	562	VAL
1	C	610	ARG
1	C	611	LEU
1	C	612	SER
1	C	619	ARG
1	C	687	CYS
1	C	692	GLN
1	C	726	GLU
1	C	727	GLU
1	C	771	THR
1	C	847	LEU
1	C	878	LYS
1	C	891	LEU
1	C	904	PHE
1	C	932	GLU
1	D	58	ARG
1	D	62	GLN
1	D	88	THR
1	D	144	GLU
1	D	206	THR
1	D	243	TYR
1	D	283	ILE
1	D	328	PHE
1	D	332	MET
1	D	350	SER
1	D	361	PHE
1	D	363	LYS
1	D	386	ARG

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Mol	Chain	Res	Type
1	D	388	ARG
1	D	484	ASP
1	D	541	SER
1	D	597	VAL
1	D	611	LEU
1	D	612	SER
1	D	619	ARG
1	D	692	GLN
1	D	825	THR
1	D	852	GLU
1	D	878	LYS
1	D	882	GLU
1	D	893	LEU
1	D	904	PHE
1	D	932	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	211	GLN
1	B	336	ASN
1	C	180	GLN
1	C	211	GLN
1	D	53	HIS
1	D	336	ASN
1	D	659	GLN
1	D	692	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GLY	A	1001	-	1,4,4	0.45	0	0,4,4	0.00	-
3	ACT	A	1002	-	1,3,3	1.52	0	0,3,3	0.00	-
3	ACT	A	1003	-	1,3,3	1.52	0	0,3,3	0.00	-
3	ACT	A	1004	-	1,3,3	1.94	0	0,3,3	0.00	-
2	GLY	B	1001	-	1,4,4	0.46	0	0,4,4	0.00	-
2	GLY	B	1002	-	1,4,4	0.42	0	0,4,4	0.00	-
3	ACT	B	1003	-	1,3,3	1.76	0	0,3,3	0.00	-
3	ACT	B	1004	-	1,3,3	1.28	0	0,3,3	0.00	-
3	ACT	B	1005	-	1,3,3	1.93	0	0,3,3	0.00	-
2	GLY	C	1001	-	1,4,4	0.47	0	0,4,4	0.00	-
3	ACT	C	1002	-	1,3,3	1.58	0	0,3,3	0.00	-
3	ACT	C	1003	-	1,3,3	1.59	0	0,3,3	0.00	-
3	ACT	C	1004	-	1,3,3	1.30	0	0,3,3	0.00	-
3	ACT	C	1005	-	1,3,3	1.55	0	0,3,3	0.00	-
2	GLY	D	1001	-	1,4,4	0.49	0	0,4,4	0.00	-
3	ACT	D	1002	-	1,3,3	2.05	1 (100%)	0,3,3	0.00	-
3	ACT	D	1003	-	1,3,3	1.33	0	0,3,3	0.00	-
3	ACT	D	1004	-	1,3,3	0.86	0	0,3,3	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
2	GLY	A	1001	-	-	0/0/2/2	0/0/0/0
3	ACT	A	1002	-	-	0/0/0/0	0/0/0/0
3	ACT	A	1003	-	-	0/0/0/0	0/0/0/0
3	ACT	A	1004	-	-	0/0/0/0	0/0/0/0
2	GLY	B	1001	-	-	0/0/2/2	0/0/0/0
2	GLY	B	1002	-	-	0/0/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	B	1003	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1004	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1005	-	-	0/0/0/0	0/0/0/0
2	GLY	C	1001	-	-	0/0/2/2	0/0/0/0
3	ACT	C	1002	-	-	0/0/0/0	0/0/0/0
3	ACT	C	1003	-	-	0/0/0/0	0/0/0/0
3	ACT	C	1004	-	-	0/0/0/0	0/0/0/0
3	ACT	C	1005	-	-	0/0/0/0	0/0/0/0
2	GLY	D	1001	-	-	0/0/2/2	0/0/0/0
3	ACT	D	1002	-	-	0/0/0/0	0/0/0/0
3	ACT	D	1003	-	-	0/0/0/0	0/0/0/0
3	ACT	D	1004	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1002	ACT	CH3-C	2.05	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	GLY	1	0
3	A	1002	ACT	1	0
3	A	1004	ACT	1	0
2	B	1002	GLY	1	0
2	C	1001	GLY	1	0
3	D	1004	ACT	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	918/970 (94%)	-0.10	12 (1%) 77 75	3, 24, 57, 85	0
1	B	917/970 (94%)	-0.23	1 (0%) 95 96	0, 17, 50, 88	0
1	C	918/970 (94%)	-0.13	9 (0%) 82 81	8, 24, 60, 101	0
1	D	918/970 (94%)	-0.04	12 (1%) 77 75	2, 30, 74, 97	0
All	All	3671/3880 (94%)	-0.13	34 (0%) 84 83	0, 23, 63, 101	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	351	GLY	4.5
1	D	352	SER	4.4
1	C	352	SER	3.9
1	D	351	GLY	3.7
1	A	353	LYS	3.5
1	D	361	PHE	3.5
1	C	354	VAL	3.2
1	A	80	LEU	3.0
1	A	351	GLY	2.9
1	D	920	THR	2.9
1	A	352	SER	2.9
1	D	764	ARG	2.8
1	D	355	THR	2.7
1	A	354	VAL	2.7
1	D	362	TRP	2.6
1	D	354	VAL	2.6
1	C	359	ILE	2.6
1	C	362	TRP	2.5
1	D	353	LYS	2.5
1	A	35	ILE	2.4
1	C	353	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	74	LYS	2.2
1	D	356	LYS	2.2
1	B	38	ASP	2.1
1	A	358	TYR	2.1
1	A	66	GLU	2.1
1	A	476	GLY	2.1
1	C	348	SER	2.1
1	A	764	ARG	2.1
1	C	358	TYR	2.1
1	C	931	ASP	2.0
1	A	350	SER	2.0
1	D	394	ALA	2.0
1	A	356	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACT	D	1003	4/4	0.91	0.28	5.01	39,39,39,39	0
3	ACT	C	1002	4/4	0.94	0.28	4.73	17,17,17,17	0
3	ACT	C	1005	4/4	0.84	0.27	2.70	37,37,37,37	0
3	ACT	C	1004	4/4	0.95	0.22	2.40	17,17,17,17	0
3	ACT	D	1004	4/4	0.91	0.24	2.37	22,22,22,22	0
3	ACT	A	1003	4/4	0.89	0.24	2.11	40,40,40,40	0
2	GLY	B	1001	5/5	0.89	0.23	1.33	22,22,22,22	0
3	ACT	B	1005	4/4	0.92	0.20	1.23	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACT	D	1002	4/4	0.87	0.21	0.28	21,21,21,21	0
2	GLY	A	1001	5/5	0.94	0.20	-0.13	9,9,9,9	0
2	GLY	B	1002	5/5	0.92	0.18	-0.15	8,8,8,8	0
3	ACT	A	1002	4/4	0.94	0.18	-0.32	16,16,16,16	0
3	ACT	C	1003	4/4	0.83	0.22	-0.33	30,30,30,30	0
2	GLY	C	1001	5/5	0.92	0.22	-0.34	18,18,18,18	0
2	GLY	D	1001	5/5	0.93	0.18	-0.72	8,8,8,8	0
3	ACT	B	1004	4/4	0.97	0.16	-0.88	10,10,10,10	0
3	ACT	A	1004	4/4	0.95	0.14	-1.74	20,20,20,20	0
3	ACT	B	1003	4/4	0.92	0.23	-	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.